Full wwPDB EM Validation Report ⓘ

May 18, 2025 – 12:45 AM JST

PDB ID	:	8YY9 / pdb_00008yy9
EMDB ID	:	EMD-39671
Title	:	Cryo-EM structure of a tri-heme cytochrome-associated RC-LH1 complex from a marine photoheterotrophic bacterium, purified with magnesium-free solutions.
Authors	:	Chen, J.H.; Zheng, Q.; Zhang, X.
Deposited on	:	2024-04-03
Resolution	:	2.70 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:

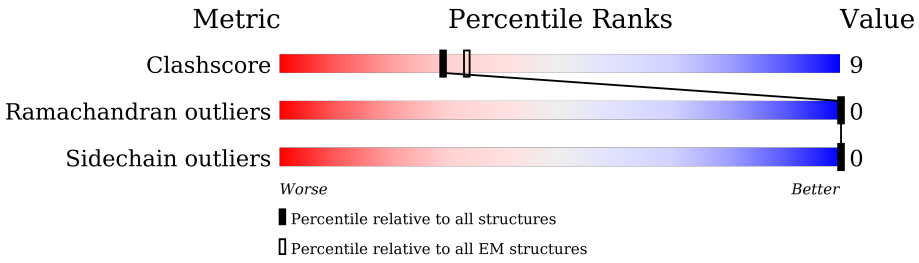
EMDB validation analysis	:	FAILED
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0rc1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

1 Overall quality at a glance

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

The reported resolution of this entry is 2.70 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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%

Mol	Chain	Length	Quality of chain
1	1	53	75% 19% 6%
1	A	53	60% 36% .
1	B	53	83% 15% .
1	D	53	83% 15% .
1	E	53	72% 26% .
1	F	53	87% 11% .
1	G	53	83% 15% .
1	I	53	75% 21% .
1	J	53	79% 15% 6%

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Mol	Chain	Length	Quality of chain
1	K	53	85% 11%
1	N	53	85% 11%
1	P	53	77% 19%
1	Q	53	77% 19%
1	R	53	75% 21%
1	S	53	77% 19%
1	T	53	64% 32%
1	V	53	83% 15%
2	O	239	17% 5% 78%
3	2	49	80% 10% 10%
3	a	49	80% 10% 10%
3	b	49	84% 6% 10%
3	d	49	82% 8% 10%
3	e	49	80% 10% 10%
3	f	49	86% 10%
3	g	49	86% 10%
3	i	49	78% 10% 12%
3	j	49	71% 16% 12%
3	k	49	73% 14% 12%
3	n	49	78% 12% 10%
3	p	49	86% 10%
3	q	49	86% 10%
3	r	49	78% 10% 12%
3	s	49	82% 8% 10%
3	t	49	71% 16% 12%

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Mol	Chain	Length	Quality of chain
3	v	49	80% 16%
4	M	330	73% 25%
5	L	279	77% 22%
6	H	256	75% 25%
7	C	360	76% 22%

2 Entry composition (i)

There are 16 unique types of molecules in this entry. The entry contains 28303 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 Antenna pigment protein alpha chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	P	51	Total	C	N	O	S	0	0
			425	291	68	64	2		
1	V	52	Total	C	N	O	S	0	0
			430	294	69	65	2		
1	S	51	Total	C	N	O	S	0	0
			422	289	68	64	1		
1	T	51	Total	C	N	O	S	0	0
			422	289	68	64	1		
1	Q	51	Total	C	N	O	S	0	0
			422	289	68	64	1		
1	R	51	Total	C	N	O	S	0	0
			422	289	68	64	1		
1	1	50	Total	C	N	O	S	0	0
			417	286	67	63	1		
1	N	51	Total	C	N	O	S	0	0
			422	289	68	64	1		
1	K	51	Total	C	N	O	S	0	0
			422	289	68	64	1		
1	J	50	Total	C	N	O	S	0	0
			417	286	67	63	1		
1	I	51	Total	C	N	O	S	0	0
			422	289	68	64	1		
1	G	52	Total	C	N	O	S	0	0
			430	294	69	65	2		
1	F	52	Total	C	N	O	S	0	0
			430	294	69	65	2		
1	E	52	Total	C	N	O	S	0	0
			430	294	69	65	2		
1	D	52	Total	C	N	O	S	0	0
			430	294	69	65	2		
1	B	52	Total	C	N	O	S	0	0
			430	294	69	65	2		
1	A	51	Total	C	N	O	S	0	0
			422	289	68	64	1		

- Molecule 2 is a protein called Reaction center protein O chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	O	52	Total	C	N	O	S	0	0
			371	249	56	59	7		

- Molecule 3 is a protein called Antenna pigment protein beta chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	v	41	Total	C	N	O	S	0	0
			332	224	53	54	1		
3	t	43	Total	C	N	O	S	0	0
			346	233	55	57	1		
3	s	44	Total	C	N	O	S	0	0
			354	237	56	60	1		
3	r	43	Total	C	N	O	S	0	0
			346	233	55	57	1		
3	q	44	Total	C	N	O	S	0	0
			354	237	56	60	1		
3	p	44	Total	C	N	O	S	0	0
			354	237	56	60	1		
3	2	44	Total	C	N	O	S	0	0
			354	237	56	60	1		
3	n	44	Total	C	N	O	S	0	0
			354	237	56	60	1		
3	k	43	Total	C	N	O	S	0	0
			346	233	55	57	1		
3	j	43	Total	C	N	O	S	0	0
			346	233	55	57	1		
3	i	43	Total	C	N	O	S	0	0
			346	233	55	57	1		
3	g	44	Total	C	N	O	S	0	0
			354	237	56	60	1		
3	f	44	Total	C	N	O	S	0	0
			354	237	56	60	1		
3	e	44	Total	C	N	O	S	0	0
			354	237	56	60	1		
3	d	44	Total	C	N	O	S	0	0
			354	237	56	60	1		
3	b	44	Total	C	N	O	S	0	0
			358	239	56	62	1		
3	a	44	Total	C	N	O	S	0	0
			358	239	56	62	1		

- Molecule 4 is a protein called Reaction center protein M chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	M	325	Total	C	N	O	S	0	0
			2633	1752	421	452	8		

- Molecule 5 is a protein called Reaction center protein L chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	L	274	Total	C	N	O	S	0	0
			2178	1469	346	354	9		

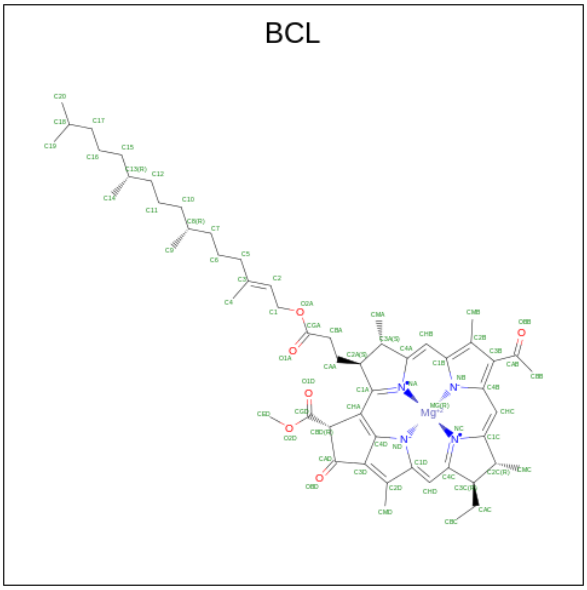
- Molecule 6 is a protein called Reaction center protein H chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	H	256	Total	C	N	O	S	0	0
			2022	1283	345	385	9		

- Molecule 7 is a protein called Photosynthetic reaction center cytochrome c subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	C	352	Total	C	N	O	S	0	0
			2740	1731	455	540	14		

- Molecule 8 is BACTERIOCHLOROPHYLL A (CCD ID: BCL) (formula: $C_{55}H_{74}MgN_4O_6$).



Mol	Chain	Residues	Atoms					AltConf
8	P	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
8	P	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	V	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	v	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	S	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	t	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	T	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	s	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	Q	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	r	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	R	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	q	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	1	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	1	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	n	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	N	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	K	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	K	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	j	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	J	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	I	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	I	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

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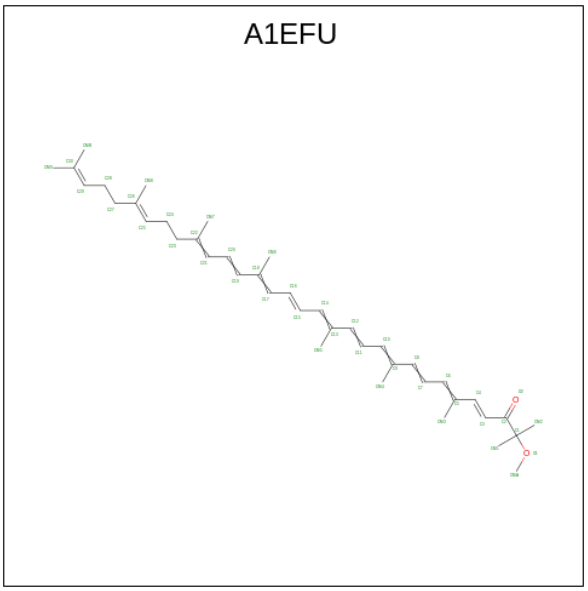
Mol	Chain	Residues	Atoms					AltConf
8	G	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	G	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	f	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	F	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	e	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	E	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	d	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	D	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	b	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	B	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	a	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	A	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	M	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	M	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	L	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	L	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

- Molecule 9 is (4 {E},16 {E},26 {E})-2-methoxy-2,6,10,14,19,23,27,31-octamethyl-dotriacont a-4,6,8,10,12,14,16,18,20,22,26,30-dodecaen-3-one (CCD ID: A1EFU) (formula: $C_{41}H_{58}O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
9	P	1	Total C O 43 41 2	0
9	v	1	Total C O 43 41 2	0
9	S	1	Total C O 43 41 2	0
9	S	1	Total C O 43 41 2	0
9	T	1	Total C O 43 41 2	0
9	T	1	Total C O 43 41 2	0
9	Q	1	Total C O 43 41 2	0
9	r	1	Total C O 43 41 2	0
9	R	1	Total C O 43 41 2	0
9	q	1	Total C O 43 41 2	0
9	p	1	Total C O 43 41 2	0
9	1	1	Total C O 43 41 2	0
9	1	1	Total C O 43 41 2	0
9	n	1	Total C O 43 41 2	0

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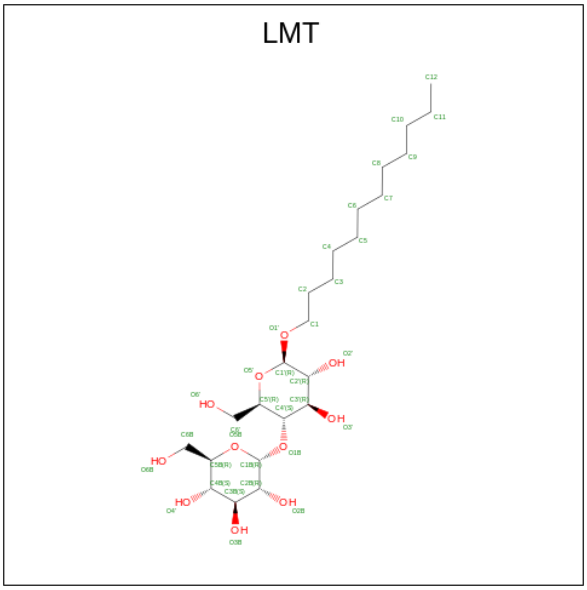
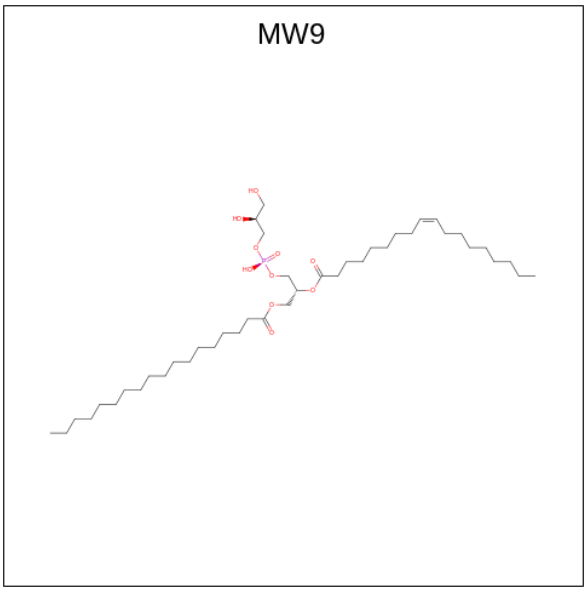
Mol	Chain	Residues	Atoms			AltConf
9	N	1	Total	C	O	0
			43	41	2	
9	K	1	Total	C	O	0
			43	41	2	
9	K	1	Total	C	O	0
			43	41	2	
9	J	1	Total	C	O	0
			43	41	2	
9	J	1	Total	C	O	0
			43	41	2	
9	i	1	Total	C	O	0
			43	41	2	
9	I	1	Total	C	O	0
			43	41	2	
9	G	1	Total	C	O	0
			43	41	2	
9	G	1	Total	C	O	0
			43	41	2	
9	F	1	Total	C	O	0
			43	41	2	
9	F	1	Total	C	O	0
			43	41	2	
9	E	1	Total	C	O	0
			43	41	2	
9	d	1	Total	C	O	0
			43	41	2	
9	D	1	Total	C	O	0
			43	41	2	
9	D	1	Total	C	O	0
			43	41	2	
9	b	1	Total	C	O	0
			43	41	2	
9	a	1	Total	C	O	0
			43	41	2	
9	a	1	Total	C	O	0
			43	41	2	
9	A	1	Total	C	O	0
			43	41	2	
9	A	1	Total	C	O	0
			43	41	2	
9	M	1	Total	C	O	0
			43	41	2	

- Molecule 10 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms	AltConf
10	S	1	Total C O 35 24 11	0
10	G	1	Total C O 24 18 6	0
10	E	1	Total C O 35 24 11	0
10	B	1	Total C O 24 19 5	0
10	L	1	Total C O 24 19 5	0
10	H	1	Total C O 24 18 6	0
10	C	1	Total C O 35 24 11	0

- Molecule 11 is (21R,24R,27S)-24,27,28-trihydroxy-18,24-dioxo-19,23,25-trioxa-24lambda 5 -phosphaoctacosan-21-yl (9Z)-octadec-9-enoate (CCD ID: MW9) (formula: $C_{42}H_{81}O_{10}P$).

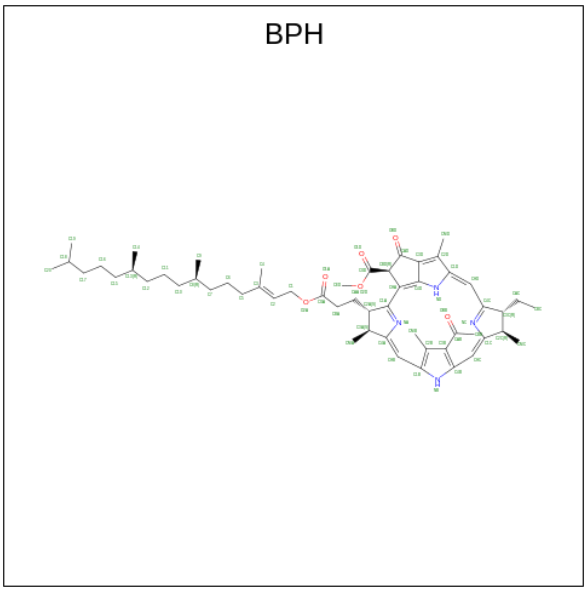


Mol	Chain	Residues	Atoms	AltConf
11	R	1	Total C O P 45 34 10 1	0
11	N	1	Total C O P 53 42 10 1	0
11	G	1	Total C O P 49 38 10 1	0
11	G	1	Total C O P 40 29 10 1	0
11	F	1	Total C O P 43 32 10 1	0
11	D	1	Total C O P 27 19 7 1	0
11	M	1	Total C O P 49 38 10 1	0
11	L	1	Total C O P 37 26 10 1	0
11	H	1	Total C O P 48 37 10 1	0
11	H	1	Total C O P 37 28 8 1	0

- Molecule 12 is FE (III) ION (CCD ID: FE) (formula: Fe).

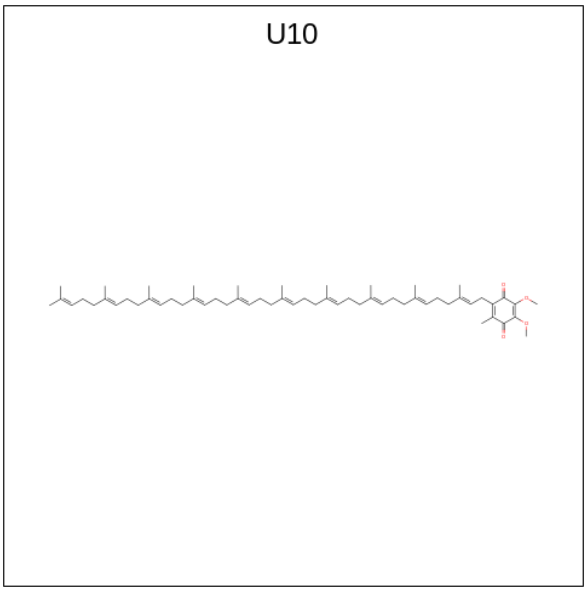
Mol	Chain	Residues	Atoms	AltConf
12	M	1	Total Fe 1 1	0

- Molecule 13 is BACTERIOPHEOPHYTIN A (CCD ID: BPH) (formula: $C_{55}H_{76}N_4O_6$).



Mol	Chain	Residues	Atoms				AltConf
13	M	1	Total	C	N	O	0
			65	55	4	6	
13	L	1	Total	C	N	O	0
			65	55	4	6	

- Molecule 14 is UBIQUINONE-10 (CCD ID: U10) (formula: $C_{59}H_{90}O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
14	M	1	Total	C	O	0
			63	59	4	

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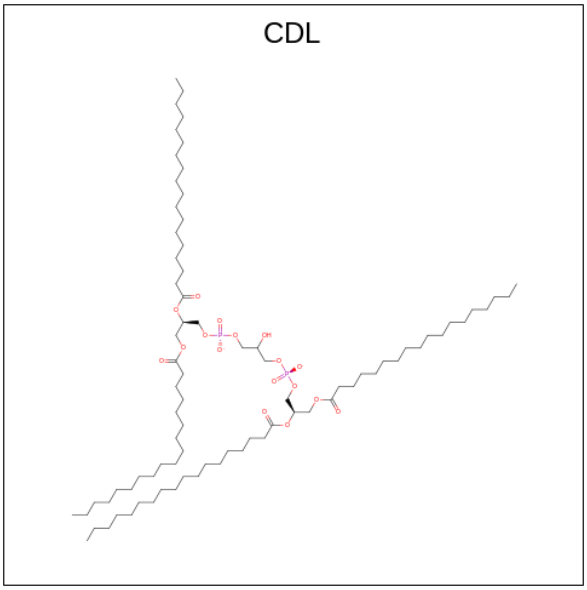
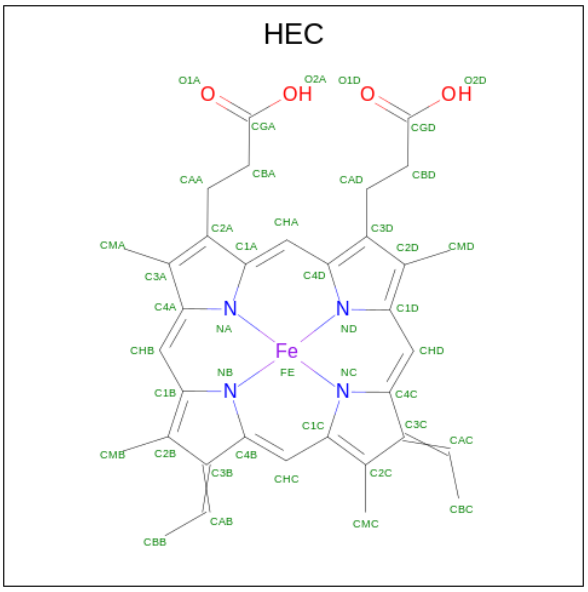
Mol	Chain	Residues	Atoms			AltConf
14	L	1	Total	C	O	0
			48	44	4	

- Molecule 15 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



Mol	Chain	Residues	Atoms				AltConf
15	M	1	Total	C	O	P	0
			67	48	17	2	
15	H	1	Total	C	O	P	0
			100	81	17	2	

- Molecule 16 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{34}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



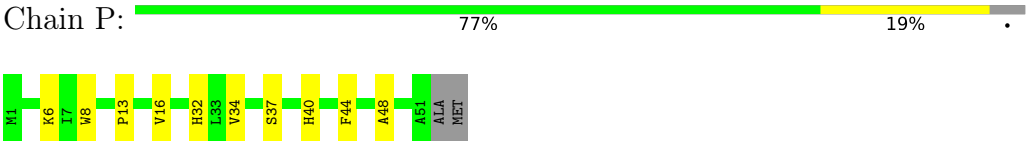
Mol	Chain	Residues	Atoms					AltConf
16	C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
16	C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
16	C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

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. 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. 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.

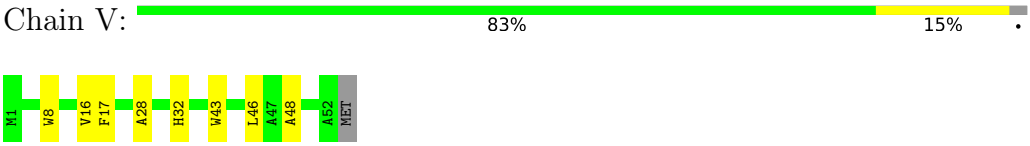
• Molecule 1: Antenna pigment protein alpha chain

Chain P:



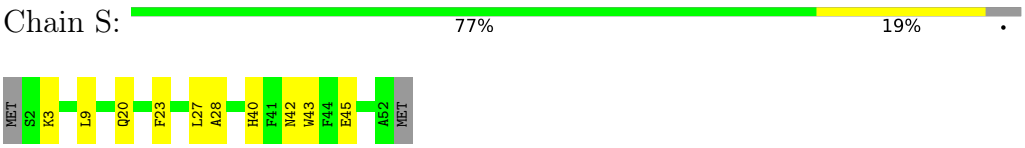
• Molecule 1: Antenna pigment protein alpha chain

Chain V:



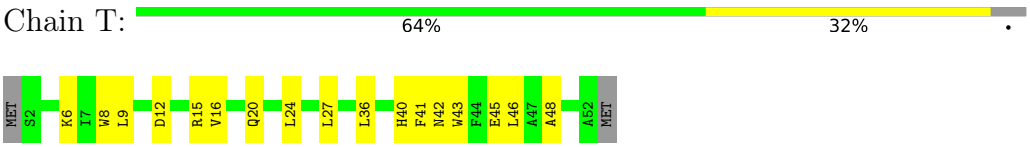
• Molecule 1: Antenna pigment protein alpha chain

Chain S:



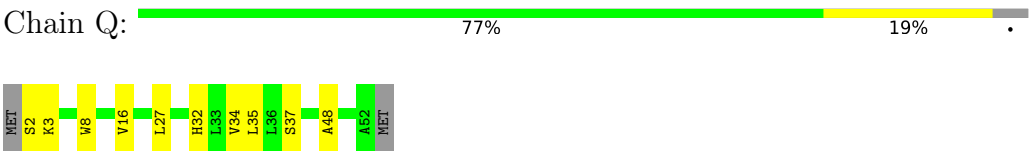
• Molecule 1: Antenna pigment protein alpha chain

Chain T:



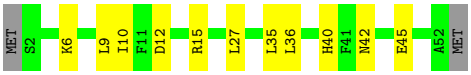
• Molecule 1: Antenna pigment protein alpha chain

Chain Q:



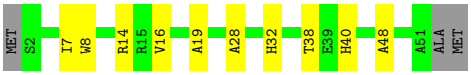
• Molecule 1: Antenna pigment protein alpha chain

Chain R:



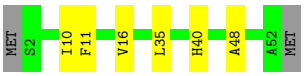
• Molecule 1: Antenna pigment protein alpha chain

Chain 1:



• Molecule 1: Antenna pigment protein alpha chain

Chain N:



• Molecule 1: Antenna pigment protein alpha chain

Chain K:

• Molecule 1: Antenna pigment protein alpha chain

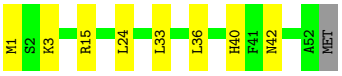
Chain J:

• Molecule 1: Antenna pigment protein alpha chain

Chain I:

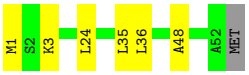
• Molecule 1: Antenna pigment protein alpha chain

Chain G:



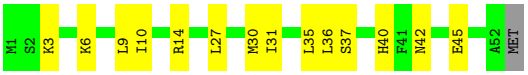
• Molecule 1: Antenna pigment protein alpha chain

Chain F:



• Molecule 1: Antenna pigment protein alpha chain

Chain E:

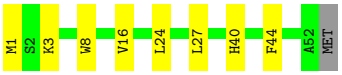


• Molecule 1: Antenna pigment protein alpha chain

Chain D:

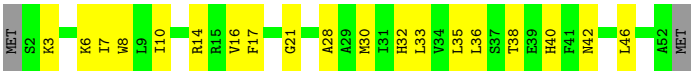
• Molecule 1: Antenna pigment protein alpha chain

Chain B:



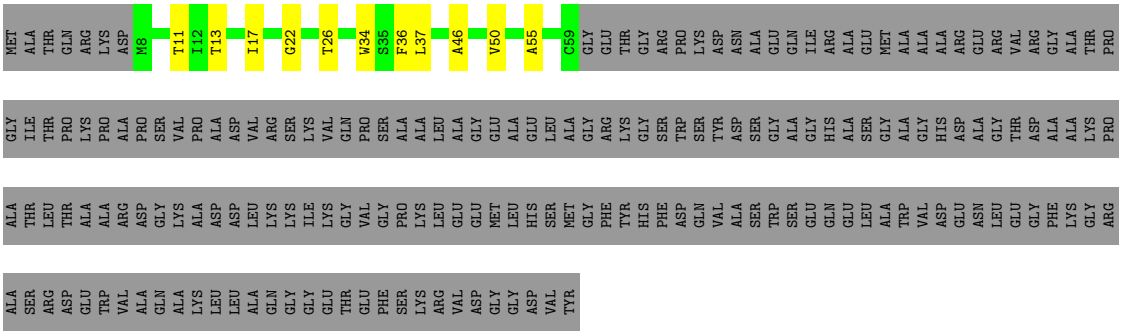
• Molecule 1: Antenna pigment protein alpha chain

Chain A:



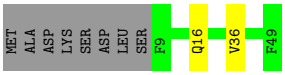
• Molecule 2: Reaction center protein O chain

Chain O:



• Molecule 3: Antenna pigment protein beta chain

Chain v:



• Molecule 3: Antenna pigment protein beta chain

Chain t:

• Molecule 3: Antenna pigment protein beta chain

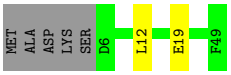
Chain s:

• Molecule 3: Antenna pigment protein beta chain

Chain r:

• Molecule 3: Antenna pigment protein beta chain

Chain q:



• Molecule 3: Antenna pigment protein beta chain

Chain p:

• Molecule 3: Antenna pigment protein beta chain

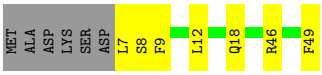
Chain 2:

• Molecule 3: Antenna pigment protein beta chain

Chain n:

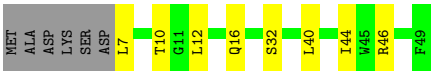
• Molecule 3: Antenna pigment protein beta chain

Chain k:



• Molecule 3: Antenna pigment protein beta chain

Chain j:

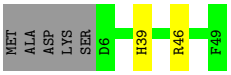


• Molecule 3: Antenna pigment protein beta chain

Chain i:

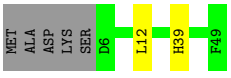
• Molecule 3: Antenna pigment protein beta chain

Chain g:



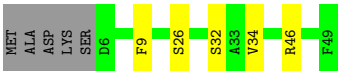
• Molecule 3: Antenna pigment protein beta chain

Chain f:



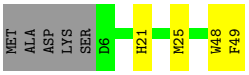
• Molecule 3: Antenna pigment protein beta chain

Chain e:



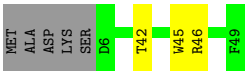
• Molecule 3: Antenna pigment protein beta chain

Chain d:



• Molecule 3: Antenna pigment protein beta chain

Chain b:

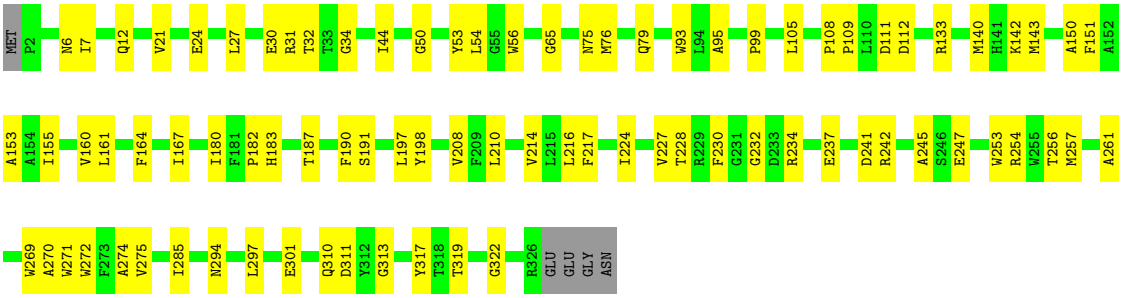


• Molecule 3: Antenna pigment protein beta chain

Chain a:

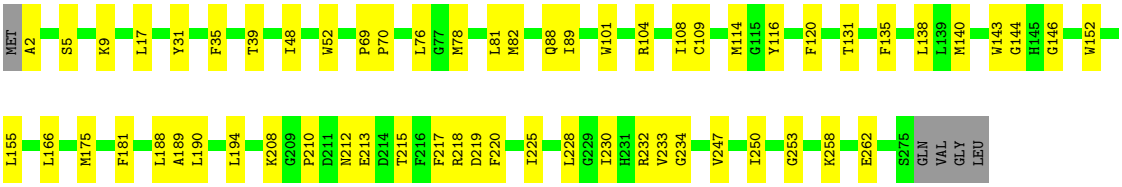
• Molecule 4: Reaction center protein M chain

Chain M:



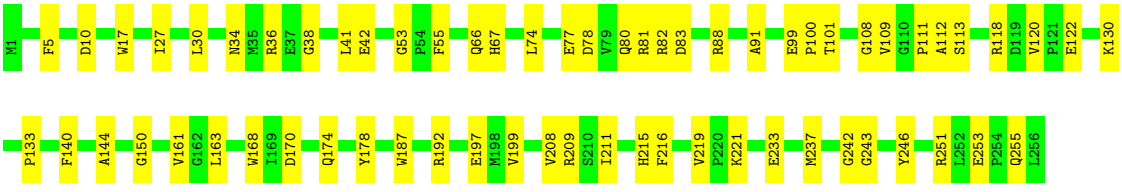
• Molecule 5: Reaction center protein L chain

Chain L:



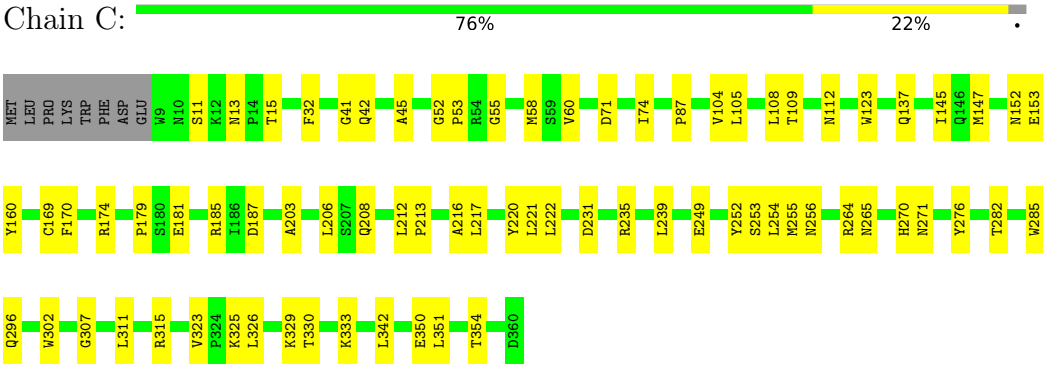
• Molecule 6: Reaction center protein H chain

Chain H:



• Molecule 7: Photosynthetic reaction center cytochrome c subunit

Chain C:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	1106552	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MW9, CDL, BCL, U10, LMT, HEC, A1EFU, FE, BPH

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	1	0.11	0/431	0.36	0/585
1	A	0.09	0/436	0.21	0/592
1	B	0.10	0/444	0.27	0/602
1	D	0.09	0/444	0.20	0/602
1	E	0.12	0/444	0.24	0/602
1	F	0.11	0/444	0.20	0/602
1	G	0.10	0/444	0.20	0/602
1	I	0.10	0/436	0.21	0/592
1	J	0.09	0/431	0.18	0/585
1	K	0.10	0/436	0.23	0/592
1	N	0.11	0/436	0.24	0/592
1	P	0.08	0/439	0.22	0/595
1	Q	0.08	0/436	0.19	0/592
1	R	0.09	0/436	0.26	0/592
1	S	0.07	0/436	0.20	0/592
1	T	0.07	0/436	0.17	0/592
1	V	0.07	0/444	0.21	0/602
2	O	0.06	0/378	0.22	0/516
3	2	0.10	0/367	0.26	0/503
3	a	0.08	0/371	0.29	0/508
3	b	0.09	0/371	0.24	0/508
3	d	0.09	0/367	0.17	0/503
3	e	0.09	0/367	0.16	0/503
3	f	0.08	0/367	0.18	0/503
3	g	0.08	0/367	0.15	0/503
3	i	0.09	0/359	0.18	0/492
3	j	0.08	0/359	0.17	0/492
3	k	0.08	0/359	0.18	0/492
3	n	0.08	0/367	0.19	0/503
3	p	0.09	0/367	0.26	0/503
3	q	0.07	0/367	0.21	0/503
3	r	0.06	0/359	0.19	0/492

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
3	s	0.07	0/367	0.17	0/503
3	t	0.08	0/359	0.19	0/492
3	v	0.06	0/345	0.16	0/473
4	M	0.13	0/2731	0.27	0/3735
5	L	0.13	0/2267	0.25	0/3105
6	H	0.13	0/2072	0.29	0/2804
7	C	0.13	0/2818	0.29	0/3868
All	All	0.11	0/23904	0.24	0/32617

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	1	417	0	421	9	0
1	A	422	0	426	14	0
1	B	430	0	438	6	0
1	D	430	0	438	8	0
1	E	430	0	438	14	0
1	F	430	0	437	5	0
1	G	430	0	438	7	0
1	I	422	0	426	6	0
1	J	417	0	421	6	0
1	K	422	0	426	10	0
1	N	422	0	426	6	0
1	P	425	0	433	9	0
1	Q	422	0	426	8	0
1	R	422	0	426	8	0
1	S	422	0	426	9	0
1	T	422	0	426	18	0
1	V	430	0	438	5	0
2	O	371	0	393	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	2	354	0	334	5	0
3	a	358	0	338	4	0
3	b	358	0	338	2	0
3	d	354	0	334	5	0
3	e	354	0	334	7	0
3	f	354	0	334	2	0
3	g	354	0	334	2	0
3	i	346	0	330	3	0
3	j	346	0	330	7	0
3	k	346	0	330	12	0
3	n	354	0	334	8	0
3	p	354	0	334	2	0
3	q	354	0	334	2	0
3	r	346	0	330	5	0
3	s	354	0	334	3	0
3	t	346	0	330	13	0
3	v	332	0	314	2	0
4	M	2633	0	2522	73	0
5	L	2178	0	2118	57	0
6	H	2022	0	1971	52	0
7	C	2740	0	2581	61	0
8	1	132	0	147	4	0
8	A	66	0	74	5	0
8	B	66	0	71	3	0
8	D	66	0	74	6	0
8	E	66	0	74	6	0
8	F	66	0	73	3	0
8	G	132	0	146	5	0
8	I	132	0	145	4	0
8	J	66	0	74	5	0
8	K	132	0	145	5	0
8	L	132	0	145	13	0
8	M	132	0	144	11	0
8	N	66	0	74	3	0
8	P	132	0	146	3	0
8	Q	66	0	74	2	0
8	R	66	0	74	4	0
8	S	66	0	74	3	0
8	T	66	0	74	4	0
8	V	66	0	73	6	0
8	a	66	0	74	4	0
8	b	66	0	71	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	d	66	0	71	9	0
8	e	66	0	74	10	0
8	f	66	0	74	4	0
8	j	66	0	74	8	0
8	n	66	0	74	6	0
8	q	66	0	74	4	0
8	r	66	0	74	6	0
8	s	66	0	72	5	0
8	t	66	0	73	9	0
8	v	66	0	74	5	0
9	1	86	0	0	0	0
9	A	86	0	0	0	0
9	D	86	0	0	0	0
9	E	43	0	0	0	0
9	F	86	0	0	0	0
9	G	86	0	0	0	0
9	I	43	0	0	0	0
9	J	86	0	0	1	0
9	K	86	0	0	0	0
9	M	43	0	0	0	0
9	N	43	0	0	0	0
9	P	43	0	0	0	0
9	Q	43	0	0	0	0
9	R	43	0	0	0	0
9	S	86	0	0	0	0
9	T	86	0	0	0	0
9	a	86	0	0	0	0
9	b	43	0	0	0	0
9	d	43	0	0	0	0
9	i	43	0	0	0	0
9	n	43	0	0	0	0
9	p	43	0	0	0	0
9	q	43	0	0	0	0
9	r	43	0	0	0	0
9	v	43	0	0	0	0
10	B	24	0	31	1	0
10	C	35	0	46	2	0
10	E	35	0	45	3	0
10	G	24	0	34	1	0
10	H	24	0	34	0	0
10	L	24	0	31	1	0
10	S	35	0	45	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	D	27	0	0	0	0
11	F	43	0	0	0	0
11	G	89	0	0	0	0
11	H	85	0	0	1	0
11	L	37	0	0	0	0
11	M	49	0	0	0	0
11	N	53	0	0	0	0
11	R	45	0	0	1	0
12	M	1	0	0	0	0
13	L	65	0	74	1	0
13	M	65	0	73	3	0
14	L	48	0	63	5	0
14	M	63	0	90	12	0
15	H	100	0	153	13	0
15	M	67	0	78	5	0
16	C	129	0	88	10	0
All	All	28303	0	26206	495	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 9.

All (495) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:131:THR:HA	5:L:135:PHE:HB2	1.62	0.82
6:H:168:TRP:HB2	6:H:178:TYR:HB2	1.67	0.77
1:B:1:MET:HG2	1:B:3:LYS:H	1.52	0.74
4:M:313:GLY:HA2	7:C:282:THR:HG23	1.67	0.74
3:d:48:TRP:CE2	8:d:102:BCL:HHC	2.22	0.73
4:M:53:TYR:O	4:M:133:ARG:NH2	2.22	0.73
7:C:185:ARG:NH1	7:C:187:ASP:OD2	2.22	0.73
5:L:140:MET:HE2	5:L:253:GLY:HA3	1.70	0.72
4:M:319:THR:HG23	4:M:322:GLY:H	1.55	0.71
8:D:101:BCL:HMA1	8:B:102:BCL:HMA1	1.73	0.70
4:M:234:ARG:NH2	6:H:233:GLU:OE2	2.24	0.69
1:Q:3:LYS:NZ	3:r:19:GLU:OE2	2.26	0.68
1:B:24:LEU:HA	1:B:27:LEU:HD12	1.76	0.68
1:G:36:LEU:O	1:G:42:ASN:ND2	2.27	0.67
1:T:6:LYS:HA	1:T:9:LEU:HD23	1.77	0.67
4:M:210:LEU:HD13	8:M:402:BCL:H3A	1.76	0.67
8:v:102:BCL:H12	8:v:102:BCL:H3A	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:256:THR:O	5:L:104:ARG:NH2	2.29	0.66
4:M:261:ALA:HB2	14:M:405:U10:H112	1.77	0.66
8:L:301:BCL:H112	8:L:304:BCL:HBB2	1.78	0.66
4:M:133:ARG:NH1	5:L:220:PHE:O	2.29	0.65
4:M:198:TYR:HB3	5:L:155:LEU:HD23	1.78	0.65
6:H:100:PRO:HB3	6:H:109:VAL:HG21	1.78	0.65
7:C:147:MET:HE2	7:C:302:TRP:HB3	1.78	0.65
6:H:10:ASP:OD1	7:C:235:ARG:NH1	2.31	0.64
1:1:8:TRP:HZ3	1:1:16:VAL:HG11	1.61	0.64
6:H:130:LYS:NZ	6:H:170:ASP:OD2	2.31	0.64
7:C:255:MET:HG2	16:C:402:HEC:NB	2.11	0.64
1:E:37:SER:HB2	5:L:82:MET:HE3	1.79	0.64
4:M:242:ARG:NH1	4:M:247:GLU:OE2	2.32	0.63
7:C:60:VAL:HG11	7:C:264:ARG:HD3	1.81	0.62
7:C:330:THR:O	7:C:333:LYS:NZ	2.31	0.62
1:G:15:ARG:NH1	6:H:53:GLY:O	2.33	0.62
5:L:31:TYR:O	5:L:104:ARG:NH1	2.32	0.62
8:f:101:BCL:HAC2	1:F:35:LEU:HD11	1.82	0.61
4:M:12:GLN:HE21	6:H:144:ALA:HB3	1.66	0.61
4:M:95:ALA:HB2	4:M:182:PRO:HG2	1.83	0.61
6:H:192:ARG:HG2	6:H:219:VAL:HB	1.82	0.61
3:r:9:PHE:HB2	1:R:10:ILE:HA	1.82	0.60
7:C:71:ASP:HB3	7:C:74:ILE:HG13	1.81	0.60
1:I:38:THR:HG22	1:I:40:HIS:H	1.67	0.59
4:M:50:GLY:HA3	5:L:218:ARG:HD3	1.84	0.59
7:C:58:MET:HE3	7:C:271:ASN:HA	1.84	0.59
7:C:206:LEU:O	7:C:208:GLN:NE2	2.34	0.59
3:t:8:SER:HA	1:T:9:LEU:HD12	1.85	0.59
1:E:6:LYS:HA	1:E:9:LEU:HD13	1.85	0.59
6:H:82:ARG:NH1	6:H:108:GLY:O	2.34	0.59
4:M:208:VAL:HG22	8:L:304:BCL:HAA2	1.83	0.59
1:A:36:LEU:O	1:A:42:ASN:ND2	2.32	0.58
8:V:101:BCL:H91	1:T:20:GLN:HG3	1.85	0.58
8:d:102:BCL:H3C	1:D:35:LEU:HD21	1.86	0.58
6:H:17:TRP:NE1	11:H:302:MW9:O3	2.31	0.58
3:d:49:PHE:HZ	8:d:102:BCL:HBB1	1.66	0.57
3:i:13:THR:HB	3:i:16:GLN:HG3	1.86	0.57
8:j:101:BCL:HED3	1:J:27:LEU:HD23	1.87	0.57
6:H:211:ILE:HG23	6:H:215:HIS:HB2	1.85	0.57
3:j:10:THR:HG23	3:j:12:LEU:HD13	1.85	0.57
4:M:269:TRP:CD1	6:H:34:ASN:HD21	2.22	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:M:405:U10:H222	8:L:304:BCL:H51	1.86	0.57
3:e:26:SER:OG	1:D:1:MET:N	2.36	0.57
4:M:21:VAL:HG22	5:L:215:THR:HG21	1.87	0.57
5:L:70:PRO:HG3	5:L:88:GLN:HE21	1.70	0.57
4:M:75:ASN:O	4:M:79:GLN:HG2	2.06	0.56
4:M:254:ARG:NH2	15:H:303:CDL:OB3	2.39	0.56
7:C:123:TRP:CG	7:C:170:PHE:HB2	2.39	0.56
7:C:152:ASN:ND2	7:C:351:LEU:O	2.38	0.56
7:C:169:CYS:HA	16:C:401:HEC:HHC	1.87	0.56
8:L:304:BCL:H102	15:H:303:CDL:H602	1.88	0.56
7:C:123:TRP:HE3	7:C:169:CYS:HB3	1.70	0.56
1:T:24:LEU:HB2	8:T:102:BCL:H42	1.87	0.56
1:I:36:LEU:O	1:I:42:ASN:ND2	2.38	0.56
4:M:7:ILE:HG13	15:M:408:CDL:H742	1.88	0.56
6:H:111:PRO:HB2	6:H:242:GLY:HA2	1.86	0.56
1:J:36:LEU:O	1:J:42:ASN:ND2	2.37	0.56
7:C:270:HIS:HE1	16:C:402:HEC:NB	2.01	0.56
3:q:12:LEU:HD11	3:p:9:PHE:HZ	1.71	0.56
3:t:48:TRP:HE1	8:t:101:BCL:HBB2	1.70	0.55
1:T:36:LEU:O	1:T:42:ASN:ND2	2.40	0.55
1:R:36:LEU:O	1:R:42:ASN:ND2	2.39	0.55
8:e:101:BCL:HHD	1:E:35:LEU:HD11	1.88	0.55
7:C:216:ALA:HB1	7:C:254:LEU:HB2	1.88	0.55
3:t:46:ARG:HH21	1:T:46:LEU:HD22	1.72	0.55
5:L:217:PHE:HA	5:L:220:PHE:HB3	1.87	0.55
1:P:6:LYS:NZ	3:q:19:GLU:OE1	2.39	0.55
4:M:161:LEU:HD23	4:M:285:ILE:HG21	1.87	0.55
1:G:33:LEU:HD21	10:G:107:LMT:H42	1.88	0.55
10:E:103:LMT:H2'	1:D:38:THR:HG22	1.87	0.54
3:e:9:PHE:HB2	1:E:10:ILE:HA	1.88	0.54
1:B:44:PHE:HB3	1:A:38:THR:HG21	1.89	0.54
8:r:101:BCL:HBC3	1:R:35:LEU:HD11	1.89	0.54
4:M:253:TRP:HB3	4:M:257:MET:HE2	1.89	0.54
5:L:190:LEU:HB2	14:L:303:U10:H1M2	1.90	0.54
1:E:45:GLU:OE1	10:E:103:LMT:O3'	2.25	0.54
5:L:208:LYS:HB3	5:L:212:ASN:HB2	1.90	0.54
8:Q:102:BCL:HBD	8:q:101:BCL:HBD	1.88	0.54
7:C:41:GLY:HA3	10:C:404:LMT:H6E	1.90	0.54
3:2:16:GLN:HB3	3:n:7:LEU:HD22	1.89	0.54
3:a:26:SER:HA	3:a:29:TRP:HB2	1.90	0.54
3:k:18:GLN:HA	1:K:5:TYR:HB2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:k:9:PHE:HD2	1:K:10:ILE:HG22	1.73	0.53
3:a:9:PHE:HB2	1:A:10:ILE:HA	1.90	0.53
4:M:270:ALA:HB1	5:L:188:LEU:HD11	1.89	0.53
7:C:52:GLY:HA3	7:C:58:MET:SD	2.49	0.53
4:M:27:LEU:HG	4:M:140:MET:HE2	1.89	0.53
8:M:402:BCL:HAA2	8:M:402:BCL:HBD	1.89	0.53
4:M:217:PHE:HB2	5:L:188:LEU:HD13	1.90	0.53
4:M:257:MET:CE	14:M:405:U10:H13	2.39	0.53
8:I:102:BCL:CAD	8:I:103:BCL:HBD	2.39	0.53
8:b:101:BCL:H171	1:A:7:ILE:HG21	1.90	0.53
5:L:69:PRO:HB2	5:L:144:GLY:HA2	1.90	0.53
4:M:30:GLU:O	4:M:54:LEU:N	2.37	0.53
4:M:160:VAL:HA	4:M:164:PHE:HB2	1.90	0.53
4:M:183:HIS:O	4:M:187:THR:OG1	2.26	0.53
6:H:55:PHE:HZ	15:H:303:CDL:H171	1.73	0.53
1:S:27:LEU:HD23	8:s:101:BCL:HED3	1.90	0.52
3:a:46:ARG:NE	1:A:40:HIS:O	2.39	0.52
7:C:212:LEU:HB3	7:C:253:SER:HB2	1.91	0.52
6:H:209:ARG:O	6:H:251:ARG:NH2	2.37	0.52
3:v:16:GLN:HE21	3:t:7:LEU:HD23	1.74	0.52
3:r:13:THR:H	3:r:16:GLN:NE2	2.07	0.52
8:r:101:BCL:HBD	8:R:101:BCL:HBD	1.91	0.52
1:I:11:PHE:HB3	1:I:16:VAL:HG21	1.92	0.52
5:L:69:PRO:HD2	7:C:55:GLY:HA2	1.92	0.52
5:L:9:LYS:HD2	6:H:113:SER:HB2	1.91	0.51
2:O:34:TRP:NE1	10:S:301:LMT:O2'	2.36	0.51
1:S:42:ASN:ND2	1:S:45:GLU:OE1	2.43	0.51
1:P:48:ALA:HB2	1:1:40:HIS:HB2	1.92	0.51
1:Q:32:HIS:HE1	8:Q:102:BCL:NA	2.09	0.51
6:H:111:PRO:HD2	6:H:246:TYR:CE2	2.45	0.51
1:Q:27:LEU:HD23	8:q:101:BCL:HED3	1.91	0.51
7:C:222:LEU:HD22	7:C:325:LYS:HE3	1.93	0.51
8:t:101:BCL:HED3	1:T:27:LEU:HD23	1.93	0.51
8:n:101:BCL:HBD	8:N:101:BCL:HBD	1.93	0.51
1:F:24:LEU:HB2	8:F:101:BCL:H42	1.92	0.51
7:C:206:LEU:HD22	7:C:217:LEU:HD12	1.93	0.51
8:G:101:BCL:CAD	8:G:102:BCL:HBD	2.40	0.50
6:H:36:ARG:HB3	6:H:74:LEU:HB3	1.92	0.50
1:1:48:ALA:HB2	1:N:40:HIS:HB2	1.94	0.50
1:D:36:LEU:O	1:D:42:ASN:ND2	2.44	0.50
14:M:405:U10:H552	15:H:303:CDL:H471	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:88:ARG:HD2	6:H:101:THR:HG22	1.92	0.50
7:C:315:ARG:NE	16:C:401:HEC:O2A	2.44	0.50
3:j:12:LEU:HA	3:j:16:GLN:HE21	1.76	0.50
3:g:39:HIS:CD2	8:G:102:BCL:HMD3	2.47	0.50
4:M:105:LEU:HD11	4:M:167:ILE:HA	1.94	0.50
4:M:65:GLY:HA3	13:M:403:BPH:H5C1	1.93	0.50
3:j:12:LEU:HD11	3:i:9:PHE:HZ	1.77	0.50
4:M:310:GLN:HB2	7:C:53:PRO:HB3	1.94	0.50
1:P:8:TRP:HZ3	1:P:16:VAL:HG11	1.77	0.50
1:P:13:PRO:HD2	3:2:9:PHE:HE2	1.76	0.50
1:P:32:HIS:HE1	8:P:101:BCL:NA	2.08	0.50
3:t:46:ARG:HD3	1:T:40:HIS:CE1	2.47	0.50
8:r:101:BCL:HED3	1:R:27:LEU:HD23	1.93	0.50
4:M:153:ALA:HB2	4:M:275:VAL:HG13	1.94	0.50
7:C:87:PRO:HB3	7:C:109:THR:HG21	1.93	0.50
4:M:261:ALA:HA	6:H:34:ASN:HB3	1.93	0.50
3:t:12:LEU:HG	3:t:16:GLN:HE22	1.77	0.49
1:Q:35:LEU:HD11	8:q:101:BCL:HHD	1.94	0.49
1:A:33:LEU:HA	1:A:36:LEU:HD12	1.94	0.49
7:C:252:TYR:CE1	16:C:402:HEC:HMB2	2.46	0.49
1:A:14:ARG:HD2	7:C:15:THR:HG21	1.94	0.49
7:C:174:ARG:HG3	7:C:333:LYS:HE2	1.93	0.49
6:H:77:GLU:O	6:H:77:GLU:HG3	2.12	0.49
1:B:8:TRP:HZ3	1:B:16:VAL:HG11	1.77	0.49
4:M:190:PHE:HD2	4:M:197:LEU:HD11	1.77	0.49
3:n:36:VAL:HG22	8:n:101:BCL:H92	1.94	0.49
3:k:12:LEU:HD11	3:j:7:LEU:HD13	1.95	0.49
3:j:32:SER:HB3	8:j:101:BCL:H72	1.93	0.49
3:j:46:ARG:NH1	1:J:40:HIS:O	2.45	0.49
7:C:137:GLN:NE2	16:C:401:HEC:O1A	2.45	0.49
5:L:225:ILE:HG22	14:L:303:U10:H3M3	1.95	0.49
3:t:48:TRP:HB3	1:T:41:PHE:CZ	2.48	0.49
4:M:257:MET:HE1	14:M:405:U10:H13	1.95	0.49
15:M:408:CDL:HB62	5:L:116:TYR:HB2	1.94	0.49
1:V:8:TRP:HZ3	1:V:16:VAL:HG11	1.78	0.49
3:p:6:ASP:OD1	3:p:6:ASP:N	2.43	0.48
5:L:225:ILE:H	14:L:303:U10:H3M3	1.75	0.48
1:S:40:HIS:HB2	1:T:48:ALA:HB2	1.94	0.48
3:t:48:TRP:CZ2	8:t:101:BCL:HHC	2.49	0.48
8:d:102:BCL:HHD	1:D:35:LEU:HD11	1.94	0.48
14:M:405:U10:H261	15:H:303:CDL:H562	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:e:101:BCL:HBD	8:E:101:BCL:HBD	1.96	0.48
4:M:30:GLU:HB2	4:M:53:TYR:CE1	2.49	0.48
7:C:221:LEU:HD13	7:C:295:VAL:HG11	1.95	0.48
3:n:16:GLN:HE22	3:k:7:LEU:HB3	1.77	0.48
10:E:103:LMT:H3'	10:E:103:LMT:H1B	1.61	0.48
2:O:11:THR:HG23	2:O:55:ALA:HB1	1.95	0.48
1:E:3:LYS:HD2	1:E:6:LYS:HE3	1.94	0.48
1:A:30:MET:HB2	7:C:32:PHE:HD1	1.78	0.48
3:n:9:PHE:HB2	1:N:10:ILE:HA	1.95	0.48
3:k:8:SER:HB3	3:k:12:LEU:H	1.79	0.48
8:a:102:BCL:HHD	1:A:35:LEU:HD11	1.96	0.48
2:O:46:ALA:O	2:O:50:VAL:HG12	2.14	0.48
3:t:24:TYR:HE1	1:T:20:GLN:HE22	1.61	0.48
1:N:48:ALA:HB2	1:K:40:HIS:HB2	1.95	0.48
7:C:179:PRO:HD2	16:C:401:HEC:HBD2	1.96	0.47
3:2:40:LEU:O	3:2:44:ILE:HD12	2.14	0.47
1:1:14:ARG:NH2	3:n:9:PHE:HB3	2.30	0.47
1:E:30:MET:SD	5:L:48:ILE:HG21	2.54	0.47
7:C:326:LEU:HD22	16:C:401:HEC:HBC2	1.95	0.47
1:K:24:LEU:HB2	8:K:102:BCL:H42	1.96	0.47
8:a:102:BCL:HBD	8:A:101:BCL:HBD	1.95	0.47
4:M:143:MET:HG2	5:L:208:LYS:HG3	1.97	0.47
8:L:304:BCL:H61	8:L:304:BCL:H41	1.70	0.47
6:H:88:ARG:NH1	6:H:99:GLU:HB3	2.30	0.47
10:C:404:LMT:H5'	10:C:404:LMT:H1B	1.44	0.47
1:P:44:PHE:HB3	1:1:38:THR:HG21	1.95	0.47
2:O:22:GLY:O	2:O:26:THR:OG1	2.29	0.47
1:Q:2:SER:OG	1:Q:3:LYS:N	2.46	0.47
1:F:48:ALA:HB2	1:E:40:HIS:HB2	1.96	0.47
6:H:178:TYR:OH	6:H:237:MET:HE3	2.15	0.47
3:s:13:THR:HG23	3:s:16:GLN:H	1.80	0.47
8:e:101:BCL:H2C	8:e:101:BCL:HBC3	1.64	0.47
1:A:8:TRP:HZ3	1:A:16:VAL:HG11	1.79	0.47
4:M:241:ASP:OD1	6:H:80:GLN:NE2	2.39	0.47
7:C:239:LEU:H	7:C:239:LEU:HD23	1.80	0.47
1:V:43:TRP:HA	1:V:46:LEU:HD12	1.97	0.47
8:v:102:BCL:H111	8:v:102:BCL:H93	1.63	0.47
3:k:46:ARG:NH2	1:K:40:HIS:O	2.47	0.47
8:E:101:BCL:HBB1	8:d:102:BCL:HMC3	1.96	0.47
8:E:101:BCL:HBC3	8:E:101:BCL:H2C	1.71	0.47
4:M:216:LEU:HD21	14:M:405:U10:H18	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:L:304:BCL:H141	8:L:304:BCL:H161	1.66	0.47
8:D:101:BCL:HAA1	8:D:101:BCL:CGD	2.45	0.47
5:L:76:LEU:O	5:L:143:TRP:NE1	2.43	0.47
5:L:194:LEU:HD22	5:L:217:PHE:HE2	1.80	0.47
1:S:43:TRP:CZ3	8:S:302:BCL:H2C	2.50	0.46
3:t:48:TRP:HZ2	8:t:101:BCL:HHC	1.79	0.46
4:M:191:SER:HB2	8:M:402:BCL:H3C	1.96	0.46
5:L:81:LEU:HD11	5:L:89:ILE:HD12	1.96	0.46
6:H:118:ARG:HB3	6:H:120:VAL:HG22	1.97	0.46
1:I:20:GLN:HA	1:I:23:PHE:HB3	1.97	0.46
4:M:311:ASP:O	4:M:317:TYR:OH	2.30	0.46
8:a:102:BCL:H121	8:a:102:BCL:H162	1.76	0.46
6:H:150:GLY:HA2	6:H:163:LEU:HD12	1.96	0.46
8:j:101:BCL:HAC2	1:J:35:LEU:HD11	1.98	0.46
8:B:102:BCL:H142	8:B:102:BCL:H111	1.70	0.46
4:M:44:ILE:O	5:L:232:ARG:HD2	2.14	0.46
3:t:48:TRP:HB3	1:T:41:PHE:HZ	1.80	0.46
8:t:101:BCL:H162	8:t:101:BCL:H141	1.70	0.46
6:H:170:ASP:O	6:H:174:GLN:N	2.48	0.46
4:M:109:PRO:HG2	4:M:112:ASP:HB3	1.98	0.46
1:S:28:ALA:HB2	8:s:101:BCL:HED2	1.97	0.46
8:F:101:BCL:HBC3	8:F:101:BCL:H2C	1.75	0.46
7:C:289:MET:SD	16:C:402:HEC:HAD1	2.56	0.46
1:R:12:ASP:HB3	1:R:15:ARG:HB3	1.98	0.46
1:G:24:LEU:HB2	8:G:102:BCL:H42	1.97	0.46
3:d:21:HIS:CE1	3:d:25:MET:HE3	2.50	0.46
4:M:32:THR:HG22	4:M:34:GLY:H	1.80	0.46
3:k:46:ARG:NH1	1:K:46:LEU:HD22	2.31	0.46
5:L:194:LEU:HD22	5:L:217:PHE:CE2	2.51	0.46
8:L:304:BCL:H8	8:L:304:BCL:H3A	1.98	0.46
8:V:101:BCL:C1B	8:t:101:BCL:HMB2	2.46	0.45
1:A:17:PHE:O	1:A:21:GLY:N	2.37	0.45
8:1:102:BCL:H162	8:1:102:BCL:H122	1.72	0.45
8:M:404:BCL:H152	8:M:404:BCL:H112	1.77	0.45
1:A:42:ASN:O	1:A:46:LEU:N	2.42	0.45
4:M:237:GLU:OE2	6:H:118:ARG:NH2	2.48	0.45
5:L:258:LYS:HD2	5:L:262:GLU:OE2	2.15	0.45
6:H:161:VAL:HG21	6:H:216:PHE:CD2	2.52	0.45
6:H:211:ILE:HD13	6:H:243:GLY:HA3	1.97	0.45
7:C:42:GLN:HG3	7:C:45:ALA:HA	1.99	0.45
3:r:46:ARG:NH1	1:R:40:HIS:O	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:27:LEU:O	1:E:31:ILE:HD12	2.16	0.45
8:b:101:BCL:H141	8:b:101:BCL:H161	1.64	0.45
4:M:151:PHE:O	4:M:155:ILE:HG12	2.17	0.45
7:C:74:ILE:HG23	7:C:342:LEU:HD22	1.98	0.45
8:e:101:BCL:H162	8:e:101:BCL:H141	1.67	0.45
1:E:14:ARG:HH22	6:H:91:ALA:HB2	1.82	0.45
8:V:101:BCL:H93	8:V:101:BCL:H111	1.71	0.45
8:s:101:BCL:H61	8:s:101:BCL:H41	1.69	0.45
8:f:101:BCL:H142	8:f:101:BCL:H111	1.69	0.45
5:L:17:LEU:HB2	5:L:35:PHE:HE2	1.81	0.45
7:C:109:THR:OG1	7:C:112:ASN:ND2	2.48	0.45
8:A:101:BCL:H61	8:A:101:BCL:H41	1.71	0.45
8:T:102:BCL:HBC3	8:T:102:BCL:H2C	1.63	0.45
1:F:1:MET:HE3	1:F:3:LYS:HD3	1.99	0.45
4:M:269:TRP:NE1	6:H:34:ASN:HD21	2.15	0.45
5:L:210:PRO:HA	5:L:213:GLU:HG2	1.98	0.45
3:d:48:TRP:CZ2	8:d:102:BCL:HHC	2.51	0.45
4:M:274:ALA:HB1	5:L:189:ALA:HB2	1.98	0.45
8:L:301:BCL:H62	8:L:301:BCL:H41	1.58	0.45
13:L:302:BPH:HHC	13:L:302:BPH:HBB2	1.99	0.45
8:r:101:BCL:H111	8:r:101:BCL:H72	1.81	0.44
1:1:19:ALA:HB2	4:M:56:TRP:CH2	2.52	0.44
5:L:225:ILE:HD13	5:L:233:VAL:HG11	1.99	0.44
1:S:3:LYS:NZ	3:t:19:GLU:OE2	2.38	0.44
8:1:102:BCL:HBC3	8:1:102:BCL:H2C	1.64	0.44
3:n:13:THR:OG1	3:n:16:GLN:HG3	2.17	0.44
4:M:93:TRP:CD1	7:C:203:ALA:HB2	2.51	0.44
1:T:43:TRP:CZ2	8:T:102:BCL:HHC	2.53	0.44
8:j:101:BCL:CAD	8:J:101:BCL:HBD	2.48	0.44
3:e:46:ARG:HH21	1:E:40:HIS:CD2	2.35	0.44
4:M:180:ILE:HG23	8:M:404:BCL:HED1	1.99	0.44
4:M:198:TYR:CE1	8:M:402:BCL:HMC2	2.53	0.44
4:M:6:ASN:HD22	4:M:228:THR:HG21	1.83	0.44
4:M:183:HIS:HD2	8:M:404:BCL:NC	2.14	0.44
4:M:272:TRP:CD1	6:H:30:LEU:HD21	2.52	0.44
7:C:307:GLY:HA2	7:C:311:LEU:HG	1.99	0.44
1:V:16:VAL:HG13	1:V:17:PHE:HD1	1.83	0.44
8:I:103:BCL:HBC3	8:I:103:BCL:H2C	1.69	0.44
8:j:101:BCL:H93	8:j:101:BCL:H62	1.83	0.44
6:H:161:VAL:HG21	6:H:216:PHE:CE2	2.52	0.44
7:C:153:GLU:OE2	7:C:354:THR:OG1	2.25	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:6:LYS:HA	1:R:9:LEU:HD23	1.99	0.44
1:R:45:GLU:OE2	11:R:103:MW9:O6	2.35	0.44
8:N:101:BCL:HBA1	8:N:101:BCL:H3A	1.72	0.44
8:P:102:BCL:H111	8:P:102:BCL:H143	1.67	0.43
8:n:101:BCL:HAC2	1:N:35:LEU:HD11	2.00	0.43
3:d:49:PHE:CZ	8:d:102:BCL:HBB1	2.51	0.43
7:C:104:VAL:HG13	7:C:105:LEU:HG	1.99	0.43
8:v:102:BCL:H62	8:v:102:BCL:H41	1.70	0.43
3:t:46:ARG:HH11	1:T:40:HIS:CE1	2.35	0.43
8:t:101:BCL:HBD	8:T:102:BCL:HBD	2.00	0.43
1:A:28:ALA:O	1:A:32:HIS:ND1	2.42	0.43
4:M:111:ASP:OD1	4:M:111:ASP:N	2.49	0.43
13:M:403:BPH:HBC3	13:M:403:BPH:HHD	2.00	0.43
8:d:102:BCL:H141	8:d:102:BCL:H161	1.73	0.43
4:M:301:GLU:OE2	7:C:235:ARG:NH1	2.51	0.43
5:L:2:ALA:HB3	6:H:41:LEU:HD13	2.00	0.43
1:S:20:GLN:HA	1:S:23:PHE:HB3	2.01	0.43
1:T:8:TRP:HZ3	1:T:16:VAL:HG11	1.84	0.43
3:i:40:LEU:O	3:i:44:ILE:HD12	2.19	0.43
8:F:101:BCL:H111	8:F:101:BCL:H91	1.64	0.43
5:L:5:SER:OG	6:H:78:ASP:OD2	2.27	0.43
8:b:101:BCL:H42	1:B:24:LEU:HB2	2.00	0.43
14:M:405:U10:H502	15:H:303:CDL:H473	1.99	0.43
15:M:408:CDL:H711	5:L:120:PHE:CG	2.53	0.43
5:L:5:SER:HB3	6:H:38:GLY:HA2	2.01	0.43
1:S:40:HIS:CD2	3:s:46:ARG:HH21	2.37	0.43
5:L:138:LEU:HD11	10:L:306:LMT:H102	2.00	0.43
7:C:123:TRP:CE3	7:C:169:CYS:HB3	2.51	0.43
7:C:307:GLY:HA3	7:C:323:VAL:HG11	2.01	0.43
3:b:46:ARG:HE	1:B:40:HIS:CD2	2.36	0.43
8:M:404:BCL:HED3	5:L:175:MET:HE3	2.00	0.43
15:H:303:CDL:H462	15:H:303:CDL:H431	1.70	0.43
8:N:101:BCL:H192	8:N:101:BCL:H162	1.84	0.43
1:E:36:LEU:O	1:E:42:ASN:ND2	2.52	0.43
5:L:166:LEU:HD21	7:C:265:ASN:HA	1.99	0.43
6:H:112:ALA:HB2	6:H:242:GLY:HA3	1.99	0.43
3:r:13:THR:OG1	3:r:16:GLN:OE1	2.37	0.43
8:n:101:BCL:HHD	1:N:35:LEU:HD11	1.99	0.43
4:M:198:TYR:O	5:L:152:TRP:HZ3	2.02	0.43
8:L:301:BCL:H161	8:L:301:BCL:H143	1.61	0.43
7:C:270:HIS:HD2	7:C:285:TRP:HD1	1.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:v:36:VAL:HG12	8:v:102:BCL:H62	1.99	0.43
3:k:49:PHE:HD2	8:K:101:BCL:H192	1.84	0.43
8:J:101:BCL:HBC3	8:J:101:BCL:H2C	1.71	0.43
14:M:405:U10:H72	14:M:405:U10:H111	1.91	0.43
5:L:225:ILE:HB	14:L:303:U10:H4M2	2.01	0.43
7:C:108:LEU:HD21	7:C:350:GLU:HG2	2.01	0.43
8:I:102:BCL:H162	8:I:102:BCL:H141	1.72	0.42
3:a:40:LEU:HA	8:a:102:BCL:H201	2.01	0.42
3:b:42:THR:HA	3:b:45:TRP:HB3	2.01	0.42
5:L:194:LEU:HG	5:L:213:GLU:HB2	2.01	0.42
5:L:228:LEU:HD11	5:L:232:ARG:HH21	1.84	0.42
6:H:27:ILE:HG21	15:H:303:CDL:H182	2.01	0.42
1:T:42:ASN:CG	1:T:45:GLU:HG3	2.44	0.42
8:K:102:BCL:H3A	9:J:102:A1EFU:C6	2.49	0.42
4:M:234:ARG:NH1	6:H:122:GLU:OE1	2.50	0.42
4:M:297:LEU:HG	7:C:276:TYR:OH	2.19	0.42
7:C:123:TRP:CD1	7:C:170:PHE:HB2	2.54	0.42
8:V:101:BCL:HBB3	8:t:101:BCL:NB	2.34	0.42
8:t:101:BCL:HBC3	8:t:101:BCL:H2C	1.84	0.42
1:Q:8:TRP:HZ3	1:Q:16:VAL:HG11	1.85	0.42
8:R:101:BCL:HBC3	8:R:101:BCL:H2C	1.68	0.42
3:e:34:VAL:HG12	8:E:101:BCL:HED1	2.02	0.42
4:M:214:VAL:HG21	5:L:181:PHE:CD2	2.53	0.42
6:H:192:ARG:HH12	6:H:221:LYS:HD3	1.84	0.42
15:H:303:CDL:H802	15:H:303:CDL:H771	1.55	0.42
3:f:12:LEU:HD11	3:e:9:PHE:HZ	1.85	0.42
4:M:227:VAL:HG23	4:M:232:GLY:HA3	2.00	0.42
4:M:228:THR:HG23	6:H:197:GLU:HG2	2.01	0.42
14:M:405:U10:H361	15:H:303:CDL:H451	2.02	0.42
8:L:301:BCL:H162	8:L:301:BCL:H202	1.75	0.42
6:H:66:GLN:HG3	6:H:67:HIS:ND1	2.35	0.42
8:K:101:BCL:CAD	8:K:102:BCL:HBD	2.50	0.42
8:J:101:BCL:H162	8:J:101:BCL:H122	1.69	0.42
1:G:1:MET:HG2	1:G:3:LYS:H	1.84	0.42
8:D:101:BCL:H161	8:D:101:BCL:H202	1.78	0.42
8:B:102:BCL:H143	8:B:102:BCL:H161	1.72	0.42
5:L:69:PRO:HG3	5:L:146:GLY:O	2.19	0.42
8:S:302:BCL:H62	8:S:302:BCL:H41	1.48	0.42
3:k:46:ARG:HH11	1:K:46:LEU:HD22	1.84	0.42
1:D:37:SER:HB2	5:L:78:MET:HB3	2.02	0.42
4:M:7:ILE:O	5:L:232:ARG:HD3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:L:304:BCL:HMA1	8:L:304:BCL:H121	2.02	0.42
6:H:42:GLU:OE2	6:H:81:ARG:NH2	2.50	0.42
3:k:46:ARG:HH21	1:K:40:HIS:CD2	2.38	0.42
8:K:101:BCL:HBB2	8:K:101:BCL:H143	2.01	0.42
3:e:32:SER:HB2	8:e:101:BCL:H61	2.00	0.42
8:A:101:BCL:H143	8:A:101:BCL:H161	1.67	0.42
4:M:150:ALA:HB2	4:M:271:TRP:NE1	2.34	0.42
6:H:133:PRO:HG3	6:H:168:TRP:CE2	2.54	0.42
1:J:8:TRP:HZ3	1:J:16:VAL:HG11	1.84	0.42
8:G:102:BCL:H162	8:G:102:BCL:H122	1.82	0.42
4:M:76:MET:HE2	4:M:95:ALA:HA	2.02	0.42
14:M:405:U10:H262	8:L:301:BCL:H201	2.02	0.42
7:C:220:TYR:O	7:C:296:GLN:NE2	2.39	0.42
8:b:101:BCL:H161	8:b:101:BCL:H202	1.79	0.41
4:M:24:GLU:OE2	4:M:142:LYS:NZ	2.37	0.41
5:L:230:ILE:HA	5:L:233:VAL:HG12	2.02	0.41
7:C:181:GLU:HG3	7:C:329:LYS:HG2	2.01	0.41
8:s:101:BCL:H93	8:s:101:BCL:H62	1.87	0.41
8:M:404:BCL:H91	8:M:404:BCL:H111	1.77	0.41
1:P:34:VAL:O	1:P:37:SER:OG	2.31	0.41
8:j:101:BCL:HBD	8:J:101:BCL:HBD	2.02	0.41
4:M:31:ARG:NE	5:L:219:ASP:OD2	2.50	0.41
8:r:101:BCL:CBD	8:R:101:BCL:HBD	2.51	0.41
3:k:9:PHE:CD2	1:K:10:ILE:HG22	2.55	0.41
8:e:101:BCL:CAD	8:E:101:BCL:HBD	2.50	0.41
1:V:48:ALA:HA	1:T:40:HIS:CD2	2.56	0.41
8:R:101:BCL:H122	8:R:101:BCL:H8	1.83	0.41
1:N:11:PHE:HB3	1:N:16:VAL:HG21	2.02	0.41
8:A:101:BCL:H102	8:A:101:BCL:H13	1.68	0.41
13:M:403:BPH:HBA2	13:M:403:BPH:H1C1	1.21	0.41
6:H:253:GLU:O	6:H:255:GLN:NE2	2.54	0.41
7:C:156:ALA:O	7:C:160:TYR:HB2	2.21	0.41
8:n:101:BCL:H2C	8:n:101:BCL:HBC3	1.82	0.41
1:I:24:LEU:HB2	8:I:103:BCL:H42	2.01	0.41
8:e:101:BCL:CBD	8:E:101:BCL:HBD	2.49	0.41
4:M:224:ILE:HD13	4:M:224:ILE:HA	1.90	0.41
5:L:39:THR:HG21	5:L:101:TRP:HE3	1.85	0.41
5:L:225:ILE:H	14:L:303:U10:H4M2	1.85	0.41
2:O:13:THR:O	2:O:17:ILE:HG12	2.20	0.41
8:V:101:BCL:H112	8:V:101:BCL:H72	1.84	0.41
3:g:46:ARG:HH21	1:G:40:HIS:CD2	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:36:LEU:HD13	5:L:52:TRP:HZ3	1.86	0.41
8:e:101:BCL:HAC2	1:E:35:LEU:HD11	2.03	0.41
8:d:102:BCL:H2C	8:d:102:BCL:HBC2	1.75	0.41
8:A:101:BCL:H111	8:A:101:BCL:H71	1.84	0.41
4:M:99:PRO:HB3	4:M:108:PRO:HG3	2.03	0.41
4:M:294:ASN:ND2	7:C:231:ASP:O	2.53	0.41
5:L:247:VAL:HA	5:L:250:ILE:HG22	2.03	0.41
6:H:163:LEU:H	6:H:163:LEU:HD23	1.84	0.41
1:T:12:ASP:HB3	1:T:15:ARG:HB3	2.02	0.41
3:n:16:GLN:NE2	3:k:7:LEU:HB3	2.35	0.41
3:j:40:LEU:O	3:j:44:ILE:HG13	2.20	0.41
1:J:33:LEU:HD22	6:H:5:PHE:CE2	2.56	0.41
1:G:33:LEU:HD23	1:G:36:LEU:HD12	2.03	0.41
1:D:45:GLU:OE1	10:B:101:LMT:O3'	2.39	0.41
14:M:405:U10:H353	15:H:303:CDL:H341	2.03	0.41
8:1:101:BCL:H111	8:1:101:BCL:H142	1.76	0.41
3:n:39:HIS:CD2	8:n:101:BCL:H111	2.56	0.41
1:I:29:ALA:O	1:I:33:LEU:HG	2.20	0.41
3:f:39:HIS:HE1	8:f:101:BCL:CHA	2.32	0.41
3:e:9:PHE:N	1:E:9:LEU:O	2.54	0.41
8:D:101:BCL:H61	8:D:101:BCL:H41	1.73	0.41
4:M:230:PHE:HB2	4:M:245:ALA:HB2	2.03	0.41
8:M:402:BCL:H192	8:M:404:BCL:H93	2.03	0.41
15:M:408:CDL:H311	15:M:408:CDL:HA62	1.90	0.41
6:H:199:VAL:HG23	6:H:208:VAL:HG13	2.03	0.41
15:H:303:CDL:H871	15:H:303:CDL:H841	1.83	0.41
7:C:11:SER:OG	7:C:13:ASN:OD1	2.37	0.41
7:C:105:LEU:HD21	7:C:145:ILE:HD13	2.02	0.41
8:v:102:BCL:H162	8:v:102:BCL:H141	1.62	0.41
8:r:101:BCL:H102	8:r:101:BCL:H13	1.89	0.41
8:D:101:BCL:H161	8:D:101:BCL:H141	1.59	0.41
5:L:104:ARG:O	5:L:108:ILE:HG12	2.20	0.41
8:L:301:BCL:CGD	8:L:301:BCL:HBA2	2.51	0.41
6:H:140:PHE:CE2	6:H:174:GLN:HG2	2.56	0.41
6:H:161:VAL:HA	6:H:187:TRP:CD1	2.55	0.41
7:C:217:LEU:HD22	7:C:221:LEU:HD12	2.03	0.41
1:V:28:ALA:O	1:V:32:HIS:ND1	2.38	0.40
1:S:9:LEU:HD23	3:s:7:LEU:O	2.21	0.40
8:S:302:BCL:HBD	8:s:101:BCL:OBD	2.21	0.40
8:q:101:BCL:H52	8:q:101:BCL:H8	1.91	0.40
3:2:46:ARG:HH21	1:1:40:HIS:CD2	2.39	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:1:101:BCL:H161	8:1:101:BCL:H141	1.79	0.40
8:j:101:BCL:CBD	8:J:101:BCL:HBD	2.51	0.40
8:f:101:BCL:H2C	8:f:101:BCL:HBC3	1.66	0.40
6:H:83:ASP:N	6:H:83:ASP:OD1	2.50	0.40
15:H:303:CDL:H382	15:H:303:CDL:H411	1.74	0.40
1:P:40:HIS:HB2	1:Q:48:ALA:HB2	2.02	0.40
1:Q:34:VAL:O	1:Q:37:SER:OG	2.32	0.40
1:1:28:ALA:O	1:1:32:HIS:ND1	2.33	0.40
8:j:101:BCL:H162	8:j:101:BCL:H141	1.78	0.40
2:O:36:PHE:HD2	2:O:37:LEU:HD22	1.86	0.40
8:V:101:BCL:H121	8:V:101:BCL:H162	1.79	0.40
8:e:101:BCL:H91	8:e:101:BCL:HAA1	2.03	0.40
8:M:402:BCL:HAA1	8:M:404:BCL:HBC1	2.02	0.40
7:C:213:PRO:HD3	7:C:249:GLU:HG2	2.02	0.40
7:C:311:LEU:HD12	7:C:323:VAL:HG13	2.03	0.40
8:P:101:BCL:H203	1:1:7:ILE:HG21	2.03	0.40
8:G:101:BCL:H162	8:G:101:BCL:H141	1.71	0.40
8:e:101:BCL:H112	8:e:101:BCL:H142	1.75	0.40
1:D:43:TRP:CZ2	8:D:101:BCL:HHC	2.55	0.40
4:M:217:PHE:CE2	5:L:234:GLY:HA3	2.56	0.40
15:M:408:CDL:H712	15:M:408:CDL:H741	1.84	0.40
5:L:109:CYS:HB2	5:L:114:MET:HG3	2.03	0.40
7:C:252:TYR:O	7:C:256:ASN:HB2	2.21	0.40
1:P:13:PRO:HD2	3:2:9:PHE:CE2	2.56	0.40
1:K:33:LEU:HD23	1:K:33:LEU:HA	1.88	0.40
1:A:3:LYS:HD2	1:A:6:LYS:HE3	2.03	0.40
7:C:159:VAL:O	16:C:403:HEC:HBD2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	48/53 (91%)	48 (100%)	0	0	100	100
1	A	49/53 (92%)	49 (100%)	0	0	100	100
1	B	50/53 (94%)	48 (96%)	2 (4%)	0	100	100
1	D	50/53 (94%)	50 (100%)	0	0	100	100
1	E	50/53 (94%)	50 (100%)	0	0	100	100
1	F	50/53 (94%)	50 (100%)	0	0	100	100
1	G	50/53 (94%)	50 (100%)	0	0	100	100
1	I	49/53 (92%)	48 (98%)	1 (2%)	0	100	100
1	J	48/53 (91%)	48 (100%)	0	0	100	100
1	K	49/53 (92%)	49 (100%)	0	0	100	100
1	N	49/53 (92%)	49 (100%)	0	0	100	100
1	P	49/53 (92%)	49 (100%)	0	0	100	100
1	Q	49/53 (92%)	49 (100%)	0	0	100	100
1	R	49/53 (92%)	49 (100%)	0	0	100	100
1	S	49/53 (92%)	49 (100%)	0	0	100	100
1	T	49/53 (92%)	48 (98%)	1 (2%)	0	100	100
1	V	50/53 (94%)	49 (98%)	1 (2%)	0	100	100
2	O	50/239 (21%)	46 (92%)	4 (8%)	0	100	100
3	2	42/49 (86%)	41 (98%)	1 (2%)	0	100	100
3	a	42/49 (86%)	41 (98%)	1 (2%)	0	100	100
3	b	42/49 (86%)	41 (98%)	1 (2%)	0	100	100
3	d	42/49 (86%)	42 (100%)	0	0	100	100
3	e	42/49 (86%)	42 (100%)	0	0	100	100
3	f	42/49 (86%)	42 (100%)	0	0	100	100
3	g	42/49 (86%)	42 (100%)	0	0	100	100
3	i	41/49 (84%)	41 (100%)	0	0	100	100
3	j	41/49 (84%)	41 (100%)	0	0	100	100
3	k	41/49 (84%)	40 (98%)	1 (2%)	0	100	100
3	n	42/49 (86%)	42 (100%)	0	0	100	100
3	p	42/49 (86%)	41 (98%)	1 (2%)	0	100	100
3	q	42/49 (86%)	39 (93%)	3 (7%)	0	100	100
3	r	41/49 (84%)	41 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	s	42/49 (86%)	42 (100%)	0	0	100	100
3	t	41/49 (84%)	41 (100%)	0	0	100	100
3	v	39/49 (80%)	39 (100%)	0	0	100	100
4	M	323/330 (98%)	316 (98%)	7 (2%)	0	100	100
5	L	272/279 (98%)	262 (96%)	10 (4%)	0	100	100
6	H	254/256 (99%)	245 (96%)	9 (4%)	0	100	100
7	C	350/360 (97%)	331 (95%)	19 (5%)	0	100	100
All	All	2792/3198 (87%)	2730 (98%)	62 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	42/44 (96%)	42 (100%)	0	100	100
1	A	42/44 (96%)	42 (100%)	0	100	100
1	B	43/44 (98%)	43 (100%)	0	100	100
1	D	43/44 (98%)	43 (100%)	0	100	100
1	E	43/44 (98%)	43 (100%)	0	100	100
1	F	43/44 (98%)	43 (100%)	0	100	100
1	G	43/44 (98%)	43 (100%)	0	100	100
1	I	42/44 (96%)	42 (100%)	0	100	100
1	J	42/44 (96%)	42 (100%)	0	100	100
1	K	42/44 (96%)	42 (100%)	0	100	100
1	N	42/44 (96%)	42 (100%)	0	100	100
1	P	43/44 (98%)	43 (100%)	0	100	100
1	Q	42/44 (96%)	42 (100%)	0	100	100
1	R	42/44 (96%)	42 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	S	42/44 (96%)	42 (100%)	0	100	100
1	T	42/44 (96%)	42 (100%)	0	100	100
1	V	43/44 (98%)	43 (100%)	0	100	100
2	O	39/174 (22%)	39 (100%)	0	100	100
3	2	36/41 (88%)	36 (100%)	0	100	100
3	a	37/41 (90%)	37 (100%)	0	100	100
3	b	37/41 (90%)	37 (100%)	0	100	100
3	d	36/41 (88%)	36 (100%)	0	100	100
3	e	36/41 (88%)	36 (100%)	0	100	100
3	f	36/41 (88%)	36 (100%)	0	100	100
3	g	36/41 (88%)	36 (100%)	0	100	100
3	i	35/41 (85%)	35 (100%)	0	100	100
3	j	35/41 (85%)	35 (100%)	0	100	100
3	k	35/41 (85%)	35 (100%)	0	100	100
3	n	36/41 (88%)	36 (100%)	0	100	100
3	p	36/41 (88%)	36 (100%)	0	100	100
3	q	36/41 (88%)	36 (100%)	0	100	100
3	r	35/41 (85%)	35 (100%)	0	100	100
3	s	36/41 (88%)	36 (100%)	0	100	100
3	t	35/41 (85%)	35 (100%)	0	100	100
3	v	33/41 (80%)	33 (100%)	0	100	100
4	M	266/270 (98%)	266 (100%)	0	100	100
5	L	218/222 (98%)	218 (100%)	0	100	100
6	H	214/214 (100%)	214 (100%)	0	100	100
7	C	298/307 (97%)	298 (100%)	0	100	100
All	All	2362/2632 (90%)	2362 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	P	20	GLN

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Mol	Chain	Res	Type
3	v	16	GLN
1	S	40	HIS
1	T	42	ASN
3	s	39	HIS
1	R	42	ASN
1	R	50	ASN
3	n	16	GLN
1	N	20	GLN
3	j	16	GLN
1	I	42	ASN
3	d	21	HIS
3	b	16	GLN
1	A	40	HIS
5	L	117	HIS
5	L	145	HIS
6	H	126	HIS
7	C	143	ASN
7	C	148	ASN
7	C	162	ASN
7	C	200	GLN
7	C	310	HIS
7	C	340	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 100 ligands modelled in this entry, 1 is monoatomic - leaving 99 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
8	BCL	j	101	-	64,74,74	1.72	11 (17%)	78,115,115	2.28	28 (35%)
9	A1EFU	1	104	-	40,42,42	1.69	9 (22%)	45,52,52	3.77	20 (44%)
8	BCL	1	102	-	64,74,74	1.73	13 (20%)	78,115,115	2.28	26 (33%)
8	BCL	d	102	-	64,74,74	1.72	11 (17%)	78,115,115	2.23	21 (26%)
11	MW9	R	103	-	44,44,52	1.48	5 (11%)	47,50,58	1.51	3 (6%)
8	BCL	D	101	-	64,74,74	1.72	12 (18%)	78,115,115	2.23	25 (32%)
10	LMT	B	101	-	24,24,36	1.03	2 (8%)	29,29,47	1.20	2 (6%)
8	BCL	J	101	-	64,74,74	1.72	11 (17%)	78,115,115	2.31	27 (34%)
14	U10	M	405	-	63,63,63	0.15	0	76,79,79	0.41	1 (1%)
10	LMT	E	103	-	36,36,36	1.15	5 (13%)	47,47,47	0.97	1 (2%)
8	BCL	a	102	-	64,74,74	1.72	11 (17%)	78,115,115	2.25	26 (33%)
8	BCL	t	101	-	64,74,74	1.76	12 (18%)	78,115,115	2.06	25 (32%)
8	BCL	r	101	-	64,74,74	1.73	13 (20%)	78,115,115	2.21	27 (34%)
15	CDL	H	303	-	99,99,99	0.88	8 (8%)	105,111,111	1.11	4 (3%)
8	BCL	V	101	-	64,74,74	1.69	11 (17%)	78,115,115	2.30	29 (37%)
11	MW9	H	301	-	47,47,52	1.39	6 (12%)	50,53,58	1.43	3 (6%)
9	A1EFU	A	102	-	40,42,42	1.69	8 (20%)	45,52,52	3.80	19 (42%)
9	A1EFU	R	102	-	40,42,42	1.69	9 (22%)	45,52,52	3.67	20 (44%)
9	A1EFU	Q	101	-	40,42,42	1.69	9 (22%)	45,52,52	3.80	20 (44%)
8	BCL	L	304	-	64,74,74	1.71	11 (17%)	78,115,115	2.33	29 (37%)
9	A1EFU	D	104	-	40,42,42	1.69	9 (22%)	45,52,52	3.77	20 (44%)
8	BCL	E	101	-	64,74,74	1.73	11 (17%)	78,115,115	2.27	27 (34%)
9	A1EFU	J	103	-	40,42,42	1.69	9 (22%)	45,52,52	3.78	20 (44%)
13	BPH	M	403	-	51,70,70	0.54	1 (1%)	52,101,101	0.77	2 (3%)
8	BCL	P	102	-	64,74,74	1.73	13 (20%)	78,115,115	2.23	25 (32%)
9	A1EFU	q	102	-	40,42,42	1.69	9 (22%)	45,52,52	3.75	20 (44%)
13	BPH	L	302	-	51,70,70	0.56	1 (1%)	52,101,101	0.68	1 (1%)
9	A1EFU	F	103	-	40,42,42	1.69	9 (22%)	45,52,52	3.81	20 (44%)
10	LMT	L	306	-	24,24,36	1.04	2 (8%)	29,29,47	1.20	2 (6%)
11	MW9	F	104	-	42,42,52	1.42	6 (14%)	45,48,58	1.47	3 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
9	A1EFU	I	101	-	40,42,42	1.68	9 (22%)	45,52,52	3.72	20 (44%)
9	A1EFU	S	304	-	40,42,42	1.70	9 (22%)	45,52,52	3.84	20 (44%)
8	BCL	B	102	-	64,74,74	1.72	13 (20%)	78,115,115	2.29	26 (33%)
9	A1EFU	P	103	-	40,42,42	1.69	9 (22%)	45,52,52	3.67	20 (44%)
9	A1EFU	n	102	-	40,42,42	1.69	9 (22%)	45,52,52	3.79	20 (44%)
16	HEC	C	403	7	32,50,50	2.02	4 (12%)	24,82,82	2.35	12 (50%)
11	MW9	L	305	-	36,36,52	1.48	5 (13%)	39,42,58	1.53	3 (7%)
8	BCL	P	101	-	64,74,74	1.71	13 (20%)	78,115,115	2.24	26 (33%)
8	BCL	M	402	-	64,74,74	1.72	12 (18%)	78,115,115	2.25	24 (30%)
11	MW9	G	106	-	39,39,52	1.42	5 (12%)	42,45,58	1.18	3 (7%)
10	LMT	C	404	-	36,36,36	1.18	5 (13%)	47,47,47	1.02	2 (4%)
9	A1EFU	v	101	-	40,42,42	1.69	9 (22%)	45,52,52	3.85	20 (44%)
9	A1EFU	a	101	-	40,42,42	1.69	9 (22%)	45,52,52	3.76	20 (44%)
9	A1EFU	i	101	-	40,42,42	1.68	8 (20%)	45,52,52	3.79	20 (44%)
16	HEC	C	401	7	32,50,50	2.01	4 (12%)	24,82,82	2.25	12 (50%)
9	A1EFU	G	103	-	40,42,42	1.68	8 (20%)	45,52,52	3.66	20 (44%)
8	BCL	N	101	-	64,74,74	1.72	12 (18%)	78,115,115	2.29	26 (33%)
9	A1EFU	a	103	-	40,42,42	1.69	9 (22%)	45,52,52	3.93	20 (44%)
8	BCL	n	101	-	64,74,74	1.74	12 (18%)	78,115,115	2.22	26 (33%)
8	BCL	G	101	-	64,74,74	1.71	11 (17%)	78,115,115	2.25	27 (34%)
9	A1EFU	F	102	-	40,42,42	1.69	9 (22%)	45,52,52	3.66	20 (44%)
9	A1EFU	T	101	-	40,42,42	1.69	9 (22%)	45,52,52	3.84	20 (44%)
9	A1EFU	J	102	-	40,42,42	1.68	8 (20%)	45,52,52	3.71	20 (44%)
9	A1EFU	M	406	-	40,42,42	1.68	7 (17%)	45,52,52	3.78	20 (44%)
8	BCL	s	101	-	64,74,74	1.70	12 (18%)	78,115,115	2.29	27 (34%)
16	HEC	C	402	7	32,50,50	2.11	4 (12%)	24,82,82	2.31	12 (50%)
9	A1EFU	K	103	-	40,42,42	1.69	9 (22%)	45,52,52	3.74	20 (44%)
9	A1EFU	p	101	-	40,42,42	1.68	9 (22%)	45,52,52	3.87	20 (44%)
8	BCL	A	101	-	64,74,74	1.73	13 (20%)	78,115,115	2.18	24 (30%)
8	BCL	q	101	-	64,74,74	1.72	11 (17%)	78,115,115	2.26	28 (35%)
11	MW9	D	102	-	25,26,52	1.20	2 (8%)	27,30,58	0.93	1 (3%)
8	BCL	Q	102	-	64,74,74	1.71	12 (18%)	78,115,115	2.22	26 (33%)
8	BCL	T	102	-	64,74,74	1.71	12 (18%)	78,115,115	2.28	27 (34%)
8	BCL	e	101	-	64,74,74	1.72	11 (17%)	78,115,115	2.28	26 (33%)
11	MW9	H	302	-	36,36,52	1.56	7 (19%)	39,41,58	1.84	4 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
8	BCL	G	102	-	64,74,74	1.73	11 (17%)	78,115,115	2.28	27 (34%)
8	BCL	K	102	-	64,74,74	1.71	12 (18%)	78,115,115	2.31	25 (32%)
9	A1EFU	K	104	-	40,42,42	1.69	9 (22%)	45,52,52	3.74	20 (44%)
9	A1EFU	D	103	-	40,42,42	1.68	9 (22%)	45,52,52	3.62	19 (42%)
8	BCL	I	102	-	64,74,74	1.71	11 (17%)	78,115,115	2.27	26 (33%)
9	A1EFU	1	103	-	40,42,42	1.68	9 (22%)	45,52,52	3.71	20 (44%)
9	A1EFU	r	102	-	40,42,42	1.68	9 (22%)	45,52,52	3.78	20 (44%)
8	BCL	f	101	-	64,74,74	1.72	10 (15%)	78,115,115	2.17	26 (33%)
9	A1EFU	T	103	-	40,42,42	1.69	9 (22%)	45,52,52	3.79	20 (44%)
8	BCL	I	103	-	64,74,74	1.72	13 (20%)	78,115,115	2.30	27 (34%)
10	LMT	H	304	-	24,24,36	1.03	2 (8%)	29,29,47	1.04	2 (6%)
8	BCL	K	101	-	64,74,74	1.72	13 (20%)	78,115,115	2.28	30 (38%)
8	BCL	v	102	-	64,74,74	1.72	12 (18%)	78,115,115	2.25	26 (33%)
14	U10	L	303	-	48,48,63	0.18	0	58,61,79	0.43	1 (1%)
8	BCL	b	101	-	64,74,74	1.73	13 (20%)	78,115,115	2.30	26 (33%)
15	CDL	M	408	-	66,66,99	1.05	8 (12%)	72,78,111	1.12	4 (5%)
9	A1EFU	E	102	-	40,42,42	1.69	9 (22%)	45,52,52	3.66	20 (44%)
8	BCL	R	101	-	64,74,74	1.71	13 (20%)	78,115,115	2.31	27 (34%)
8	BCL	M	404	-	64,74,74	1.70	12 (18%)	78,115,115	2.28	26 (33%)
8	BCL	S	302	-	64,74,74	1.71	14 (21%)	78,115,115	2.22	27 (34%)
9	A1EFU	A	103	-	40,42,42	1.70	9 (22%)	45,52,52	3.81	20 (44%)
8	BCL	L	301	-	64,74,74	1.71	12 (18%)	78,115,115	2.30	30 (38%)
8	BCL	F	101	-	64,74,74	1.74	10 (15%)	78,115,115	2.27	27 (34%)
11	MW9	G	105	-	48,48,52	1.49	6 (12%)	51,54,58	1.48	4 (7%)
9	A1EFU	S	303	-	40,42,42	1.69	9 (22%)	45,52,52	3.81	20 (44%)
9	A1EFU	b	102	-	40,42,42	1.69	8 (20%)	45,52,52	3.81	20 (44%)
10	LMT	G	107	-	24,24,36	1.03	2 (8%)	29,29,47	1.07	2 (6%)
11	MW9	M	407	-	48,48,52	1.48	6 (12%)	51,54,58	1.51	5 (9%)
9	A1EFU	N	102	-	40,42,42	1.68	9 (22%)	45,52,52	3.68	20 (44%)
8	BCL	1	101	-	64,74,74	1.71	11 (17%)	78,115,115	2.26	28 (35%)
10	LMT	S	301	-	36,36,36	1.15	5 (13%)	47,47,47	0.97	2 (4%)
9	A1EFU	G	104	-	40,42,42	1.69	9 (22%)	45,52,52	3.75	20 (44%)
11	MW9	N	103	-	52,52,52	1.44	6 (11%)	55,58,58	1.43	3 (5%)
9	A1EFU	d	101	-	40,42,42	1.68	9 (22%)	45,52,52	3.74	20 (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
8	BCL	j	101	-	-	18/37/137/137	-
9	A1EFU	1	104	-	-	24/50/51/51	-
8	BCL	1	102	-	-	16/37/137/137	-
8	BCL	d	102	-	-	23/37/137/137	-
11	MW9	R	103	-	-	31/49/49/57	-
8	BCL	D	101	-	-	15/37/137/137	-
10	LMT	B	101	-	-	7/15/35/61	0/1/1/2
8	BCL	J	101	-	-	13/37/137/137	-
14	U10	M	405	-	-	11/63/87/87	0/1/1/1
10	LMT	E	103	-	-	11/21/61/61	0/2/2/2
8	BCL	a	102	-	-	11/37/137/137	-
8	BCL	t	101	-	-	11/37/137/137	-
8	BCL	r	101	-	-	12/37/137/137	-
15	CDL	H	303	-	-	55/110/110/110	-
8	BCL	V	101	-	-	11/37/137/137	-
11	MW9	H	301	-	-	25/52/52/57	-
9	A1EFU	A	102	-	-	21/50/51/51	-
9	A1EFU	R	102	-	-	22/50/51/51	-
9	A1EFU	Q	101	-	-	21/50/51/51	-
8	BCL	L	304	-	-	21/37/137/137	-
9	A1EFU	D	104	-	-	22/50/51/51	-
8	BCL	E	101	-	-	11/37/137/137	-
9	A1EFU	J	103	-	-	17/50/51/51	-
13	BPH	M	403	-	-	16/37/105/105	0/5/6/6
8	BCL	P	102	-	-	13/37/137/137	-
9	A1EFU	q	102	-	-	22/50/51/51	-
13	BPH	L	302	-	-	4/37/105/105	0/5/6/6
9	A1EFU	F	103	-	-	18/50/51/51	-
10	LMT	L	306	-	-	5/15/35/61	0/1/1/2
11	MW9	F	104	-	-	31/47/47/57	-
9	A1EFU	I	101	-	-	18/50/51/51	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	A1EFU	S	304	-	-	23/50/51/51	-
8	BCL	B	102	-	-	6/37/137/137	-
9	A1EFU	P	103	-	-	21/50/51/51	-
9	A1EFU	n	102	-	-	19/50/51/51	-
16	HEC	C	403	7	-	3/10/54/54	-
11	MW9	L	305	-	-	17/41/41/57	-
8	BCL	P	101	-	-	12/37/137/137	-
8	BCL	M	402	-	-	14/37/137/137	-
11	MW9	G	106	-	-	29/44/44/57	-
10	LMT	C	404	-	-	10/21/61/61	0/2/2/2
9	A1EFU	v	101	-	-	18/50/51/51	-
9	A1EFU	a	101	-	-	17/50/51/51	-
9	A1EFU	i	101	-	-	17/50/51/51	-
16	HEC	C	401	7	-	3/10/54/54	-
9	A1EFU	G	103	-	-	16/50/51/51	-
8	BCL	N	101	-	-	12/37/137/137	-
9	A1EFU	a	103	-	-	28/50/51/51	-
8	BCL	n	101	-	-	13/37/137/137	-
8	BCL	G	101	-	-	14/37/137/137	-
9	A1EFU	F	102	-	-	22/50/51/51	-
9	A1EFU	T	101	-	-	16/50/51/51	-
9	A1EFU	J	102	-	-	16/50/51/51	-
9	A1EFU	M	406	-	-	19/50/51/51	-
8	BCL	s	101	-	-	18/37/137/137	-
16	HEC	C	402	7	-	4/10/54/54	-
9	A1EFU	K	103	-	-	16/50/51/51	-
9	A1EFU	p	101	-	-	23/50/51/51	-
8	BCL	A	101	-	-	15/37/137/137	-
8	BCL	q	101	-	-	17/37/137/137	-
11	MW9	D	102	-	-	13/27/27/57	-
8	BCL	Q	102	-	-	9/37/137/137	-
8	BCL	T	102	-	-	17/37/137/137	-
8	BCL	e	101	-	-	11/37/137/137	-
11	MW9	H	302	-	-	22/38/38/57	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	BCL	G	102	-	-	11/37/137/137	-
8	BCL	K	102	-	-	10/37/137/137	-
9	A1EFU	K	104	-	-	26/50/51/51	-
9	A1EFU	D	103	-	-	20/50/51/51	-
8	BCL	I	102	-	-	22/37/137/137	-
9	A1EFU	1	103	-	-	19/50/51/51	-
9	A1EFU	r	102	-	-	20/50/51/51	-
8	BCL	f	101	-	-	9/37/137/137	-
9	A1EFU	T	103	-	-	16/50/51/51	-
8	BCL	I	103	-	-	14/37/137/137	-
10	LMT	H	304	-	-	7/15/35/61	0/1/1/2
8	BCL	K	101	-	-	8/37/137/137	-
8	BCL	v	102	-	-	19/37/137/137	-
14	U10	L	303	-	-	10/45/69/87	0/1/1/1
8	BCL	b	101	-	-	23/37/137/137	-
15	CDL	M	408	-	-	38/77/77/110	-
9	A1EFU	E	102	-	-	23/50/51/51	-
8	BCL	R	101	-	-	6/37/137/137	-
8	BCL	M	404	-	-	14/37/137/137	-
8	BCL	S	302	-	-	16/37/137/137	-
9	A1EFU	A	103	-	-	15/50/51/51	-
8	BCL	L	301	-	-	18/37/137/137	-
8	BCL	F	101	-	-	14/37/137/137	-
11	MW9	G	105	-	-	30/53/53/57	-
9	A1EFU	S	303	-	-	20/50/51/51	-
9	A1EFU	b	102	-	-	17/50/51/51	-
10	LMT	G	107	-	-	4/15/35/61	0/1/1/2
11	MW9	M	407	-	-	28/53/53/57	-
9	A1EFU	N	102	-	-	16/50/51/51	-
8	BCL	1	101	-	-	17/37/137/137	-
10	LMT	S	301	-	-	9/21/61/61	0/2/2/2
9	A1EFU	G	104	-	-	22/50/51/51	-
11	MW9	N	103	-	-	35/57/57/57	-
9	A1EFU	d	101	-	-	18/50/51/51	-

All (866) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	C	402	HEC	C3C-C2C	-6.97	1.33	1.40
16	C	403	HEC	C3C-C2C	-6.55	1.33	1.40
16	C	402	HEC	C2B-C3B	-6.51	1.34	1.40
16	C	401	HEC	C3C-C2C	-6.42	1.34	1.40
8	t	101	BCL	MG-ND	-6.15	1.93	2.05
8	F	101	BCL	MG-ND	-6.09	1.93	2.05
8	f	101	BCL	MG-ND	-6.00	1.93	2.05
8	d	102	BCL	MG-ND	-5.95	1.94	2.05
8	D	101	BCL	MG-ND	-5.94	1.94	2.05
16	C	403	HEC	C2B-C3B	-5.92	1.34	1.40
16	C	401	HEC	C2B-C3B	-5.92	1.34	1.40
8	G	102	BCL	MG-ND	-5.90	1.94	2.05
8	J	101	BCL	MG-ND	-5.88	1.94	2.05
8	E	101	BCL	MG-ND	-5.84	1.94	2.05
8	b	101	BCL	MG-ND	-5.83	1.94	2.05
8	I	103	BCL	MG-ND	-5.82	1.94	2.05
8	1	102	BCL	MG-ND	-5.80	1.94	2.05
8	j	101	BCL	MG-ND	-5.76	1.94	2.05
8	q	101	BCL	MG-ND	-5.74	1.94	2.05
8	e	101	BCL	MG-ND	-5.71	1.94	2.05
8	I	102	BCL	MG-ND	-5.70	1.94	2.05
8	n	101	BCL	MG-ND	-5.69	1.94	2.05
8	A	101	BCL	MG-ND	-5.69	1.94	2.05
8	M	402	BCL	MG-ND	-5.68	1.94	2.05
8	K	102	BCL	MG-ND	-5.67	1.94	2.05
8	G	101	BCL	MG-ND	-5.66	1.94	2.05
8	Q	102	BCL	MG-ND	-5.66	1.94	2.05
8	N	101	BCL	MG-ND	-5.66	1.94	2.05
8	K	101	BCL	MG-ND	-5.65	1.94	2.05
9	A	103	A1EFU	C19-C18	-5.65	1.33	1.45
8	P	101	BCL	MG-ND	-5.65	1.94	2.05
8	r	101	BCL	MG-ND	-5.64	1.94	2.05
8	T	102	BCL	MG-ND	-5.64	1.94	2.05
8	s	101	BCL	MG-ND	-5.63	1.94	2.05
8	S	302	BCL	MG-ND	-5.63	1.94	2.05
9	A	102	A1EFU	C19-C18	-5.61	1.33	1.45
8	L	304	BCL	MG-ND	-5.61	1.94	2.05
9	M	406	A1EFU	C19-C18	-5.61	1.33	1.45
8	a	102	BCL	MG-ND	-5.61	1.94	2.05
9	F	103	A1EFU	C19-C18	-5.60	1.33	1.45
9	b	102	A1EFU	C19-C18	-5.60	1.33	1.45
8	v	102	BCL	MG-ND	-5.60	1.94	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	R	101	BCL	MG-ND	-5.59	1.94	2.05
9	K	104	A1EFU	C19-C18	-5.58	1.34	1.45
8	1	101	BCL	MG-ND	-5.58	1.94	2.05
9	n	102	A1EFU	C19-C18	-5.57	1.34	1.45
9	i	101	A1EFU	C19-C18	-5.57	1.34	1.45
9	G	104	A1EFU	C19-C18	-5.57	1.34	1.45
9	Q	101	A1EFU	C19-C18	-5.57	1.34	1.45
8	V	101	BCL	MG-ND	-5.57	1.94	2.05
9	S	303	A1EFU	C19-C18	-5.56	1.34	1.45
9	D	104	A1EFU	C19-C18	-5.56	1.34	1.45
9	I	101	A1EFU	C19-C18	-5.56	1.34	1.45
8	P	102	BCL	MG-ND	-5.55	1.94	2.05
8	M	404	BCL	MG-ND	-5.55	1.94	2.05
9	1	103	A1EFU	C19-C18	-5.55	1.34	1.45
8	L	301	BCL	MG-ND	-5.55	1.94	2.05
9	p	101	A1EFU	C19-C18	-5.54	1.34	1.45
9	1	104	A1EFU	C19-C18	-5.54	1.34	1.45
9	S	304	A1EFU	C19-C18	-5.53	1.34	1.45
9	N	102	A1EFU	C19-C18	-5.53	1.34	1.45
9	T	103	A1EFU	C19-C18	-5.53	1.34	1.45
9	J	103	A1EFU	C19-C18	-5.52	1.34	1.45
9	R	102	A1EFU	C19-C18	-5.52	1.34	1.45
8	B	102	BCL	MG-ND	-5.52	1.94	2.05
9	r	102	A1EFU	C19-C18	-5.52	1.34	1.45
9	E	102	A1EFU	C19-C18	-5.52	1.34	1.45
9	T	101	A1EFU	C19-C18	-5.51	1.34	1.45
9	q	102	A1EFU	C19-C18	-5.51	1.34	1.45
9	P	103	A1EFU	C19-C18	-5.51	1.34	1.45
9	F	102	A1EFU	C19-C18	-5.50	1.34	1.45
9	v	101	A1EFU	C19-C18	-5.49	1.34	1.45
9	G	103	A1EFU	C19-C18	-5.49	1.34	1.45
9	a	103	A1EFU	C19-C18	-5.49	1.34	1.45
9	K	103	A1EFU	C19-C18	-5.47	1.34	1.45
9	a	101	A1EFU	C19-C18	-5.47	1.34	1.45
9	D	103	A1EFU	C19-C18	-5.47	1.34	1.45
9	d	101	A1EFU	C19-C18	-5.47	1.34	1.45
9	J	102	A1EFU	C19-C18	-5.46	1.34	1.45
8	F	101	BCL	OBD-CAD	4.79	1.30	1.22
8	f	101	BCL	OBD-CAD	4.79	1.30	1.22
8	R	101	BCL	OBD-CAD	4.76	1.30	1.22
8	T	102	BCL	OBD-CAD	4.76	1.30	1.22
8	1	102	BCL	OBD-CAD	4.76	1.30	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	v	102	BCL	OBD-CAD	4.75	1.30	1.22
8	n	101	BCL	OBD-CAD	4.75	1.30	1.22
8	s	101	BCL	OBD-CAD	4.72	1.30	1.22
8	t	101	BCL	OBD-CAD	4.72	1.30	1.22
8	P	101	BCL	OBD-CAD	4.72	1.30	1.22
8	D	101	BCL	OBD-CAD	4.72	1.30	1.22
8	V	101	BCL	OBD-CAD	4.71	1.30	1.22
8	L	301	BCL	OBD-CAD	4.70	1.30	1.22
8	A	101	BCL	OBD-CAD	4.70	1.30	1.22
8	j	101	BCL	OBD-CAD	4.70	1.30	1.22
8	a	102	BCL	OBD-CAD	4.69	1.30	1.22
8	G	102	BCL	OBD-CAD	4.69	1.30	1.22
8	N	101	BCL	OBD-CAD	4.69	1.30	1.22
8	1	101	BCL	OBD-CAD	4.69	1.30	1.22
8	E	101	BCL	OBD-CAD	4.69	1.30	1.22
8	K	102	BCL	OBD-CAD	4.69	1.30	1.22
8	q	101	BCL	OBD-CAD	4.68	1.30	1.22
8	e	101	BCL	OBD-CAD	4.68	1.30	1.22
8	r	101	BCL	OBD-CAD	4.68	1.30	1.22
8	P	102	BCL	OBD-CAD	4.68	1.30	1.22
8	F	101	BCL	C4D-ND	-4.67	1.31	1.37
8	J	101	BCL	OBD-CAD	4.67	1.30	1.22
8	B	102	BCL	OBD-CAD	4.66	1.30	1.22
8	t	101	BCL	C4D-ND	-4.66	1.31	1.37
8	S	302	BCL	OBD-CAD	4.65	1.30	1.22
8	Q	102	BCL	OBD-CAD	4.65	1.30	1.22
8	M	402	BCL	OBD-CAD	4.64	1.30	1.22
8	b	101	BCL	OBD-CAD	4.64	1.30	1.22
8	K	101	BCL	OBD-CAD	4.63	1.30	1.22
8	L	304	BCL	OBD-CAD	4.62	1.30	1.22
8	M	404	BCL	OBD-CAD	4.61	1.30	1.22
8	I	103	BCL	OBD-CAD	4.61	1.30	1.22
8	G	101	BCL	OBD-CAD	4.57	1.30	1.22
8	d	102	BCL	OBD-CAD	4.55	1.30	1.22
11	M	407	MW9	C35-C34	-4.49	1.34	1.52
11	R	103	MW9	C35-C34	-4.49	1.34	1.52
11	N	103	MW9	C35-C34	-4.48	1.34	1.52
8	I	102	BCL	OBD-CAD	4.48	1.30	1.22
8	M	402	BCL	C4D-ND	-4.47	1.31	1.37
8	K	101	BCL	C4D-ND	-4.40	1.31	1.37
8	n	101	BCL	C4D-ND	-4.39	1.31	1.37
8	e	101	BCL	C4D-ND	-4.38	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	q	101	BCL	C4D-ND	-4.37	1.31	1.37
8	E	101	BCL	C4D-ND	-4.36	1.31	1.37
8	G	102	BCL	C4D-ND	-4.34	1.31	1.37
8	j	101	BCL	C4D-ND	-4.34	1.31	1.37
8	b	101	BCL	C4D-ND	-4.33	1.31	1.37
8	v	102	BCL	C4D-ND	-4.33	1.31	1.37
8	a	102	BCL	C4D-ND	-4.32	1.31	1.37
8	I	103	BCL	C4D-ND	-4.32	1.31	1.37
11	G	105	MW9	C35-C34	-4.32	1.35	1.52
8	J	101	BCL	C4D-ND	-4.32	1.31	1.37
8	1	102	BCL	C4D-ND	-4.30	1.31	1.37
8	d	102	BCL	C4D-ND	-4.29	1.31	1.37
8	R	101	BCL	C4D-ND	-4.28	1.31	1.37
8	T	102	BCL	C4D-ND	-4.26	1.31	1.37
8	N	101	BCL	C4D-ND	-4.25	1.31	1.37
8	A	101	BCL	C4D-ND	-4.23	1.31	1.37
8	M	404	BCL	C4D-ND	-4.22	1.31	1.37
8	1	101	BCL	C4D-ND	-4.22	1.31	1.37
8	r	101	BCL	C4D-ND	-4.21	1.31	1.37
8	V	101	BCL	C4D-ND	-4.21	1.31	1.37
8	P	102	BCL	C4D-ND	-4.20	1.31	1.37
8	S	302	BCL	C4D-ND	-4.20	1.31	1.37
8	P	101	BCL	C4D-ND	-4.20	1.31	1.37
8	Q	102	BCL	C4D-ND	-4.19	1.31	1.37
8	B	102	BCL	C4D-ND	-4.18	1.32	1.37
8	G	101	BCL	C4D-ND	-4.18	1.32	1.37
8	L	301	BCL	C4D-ND	-4.17	1.32	1.37
8	s	101	BCL	C4D-ND	-4.17	1.32	1.37
8	K	102	BCL	C4D-ND	-4.15	1.32	1.37
11	F	104	MW9	C33-C32	4.14	1.55	1.31
8	I	102	BCL	C4D-ND	-4.13	1.32	1.37
11	G	105	MW9	C33-C32	4.13	1.55	1.31
11	R	103	MW9	C33-C32	4.12	1.55	1.31
8	D	101	BCL	C4D-ND	-4.12	1.32	1.37
8	L	304	BCL	C4D-ND	-4.12	1.32	1.37
8	f	101	BCL	C4D-ND	-4.12	1.32	1.37
11	L	305	MW9	C33-C32	4.11	1.55	1.31
11	H	301	MW9	C33-C32	4.11	1.55	1.31
11	M	407	MW9	C33-C32	4.11	1.55	1.31
11	N	103	MW9	C33-C32	4.11	1.55	1.31
11	H	302	MW9	C33-C32	4.08	1.55	1.31
8	B	102	BCL	O1D-CGD	-4.06	1.11	1.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	n	101	BCL	O1D-CGD	-4.03	1.11	1.21
8	L	301	BCL	O1D-CGD	-4.02	1.11	1.21
8	L	304	BCL	O1D-CGD	-4.02	1.11	1.21
8	G	102	BCL	O1D-CGD	-4.01	1.11	1.21
8	e	101	BCL	O1D-CGD	-4.01	1.11	1.21
8	K	101	BCL	O1D-CGD	-4.01	1.11	1.21
8	N	101	BCL	O1D-CGD	-4.01	1.11	1.21
8	M	402	BCL	O1D-CGD	-4.01	1.11	1.21
11	G	106	MW9	C33-C32	4.00	1.55	1.28
8	v	102	BCL	O1D-CGD	-4.00	1.11	1.21
8	M	404	BCL	O1D-CGD	-4.00	1.11	1.21
8	q	101	BCL	O1D-CGD	-4.00	1.11	1.21
8	F	101	BCL	O1D-CGD	-4.00	1.11	1.21
8	1	102	BCL	O1D-CGD	-4.00	1.11	1.21
8	P	101	BCL	O1D-CGD	-3.99	1.11	1.21
8	j	101	BCL	O1D-CGD	-3.99	1.11	1.21
8	T	102	BCL	O1D-CGD	-3.99	1.11	1.21
8	I	103	BCL	O1D-CGD	-3.99	1.11	1.21
8	E	101	BCL	O1D-CGD	-3.98	1.11	1.21
8	V	101	BCL	O1D-CGD	-3.98	1.11	1.21
8	R	101	BCL	O1D-CGD	-3.98	1.11	1.21
8	b	101	BCL	O1D-CGD	-3.98	1.11	1.21
8	a	102	BCL	O1D-CGD	-3.98	1.11	1.21
8	J	101	BCL	O1D-CGD	-3.97	1.11	1.21
8	r	101	BCL	O1D-CGD	-3.97	1.11	1.21
8	1	101	BCL	O1D-CGD	-3.97	1.11	1.21
8	Q	102	BCL	O1D-CGD	-3.97	1.11	1.21
8	S	302	BCL	O1D-CGD	-3.97	1.11	1.21
8	s	101	BCL	O1D-CGD	-3.96	1.11	1.21
8	K	102	BCL	O1D-CGD	-3.96	1.11	1.21
8	I	102	BCL	O1D-CGD	-3.96	1.11	1.21
8	t	101	BCL	O1D-CGD	-3.95	1.11	1.21
8	A	101	BCL	O1D-CGD	-3.95	1.11	1.21
8	G	101	BCL	O1D-CGD	-3.95	1.11	1.21
8	P	102	BCL	O1D-CGD	-3.94	1.11	1.21
8	f	101	BCL	O1D-CGD	-3.92	1.11	1.21
8	D	101	BCL	O1D-CGD	-3.92	1.11	1.21
8	B	102	BCL	O2D-CED	3.89	1.54	1.45
8	d	102	BCL	O1D-CGD	-3.86	1.11	1.21
8	I	102	BCL	O2D-CED	3.75	1.54	1.45
8	d	102	BCL	O2D-CED	3.71	1.54	1.45
8	G	101	BCL	O2D-CED	3.57	1.53	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	102	A1EFU	C7-C6	3.57	1.54	1.43
9	D	103	A1EFU	C7-C6	3.56	1.54	1.43
9	a	103	A1EFU	C7-C6	3.53	1.54	1.43
9	G	104	A1EFU	C7-C6	3.53	1.54	1.43
9	A	103	A1EFU	C7-C6	3.53	1.54	1.43
9	G	103	A1EFU	C7-C6	3.53	1.54	1.43
9	S	304	A1EFU	C7-C6	3.52	1.54	1.43
8	P	102	BCL	O2D-CED	3.52	1.53	1.45
9	P	103	A1EFU	C7-C6	3.52	1.54	1.43
9	1	104	A1EFU	C7-C6	3.52	1.54	1.43
9	T	101	A1EFU	C7-C6	3.52	1.54	1.43
9	1	103	A1EFU	C7-C6	3.51	1.54	1.43
9	K	103	A1EFU	C7-C6	3.51	1.54	1.43
9	N	102	A1EFU	C7-C6	3.51	1.54	1.43
9	F	102	A1EFU	C7-C6	3.51	1.54	1.43
9	J	102	A1EFU	C7-C6	3.51	1.54	1.43
9	a	101	A1EFU	C7-C6	3.50	1.54	1.43
9	v	101	A1EFU	C7-C6	3.50	1.54	1.43
9	q	102	A1EFU	C7-C6	3.50	1.54	1.43
9	E	102	A1EFU	C7-C6	3.50	1.54	1.43
9	T	103	A1EFU	C7-C6	3.50	1.54	1.43
9	J	103	A1EFU	C7-C6	3.50	1.54	1.43
9	D	104	A1EFU	C7-C6	3.49	1.54	1.43
9	J	102	A1EFU	C11-C10	3.49	1.54	1.43
9	F	103	A1EFU	C7-C6	3.49	1.54	1.43
9	a	101	A1EFU	C11-C10	3.49	1.54	1.43
9	R	102	A1EFU	C11-C10	3.49	1.54	1.43
8	1	101	BCL	O2D-CED	3.48	1.53	1.45
9	S	303	A1EFU	C7-C6	3.48	1.54	1.43
9	r	102	A1EFU	C7-C6	3.48	1.54	1.43
9	R	102	A1EFU	C7-C6	3.48	1.54	1.43
9	i	101	A1EFU	C7-C6	3.48	1.54	1.43
9	d	101	A1EFU	C7-C6	3.47	1.54	1.43
9	Q	101	A1EFU	C11-C10	3.47	1.54	1.43
9	d	101	A1EFU	C11-C10	3.47	1.54	1.43
9	n	102	A1EFU	C7-C6	3.47	1.54	1.43
8	q	101	BCL	O2D-CED	3.47	1.53	1.45
9	A	102	A1EFU	C11-C10	3.47	1.54	1.43
9	K	104	A1EFU	C7-C6	3.47	1.54	1.43
8	v	102	BCL	O2D-CED	3.47	1.53	1.45
9	1	104	A1EFU	C11-C10	3.47	1.54	1.43
9	q	102	A1EFU	C11-C10	3.47	1.54	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	Q	101	A1EFU	C7-C6	3.47	1.54	1.43
9	D	103	A1EFU	C11-C10	3.47	1.54	1.43
9	p	101	A1EFU	C7-C6	3.47	1.54	1.43
9	I	101	A1EFU	C7-C6	3.47	1.54	1.43
9	T	101	A1EFU	C11-C10	3.46	1.54	1.43
8	r	101	BCL	O2D-CED	3.46	1.53	1.45
8	S	302	BCL	O2D-CED	3.46	1.53	1.45
8	V	101	BCL	O2D-CED	3.46	1.53	1.45
9	v	101	A1EFU	C11-C10	3.46	1.54	1.43
8	I	103	BCL	O2D-CED	3.46	1.53	1.45
9	T	103	A1EFU	C11-C10	3.46	1.54	1.43
9	S	303	A1EFU	C11-C10	3.46	1.54	1.43
8	t	101	BCL	O2D-CED	3.46	1.53	1.45
9	n	102	A1EFU	C11-C10	3.46	1.54	1.43
9	F	102	A1EFU	C11-C10	3.46	1.54	1.43
8	A	101	BCL	O2D-CED	3.45	1.53	1.45
9	P	103	A1EFU	C11-C10	3.45	1.54	1.43
9	K	103	A1EFU	C11-C10	3.45	1.54	1.43
9	G	103	A1EFU	C11-C10	3.45	1.54	1.43
9	b	102	A1EFU	C11-C10	3.45	1.54	1.43
9	S	304	A1EFU	C11-C10	3.45	1.54	1.43
9	b	102	A1EFU	C7-C6	3.45	1.54	1.43
9	D	104	A1EFU	C11-C10	3.45	1.54	1.43
9	E	102	A1EFU	C11-C10	3.45	1.54	1.43
8	F	101	BCL	O2D-CED	3.45	1.53	1.45
9	A	103	A1EFU	C11-C10	3.44	1.54	1.43
9	I	101	A1EFU	C11-C10	3.44	1.54	1.43
8	G	102	BCL	O2D-CED	3.44	1.53	1.45
9	p	101	A1EFU	C11-C10	3.44	1.54	1.43
9	r	102	A1EFU	C11-C10	3.44	1.54	1.43
9	M	406	A1EFU	C7-C6	3.44	1.54	1.43
8	N	101	BCL	O2D-CED	3.43	1.53	1.45
8	K	102	BCL	O2D-CED	3.43	1.53	1.45
8	P	101	BCL	O2D-CED	3.43	1.53	1.45
8	Q	102	BCL	O2D-CED	3.43	1.53	1.45
8	1	102	BCL	O2D-CED	3.43	1.53	1.45
9	G	104	A1EFU	C11-C10	3.43	1.54	1.43
8	s	101	BCL	O2D-CED	3.43	1.53	1.45
9	1	103	A1EFU	C11-C10	3.43	1.54	1.43
9	K	104	A1EFU	C11-C10	3.43	1.54	1.43
8	j	101	BCL	O2D-CED	3.43	1.53	1.45
8	E	101	BCL	O2D-CED	3.43	1.53	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	N	102	A1EFU	C11-C10	3.43	1.54	1.43
9	J	103	A1EFU	C11-C10	3.43	1.54	1.43
8	K	101	BCL	O2D-CED	3.43	1.53	1.45
8	n	101	BCL	O2D-CED	3.42	1.53	1.45
9	i	101	A1EFU	C11-C10	3.42	1.54	1.43
8	T	102	BCL	O2D-CED	3.42	1.53	1.45
8	J	101	BCL	O2D-CED	3.42	1.53	1.45
8	a	102	BCL	O2D-CED	3.42	1.53	1.45
8	f	101	BCL	O2D-CED	3.42	1.53	1.45
9	a	103	A1EFU	C11-C10	3.41	1.54	1.43
9	M	406	A1EFU	C11-C10	3.41	1.54	1.43
8	e	101	BCL	O2D-CED	3.41	1.53	1.45
9	F	103	A1EFU	C11-C10	3.40	1.54	1.43
8	L	304	BCL	O2D-CED	3.40	1.53	1.45
16	C	402	HEC	CBC-CAC	-3.40	1.36	1.49
8	R	101	BCL	O2D-CED	3.40	1.53	1.45
8	M	402	BCL	O2D-CED	3.39	1.53	1.45
16	C	403	HEC	CBC-CAC	-3.39	1.36	1.49
8	b	101	BCL	O2D-CED	3.39	1.53	1.45
16	C	401	HEC	CBC-CAC	-3.38	1.36	1.49
9	J	103	A1EFU	C20-C21	3.37	1.53	1.43
8	L	301	BCL	O2D-CED	3.37	1.53	1.45
9	a	101	A1EFU	C20-C21	3.34	1.53	1.43
8	D	101	BCL	O2D-CED	3.33	1.53	1.45
9	v	101	A1EFU	C20-C21	3.33	1.53	1.43
9	F	102	A1EFU	C20-C21	3.33	1.53	1.43
9	S	304	A1EFU	C20-C21	3.33	1.53	1.43
9	G	103	A1EFU	C20-C21	3.33	1.53	1.43
9	R	102	A1EFU	C20-C21	3.33	1.53	1.43
9	d	101	A1EFU	C20-C21	3.33	1.53	1.43
9	J	102	A1EFU	C20-C21	3.32	1.53	1.43
9	R	102	A1EFU	C16-C17	3.32	1.53	1.43
9	F	102	A1EFU	C16-C17	3.32	1.53	1.43
9	K	103	A1EFU	C20-C21	3.31	1.53	1.43
9	D	103	A1EFU	C20-C21	3.31	1.53	1.43
9	G	104	A1EFU	C20-C21	3.31	1.53	1.43
9	d	101	A1EFU	C15-C14	3.31	1.53	1.43
9	r	102	A1EFU	C20-C21	3.31	1.53	1.43
9	G	103	A1EFU	C16-C17	3.31	1.53	1.43
9	a	103	A1EFU	C20-C21	3.30	1.53	1.43
9	P	103	A1EFU	C16-C17	3.30	1.53	1.43
9	I	101	A1EFU	C16-C17	3.30	1.53	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	E	102	A1EFU	C16-C17	3.30	1.53	1.43
9	R	102	A1EFU	C15-C14	3.30	1.53	1.43
9	E	102	A1EFU	C20-C21	3.29	1.53	1.43
9	T	101	A1EFU	C20-C21	3.29	1.53	1.43
9	T	103	A1EFU	C15-C14	3.29	1.53	1.43
9	n	102	A1EFU	C20-C21	3.29	1.53	1.43
9	v	101	A1EFU	C15-C14	3.29	1.53	1.43
9	N	102	A1EFU	C20-C21	3.28	1.53	1.43
9	q	102	A1EFU	C20-C21	3.28	1.53	1.43
9	Q	101	A1EFU	C20-C21	3.28	1.53	1.43
9	K	103	A1EFU	C16-C17	3.28	1.53	1.43
9	T	103	A1EFU	C20-C21	3.28	1.53	1.43
9	F	102	A1EFU	C15-C14	3.28	1.53	1.43
9	N	102	A1EFU	C16-C17	3.28	1.53	1.43
9	Q	101	A1EFU	C16-C17	3.28	1.53	1.43
9	P	103	A1EFU	C20-C21	3.28	1.53	1.43
9	D	104	A1EFU	C20-C21	3.28	1.53	1.43
9	D	103	A1EFU	C16-C17	3.27	1.53	1.43
9	S	303	A1EFU	C20-C21	3.27	1.53	1.43
9	p	101	A1EFU	C20-C21	3.27	1.53	1.43
9	a	103	A1EFU	C15-C14	3.27	1.53	1.43
9	E	102	A1EFU	C15-C14	3.27	1.53	1.43
9	1	103	A1EFU	C20-C21	3.27	1.53	1.43
9	1	104	A1EFU	C20-C21	3.27	1.53	1.43
9	K	104	A1EFU	C20-C21	3.27	1.53	1.43
9	i	101	A1EFU	C20-C21	3.27	1.53	1.43
9	J	102	A1EFU	C16-C17	3.27	1.53	1.43
9	J	103	A1EFU	C15-C14	3.27	1.53	1.43
9	r	102	A1EFU	C15-C14	3.27	1.53	1.43
9	T	101	A1EFU	C15-C14	3.26	1.53	1.43
9	d	101	A1EFU	C16-C17	3.26	1.53	1.43
9	M	406	A1EFU	C15-C14	3.26	1.53	1.43
9	a	103	A1EFU	C16-C17	3.26	1.53	1.43
8	M	404	BCL	O2D-CED	3.26	1.53	1.45
9	P	103	A1EFU	C15-C14	3.26	1.53	1.43
9	G	103	A1EFU	C15-C14	3.26	1.53	1.43
9	a	101	A1EFU	C15-C14	3.26	1.53	1.43
9	I	101	A1EFU	C20-C21	3.26	1.53	1.43
9	J	102	A1EFU	C15-C14	3.26	1.53	1.43
9	T	101	A1EFU	C16-C17	3.26	1.53	1.43
9	1	103	A1EFU	C16-C17	3.26	1.53	1.43
9	a	101	A1EFU	C16-C17	3.26	1.53	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	G	104	A1EFU	C15-C14	3.26	1.53	1.43
9	F	103	A1EFU	C20-C21	3.26	1.53	1.43
9	Q	101	A1EFU	C15-C14	3.25	1.53	1.43
9	v	101	A1EFU	C16-C17	3.25	1.53	1.43
9	S	304	A1EFU	C15-C14	3.25	1.53	1.43
9	D	103	A1EFU	C15-C14	3.25	1.53	1.43
9	r	102	A1EFU	C16-C17	3.25	1.53	1.43
9	J	103	A1EFU	C16-C17	3.25	1.53	1.43
9	n	102	A1EFU	C15-C14	3.25	1.53	1.43
9	b	102	A1EFU	C15-C14	3.25	1.53	1.43
9	M	406	A1EFU	C20-C21	3.25	1.53	1.43
9	T	103	A1EFU	C16-C17	3.25	1.53	1.43
9	1	104	A1EFU	C15-C14	3.25	1.53	1.43
9	D	104	A1EFU	C16-C17	3.25	1.53	1.43
9	K	104	A1EFU	C15-C14	3.25	1.53	1.43
9	A	102	A1EFU	C20-C21	3.24	1.53	1.43
9	S	303	A1EFU	C15-C14	3.24	1.53	1.43
9	A	103	A1EFU	C15-C14	3.24	1.53	1.43
9	S	304	A1EFU	C16-C17	3.24	1.53	1.43
9	A	103	A1EFU	C20-C21	3.24	1.53	1.43
9	1	103	A1EFU	C15-C14	3.24	1.53	1.43
9	S	303	A1EFU	C16-C17	3.24	1.53	1.43
9	A	103	A1EFU	C16-C17	3.24	1.53	1.43
9	b	102	A1EFU	C20-C21	3.24	1.53	1.43
9	q	102	A1EFU	C16-C17	3.24	1.53	1.43
9	p	101	A1EFU	C15-C14	3.23	1.53	1.43
9	G	104	A1EFU	C16-C17	3.23	1.53	1.43
9	b	102	A1EFU	C16-C17	3.23	1.53	1.43
9	I	101	A1EFU	C15-C14	3.23	1.53	1.43
9	K	104	A1EFU	C16-C17	3.23	1.53	1.43
9	F	103	A1EFU	C15-C14	3.23	1.53	1.43
9	i	101	A1EFU	C16-C17	3.23	1.53	1.43
9	n	102	A1EFU	C16-C17	3.23	1.53	1.43
9	D	104	A1EFU	C15-C14	3.23	1.53	1.43
9	N	102	A1EFU	C15-C14	3.22	1.53	1.43
9	i	101	A1EFU	C15-C14	3.22	1.53	1.43
9	A	102	A1EFU	C16-C17	3.22	1.53	1.43
9	1	104	A1EFU	C16-C17	3.22	1.53	1.43
9	M	406	A1EFU	C16-C17	3.21	1.53	1.43
9	K	103	A1EFU	C15-C14	3.21	1.53	1.43
9	p	101	A1EFU	C16-C17	3.21	1.53	1.43
9	q	102	A1EFU	C15-C14	3.21	1.53	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	F	103	A1EFU	C16-C17	3.20	1.53	1.43
9	A	102	A1EFU	C15-C14	3.20	1.53	1.43
11	N	103	MW9	C7-C6	-3.14	1.34	1.51
11	H	301	MW9	C7-C6	-3.13	1.34	1.51
11	M	407	MW9	C7-C6	-3.13	1.34	1.51
11	G	105	MW9	C7-C6	-3.12	1.34	1.51
11	L	305	MW9	O1-C17	3.06	1.42	1.33
11	H	302	MW9	P-O5	3.05	1.66	1.54
8	N	101	BCL	O2A-CGA	-3.04	1.24	1.33
8	G	102	BCL	O2A-CGA	-3.03	1.24	1.33
8	b	101	BCL	O2A-CGA	-3.03	1.24	1.33
8	V	101	BCL	O2A-CGA	-3.03	1.24	1.33
8	J	101	BCL	O2A-CGA	-3.02	1.24	1.33
8	L	304	BCL	O2A-CGA	-3.02	1.24	1.33
11	G	105	MW9	O1-C17	3.01	1.42	1.33
8	1	102	BCL	O2A-CGA	-3.01	1.24	1.33
11	G	106	MW9	O1-C17	3.01	1.42	1.33
8	d	102	BCL	O2A-CGA	-3.01	1.24	1.33
11	N	103	MW9	O1-C17	3.00	1.42	1.33
8	M	402	BCL	O2A-CGA	-3.00	1.24	1.33
8	R	101	BCL	O2A-CGA	-3.00	1.24	1.33
8	K	102	BCL	O2A-CGA	-3.00	1.24	1.33
8	f	101	BCL	O2D-CGD	-2.99	1.25	1.33
8	Q	102	BCL	O2A-CGA	-2.99	1.24	1.33
11	R	103	MW9	O1-C17	2.99	1.42	1.33
8	P	101	BCL	O2A-CGA	-2.99	1.24	1.33
8	M	404	BCL	O2A-CGA	-2.99	1.24	1.33
8	E	101	BCL	O2A-CGA	-2.99	1.24	1.33
8	L	301	BCL	O2A-CGA	-2.98	1.24	1.33
8	j	101	BCL	O2A-CGA	-2.98	1.24	1.33
8	I	103	BCL	O2A-CGA	-2.98	1.24	1.33
8	e	101	BCL	O2A-CGA	-2.98	1.24	1.33
8	D	101	BCL	O2A-CGA	-2.98	1.24	1.33
8	S	302	BCL	O2A-CGA	-2.98	1.24	1.33
8	n	101	BCL	O2A-CGA	-2.98	1.24	1.33
11	M	407	MW9	O1-C17	2.98	1.42	1.33
8	q	101	BCL	O2A-CGA	-2.98	1.24	1.33
8	P	102	BCL	O2A-CGA	-2.97	1.24	1.33
11	H	302	MW9	O1-C17	2.97	1.42	1.33
8	t	101	BCL	O2A-CGA	-2.97	1.24	1.33
8	v	102	BCL	O2A-CGA	-2.96	1.24	1.33
8	s	101	BCL	O2A-CGA	-2.96	1.24	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	101	BCL	O2A-CGA	-2.96	1.24	1.33
8	B	102	BCL	O2A-CGA	-2.96	1.24	1.33
8	r	101	BCL	O2A-CGA	-2.96	1.24	1.33
8	T	102	BCL	O2A-CGA	-2.96	1.24	1.33
11	D	102	MW9	O1-C17	2.96	1.42	1.33
8	f	101	BCL	O2A-CGA	-2.96	1.24	1.33
8	I	102	BCL	O2A-CGA	-2.96	1.24	1.33
8	a	102	BCL	O2A-CGA	-2.95	1.24	1.33
8	D	101	BCL	O2D-CGD	-2.95	1.26	1.33
11	F	104	MW9	O1-C17	2.95	1.41	1.33
11	H	301	MW9	O1-C17	2.94	1.41	1.33
8	1	101	BCL	O2A-CGA	-2.94	1.24	1.33
8	F	101	BCL	O2A-CGA	-2.94	1.24	1.33
8	E	101	BCL	O2D-CGD	-2.94	1.26	1.33
8	I	103	BCL	O2D-CGD	-2.93	1.26	1.33
8	b	101	BCL	O2D-CGD	-2.93	1.26	1.33
8	M	404	BCL	O2D-CGD	-2.93	1.26	1.33
8	G	101	BCL	O2A-CGA	-2.92	1.24	1.33
8	J	101	BCL	O2D-CGD	-2.92	1.26	1.33
8	K	101	BCL	O2A-CGA	-2.92	1.24	1.33
8	G	102	BCL	O2D-CGD	-2.92	1.26	1.33
8	K	102	BCL	O2D-CGD	-2.91	1.26	1.33
8	L	304	BCL	O2D-CGD	-2.90	1.26	1.33
8	A	101	BCL	O2D-CGD	-2.90	1.26	1.33
8	1	102	BCL	O2D-CGD	-2.90	1.26	1.33
8	L	301	BCL	O1A-CGA	-2.89	1.13	1.22
8	n	101	BCL	O2D-CGD	-2.89	1.26	1.33
8	T	102	BCL	O2D-CGD	-2.88	1.26	1.33
8	K	101	BCL	O2D-CGD	-2.88	1.26	1.33
8	D	101	BCL	O1A-CGA	-2.87	1.14	1.22
8	S	302	BCL	O2D-CGD	-2.87	1.26	1.33
8	N	101	BCL	O2D-CGD	-2.87	1.26	1.33
8	P	101	BCL	O2D-CGD	-2.86	1.26	1.33
8	e	101	BCL	O2D-CGD	-2.86	1.26	1.33
8	R	101	BCL	O2D-CGD	-2.86	1.26	1.33
8	F	101	BCL	O2D-CGD	-2.86	1.26	1.33
8	M	402	BCL	O2D-CGD	-2.85	1.26	1.33
8	N	101	BCL	O1A-CGA	-2.84	1.14	1.22
8	j	101	BCL	O2D-CGD	-2.84	1.26	1.33
8	q	101	BCL	O2D-CGD	-2.83	1.26	1.33
8	1	101	BCL	O2D-CGD	-2.83	1.26	1.33
8	I	103	BCL	O1A-CGA	-2.83	1.14	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	L	301	BCL	O2D-CGD	-2.83	1.26	1.33
11	N	103	MW9	O8-C24	2.83	1.42	1.34
8	G	102	BCL	O1A-CGA	-2.83	1.14	1.22
8	Q	102	BCL	O2D-CGD	-2.83	1.26	1.33
8	V	101	BCL	O2D-CGD	-2.83	1.26	1.33
8	K	102	BCL	O1A-CGA	-2.82	1.14	1.22
8	M	404	BCL	O1A-CGA	-2.82	1.14	1.22
8	t	101	BCL	O2D-CGD	-2.82	1.26	1.33
8	b	101	BCL	O1A-CGA	-2.82	1.14	1.22
8	J	101	BCL	O1A-CGA	-2.82	1.14	1.22
8	r	101	BCL	O2D-CGD	-2.82	1.26	1.33
8	a	102	BCL	O2D-CGD	-2.82	1.26	1.33
8	v	102	BCL	O2D-CGD	-2.82	1.26	1.33
8	L	304	BCL	O1A-CGA	-2.82	1.14	1.22
8	j	101	BCL	O1A-CGA	-2.81	1.14	1.22
8	S	302	BCL	O1A-CGA	-2.81	1.14	1.22
8	T	102	BCL	O1A-CGA	-2.81	1.14	1.22
8	a	102	BCL	O1A-CGA	-2.81	1.14	1.22
8	1	101	BCL	O1A-CGA	-2.80	1.14	1.22
8	s	101	BCL	O2D-CGD	-2.80	1.26	1.33
8	1	102	BCL	O1A-CGA	-2.80	1.14	1.22
8	M	402	BCL	O1A-CGA	-2.80	1.14	1.22
8	P	102	BCL	O1A-CGA	-2.79	1.14	1.22
8	P	101	BCL	O1A-CGA	-2.79	1.14	1.22
8	d	102	BCL	O1A-CGA	-2.79	1.14	1.22
8	f	101	BCL	O1A-CGA	-2.79	1.14	1.22
8	G	101	BCL	O1A-CGA	-2.79	1.14	1.22
8	n	101	BCL	O1A-CGA	-2.79	1.14	1.22
8	I	102	BCL	O1A-CGA	-2.79	1.14	1.22
8	Q	102	BCL	O1A-CGA	-2.79	1.14	1.22
8	q	101	BCL	O1A-CGA	-2.79	1.14	1.22
8	e	101	BCL	O1A-CGA	-2.79	1.14	1.22
8	r	101	BCL	O1A-CGA	-2.78	1.14	1.22
8	P	102	BCL	O2D-CGD	-2.78	1.26	1.33
8	V	101	BCL	O1A-CGA	-2.78	1.14	1.22
8	K	101	BCL	O1A-CGA	-2.78	1.14	1.22
8	A	101	BCL	O1A-CGA	-2.78	1.14	1.22
8	G	101	BCL	O2D-CGD	-2.78	1.26	1.33
8	B	102	BCL	O1A-CGA	-2.78	1.14	1.22
8	R	101	BCL	O1A-CGA	-2.78	1.14	1.22
8	s	101	BCL	O1A-CGA	-2.77	1.14	1.22
8	v	102	BCL	O1A-CGA	-2.77	1.14	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	d	102	BCL	O2D-CGD	-2.76	1.26	1.33
8	t	101	BCL	O1A-CGA	-2.75	1.14	1.22
11	R	103	MW9	O8-C24	2.74	1.42	1.34
11	G	105	MW9	O8-C24	2.72	1.42	1.34
11	G	106	MW9	O8-C24	2.71	1.42	1.34
10	G	107	LMT	O3'-C3'	-2.71	1.36	1.43
10	H	304	LMT	O3'-C3'	-2.70	1.36	1.43
8	b	101	BCL	C1D-C2D	-2.70	1.40	1.45
11	H	301	MW9	O8-C24	2.68	1.41	1.34
10	S	301	LMT	O3'-C3'	-2.67	1.36	1.43
10	B	101	LMT	O3'-C3'	-2.67	1.36	1.43
10	L	306	LMT	O3'-C3'	-2.66	1.36	1.43
8	E	101	BCL	O1A-CGA	-2.66	1.14	1.22
10	E	103	LMT	O3'-C3'	-2.65	1.36	1.43
11	L	305	MW9	O8-C24	2.65	1.41	1.34
11	F	104	MW9	O8-C24	2.65	1.41	1.34
8	I	102	BCL	O2D-CGD	-2.65	1.26	1.33
8	D	101	BCL	C1D-C2D	-2.64	1.40	1.45
11	H	302	MW9	O8-C24	2.64	1.41	1.34
8	n	101	BCL	C4B-NB	2.63	1.37	1.35
8	F	101	BCL	O1A-CGA	-2.63	1.14	1.22
11	M	407	MW9	O8-C24	2.62	1.41	1.34
8	r	101	BCL	C4B-NB	2.62	1.37	1.35
15	H	303	CDL	OB6-CB4	-2.59	1.40	1.46
8	P	102	BCL	C4B-NB	2.58	1.37	1.35
10	C	404	LMT	O3'-C3'	-2.57	1.36	1.43
11	M	407	MW9	O8-C19	-2.56	1.40	1.46
11	H	302	MW9	O8-C19	-2.55	1.40	1.46
11	F	104	MW9	O8-C19	-2.54	1.40	1.46
8	d	102	BCL	C1D-C2D	-2.53	1.40	1.45
11	H	301	MW9	O8-C19	-2.53	1.40	1.46
11	L	305	MW9	O8-C19	-2.50	1.40	1.46
11	R	103	MW9	O8-C19	-2.49	1.40	1.46
11	G	106	MW9	O8-C19	-2.49	1.40	1.46
11	D	102	MW9	C6-C7	-2.49	1.34	1.51
11	F	104	MW9	C6-C7	-2.49	1.34	1.51
11	G	106	MW9	C6-C7	-2.48	1.34	1.51
11	G	105	MW9	O8-C19	-2.48	1.40	1.46
11	H	302	MW9	C6-C7	-2.48	1.34	1.51
8	Q	102	BCL	C1D-C2D	-2.45	1.40	1.45
8	I	102	BCL	C1D-C2D	-2.45	1.40	1.45
8	F	101	BCL	C3D-C4D	-2.44	1.38	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	H	303	CDL	OA8-CA7	2.44	1.40	1.33
15	M	408	CDL	OB6-CB4	-2.44	1.40	1.46
8	A	101	BCL	C4B-NB	2.44	1.37	1.35
8	E	101	BCL	C1D-C2D	-2.43	1.40	1.45
8	L	301	BCL	C1D-C2D	-2.42	1.40	1.45
15	M	408	CDL	OA8-CA7	2.42	1.40	1.33
11	L	305	MW9	C35-C34	-2.42	1.34	1.51
11	H	301	MW9	C35-C34	-2.41	1.34	1.51
8	1	101	BCL	C1D-C2D	-2.41	1.40	1.45
8	B	102	BCL	O2D-CGD	-2.41	1.27	1.33
8	G	102	BCL	C1D-C2D	-2.41	1.40	1.45
10	G	107	LMT	O2'-C2'	-2.40	1.37	1.43
8	1	102	BCL	C1D-C2D	-2.40	1.40	1.45
11	F	104	MW9	C35-C34	-2.40	1.34	1.51
15	M	408	CDL	OB8-CB7	2.40	1.40	1.33
8	G	101	BCL	C1D-C2D	-2.39	1.40	1.45
8	P	101	BCL	C1D-C2D	-2.38	1.40	1.45
8	v	102	BCL	C1D-C2D	-2.38	1.40	1.45
8	N	101	BCL	C1D-C2D	-2.38	1.40	1.45
8	j	101	BCL	C1D-C2D	-2.37	1.40	1.45
8	L	301	BCL	C4B-NB	2.37	1.37	1.35
8	b	101	BCL	C4B-NB	2.36	1.37	1.35
10	S	301	LMT	O2B-C2B	-2.35	1.37	1.43
8	s	101	BCL	C1D-C2D	-2.35	1.40	1.45
13	L	302	BPH	C3B-C2B	2.35	1.43	1.39
8	K	102	BCL	C1D-C2D	-2.35	1.40	1.45
10	S	301	LMT	O2'-C2'	-2.35	1.37	1.43
16	C	402	HEC	CBB-CAB	-2.35	1.40	1.49
8	T	102	BCL	C1D-C2D	-2.34	1.40	1.45
10	E	103	LMT	O2B-C2B	-2.34	1.37	1.43
15	H	303	CDL	OA6-CA4	-2.34	1.40	1.46
10	E	103	LMT	O3B-C3B	-2.34	1.37	1.43
13	M	403	BPH	C3B-C2B	2.34	1.43	1.39
10	C	404	LMT	O2B-C2B	-2.33	1.37	1.43
8	I	103	BCL	C1D-C2D	-2.33	1.40	1.45
8	L	304	BCL	C1D-C2D	-2.32	1.40	1.45
15	H	303	CDL	OB8-CB7	2.32	1.40	1.33
8	J	101	BCL	C1D-C2D	-2.32	1.40	1.45
8	A	101	BCL	C1D-C2D	-2.32	1.40	1.45
10	B	101	LMT	O2'-C2'	-2.31	1.37	1.43
8	n	101	BCL	C1D-C2D	-2.31	1.40	1.45
8	1	102	BCL	C4B-NB	2.31	1.37	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	C	403	HEC	CBB-CAB	-2.31	1.40	1.49
10	H	304	LMT	O2'-C2'	-2.31	1.37	1.43
8	a	102	BCL	C1D-C2D	-2.30	1.40	1.45
15	M	408	CDL	OA6-CA5	2.30	1.40	1.34
10	E	103	LMT	O2'-C2'	-2.29	1.37	1.43
10	C	404	LMT	O3B-C3B	-2.29	1.37	1.43
8	S	302	BCL	C1D-C2D	-2.29	1.40	1.45
10	S	301	LMT	O3B-C3B	-2.29	1.37	1.43
8	v	102	BCL	C4B-NB	2.29	1.37	1.35
16	C	401	HEC	CBB-CAB	-2.28	1.41	1.49
15	H	303	CDL	OB8-CB6	-2.27	1.40	1.45
8	V	101	BCL	C1D-C2D	-2.27	1.40	1.45
8	P	102	BCL	C1D-C2D	-2.27	1.40	1.45
11	H	302	MW9	C35-C34	-2.27	1.34	1.49
8	F	101	BCL	C1D-C2D	-2.27	1.40	1.45
15	M	408	CDL	OA6-CA4	-2.26	1.40	1.46
8	n	101	BCL	C3B-C2B	-2.26	1.35	1.39
8	R	101	BCL	C1D-C2D	-2.26	1.40	1.45
8	q	101	BCL	C1D-C2D	-2.26	1.40	1.45
8	P	102	BCL	C3B-C2B	-2.26	1.35	1.39
8	t	101	BCL	C3D-C4D	-2.26	1.39	1.44
8	e	101	BCL	C1D-C2D	-2.26	1.40	1.45
10	L	306	LMT	O2'-C2'	-2.25	1.37	1.43
8	t	101	BCL	C1D-C2D	-2.25	1.40	1.45
8	f	101	BCL	C1D-C2D	-2.25	1.40	1.45
8	M	402	BCL	C1D-C2D	-2.25	1.40	1.45
15	H	303	CDL	OA6-CA5	2.25	1.40	1.34
11	N	103	MW9	O8-C19	-2.25	1.41	1.46
8	r	101	BCL	C1D-C2D	-2.25	1.40	1.45
8	B	102	BCL	C1D-C2D	-2.24	1.40	1.45
8	M	404	BCL	C1D-C2D	-2.23	1.40	1.45
8	L	304	BCL	C4B-NB	2.23	1.37	1.35
8	s	101	BCL	C4B-NB	2.22	1.37	1.35
8	A	101	BCL	C3B-C2B	-2.22	1.35	1.39
10	C	404	LMT	O2'-C2'	-2.21	1.37	1.43
8	K	101	BCL	C3D-C4D	-2.21	1.39	1.44
8	E	101	BCL	C4B-NB	2.21	1.37	1.35
8	M	402	BCL	C3D-C4D	-2.21	1.39	1.44
8	B	102	BCL	C4B-NB	2.20	1.37	1.35
8	a	102	BCL	C4B-NB	2.20	1.37	1.35
8	d	102	BCL	C3B-CAB	2.20	1.55	1.49
8	I	102	BCL	C3D-C4D	-2.20	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	K	102	BCL	C4B-NB	2.19	1.37	1.35
8	q	101	BCL	C3D-C4D	-2.19	1.39	1.44
8	N	101	BCL	C4B-NB	2.19	1.37	1.35
8	E	101	BCL	C3D-C4D	-2.19	1.39	1.44
8	G	102	BCL	C3D-C4D	-2.19	1.39	1.44
8	n	101	BCL	C3D-C4D	-2.19	1.39	1.44
8	d	102	BCL	C3D-C4D	-2.18	1.39	1.44
8	t	101	BCL	C3B-C2B	-2.18	1.35	1.39
8	r	101	BCL	C3B-C2B	-2.18	1.35	1.39
8	I	103	BCL	C3D-C4D	-2.18	1.39	1.44
8	R	101	BCL	C4B-NB	2.18	1.37	1.35
9	R	102	A1EFU	C12-C13	2.18	1.50	1.45
8	B	102	BCL	C3D-C4D	-2.17	1.39	1.44
8	j	101	BCL	C3D-C4D	-2.17	1.39	1.44
8	j	101	BCL	C4B-NB	2.17	1.37	1.35
15	M	408	CDL	OB6-CB5	2.17	1.40	1.34
8	e	101	BCL	C3D-C4D	-2.17	1.39	1.44
8	1	101	BCL	C3D-C4D	-2.17	1.39	1.44
8	1	101	BCL	C4B-NB	2.17	1.37	1.35
8	a	102	BCL	C3D-C4D	-2.16	1.39	1.44
8	T	102	BCL	C4B-NB	2.16	1.37	1.35
8	G	101	BCL	C4B-NB	2.16	1.37	1.35
8	G	101	BCL	C3D-C4D	-2.16	1.39	1.44
8	P	102	BCL	C3D-C4D	-2.16	1.39	1.44
8	M	404	BCL	C3D-C4D	-2.16	1.39	1.44
8	t	101	BCL	C3B-CAB	2.16	1.54	1.49
15	M	408	CDL	OB8-CB6	-2.15	1.40	1.45
15	H	303	CDL	OA8-CA6	-2.15	1.40	1.45
8	b	101	BCL	C3D-C4D	-2.15	1.39	1.44
8	S	302	BCL	C4B-NB	2.15	1.37	1.35
8	J	101	BCL	C3D-C4D	-2.15	1.39	1.44
8	e	101	BCL	C4B-NB	2.15	1.37	1.35
8	q	101	BCL	C4B-NB	2.14	1.37	1.35
8	R	101	BCL	C3D-C4D	-2.14	1.39	1.44
9	T	101	A1EFU	C12-C13	2.13	1.50	1.45
8	P	101	BCL	C4B-NB	2.13	1.37	1.35
8	Q	102	BCL	C3D-C4D	-2.13	1.39	1.44
9	S	304	A1EFU	C8-C9	2.13	1.50	1.45
8	r	101	BCL	C3D-C4D	-2.13	1.39	1.44
8	f	101	BCL	C3D-C4D	-2.13	1.39	1.44
9	v	101	A1EFU	C8-C9	2.13	1.50	1.45
8	A	101	BCL	C3D-C4D	-2.12	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	K	101	BCL	C4B-NB	2.12	1.37	1.35
8	T	102	BCL	C3D-C4D	-2.12	1.39	1.44
9	v	101	A1EFU	C4-C5	2.12	1.50	1.45
9	J	102	A1EFU	C12-C13	2.12	1.50	1.45
8	K	101	BCL	C1D-C2D	-2.12	1.41	1.45
9	R	102	A1EFU	C4-C5	2.12	1.50	1.45
9	S	304	A1EFU	C4-C5	2.12	1.50	1.45
15	M	408	CDL	OA8-CA6	-2.12	1.40	1.45
9	r	102	A1EFU	C4-C5	2.11	1.50	1.45
9	F	102	A1EFU	C12-C13	2.11	1.50	1.45
9	E	102	A1EFU	C12-C13	2.11	1.50	1.45
8	v	102	BCL	C3D-C4D	-2.11	1.39	1.44
9	v	101	A1EFU	C12-C13	2.11	1.50	1.45
9	K	103	A1EFU	C12-C13	2.11	1.50	1.45
9	F	103	A1EFU	C4-C5	2.11	1.50	1.45
8	N	101	BCL	C3D-C4D	-2.11	1.39	1.44
8	Q	102	BCL	C4B-NB	2.11	1.37	1.35
8	I	102	BCL	C4B-NB	2.11	1.37	1.35
8	V	101	BCL	C3D-C4D	-2.11	1.39	1.44
9	P	103	A1EFU	C8-C9	2.11	1.50	1.45
9	D	103	A1EFU	C8-C9	2.11	1.50	1.45
9	S	303	A1EFU	C8-C9	2.10	1.50	1.45
9	T	103	A1EFU	C8-C9	2.10	1.50	1.45
9	G	103	A1EFU	C12-C13	2.10	1.50	1.45
9	K	104	A1EFU	C4-C5	2.10	1.50	1.45
9	T	103	A1EFU	C12-C13	2.10	1.50	1.45
8	S	302	BCL	C3D-C4D	-2.10	1.39	1.44
9	i	101	A1EFU	C4-C5	2.10	1.50	1.45
9	I	101	A1EFU	C12-C13	2.10	1.50	1.45
9	G	103	A1EFU	C8-C9	2.10	1.50	1.45
8	1	102	BCL	C3D-C4D	-2.10	1.39	1.44
9	a	101	A1EFU	C4-C5	2.10	1.50	1.45
9	P	103	A1EFU	C12-C13	2.10	1.50	1.45
10	C	404	LMT	O4'-C4B	-2.10	1.38	1.43
9	T	101	A1EFU	C8-C9	2.10	1.50	1.45
9	q	102	A1EFU	C4-C5	2.10	1.50	1.45
9	d	101	A1EFU	C12-C13	2.10	1.50	1.45
8	P	101	BCL	C3D-C4D	-2.10	1.39	1.44
9	a	101	A1EFU	C8-C9	2.10	1.50	1.45
9	Q	101	A1EFU	C4-C5	2.10	1.50	1.45
9	1	104	A1EFU	C4-C5	2.10	1.50	1.45
8	b	101	BCL	C3D-C2D	-2.10	1.33	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	E	102	A1EFU	C8-C9	2.10	1.50	1.45
8	L	304	BCL	C3D-C4D	-2.09	1.39	1.44
9	q	102	A1EFU	C8-C9	2.09	1.50	1.45
9	Q	101	A1EFU	C12-C13	2.09	1.50	1.45
9	p	101	A1EFU	C4-C5	2.09	1.50	1.45
8	M	404	BCL	C4B-NB	2.09	1.37	1.35
9	q	102	A1EFU	C12-C13	2.09	1.50	1.45
9	n	102	A1EFU	C4-C5	2.09	1.50	1.45
9	1	104	A1EFU	C8-C9	2.09	1.50	1.45
9	a	103	A1EFU	C4-C5	2.09	1.50	1.45
8	I	103	BCL	C4B-NB	2.09	1.37	1.35
9	G	104	A1EFU	C4-C5	2.09	1.50	1.45
8	M	402	BCL	C4B-NB	2.09	1.37	1.35
9	S	303	A1EFU	C12-C13	2.09	1.50	1.45
9	J	103	A1EFU	C4-C5	2.09	1.50	1.45
9	b	102	A1EFU	C12-C13	2.09	1.50	1.45
9	n	102	A1EFU	C8-C9	2.09	1.50	1.45
9	K	103	A1EFU	C8-C9	2.09	1.50	1.45
9	T	103	A1EFU	C4-C5	2.08	1.50	1.45
9	R	102	A1EFU	C8-C9	2.08	1.50	1.45
9	P	103	A1EFU	C4-C5	2.08	1.50	1.45
9	A	103	A1EFU	C4-C5	2.08	1.50	1.45
8	J	101	BCL	C4B-NB	2.08	1.37	1.35
8	L	301	BCL	C3D-C2D	-2.08	1.33	1.39
9	d	101	A1EFU	C4-C5	2.08	1.50	1.45
9	F	102	A1EFU	C4-C5	2.08	1.50	1.45
9	S	304	A1EFU	C12-C13	2.08	1.50	1.45
9	T	101	A1EFU	C4-C5	2.08	1.50	1.45
9	p	101	A1EFU	C8-C9	2.08	1.50	1.45
9	D	103	A1EFU	C12-C13	2.08	1.50	1.45
9	N	102	A1EFU	C4-C5	2.08	1.50	1.45
9	d	101	A1EFU	C8-C9	2.08	1.50	1.45
9	K	104	A1EFU	C8-C9	2.07	1.50	1.45
9	D	104	A1EFU	C4-C5	2.07	1.50	1.45
9	1	104	A1EFU	C12-C13	2.07	1.50	1.45
9	N	102	A1EFU	C8-C9	2.07	1.50	1.45
9	D	103	A1EFU	C4-C5	2.07	1.50	1.45
10	S	301	LMT	O4'-C4B	-2.07	1.38	1.43
9	A	102	A1EFU	C8-C9	2.07	1.50	1.45
9	K	103	A1EFU	C4-C5	2.07	1.50	1.45
9	A	103	A1EFU	C12-C13	2.07	1.50	1.45
9	S	303	A1EFU	C4-C5	2.06	1.50	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	1	103	A1EFU	C4-C5	2.06	1.50	1.45
9	N	102	A1EFU	C12-C13	2.06	1.50	1.45
10	E	103	LMT	O4'-C4B	-2.06	1.38	1.43
8	S	302	BCL	C3D-C2D	-2.06	1.33	1.39
9	a	101	A1EFU	C12-C13	2.06	1.50	1.45
9	a	103	A1EFU	C12-C13	2.06	1.50	1.45
9	J	102	A1EFU	C8-C9	2.06	1.50	1.45
8	T	102	BCL	C3B-CAB	2.06	1.54	1.49
9	Q	101	A1EFU	C8-C9	2.06	1.50	1.45
9	D	104	A1EFU	C12-C13	2.06	1.50	1.45
9	F	102	A1EFU	C8-C9	2.06	1.50	1.45
9	r	102	A1EFU	C8-C9	2.05	1.50	1.45
9	A	103	A1EFU	C8-C9	2.05	1.50	1.45
8	D	101	BCL	C3D-C2D	-2.05	1.33	1.39
9	D	104	A1EFU	C8-C9	2.05	1.50	1.45
15	H	303	CDL	OB6-CB5	2.05	1.40	1.34
8	G	102	BCL	C3D-C2D	-2.05	1.33	1.39
9	p	101	A1EFU	C12-C13	2.05	1.50	1.45
9	1	103	A1EFU	C12-C13	2.04	1.50	1.45
9	G	104	A1EFU	C12-C13	2.04	1.50	1.45
9	1	103	A1EFU	C8-C9	2.04	1.50	1.45
8	S	302	BCL	C3B-CAB	2.04	1.54	1.49
9	E	102	A1EFU	C4-C5	2.04	1.50	1.45
9	A	102	A1EFU	C12-C13	2.04	1.50	1.45
9	i	101	A1EFU	C8-C9	2.04	1.50	1.45
9	b	102	A1EFU	C8-C9	2.04	1.50	1.45
9	a	103	A1EFU	C8-C9	2.04	1.50	1.45
9	J	103	A1EFU	C8-C9	2.03	1.50	1.45
9	r	102	A1EFU	C12-C13	2.03	1.50	1.45
8	N	101	BCL	C3D-C2D	-2.03	1.33	1.39
8	K	101	BCL	C3B-CAB	2.03	1.54	1.49
9	G	104	A1EFU	C8-C9	2.03	1.50	1.45
8	P	102	BCL	C3B-CAB	2.03	1.54	1.49
9	J	103	A1EFU	C12-C13	2.03	1.50	1.45
8	L	301	BCL	C3D-C4D	-2.03	1.39	1.44
8	R	101	BCL	C3B-CAB	2.03	1.54	1.49
9	n	102	A1EFU	C12-C13	2.02	1.50	1.45
8	I	103	BCL	C3D-C2D	-2.02	1.33	1.39
8	M	402	BCL	C3B-CAB	2.02	1.54	1.49
8	B	102	BCL	C1A-CHA	-2.02	1.34	1.43
9	F	103	A1EFU	C8-C9	2.02	1.50	1.45
8	K	102	BCL	C3D-C2D	-2.02	1.33	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	s	101	BCL	C3D-C4D	-2.02	1.39	1.44
8	K	101	BCL	C3D-C2D	-2.02	1.33	1.39
8	M	404	BCL	C3D-C2D	-2.02	1.33	1.39
8	1	102	BCL	C3D-C2D	-2.02	1.33	1.39
8	1	102	BCL	C3B-CAB	2.02	1.54	1.49
8	V	101	BCL	C3B-CAB	2.02	1.54	1.49
9	I	101	A1EFU	C4-C5	2.02	1.50	1.45
8	P	101	BCL	C3D-C2D	-2.02	1.33	1.39
8	b	101	BCL	C3B-CAB	2.02	1.54	1.49
9	K	104	A1EFU	C12-C13	2.02	1.50	1.45
8	S	302	BCL	C5-C3	2.02	1.55	1.51
8	v	102	BCL	C3B-CAB	2.01	1.54	1.49
8	I	103	BCL	C3B-CAB	2.01	1.54	1.49
8	Q	102	BCL	C3B-CAB	2.01	1.54	1.49
8	D	101	BCL	C3D-C4D	-2.01	1.39	1.44
8	K	102	BCL	C3D-C4D	-2.01	1.39	1.44
8	A	101	BCL	C3B-CAB	2.01	1.54	1.49
8	R	101	BCL	C3D-C2D	-2.01	1.33	1.39
8	B	102	BCL	C3B-C2B	-2.01	1.35	1.39
9	F	103	A1EFU	C12-C13	2.01	1.50	1.45
8	s	101	BCL	C3B-CAB	2.01	1.54	1.49
9	I	101	A1EFU	C8-C9	2.01	1.50	1.45
8	P	101	BCL	C3B-CAB	2.00	1.54	1.49
8	r	101	BCL	C3B-CAB	2.00	1.54	1.49
9	M	406	A1EFU	C12-C13	2.00	1.50	1.45
8	D	101	BCL	C4B-NB	2.00	1.37	1.35

All (1798) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	A	103	A1EFU	C11-C10-C9	-10.55	112.26	127.31
9	r	102	A1EFU	C11-C10-C9	-10.16	112.82	127.31
9	A	102	A1EFU	C11-C10-C9	-10.14	112.84	127.31
9	Q	101	A1EFU	C15-C14-C13	-10.10	112.90	127.31
9	p	101	A1EFU	C11-C10-C9	-10.08	112.92	127.31
9	A	103	A1EFU	C15-C14-C13	-10.07	112.94	127.31
9	J	103	A1EFU	C7-C6-C5	-10.04	112.98	127.31
9	n	102	A1EFU	C7-C6-C5	-10.04	112.98	127.31
9	A	102	A1EFU	C15-C14-C13	-10.04	112.99	127.31
9	a	103	A1EFU	C11-C10-C9	-10.01	113.03	127.31
9	G	104	A1EFU	C11-C10-C9	-9.97	113.08	127.31
9	F	103	A1EFU	C11-C10-C9	-9.96	113.09	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	1	104	A1EFU	C7-C6-C5	-9.95	113.11	127.31
9	b	102	A1EFU	C15-C14-C13	-9.93	113.13	127.31
9	v	101	A1EFU	C7-C6-C5	-9.89	113.20	127.31
9	S	304	A1EFU	C7-C6-C5	-9.87	113.22	127.31
9	Q	101	A1EFU	C11-C10-C9	-9.83	113.28	127.31
9	M	406	A1EFU	C7-C6-C5	-9.80	113.32	127.31
9	K	104	A1EFU	C7-C6-C5	-9.78	113.36	127.31
9	a	103	A1EFU	C7-C6-C5	-9.75	113.40	127.31
9	T	101	A1EFU	C11-C10-C9	-9.73	113.42	127.31
9	i	101	A1EFU	C11-C10-C9	-9.73	113.43	127.31
9	I	101	A1EFU	C11-C10-C9	-9.73	113.43	127.31
9	D	104	A1EFU	C15-C14-C13	-9.72	113.44	127.31
9	I	101	A1EFU	C15-C14-C13	-9.70	113.47	127.31
9	q	102	A1EFU	C7-C6-C5	-9.69	113.48	127.31
9	T	101	A1EFU	C15-C14-C13	-9.69	113.48	127.31
9	T	103	A1EFU	C11-C10-C9	-9.68	113.49	127.31
9	a	101	A1EFU	C7-C6-C5	-9.67	113.51	127.31
9	d	101	A1EFU	C7-C6-C5	-9.66	113.52	127.31
9	N	102	A1EFU	C11-C10-C9	-9.66	113.53	127.31
9	b	102	A1EFU	C11-C10-C9	-9.64	113.55	127.31
9	S	303	A1EFU	C11-C10-C9	-9.64	113.55	127.31
9	M	406	A1EFU	C11-C10-C9	-9.63	113.57	127.31
9	T	103	A1EFU	C7-C6-C5	-9.63	113.57	127.31
9	a	101	A1EFU	C16-C17-C18	-9.60	113.61	127.31
9	p	101	A1EFU	C15-C14-C13	-9.58	113.64	127.31
9	r	102	A1EFU	C7-C6-C5	-9.57	113.65	127.31
9	G	104	A1EFU	C7-C6-C5	-9.55	113.68	127.31
9	D	104	A1EFU	C11-C10-C9	-9.53	113.71	127.31
9	p	101	A1EFU	C7-C6-C5	-9.53	113.71	127.31
9	1	103	A1EFU	C11-C10-C9	-9.52	113.73	127.31
9	J	102	A1EFU	C15-C14-C13	-9.51	113.73	127.31
9	n	102	A1EFU	C11-C10-C9	-9.51	113.74	127.31
9	a	103	A1EFU	C15-C14-C13	-9.50	113.75	127.31
9	J	102	A1EFU	C11-C10-C9	-9.49	113.77	127.31
9	d	101	A1EFU	C11-C10-C9	-9.46	113.81	127.31
9	S	304	A1EFU	C16-C17-C18	-9.45	113.83	127.31
9	v	101	A1EFU	C11-C10-C9	-9.45	113.83	127.31
9	R	102	A1EFU	C11-C10-C9	-9.45	113.83	127.31
9	1	103	A1EFU	C15-C14-C13	-9.44	113.84	127.31
9	E	102	A1EFU	C11-C10-C9	-9.43	113.85	127.31
9	D	103	A1EFU	C7-C6-C5	-9.42	113.87	127.31
9	v	101	A1EFU	C16-C17-C18	-9.41	113.88	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	K	103	A1EFU	C11-C10-C9	-9.40	113.89	127.31
9	F	103	A1EFU	C7-C6-C5	-9.39	113.91	127.31
9	G	103	A1EFU	C11-C10-C9	-9.38	113.92	127.31
9	i	101	A1EFU	C7-C6-C5	-9.35	113.96	127.31
9	S	303	A1EFU	C15-C14-C13	-9.32	114.00	127.31
9	F	102	A1EFU	C15-C14-C13	-9.30	114.04	127.31
9	K	103	A1EFU	C15-C14-C13	-9.23	114.13	127.31
9	F	102	A1EFU	C11-C10-C9	-9.21	114.17	127.31
9	G	103	A1EFU	C15-C14-C13	-9.18	114.21	127.31
9	T	101	A1EFU	C7-C6-C5	-9.18	114.21	127.31
9	a	103	A1EFU	C16-C17-C18	-9.15	114.26	127.31
9	E	102	A1EFU	C15-C14-C13	-9.14	114.26	127.31
9	S	303	A1EFU	C7-C6-C5	-9.00	114.47	127.31
9	P	103	A1EFU	C11-C10-C9	-8.89	114.62	127.31
9	p	101	A1EFU	C16-C17-C18	-8.89	114.62	127.31
9	M	406	A1EFU	C16-C17-C18	-8.89	114.62	127.31
9	F	103	A1EFU	C16-C17-C18	-8.87	114.64	127.31
9	v	101	A1EFU	C15-C14-C13	-8.87	114.65	127.31
9	K	103	A1EFU	C7-C6-C5	-8.85	114.68	127.31
9	K	104	A1EFU	C15-C14-C13	-8.85	114.68	127.31
9	R	102	A1EFU	C15-C14-C13	-8.85	114.68	127.31
9	i	101	A1EFU	C15-C14-C13	-8.79	114.77	127.31
9	S	304	A1EFU	C15-C14-C13	-8.78	114.78	127.31
9	P	103	A1EFU	C15-C14-C13	-8.77	114.80	127.31
9	S	304	A1EFU	C11-C10-C9	-8.75	114.83	127.31
9	P	103	A1EFU	C7-C6-C5	-8.72	114.86	127.31
9	F	103	A1EFU	C15-C14-C13	-8.72	114.87	127.31
9	T	103	A1EFU	C15-C14-C13	-8.71	114.88	127.31
9	N	102	A1EFU	C15-C14-C13	-8.71	114.88	127.31
9	R	102	A1EFU	C7-C6-C5	-8.68	114.92	127.31
9	J	103	A1EFU	C15-C14-C13	-8.68	114.92	127.31
9	1	104	A1EFU	C15-C14-C13	-8.68	114.93	127.31
9	q	102	A1EFU	C16-C17-C18	-8.67	114.94	127.31
9	G	104	A1EFU	C15-C14-C13	-8.67	114.94	127.31
9	S	303	A1EFU	C16-C17-C18	-8.65	114.97	127.31
9	J	103	A1EFU	C11-C10-C9	-8.62	115.01	127.31
9	d	101	A1EFU	C16-C17-C18	-8.61	115.02	127.31
9	b	102	A1EFU	C7-C6-C5	-8.61	115.02	127.31
9	K	104	A1EFU	C16-C17-C18	-8.60	115.03	127.31
9	1	104	A1EFU	C11-C10-C9	-8.59	115.04	127.31
9	G	103	A1EFU	C7-C6-C5	-8.59	115.06	127.31
9	q	102	A1EFU	C15-C14-C13	-8.58	115.07	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	n	102	A1EFU	C16-C17-C18	-8.55	115.11	127.31
9	J	103	A1EFU	C16-C17-C18	-8.55	115.11	127.31
9	J	102	A1EFU	C7-C6-C5	-8.54	115.12	127.31
9	r	102	A1EFU	C15-C14-C13	-8.53	115.14	127.31
9	A	102	A1EFU	C7-C6-C5	-8.51	115.16	127.31
9	n	102	A1EFU	C15-C14-C13	-8.50	115.19	127.31
11	H	302	MW9	C35-C34-C33	8.50	151.60	112.71
9	Q	101	A1EFU	C7-C6-C5	-8.48	115.21	127.31
9	N	102	A1EFU	C7-C6-C5	-8.43	115.27	127.31
9	A	103	A1EFU	C16-C17-C18	-8.39	115.34	127.31
9	r	102	A1EFU	C16-C17-C18	-8.37	115.36	127.31
9	i	101	A1EFU	C16-C17-C18	-8.36	115.38	127.31
9	M	406	A1EFU	C15-C14-C13	-8.36	115.38	127.31
9	q	102	A1EFU	C11-C10-C9	-8.34	115.41	127.31
9	d	101	A1EFU	C15-C14-C13	-8.33	115.43	127.31
9	T	103	A1EFU	C16-C17-C18	-8.29	115.48	127.31
9	b	102	A1EFU	C16-C17-C18	-8.27	115.50	127.31
9	K	104	A1EFU	C11-C10-C9	-8.20	115.60	127.31
9	D	103	A1EFU	C16-C17-C18	-8.19	115.62	127.31
9	D	103	A1EFU	C15-C14-C13	-8.18	115.63	127.31
9	D	104	A1EFU	C7-C6-C5	-8.17	115.64	127.31
9	1	103	A1EFU	C7-C6-C5	-8.15	115.68	127.31
9	T	101	A1EFU	C16-C17-C18	-8.14	115.69	127.31
9	A	102	A1EFU	C16-C17-C18	-8.11	115.74	127.31
9	Q	101	A1EFU	C16-C17-C18	-8.10	115.75	127.31
9	K	103	A1EFU	C16-C17-C18	-8.09	115.76	127.31
9	G	104	A1EFU	C16-C17-C18	-8.09	115.76	127.31
9	1	104	A1EFU	C16-C17-C18	-8.09	115.77	127.31
9	a	101	A1EFU	C15-C14-C13	-8.06	115.80	127.31
9	A	103	A1EFU	C7-C6-C5	-8.00	115.89	127.31
9	N	102	A1EFU	C16-C17-C18	-7.99	115.91	127.31
9	a	101	A1EFU	C11-C10-C9	-7.98	115.92	127.31
9	D	103	A1EFU	C11-C10-C9	-7.96	115.94	127.31
9	D	104	A1EFU	C16-C17-C18	-7.94	115.98	127.31
9	I	101	A1EFU	C16-C17-C18	-7.93	115.99	127.31
9	F	102	A1EFU	C16-C17-C18	-7.91	116.02	127.31
9	E	102	A1EFU	C16-C17-C18	-7.83	116.14	127.31
9	I	101	A1EFU	C7-C6-C5	-7.82	116.15	127.31
9	F	102	A1EFU	C7-C6-C5	-7.82	116.16	127.31
9	E	102	A1EFU	C7-C6-C5	-7.78	116.21	127.31
9	R	102	A1EFU	C16-C17-C18	-7.74	116.27	127.31
9	P	103	A1EFU	C16-C17-C18	-7.67	116.36	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	G	103	A1EFU	C16-C17-C18	-7.61	116.45	127.31
9	J	102	A1EFU	C16-C17-C18	-7.55	116.54	127.31
9	1	103	A1EFU	C16-C17-C18	-7.50	116.61	127.31
11	G	105	MW9	C35-C34-C33	7.05	152.85	112.43
11	M	407	MW9	C35-C34-C33	7.02	152.69	112.43
11	N	103	MW9	C35-C34-C33	7.00	152.58	112.43
11	R	103	MW9	C35-C34-C33	6.99	152.49	112.43
8	P	102	BCL	C1D-ND-C4D	-6.53	101.70	106.33
8	B	102	BCL	CMB-C2B-C1B	-6.50	118.48	128.46
8	d	102	BCL	CMB-C2B-C1B	-6.44	118.56	128.46
8	L	301	BCL	C1D-ND-C4D	-6.42	101.77	106.33
8	B	102	BCL	C1D-ND-C4D	-6.39	101.80	106.33
8	1	101	BCL	C1D-ND-C4D	-6.39	101.80	106.33
8	s	101	BCL	CMB-C2B-C1B	-6.36	118.69	128.46
8	r	101	BCL	C1D-ND-C4D	-6.35	101.82	106.33
8	L	304	BCL	CMB-C2B-C1B	-6.35	118.71	128.46
8	v	102	BCL	C1D-ND-C4D	-6.33	101.84	106.33
8	b	101	BCL	C1D-ND-C4D	-6.33	101.84	106.33
8	T	102	BCL	CMB-C2B-C1B	-6.32	118.75	128.46
8	N	101	BCL	CMB-C2B-C1B	-6.32	118.75	128.46
8	b	101	BCL	CMB-C2B-C1B	-6.29	118.80	128.46
8	q	101	BCL	CMB-C2B-C1B	-6.29	118.80	128.46
8	K	102	BCL	CMB-C2B-C1B	-6.29	118.80	128.46
8	J	101	BCL	CMB-C2B-C1B	-6.28	118.81	128.46
8	a	102	BCL	CMB-C2B-C1B	-6.28	118.81	128.46
8	e	101	BCL	C1D-ND-C4D	-6.28	101.87	106.33
8	G	101	BCL	CMB-C2B-C1B	-6.28	118.82	128.46
8	M	404	BCL	CMB-C2B-C1B	-6.28	118.82	128.46
8	q	101	BCL	C1D-ND-C4D	-6.27	101.88	106.33
8	P	101	BCL	CMB-C2B-C1B	-6.27	118.83	128.46
8	F	101	BCL	CMB-C2B-C1B	-6.27	118.83	128.46
8	I	102	BCL	CMB-C2B-C1B	-6.26	118.84	128.46
8	Q	102	BCL	CMB-C2B-C1B	-6.26	118.85	128.46
8	K	101	BCL	CMB-C2B-C1B	-6.25	118.85	128.46
8	E	101	BCL	CMB-C2B-C1B	-6.24	118.87	128.46
8	a	102	BCL	C1D-ND-C4D	-6.23	101.91	106.33
8	R	101	BCL	CMB-C2B-C1B	-6.23	118.89	128.46
8	n	101	BCL	C1D-ND-C4D	-6.23	101.91	106.33
8	L	301	BCL	CMB-C2B-C1B	-6.22	118.91	128.46
8	1	102	BCL	CMB-C2B-C1B	-6.21	118.92	128.46
8	R	101	BCL	C1D-ND-C4D	-6.21	101.92	106.33
8	v	102	BCL	CMB-C2B-C1B	-6.21	118.92	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	K	101	BCL	C1D-ND-C4D	-6.21	101.93	106.33
8	f	101	BCL	CMB-C2B-C1B	-6.20	118.93	128.46
8	j	101	BCL	CMB-C2B-C1B	-6.20	118.93	128.46
8	S	302	BCL	CMB-C2B-C1B	-6.20	118.94	128.46
8	G	101	BCL	C1D-ND-C4D	-6.20	101.93	106.33
8	G	102	BCL	CMB-C2B-C1B	-6.19	118.95	128.46
8	M	404	BCL	C1D-ND-C4D	-6.18	101.94	106.33
11	F	104	MW9	C35-C34-C33	6.18	152.69	112.55
8	1	101	BCL	CMB-C2B-C1B	-6.18	118.97	128.46
8	e	101	BCL	CMB-C2B-C1B	-6.17	118.98	128.46
8	M	402	BCL	CMB-C2B-C1B	-6.16	118.99	128.46
8	V	101	BCL	C1D-ND-C4D	-6.16	101.96	106.33
8	S	302	BCL	C1D-ND-C4D	-6.15	101.96	106.33
8	D	101	BCL	CMB-C2B-C1B	-6.15	119.01	128.46
8	L	304	BCL	C1D-ND-C4D	-6.15	101.96	106.33
8	I	103	BCL	CMB-C2B-C1B	-6.15	119.02	128.46
11	L	305	MW9	C35-C34-C33	6.14	152.40	112.55
8	j	101	BCL	C1D-ND-C4D	-6.10	102.00	106.33
11	H	301	MW9	C35-C34-C33	6.10	152.17	112.55
8	A	101	BCL	C1D-ND-C4D	-6.10	102.00	106.33
8	M	402	BCL	C1D-ND-C4D	-6.09	102.01	106.33
8	s	101	BCL	C1D-ND-C4D	-6.07	102.02	106.33
8	N	101	BCL	C1D-ND-C4D	-6.06	102.03	106.33
8	T	102	BCL	C1D-ND-C4D	-6.05	102.03	106.33
8	P	101	BCL	C1D-ND-C4D	-6.03	102.05	106.33
9	b	102	A1EFU	C15-C16-C17	-6.01	111.17	123.47
9	D	104	A1EFU	C15-C16-C17	-6.00	111.19	123.47
8	I	102	BCL	C1D-ND-C4D	-5.97	102.09	106.33
9	A	103	A1EFU	C15-C16-C17	-5.96	111.25	123.47
9	a	101	A1EFU	C16-C15-C14	-5.95	111.28	123.47
8	Q	102	BCL	C1D-ND-C4D	-5.94	102.12	106.33
8	K	102	BCL	C1D-ND-C4D	-5.93	102.12	106.33
8	V	101	BCL	CMB-C2B-C1B	-5.93	119.36	128.46
8	b	101	BCL	C2D-C1D-ND	5.92	114.47	110.10
9	1	103	A1EFU	C15-C16-C17	-5.92	111.35	123.47
9	Q	101	A1EFU	C15-C16-C17	-5.91	111.38	123.47
8	I	103	BCL	C1D-ND-C4D	-5.89	102.15	106.33
8	1	102	BCL	C1D-ND-C4D	-5.87	102.16	106.33
8	E	101	BCL	C1D-ND-C4D	-5.87	102.17	106.33
8	L	301	BCL	C2D-C1D-ND	5.86	114.42	110.10
9	A	102	A1EFU	C15-C16-C17	-5.86	111.48	123.47
9	J	102	A1EFU	C15-C16-C17	-5.84	111.52	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	I	101	A1EFU	C15-C16-C17	-5.79	111.60	123.47
9	T	101	A1EFU	C15-C16-C17	-5.77	111.66	123.47
9	a	101	A1EFU	CM6-C18-C17	-5.76	114.85	122.92
9	S	304	A1EFU	CM6-C18-C17	-5.74	114.88	122.92
9	T	103	A1EFU	C15-C16-C17	-5.71	111.77	123.47
9	v	101	A1EFU	CM6-C18-C17	-5.71	114.92	122.92
8	b	101	BCL	C1C-NC-C4C	-5.71	104.14	106.71
9	G	104	A1EFU	C15-C16-C17	-5.68	111.84	123.47
9	d	101	A1EFU	CM6-C18-C17	-5.68	114.97	122.92
8	J	101	BCL	C1D-ND-C4D	-5.67	102.31	106.33
9	F	103	A1EFU	C16-C15-C14	-5.66	111.88	123.47
9	q	102	A1EFU	CM3-C5-C6	-5.66	115.00	122.92
9	F	102	A1EFU	C15-C16-C17	-5.65	111.90	123.47
9	G	103	A1EFU	C15-C16-C17	-5.65	111.90	123.47
8	1	102	BCL	C1C-NC-C4C	-5.64	104.17	106.71
8	K	102	BCL	C1C-NC-C4C	-5.64	104.17	106.71
9	r	102	A1EFU	C15-C16-C17	-5.63	111.94	123.47
8	d	102	BCL	C1D-ND-C4D	-5.63	102.33	106.33
9	1	104	A1EFU	C15-C16-C17	-5.60	112.00	123.47
8	F	101	BCL	C1D-ND-C4D	-5.59	102.36	106.33
9	a	103	A1EFU	CM3-C5-C6	-5.58	115.10	122.92
9	S	304	A1EFU	CM3-C5-C6	-5.56	115.14	122.92
9	J	103	A1EFU	CM3-C5-C6	-5.56	115.14	122.92
8	G	102	BCL	C1D-ND-C4D	-5.55	102.39	106.33
9	a	101	A1EFU	CM3-C5-C6	-5.54	115.16	122.92
8	P	102	BCL	CMB-C2B-C1B	-5.54	119.94	128.46
9	1	104	A1EFU	CM3-C5-C6	-5.54	115.16	122.92
9	K	103	A1EFU	C15-C16-C17	-5.54	112.12	123.47
8	P	102	BCL	C2D-C1D-ND	5.54	114.19	110.10
9	E	102	A1EFU	C15-C16-C17	-5.54	112.12	123.47
9	n	102	A1EFU	CM3-C5-C6	-5.52	115.19	122.92
8	D	101	BCL	C1D-ND-C4D	-5.52	102.41	106.33
9	S	304	A1EFU	C16-C15-C14	-5.51	112.18	123.47
8	I	102	BCL	O2D-CGD-CBD	5.51	121.06	111.27
9	a	103	A1EFU	CM6-C18-C17	-5.51	115.21	122.92
9	A	103	A1EFU	CM4-C9-C10	-5.51	115.21	122.92
8	s	101	BCL	C2D-C1D-ND	5.51	114.16	110.10
9	J	103	A1EFU	CM6-C18-C17	-5.50	115.21	122.92
9	a	103	A1EFU	CM5-C13-C14	-5.50	115.22	122.92
8	n	101	BCL	CMB-C2B-C1B	-5.50	120.01	128.46
8	v	102	BCL	C2D-C1D-ND	5.50	114.16	110.10
9	n	102	A1EFU	C15-C16-C17	-5.50	112.22	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	A	102	A1EFU	CM5-C13-C14	-5.49	115.23	122.92
8	R	101	BCL	C1C-NC-C4C	-5.49	104.24	106.71
9	Q	101	A1EFU	CM5-C13-C14	-5.49	115.23	122.92
9	K	104	A1EFU	C15-C16-C17	-5.49	112.22	123.47
9	T	103	A1EFU	CM3-C5-C6	-5.49	115.24	122.92
9	d	101	A1EFU	C15-C16-C17	-5.49	112.24	123.47
9	q	102	A1EFU	C15-C16-C17	-5.48	112.25	123.47
9	K	104	A1EFU	CM3-C5-C6	-5.48	115.25	122.92
9	N	102	A1EFU	CM4-C9-C10	-5.48	115.25	122.92
9	i	101	A1EFU	C16-C15-C14	-5.48	112.26	123.47
9	M	406	A1EFU	CM6-C18-C17	-5.47	115.26	122.92
8	r	101	BCL	CMB-C2B-C1B	-5.47	120.05	128.46
8	D	101	BCL	C2D-C1D-ND	5.47	114.14	110.10
9	T	101	A1EFU	CM5-C13-C14	-5.47	115.27	122.92
8	K	102	BCL	C2D-C1D-ND	5.46	114.13	110.10
9	M	406	A1EFU	CM3-C5-C6	-5.46	115.27	122.92
9	I	101	A1EFU	CM5-C13-C14	-5.46	115.28	122.92
8	A	101	BCL	C2D-C1D-ND	5.46	114.12	110.10
9	A	103	A1EFU	CM5-C13-C14	-5.45	115.28	122.92
8	A	101	BCL	CMB-C2B-C1B	-5.45	120.09	128.46
9	S	303	A1EFU	CM5-C13-C14	-5.45	115.29	122.92
8	q	101	BCL	C2D-C1D-ND	5.45	114.12	110.10
9	D	103	A1EFU	CM6-C18-C17	-5.45	115.30	122.92
9	p	101	A1EFU	CM5-C13-C14	-5.44	115.30	122.92
9	q	102	A1EFU	CM6-C18-C17	-5.44	115.30	122.92
8	G	101	BCL	C2D-C1D-ND	5.44	114.11	110.10
9	p	101	A1EFU	CM6-C18-C17	-5.43	115.31	122.92
8	1	101	BCL	C2D-C1D-ND	5.43	114.11	110.10
9	b	102	A1EFU	CM5-C13-C14	-5.43	115.31	122.92
9	T	101	A1EFU	CM6-C18-C17	-5.43	115.32	122.92
9	q	102	A1EFU	C16-C15-C14	-5.43	112.35	123.47
9	v	101	A1EFU	C16-C15-C14	-5.43	112.36	123.47
9	P	103	A1EFU	C15-C16-C17	-5.42	112.36	123.47
9	J	103	A1EFU	C16-C15-C14	-5.42	112.37	123.47
9	D	104	A1EFU	CM5-C13-C14	-5.42	115.33	122.92
9	n	102	A1EFU	CM6-C18-C17	-5.42	115.34	122.92
9	F	102	A1EFU	CM5-C13-C14	-5.41	115.34	122.92
9	r	102	A1EFU	CM6-C18-C17	-5.40	115.36	122.92
9	K	104	A1EFU	CM6-C18-C17	-5.40	115.36	122.92
8	r	101	BCL	C2D-C1D-ND	5.40	114.08	110.10
9	b	102	A1EFU	CM4-C9-C10	-5.39	115.38	122.92
9	d	101	A1EFU	CM3-C5-C6	-5.39	115.38	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	a	103	A1EFU	C15-C16-C17	-5.38	112.45	123.47
9	v	101	A1EFU	CM3-C5-C6	-5.38	115.39	122.92
9	J	102	A1EFU	CM5-C13-C14	-5.37	115.40	122.92
8	S	302	BCL	C2D-C1D-ND	5.37	114.06	110.10
8	e	101	BCL	C2D-C1D-ND	5.37	114.06	110.10
8	d	102	BCL	O2D-CGD-CBD	5.36	120.80	111.27
9	E	102	A1EFU	CM4-C9-C10	-5.36	115.41	122.92
8	P	101	BCL	C2D-C1D-ND	5.36	114.06	110.10
8	N	101	BCL	C2D-C1D-ND	5.36	114.06	110.10
9	p	101	A1EFU	CM4-C9-C10	-5.36	115.41	122.92
8	R	101	BCL	C2D-C1D-ND	5.36	114.05	110.10
8	K	101	BCL	C2D-C1D-ND	5.35	114.05	110.10
9	N	102	A1EFU	C16-C15-C14	-5.35	112.51	123.47
8	n	101	BCL	C2D-C1D-ND	5.35	114.05	110.10
9	D	103	A1EFU	C15-C16-C17	-5.34	112.53	123.47
9	i	101	A1EFU	CM3-C5-C6	-5.34	115.44	122.92
9	T	103	A1EFU	CM6-C18-C17	-5.34	115.44	122.92
8	L	304	BCL	C2D-C1D-ND	5.34	114.04	110.10
9	1	103	A1EFU	CM4-C9-C10	-5.33	115.45	122.92
9	G	104	A1EFU	CM4-C9-C10	-5.33	115.45	122.92
8	Q	102	BCL	C2D-C1D-ND	5.33	114.03	110.10
9	F	103	A1EFU	CM6-C18-C17	-5.33	115.46	122.92
8	V	101	BCL	C2D-C1D-ND	5.33	114.03	110.10
9	G	103	A1EFU	CM5-C13-C14	-5.33	115.46	122.92
9	A	102	A1EFU	CM4-C9-C10	-5.33	115.46	122.92
9	r	102	A1EFU	CM3-C5-C6	-5.32	115.47	122.92
9	S	303	A1EFU	C15-C16-C17	-5.32	112.57	123.47
9	F	103	A1EFU	CM4-C9-C10	-5.32	115.47	122.92
9	i	101	A1EFU	C15-C16-C17	-5.32	112.58	123.47
9	K	103	A1EFU	CM4-C9-C10	-5.32	115.47	122.92
9	T	101	A1EFU	CM4-C9-C10	-5.32	115.47	122.92
9	1	103	A1EFU	CM5-C13-C14	-5.32	115.47	122.92
9	R	102	A1EFU	C15-C16-C17	-5.32	112.58	123.47
9	Q	101	A1EFU	CM6-C18-C17	-5.31	115.48	122.92
8	j	101	BCL	C2D-C1D-ND	5.31	114.02	110.10
9	D	104	A1EFU	CM4-C9-C10	-5.31	115.48	122.92
9	K	104	A1EFU	C16-C15-C14	-5.31	112.60	123.47
9	F	102	A1EFU	CM6-C18-C17	-5.31	115.49	122.92
9	p	101	A1EFU	C15-C16-C17	-5.31	112.60	123.47
9	K	103	A1EFU	CM5-C13-C14	-5.31	115.49	122.92
9	T	103	A1EFU	CM4-C9-C10	-5.31	115.49	122.92
9	J	102	A1EFU	CM4-C9-C10	-5.30	115.49	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	I	102	BCL	C2D-C1D-ND	5.30	114.01	110.10
9	v	101	A1EFU	CM4-C9-C10	-5.30	115.50	122.92
9	i	101	A1EFU	CM4-C9-C10	-5.30	115.50	122.92
9	1	104	A1EFU	C16-C15-C14	-5.30	112.62	123.47
9	J	103	A1EFU	C15-C16-C17	-5.30	112.62	123.47
9	E	102	A1EFU	CM5-C13-C14	-5.30	115.50	122.92
8	G	102	BCL	O2D-CGD-CBD	5.29	120.67	111.27
8	G	102	BCL	C1C-NC-C4C	-5.29	104.33	106.71
8	T	102	BCL	C2D-C1D-ND	5.28	114.00	110.10
9	G	103	A1EFU	CM4-C9-C10	-5.28	115.53	122.92
8	M	404	BCL	C2D-C1D-ND	5.28	113.99	110.10
9	S	304	A1EFU	CM5-C13-C14	-5.28	115.53	122.92
9	S	303	A1EFU	CM4-C9-C10	-5.27	115.54	122.92
8	f	101	BCL	O2D-CGD-CBD	5.27	120.64	111.27
9	a	103	A1EFU	CM4-C9-C10	-5.27	115.54	122.92
8	a	102	BCL	C2D-C1D-ND	5.27	113.99	110.10
9	n	102	A1EFU	C16-C15-C14	-5.26	112.70	123.47
9	a	103	A1EFU	C16-C15-C14	-5.26	112.70	123.47
9	b	102	A1EFU	CM6-C18-C17	-5.25	115.56	122.92
9	S	303	A1EFU	C16-C15-C14	-5.25	112.72	123.47
9	R	102	A1EFU	CM5-C13-C14	-5.25	115.57	122.92
9	D	103	A1EFU	C16-C15-C14	-5.25	112.72	123.47
8	B	102	BCL	C2D-C1D-ND	5.25	113.97	110.10
9	r	102	A1EFU	CM4-C9-C10	-5.25	115.57	122.92
9	M	406	A1EFU	CM4-C9-C10	-5.25	115.57	122.92
8	E	101	BCL	O2D-CGD-CBD	5.24	120.59	111.27
9	D	103	A1EFU	CM3-C5-C6	-5.23	115.59	122.92
8	1	102	BCL	C2D-C1D-ND	5.23	113.96	110.10
9	S	303	A1EFU	CM6-C18-C17	-5.23	115.60	122.92
9	P	103	A1EFU	CM3-C5-C6	-5.23	115.60	122.92
9	N	102	A1EFU	C15-C16-C17	-5.22	112.77	123.47
9	P	103	A1EFU	C16-C15-C14	-5.22	112.78	123.47
9	v	101	A1EFU	CM5-C13-C14	-5.22	115.61	122.92
8	I	103	BCL	C1C-NC-C4C	-5.22	104.36	106.71
9	R	102	A1EFU	CM4-C9-C10	-5.22	115.62	122.92
8	I	103	BCL	C2D-C1D-ND	5.21	113.95	110.10
9	p	101	A1EFU	CM3-C5-C6	-5.21	115.62	122.92
9	F	103	A1EFU	CM3-C5-C6	-5.21	115.63	122.92
9	A	103	A1EFU	CM6-C18-C17	-5.20	115.63	122.92
9	I	101	A1EFU	CM4-C9-C10	-5.20	115.63	122.92
9	D	104	A1EFU	CM6-C18-C17	-5.20	115.64	122.92
8	J	101	BCL	C2D-C1D-ND	5.20	113.94	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	1	104	A1EFU	CM6-C18-C17	-5.19	115.65	122.92
9	G	104	A1EFU	CM6-C18-C17	-5.19	115.65	122.92
9	P	103	A1EFU	CM4-C9-C10	-5.19	115.65	122.92
8	I	103	BCL	O2D-CGD-CBD	5.18	120.48	111.27
8	M	402	BCL	C2D-C1D-ND	5.18	113.92	110.10
9	i	101	A1EFU	CM5-C13-C14	-5.18	115.67	122.92
9	R	102	A1EFU	C16-C15-C14	-5.17	112.87	123.47
9	P	103	A1EFU	CM5-C13-C14	-5.17	115.68	122.92
9	T	101	A1EFU	CM3-C5-C6	-5.17	115.68	122.92
9	F	103	A1EFU	C15-C16-C17	-5.17	112.88	123.47
9	S	303	A1EFU	CM3-C5-C6	-5.15	115.70	122.92
8	J	101	BCL	O2D-CGD-CBD	5.15	120.42	111.27
8	L	304	BCL	CAC-C3C-C2C	-5.15	101.40	114.26
9	K	103	A1EFU	CM6-C18-C17	-5.14	115.72	122.92
9	A	102	A1EFU	CM6-C18-C17	-5.14	115.73	122.92
8	K	102	BCL	O2D-CGD-CBD	5.14	120.39	111.27
9	F	102	A1EFU	CM4-C9-C10	-5.13	115.74	122.92
9	i	101	A1EFU	CM6-C18-C17	-5.13	115.74	122.92
9	K	103	A1EFU	CM3-C5-C6	-5.13	115.74	122.92
9	G	104	A1EFU	CM3-C5-C6	-5.12	115.74	122.92
9	Q	101	A1EFU	CM4-C9-C10	-5.12	115.75	122.92
9	G	104	A1EFU	C16-C15-C14	-5.12	112.99	123.47
8	E	101	BCL	C2D-C1D-ND	5.11	113.87	110.10
9	J	103	A1EFU	CM4-C9-C10	-5.11	115.76	122.92
9	1	104	A1EFU	CM4-C9-C10	-5.11	115.76	122.92
9	I	101	A1EFU	CM6-C18-C17	-5.11	115.77	122.92
8	M	404	BCL	CAC-C3C-C2C	-5.11	101.50	114.26
9	J	103	A1EFU	CM5-C13-C14	-5.11	115.77	122.92
9	S	304	A1EFU	CM4-C9-C10	-5.10	115.77	122.92
8	B	102	BCL	O2D-CGD-CBD	5.10	120.33	111.27
9	r	102	A1EFU	C16-C15-C14	-5.10	113.02	123.47
9	R	102	A1EFU	CM3-C5-C6	-5.10	115.78	122.92
8	d	102	BCL	C2D-C1D-ND	5.10	113.86	110.10
9	K	103	A1EFU	C16-C15-C14	-5.09	113.04	123.47
9	a	101	A1EFU	CM5-C13-C14	-5.09	115.79	122.92
9	F	103	A1EFU	CM5-C13-C14	-5.06	115.83	122.92
8	G	101	BCL	O2D-CGD-CBD	5.06	120.26	111.27
8	J	101	BCL	C1C-NC-C4C	-5.06	104.43	106.71
9	J	102	A1EFU	CM6-C18-C17	-5.06	115.84	122.92
8	e	101	BCL	CAC-C3C-C2C	-5.05	101.64	114.26
9	d	101	A1EFU	C16-C15-C14	-5.05	113.13	123.47
9	S	304	A1EFU	C15-C16-C17	-5.05	113.14	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	K	104	A1EFU	CM5-C13-C14	-5.05	115.86	122.92
9	G	103	A1EFU	CM6-C18-C17	-5.05	115.86	122.92
9	1	104	A1EFU	CM5-C13-C14	-5.04	115.86	122.92
8	N	101	BCL	C1C-NC-C4C	-5.03	104.44	106.71
9	N	102	A1EFU	CM5-C13-C14	-5.03	115.88	122.92
8	d	102	BCL	CAC-C3C-C2C	-5.03	101.70	114.26
9	v	101	A1EFU	C15-C16-C17	-5.02	113.18	123.47
9	Q	101	A1EFU	CM3-C5-C6	-5.02	115.89	122.92
9	M	406	A1EFU	C16-C15-C14	-5.02	113.20	123.47
9	p	101	A1EFU	C16-C15-C14	-5.02	113.20	123.47
9	A	102	A1EFU	C16-C15-C14	-5.01	113.20	123.47
9	N	102	A1EFU	CM3-C5-C6	-5.01	115.91	122.92
9	b	102	A1EFU	CM3-C5-C6	-5.01	115.91	122.92
9	n	102	A1EFU	CM4-C9-C10	-5.00	115.91	122.92
8	G	102	BCL	C2D-C1D-ND	4.99	113.78	110.10
9	E	102	A1EFU	C16-C15-C14	-4.99	113.26	123.47
16	C	402	HEC	CBD-CAD-C3D	4.98	121.12	112.62
9	M	406	A1EFU	C15-C16-C17	-4.97	113.30	123.47
9	T	103	A1EFU	C16-C15-C14	-4.96	113.32	123.47
8	f	101	BCL	CAC-C3C-C2C	-4.94	101.91	114.26
9	n	102	A1EFU	CM5-C13-C14	-4.93	116.02	122.92
8	P	102	BCL	O2D-CGD-CBD	4.93	120.03	111.27
9	q	102	A1EFU	CM5-C13-C14	-4.92	116.03	122.92
9	G	103	A1EFU	C16-C15-C14	-4.91	113.41	123.47
9	d	101	A1EFU	CM4-C9-C10	-4.91	116.05	122.92
9	E	102	A1EFU	CM6-C18-C17	-4.91	116.05	122.92
9	T	101	A1EFU	C16-C15-C14	-4.91	113.42	123.47
9	T	103	A1EFU	CM5-C13-C14	-4.90	116.06	122.92
8	M	402	BCL	CAC-C3C-C2C	-4.89	102.03	114.26
8	v	102	BCL	O2D-CGD-CBD	4.89	119.96	111.27
9	q	102	A1EFU	CM4-C9-C10	-4.88	116.08	122.92
9	1	103	A1EFU	CM3-C5-C6	-4.88	116.09	122.92
9	N	102	A1EFU	CM6-C18-C17	-4.88	116.09	122.92
9	D	104	A1EFU	CM3-C5-C6	-4.87	116.09	122.92
9	R	102	A1EFU	CM6-C18-C17	-4.87	116.10	122.92
8	F	101	BCL	C2D-C1D-ND	4.87	113.69	110.10
8	B	102	BCL	CAC-C3C-C2C	-4.86	102.11	114.26
8	S	302	BCL	CAC-C3C-C2C	-4.86	102.11	114.26
9	J	102	A1EFU	CM3-C5-C6	-4.86	116.12	122.92
8	T	102	BCL	C1C-NC-C4C	-4.86	104.52	106.71
8	b	101	BCL	O2D-CGD-CBD	4.85	119.89	111.27
9	G	104	A1EFU	CM5-C13-C14	-4.85	116.13	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	Q	102	BCL	CAC-C3C-C2C	-4.85	102.15	114.26
8	j	101	BCL	O2D-CGD-CBD	4.85	119.88	111.27
8	K	101	BCL	O2D-CGD-CBD	4.84	119.87	111.27
9	K	104	A1EFU	CM4-C9-C10	-4.84	116.14	122.92
9	1	103	A1EFU	C16-C15-C14	-4.83	113.59	123.47
8	1	101	BCL	O2D-CGD-CBD	4.83	119.84	111.27
8	1	101	BCL	CAC-C3C-C2C	-4.82	102.20	114.26
9	G	103	A1EFU	CM3-C5-C6	-4.82	116.17	122.92
8	a	102	BCL	CAC-C3C-C2C	-4.82	102.22	114.26
8	s	101	BCL	O2D-CGD-CBD	4.82	119.83	111.27
8	P	101	BCL	CAC-C3C-C2C	-4.81	102.23	114.26
8	A	101	BCL	O2D-CGD-CBD	4.81	119.82	111.27
9	I	101	A1EFU	C16-C15-C14	-4.81	113.62	123.47
9	A	103	A1EFU	C16-C15-C14	-4.80	113.64	123.47
8	f	101	BCL	C1D-ND-C4D	-4.80	102.92	106.33
9	1	103	A1EFU	CM6-C18-C17	-4.80	116.20	122.92
9	r	102	A1EFU	CM5-C13-C14	-4.80	116.20	122.92
8	G	101	BCL	CAC-C3C-C2C	-4.80	102.28	114.26
8	n	101	BCL	O2D-CGD-CBD	4.79	119.79	111.27
8	V	101	BCL	CAC-C3C-C2C	-4.79	102.29	114.26
8	a	102	BCL	O2D-CGD-CBD	4.79	119.78	111.27
8	Q	102	BCL	O2D-CGD-CBD	4.79	119.77	111.27
9	D	103	A1EFU	CM5-C13-C14	-4.78	116.22	122.92
8	q	101	BCL	O2D-CGD-CBD	4.78	119.77	111.27
9	D	104	A1EFU	C16-C15-C14	-4.78	113.68	123.47
8	P	101	BCL	O2D-CGD-CBD	4.78	119.76	111.27
8	q	101	BCL	CAC-C3C-C2C	-4.78	102.31	114.26
8	P	102	BCL	CAC-C3C-C2C	-4.78	102.32	114.26
8	r	101	BCL	O2D-CGD-CBD	4.77	119.75	111.27
9	D	103	A1EFU	CM4-C9-C10	-4.76	116.25	122.92
9	J	102	A1EFU	C16-C15-C14	-4.76	113.72	123.47
8	B	102	BCL	C4A-NA-C1A	-4.76	104.57	106.71
8	t	101	BCL	C1D-ND-C4D	-4.76	102.95	106.33
8	v	102	BCL	CAC-C3C-C2C	-4.76	102.38	114.26
8	I	102	BCL	CAC-C3C-C2C	-4.76	102.38	114.26
8	V	101	BCL	O2D-CGD-CBD	4.75	119.72	111.27
9	d	101	A1EFU	CM5-C13-C14	-4.75	116.27	122.92
9	F	102	A1EFU	CM3-C5-C6	-4.75	116.27	122.92
8	s	101	BCL	CAC-C3C-C2C	-4.74	102.41	114.26
8	K	101	BCL	CAC-C3C-C2C	-4.74	102.41	114.26
9	F	102	A1EFU	C16-C15-C14	-4.74	113.76	123.47
9	E	102	A1EFU	CM3-C5-C6	-4.74	116.28	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	P	103	A1EFU	CM6-C18-C17	-4.74	116.28	122.92
9	b	102	A1EFU	C16-C15-C14	-4.74	113.77	123.47
8	L	304	BCL	O2D-CGD-CBD	4.74	119.68	111.27
8	t	101	BCL	O2D-CGD-CBD	4.72	119.66	111.27
9	I	101	A1EFU	CM3-C5-C6	-4.72	116.31	122.92
8	D	101	BCL	O2D-CGD-CBD	4.72	119.66	111.27
8	N	101	BCL	O2D-CGD-CBD	4.71	119.64	111.27
8	T	102	BCL	O2D-CGD-CBD	4.71	119.63	111.27
8	A	101	BCL	CAC-C3C-C2C	-4.70	102.50	114.26
8	L	301	BCL	CAC-C3C-C2C	-4.70	102.52	114.26
8	r	101	BCL	CAC-C3C-C2C	-4.69	102.55	114.26
8	E	101	BCL	C1C-NC-C4C	-4.68	104.60	106.71
8	R	101	BCL	O2D-CGD-CBD	4.68	119.58	111.27
8	1	102	BCL	O2D-CGD-CBD	4.67	119.57	111.27
8	e	101	BCL	O2D-CGD-CBD	4.67	119.57	111.27
9	a	101	A1EFU	CM4-C9-C10	-4.66	116.40	122.92
9	a	101	A1EFU	C15-C16-C17	-4.65	113.94	123.47
8	j	101	BCL	CAC-C3C-C2C	-4.63	102.68	114.26
9	Q	101	A1EFU	C16-C15-C14	-4.63	114.00	123.47
8	L	304	BCL	C1C-NC-C4C	-4.62	104.63	106.71
9	M	406	A1EFU	CM5-C13-C14	-4.61	116.47	122.92
8	S	302	BCL	O2D-CGD-CBD	4.60	119.44	111.27
8	F	101	BCL	O2D-CGD-CBD	4.57	119.38	111.27
8	D	101	BCL	CAC-C3C-C2C	-4.53	102.93	114.26
8	E	101	BCL	CAC-C3C-C2C	-4.53	102.95	114.26
8	J	101	BCL	CAC-C3C-C2C	-4.53	102.95	114.26
8	n	101	BCL	CAC-C3C-C2C	-4.52	102.96	114.26
8	d	102	BCL	C1C-NC-C4C	-4.51	104.68	106.71
8	F	101	BCL	CAC-C3C-C2C	-4.49	103.04	114.26
9	A	102	A1EFU	CM3-C5-C6	-4.49	116.64	122.92
8	t	101	BCL	CAC-C3C-C2C	-4.48	103.07	114.26
8	M	402	BCL	O2D-CGD-CBD	4.46	119.19	111.27
9	d	101	A1EFU	CM7-C22-C21	-4.45	111.11	122.59
8	T	102	BCL	CAC-C3C-C2C	-4.44	103.17	114.26
8	t	101	BCL	C2D-C1D-ND	4.43	113.37	110.10
8	f	101	BCL	C2D-C1D-ND	4.42	113.36	110.10
8	I	102	BCL	O2D-CGD-O1D	-4.40	115.23	123.84
8	I	103	BCL	CAC-C3C-C2C	-4.40	103.28	114.26
9	r	102	A1EFU	CM7-C22-C21	-4.38	111.28	122.59
8	K	102	BCL	CAC-C3C-C2C	-4.38	103.32	114.26
9	A	102	A1EFU	CM7-C22-C21	-4.37	111.32	122.59
9	n	102	A1EFU	CM7-C22-C21	-4.36	111.34	122.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	P	103	A1EFU	CM3-C5-C4	4.36	124.94	118.08
9	A	103	A1EFU	CM3-C5-C6	-4.35	116.83	122.92
9	i	101	A1EFU	CM3-C5-C4	4.35	124.92	118.08
9	J	102	A1EFU	CM7-C22-C21	-4.34	111.38	122.59
8	J	101	BCL	O2D-CGD-O1D	-4.33	115.36	123.84
8	N	101	BCL	CAC-C3C-C2C	-4.33	103.43	114.26
9	1	104	A1EFU	CM7-C22-C21	-4.33	111.42	122.59
8	G	102	BCL	CAC-C3C-C2C	-4.33	103.44	114.26
9	D	104	A1EFU	C6-C7-C8	-4.32	109.73	123.22
8	R	101	BCL	CAC-C3C-C2C	-4.32	103.46	114.26
9	p	101	A1EFU	CM7-C22-C21	-4.32	111.45	122.59
9	I	101	A1EFU	CM3-C5-C4	4.31	124.87	118.08
9	T	101	A1EFU	CM3-C5-C4	4.31	124.86	118.08
9	T	103	A1EFU	CM7-C22-C21	-4.30	111.49	122.59
8	G	102	BCL	O2D-CGD-O1D	-4.30	115.43	123.84
8	M	402	BCL	C1C-NC-C4C	-4.29	104.78	106.71
9	K	104	A1EFU	CM7-C22-C21	-4.29	111.52	122.59
8	E	101	BCL	O2D-CGD-O1D	-4.29	115.45	123.84
9	q	102	A1EFU	C10-C11-C12	-4.29	109.84	123.22
8	f	101	BCL	O2D-CGD-O1D	-4.28	115.46	123.84
8	I	103	BCL	O2D-CGD-O1D	-4.28	115.47	123.84
8	e	101	BCL	C1C-NC-C4C	-4.28	104.78	106.71
9	E	102	A1EFU	C6-C7-C8	-4.28	109.87	123.22
8	K	102	BCL	O2D-CGD-O1D	-4.27	115.48	123.84
8	b	101	BCL	O2D-CGD-O1D	-4.27	115.48	123.84
9	G	104	A1EFU	CM7-C22-C21	-4.27	111.57	122.59
9	i	101	A1EFU	CM7-C22-C21	-4.27	111.57	122.59
9	I	101	A1EFU	CM7-C22-C21	-4.27	111.58	122.59
8	d	102	BCL	O2D-CGD-O1D	-4.26	115.50	123.84
9	F	102	A1EFU	CM7-C22-C21	-4.26	111.59	122.59
9	J	103	A1EFU	CM3-C5-C4	4.26	124.79	118.08
9	q	102	A1EFU	CM7-C22-C21	-4.26	111.60	122.59
9	a	101	A1EFU	C10-C11-C12	-4.26	109.93	123.22
9	K	103	A1EFU	CM7-C22-C21	-4.25	111.62	122.59
9	b	102	A1EFU	CM7-C22-C21	-4.25	111.62	122.59
9	G	103	A1EFU	CM7-C22-C21	-4.25	111.62	122.59
9	I	101	A1EFU	C6-C7-C8	-4.25	109.95	123.22
9	K	104	A1EFU	CM3-C5-C4	4.25	124.77	118.08
9	K	104	A1EFU	C10-C11-C12	-4.25	109.96	123.22
9	T	103	A1EFU	CM3-C5-C4	4.25	124.77	118.08
16	C	403	HEC	CMD-C2D-C1D	-4.25	121.94	128.46
9	D	103	A1EFU	CM7-C22-C21	-4.24	111.64	122.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	1	103	A1EFU	CM7-C22-C21	-4.24	111.65	122.59
9	r	102	A1EFU	CM3-C5-C4	4.24	124.75	118.08
9	E	102	A1EFU	CM3-C5-C4	4.24	124.75	118.08
8	M	404	BCL	CHD-C1D-ND	-4.23	120.56	124.45
9	T	101	A1EFU	CM7-C22-C21	-4.23	111.68	122.59
9	F	103	A1EFU	CM3-C5-C4	4.23	124.74	118.08
9	Q	101	A1EFU	CM7-C22-C21	-4.23	111.68	122.59
9	n	102	A1EFU	CM3-C5-C4	4.23	124.74	118.08
8	B	102	BCL	CMB-C2B-C3B	4.23	132.58	124.68
8	t	101	BCL	CHD-C1D-ND	-4.22	120.57	124.45
8	G	101	BCL	O2D-CGD-O1D	-4.22	115.58	123.84
16	C	402	HEC	CMD-C2D-C1D	-4.22	121.98	128.46
9	F	103	A1EFU	CM7-C22-C21	-4.22	111.71	122.59
9	P	103	A1EFU	CM7-C22-C21	-4.21	111.72	122.59
8	j	101	BCL	C1C-NC-C4C	-4.21	104.81	106.71
9	D	104	A1EFU	CM3-C5-C4	4.21	124.71	118.08
9	M	406	A1EFU	CM7-C22-C21	-4.21	111.73	122.59
9	Q	101	A1EFU	CM3-C5-C4	4.20	124.70	118.08
8	M	404	BCL	CMB-C2B-C3B	4.20	132.53	124.68
9	D	103	A1EFU	C10-C11-C12	-4.19	110.14	123.22
8	P	102	BCL	O2D-CGD-O1D	-4.19	115.65	123.84
9	P	103	A1EFU	C6-C7-C8	-4.19	110.15	123.22
9	q	102	A1EFU	CM3-C5-C4	4.19	124.67	118.08
8	L	301	BCL	O2D-CGD-CBD	4.19	118.70	111.27
9	a	103	A1EFU	CM7-C22-C21	-4.18	111.80	122.59
9	F	102	A1EFU	C6-C7-C8	-4.18	110.18	123.22
8	K	101	BCL	CHD-C1D-ND	-4.18	120.61	124.45
9	D	104	A1EFU	CM7-C22-C21	-4.18	111.81	122.59
9	A	103	A1EFU	CM7-C22-C21	-4.18	111.81	122.59
9	S	303	A1EFU	CM7-C22-C21	-4.18	111.81	122.59
16	C	403	HEC	CMB-C2B-C3B	4.17	130.73	125.82
9	N	102	A1EFU	CM4-C9-C8	4.17	124.65	118.08
9	S	303	A1EFU	CM3-C5-C4	4.17	124.65	118.08
9	M	406	A1EFU	CM3-C5-C4	4.17	124.65	118.08
9	1	103	A1EFU	CM4-C9-C8	4.17	124.65	118.08
9	S	304	A1EFU	CM3-C5-C4	4.17	124.65	118.08
9	a	103	A1EFU	CM4-C9-C8	4.17	124.65	118.08
9	1	104	A1EFU	CM3-C5-C4	4.17	124.64	118.08
9	E	102	A1EFU	CM7-C22-C21	-4.16	111.85	122.59
9	d	101	A1EFU	CM3-C5-C4	4.16	124.64	118.08
9	1	103	A1EFU	CM3-C5-C4	4.16	124.63	118.08
8	v	102	BCL	C1C-NC-C4C	-4.16	104.84	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	R	102	A1EFU	CM3-C5-C4	4.16	124.63	118.08
9	1	104	A1EFU	C10-C11-C12	-4.16	110.25	123.22
9	1	103	A1EFU	C6-C7-C8	-4.16	110.25	123.22
9	R	102	A1EFU	CM7-C22-C21	-4.15	111.88	122.59
9	N	102	A1EFU	CM7-C22-C21	-4.15	111.88	122.59
9	A	102	A1EFU	C23-C22-C21	-4.15	109.42	121.98
9	P	103	A1EFU	CM4-C9-C8	4.15	124.61	118.08
8	L	304	BCL	CMB-C2B-C3B	4.15	132.44	124.68
9	K	103	A1EFU	CM3-C5-C4	4.14	124.61	118.08
8	N	101	BCL	CMB-C2B-C3B	4.14	132.43	124.68
9	K	104	A1EFU	CM4-C9-C8	4.14	124.59	118.08
8	1	102	BCL	CAC-C3C-C2C	-4.13	103.94	114.26
9	S	304	A1EFU	CM4-C9-C8	4.13	124.58	118.08
8	s	101	BCL	CMB-C2B-C3B	4.13	132.40	124.68
8	P	101	BCL	CMB-C2B-C3B	4.13	132.40	124.68
9	D	104	A1EFU	CM4-C9-C8	4.12	124.58	118.08
8	V	101	BCL	CMB-C2B-C3B	4.12	132.39	124.68
8	Q	102	BCL	CMB-C2B-C3B	4.12	132.39	124.68
8	F	101	BCL	CMB-C2B-C3B	4.12	132.39	124.68
11	G	106	MW9	O8-C24-C25	4.12	120.38	111.50
8	V	101	BCL	C4B-CHC-C1C	-4.12	121.97	130.12
8	R	101	BCL	CMB-C2B-C3B	4.11	132.38	124.68
8	D	101	BCL	C1C-NC-C4C	-4.11	104.86	106.71
9	a	101	A1EFU	CM3-C5-C4	4.11	124.56	118.08
8	q	101	BCL	CMB-C2B-C3B	4.11	132.37	124.68
8	s	101	BCL	O2D-CGD-O1D	-4.11	115.80	123.84
8	s	101	BCL	CHD-C1D-ND	-4.11	120.68	124.45
8	T	102	BCL	CMB-C2B-C3B	4.11	132.36	124.68
9	i	101	A1EFU	CM4-C9-C8	4.11	124.55	118.08
9	b	102	A1EFU	CM4-C9-C8	4.11	124.55	118.08
8	j	101	BCL	O2D-CGD-O1D	-4.10	115.82	123.84
8	F	101	BCL	O2D-CGD-O1D	-4.10	115.82	123.84
8	b	101	BCL	CMB-C2B-C3B	4.10	132.35	124.68
8	F	101	BCL	CHD-C1D-ND	-4.10	120.69	124.45
9	q	102	A1EFU	CM4-C9-C8	4.10	124.54	118.08
9	F	102	A1EFU	CM3-C5-C4	4.10	124.54	118.08
9	v	101	A1EFU	CM7-C22-C21	-4.10	112.01	122.59
16	C	401	HEC	CMD-C2D-C1D	-4.10	122.16	128.46
9	J	103	A1EFU	C10-C11-C12	-4.10	110.43	123.22
8	J	101	BCL	CMB-C2B-C3B	4.10	132.34	124.68
8	V	101	BCL	C4A-NA-C1A	-4.09	104.86	106.71
8	I	102	BCL	CMB-C2B-C3B	4.09	132.32	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	1	104	A1EFU	CM4-C9-C8	4.09	124.52	118.08
11	L	305	MW9	O8-C24-C25	4.09	120.31	111.50
11	H	301	MW9	O8-C24-C25	4.09	120.31	111.50
8	K	102	BCL	CMB-C2B-C3B	4.09	132.32	124.68
8	a	102	BCL	CMB-C2B-C3B	4.08	132.32	124.68
9	Q	101	A1EFU	C6-C7-C8	-4.08	110.47	123.22
9	J	103	A1EFU	CM4-C9-C8	4.08	124.51	118.08
8	K	101	BCL	O2D-CGD-O1D	-4.08	115.86	123.84
9	p	101	A1EFU	CM3-C5-C4	4.08	124.50	118.08
9	S	303	A1EFU	CM4-C9-C8	4.08	124.50	118.08
9	K	103	A1EFU	CM4-C9-C8	4.08	124.50	118.08
8	L	301	BCL	CMB-C2B-C3B	4.07	132.30	124.68
9	E	102	A1EFU	CM4-C9-C8	4.07	124.49	118.08
8	r	101	BCL	O2D-CGD-O1D	-4.07	115.88	123.84
9	b	102	A1EFU	C6-C7-C8	-4.07	110.52	123.22
8	v	102	BCL	CMB-C2B-C3B	4.07	132.29	124.68
8	K	101	BCL	CMB-C2B-C3B	4.06	132.28	124.68
8	t	101	BCL	O2D-CGD-O1D	-4.06	115.89	123.84
8	1	101	BCL	O2D-CGD-O1D	-4.06	115.89	123.84
8	M	402	BCL	CMB-C2B-C3B	4.06	132.28	124.68
11	G	105	MW9	O8-C24-C25	4.06	120.25	111.50
8	a	102	BCL	O2D-CGD-O1D	-4.06	115.90	123.84
8	G	101	BCL	CMB-C2B-C3B	4.06	132.27	124.68
8	n	101	BCL	O2D-CGD-O1D	-4.06	115.91	123.84
8	L	304	BCL	O2D-CGD-O1D	-4.06	115.91	123.84
8	N	101	BCL	O2D-CGD-O1D	-4.05	115.91	123.84
11	M	407	MW9	O8-C24-C25	4.05	120.24	111.50
8	t	101	BCL	OBB-CAB-CBB	-4.05	111.05	120.17
8	d	102	BCL	CMB-C2B-C3B	4.05	132.26	124.68
8	v	102	BCL	O2D-CGD-O1D	-4.05	115.92	123.84
8	R	101	BCL	O2D-CGD-O1D	-4.05	115.92	123.84
8	A	101	BCL	O2D-CGD-O1D	-4.05	115.92	123.84
9	T	101	A1EFU	CM4-C9-C8	4.05	124.45	118.08
8	e	101	BCL	O2D-CGD-O1D	-4.05	115.93	123.84
9	S	304	A1EFU	C10-C11-C12	-4.04	110.59	123.22
8	q	101	BCL	O2D-CGD-O1D	-4.04	115.94	123.84
8	S	302	BCL	CMB-C2B-C3B	4.04	132.24	124.68
9	a	101	A1EFU	CM5-C13-C12	4.04	124.44	118.08
8	1	102	BCL	O2D-CGD-O1D	-4.04	115.94	123.84
8	P	101	BCL	O2D-CGD-O1D	-4.04	115.94	123.84
8	G	102	BCL	CMB-C2B-C3B	4.03	132.22	124.68
8	E	101	BCL	CMB-C2B-C3B	4.03	132.22	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	D	103	A1EFU	CM4-C9-C8	4.03	124.42	118.08
8	Q	102	BCL	O2D-CGD-O1D	-4.03	115.96	123.84
15	H	303	CDL	OB6-CB5-C51	4.02	120.17	111.50
8	1	102	BCL	CMB-C2B-C3B	4.02	132.20	124.68
8	D	101	BCL	CMB-C2B-C3B	4.02	132.20	124.68
8	M	402	BCL	CHD-C1D-ND	-4.02	120.76	124.45
8	1	101	BCL	CMB-C2B-C3B	4.02	132.19	124.68
16	C	403	HEC	CMB-C2B-C1B	-4.02	122.29	128.46
9	K	103	A1EFU	C6-C7-C8	-4.01	110.69	123.22
11	H	302	MW9	O8-C24-C25	4.01	120.15	111.50
8	j	101	BCL	CMB-C2B-C3B	4.01	132.19	124.68
9	S	304	A1EFU	CM7-C22-C21	-4.01	112.24	122.59
8	V	101	BCL	O2D-CGD-O1D	-4.01	116.00	123.84
9	J	102	A1EFU	CM3-C5-C4	4.01	124.40	118.08
9	A	102	A1EFU	CM5-C13-C12	4.01	124.39	118.08
8	f	101	BCL	CMB-C2B-C3B	4.01	132.17	124.68
8	D	101	BCL	O2D-CGD-O1D	-4.00	116.01	123.84
11	R	103	MW9	O8-C24-C25	4.00	120.12	111.50
9	D	104	A1EFU	CM6-C18-C19	4.00	124.38	118.08
9	G	103	A1EFU	CM4-C9-C8	4.00	124.37	118.08
9	a	101	A1EFU	CM7-C22-C21	-3.99	112.29	122.59
8	V	101	BCL	OBB-CAB-CBB	-3.99	111.18	120.17
9	J	102	A1EFU	C6-C7-C8	-3.99	110.77	123.22
8	M	404	BCL	O2D-CGD-CBD	3.99	118.35	111.27
9	S	303	A1EFU	CM5-C13-C12	3.99	124.36	118.08
9	P	103	A1EFU	C10-C11-C12	-3.99	110.78	123.22
8	M	402	BCL	O2D-CGD-O1D	-3.98	116.06	123.84
9	a	101	A1EFU	C6-C7-C8	-3.98	110.80	123.22
9	1	104	A1EFU	CM6-C18-C19	3.98	124.35	118.08
8	I	103	BCL	CMB-C2B-C3B	3.98	132.12	124.68
9	a	101	A1EFU	CM4-C9-C8	3.98	124.34	118.08
8	S	302	BCL	O2D-CGD-O1D	-3.98	116.06	123.84
9	Q	101	A1EFU	CM4-C9-C8	3.98	124.34	118.08
9	a	103	A1EFU	CM6-C18-C19	3.97	124.34	118.08
9	i	101	A1EFU	C6-C7-C8	-3.97	110.83	123.22
9	J	102	A1EFU	CM4-C9-C8	3.97	124.33	118.08
8	T	102	BCL	O2D-CGD-O1D	-3.97	116.08	123.84
9	a	103	A1EFU	C23-C22-C21	-3.97	109.97	121.98
9	F	103	A1EFU	CM4-C9-C8	3.96	124.32	118.08
9	R	102	A1EFU	C6-C7-C8	-3.96	110.85	123.22
8	e	101	BCL	CMB-C2B-C3B	3.96	132.09	124.68
9	T	103	A1EFU	CM4-C9-C8	3.96	124.31	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	F	102	A1EFU	CM4-C9-C8	3.96	124.31	118.08
9	N	102	A1EFU	C6-C7-C8	-3.95	110.89	123.22
9	N	102	A1EFU	CM5-C13-C12	3.95	124.30	118.08
9	A	102	A1EFU	CM6-C18-C19	3.95	124.30	118.08
15	H	303	CDL	OA6-CA5-C11	3.95	120.01	111.50
8	M	404	BCL	C1C-NC-C4C	-3.94	104.93	106.71
9	S	303	A1EFU	C6-C7-C8	-3.94	110.92	123.22
9	P	103	A1EFU	CM5-C13-C12	3.94	124.29	118.08
11	F	104	MW9	O8-C24-C25	3.94	119.99	111.50
8	e	101	BCL	OBB-CAB-CBB	-3.93	111.31	120.17
9	b	102	A1EFU	C23-C22-C21	-3.93	110.08	121.98
9	D	103	A1EFU	CM6-C18-C19	3.93	124.27	118.08
9	q	102	A1EFU	C6-C7-C8	-3.93	110.96	123.22
9	N	102	A1EFU	CM3-C5-C4	3.93	124.26	118.08
9	T	101	A1EFU	CM6-C18-C19	3.92	124.26	118.08
9	M	406	A1EFU	CM6-C18-C19	3.92	124.26	118.08
9	p	101	A1EFU	CM4-C9-C8	3.92	124.25	118.08
9	v	101	A1EFU	CM3-C5-C4	3.92	124.25	118.08
9	1	104	A1EFU	CM5-C13-C12	3.92	124.25	118.08
9	v	101	A1EFU	C23-C22-C21	-3.91	110.13	121.98
9	b	102	A1EFU	CM3-C5-C4	3.91	124.24	118.08
9	n	102	A1EFU	CM6-C18-C19	3.91	124.24	118.08
15	M	408	CDL	OB6-CB5-C51	3.91	119.93	111.50
9	J	103	A1EFU	CM7-C22-C21	-3.91	112.50	122.59
9	T	101	A1EFU	C6-C7-C8	-3.91	111.03	123.22
15	M	408	CDL	OA6-CA5-C11	3.91	119.92	111.50
9	S	304	A1EFU	C23-C22-C21	-3.91	110.15	121.98
9	T	103	A1EFU	CM6-C18-C19	3.90	124.23	118.08
9	A	103	A1EFU	CM4-C9-C8	3.90	124.23	118.08
8	1	101	BCL	OBB-CAB-CBB	-3.90	111.39	120.17
9	Q	101	A1EFU	CM6-C18-C19	3.90	124.22	118.08
9	a	103	A1EFU	CM3-C5-C4	3.90	124.22	118.08
9	a	103	A1EFU	CM5-C13-C12	3.90	124.22	118.08
9	R	102	A1EFU	CM4-C9-C8	3.90	124.22	118.08
9	1	104	A1EFU	C23-C22-C21	-3.89	110.19	121.98
9	v	101	A1EFU	CM6-C18-C19	3.89	124.21	118.08
8	f	101	BCL	CHD-C1D-ND	-3.89	120.88	124.45
9	S	304	A1EFU	CM6-C18-C19	3.89	124.21	118.08
9	b	102	A1EFU	CM6-C18-C19	3.89	124.20	118.08
9	q	102	A1EFU	CM5-C13-C12	3.89	124.20	118.08
9	a	101	A1EFU	C23-C22-C21	-3.89	110.21	121.98
8	G	101	BCL	OBB-CAB-CBB	-3.89	111.42	120.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	K	104	A1EFU	C6-C7-C8	-3.89	111.09	123.22
9	G	104	A1EFU	CM6-C18-C19	3.89	124.20	118.08
9	M	406	A1EFU	CM4-C9-C8	3.89	124.20	118.08
9	r	102	A1EFU	CM4-C9-C8	3.88	124.20	118.08
8	L	304	BCL	CHD-C1D-ND	-3.88	120.88	124.45
9	v	101	A1EFU	CM5-C13-C12	3.88	124.19	118.08
8	a	102	BCL	OBB-CAB-CBB	-3.88	111.43	120.17
9	G	104	A1EFU	CM4-C9-C8	3.88	124.19	118.08
9	T	101	A1EFU	CM5-C13-C12	3.88	124.19	118.08
9	J	103	A1EFU	C23-C22-C21	-3.88	110.25	121.98
9	S	304	A1EFU	C6-C7-C8	-3.88	111.12	123.22
8	T	102	BCL	OBB-CAB-CBB	-3.88	111.45	120.17
9	a	103	A1EFU	C6-C7-C8	-3.87	111.12	123.22
9	N	102	A1EFU	C10-C11-C12	-3.87	111.14	123.22
9	A	103	A1EFU	C23-C22-C21	-3.87	110.26	121.98
9	d	101	A1EFU	CM6-C18-C19	3.87	124.17	118.08
8	L	301	BCL	O2D-CGD-O1D	-3.87	116.28	123.84
8	K	101	BCL	OBB-CAB-CBB	-3.87	111.47	120.17
8	j	101	BCL	OBB-CAB-CBB	-3.87	111.47	120.17
9	D	104	A1EFU	CM5-C13-C12	3.87	124.17	118.08
9	R	102	A1EFU	CM5-C13-C12	3.86	124.17	118.08
9	D	103	A1EFU	CM3-C5-C4	3.86	124.16	118.08
8	M	402	BCL	OBB-CAB-CBB	-3.86	111.48	120.17
8	L	301	BCL	OBB-CAB-CBB	-3.86	111.48	120.17
9	D	103	A1EFU	C6-C7-C8	-3.86	111.17	123.22
9	K	103	A1EFU	CM5-C13-C12	3.86	124.15	118.08
9	D	104	A1EFU	C23-C22-C21	-3.85	110.31	121.98
9	1	103	A1EFU	C23-C22-C21	-3.85	110.31	121.98
8	I	102	BCL	OBB-CAB-CBB	-3.85	111.50	120.17
9	i	101	A1EFU	C23-C22-C21	-3.85	110.32	121.98
9	I	101	A1EFU	CM4-C9-C8	3.85	124.14	118.08
8	1	102	BCL	C2C-C3C-C4C	-3.85	95.58	101.34
8	v	102	BCL	OBB-CAB-CBB	-3.85	111.51	120.17
8	R	101	BCL	OBB-CAB-CBB	-3.85	111.51	120.17
9	1	103	A1EFU	CM6-C18-C19	3.85	124.14	118.08
8	K	102	BCL	OBB-CAB-CBB	-3.84	111.52	120.17
9	F	103	A1EFU	C6-C7-C8	-3.84	111.23	123.22
9	b	102	A1EFU	CM5-C13-C12	3.84	124.13	118.08
11	N	103	MW9	O8-C24-C25	3.84	119.77	111.50
9	a	101	A1EFU	CM6-C18-C19	3.84	124.12	118.08
8	q	101	BCL	OBB-CAB-CBB	-3.84	111.53	120.17
9	M	406	A1EFU	C6-C7-C8	-3.84	111.25	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	S	302	BCL	OBB-CAB-CBB	-3.83	111.54	120.17
8	L	304	BCL	OBB-CAB-CBB	-3.83	111.54	120.17
9	A	102	A1EFU	CM4-C9-C8	3.83	124.12	118.08
9	n	102	A1EFU	C23-C22-C21	-3.83	110.38	121.98
9	T	103	A1EFU	C6-C7-C8	-3.83	111.26	123.22
9	1	104	A1EFU	C6-C7-C8	-3.83	111.26	123.22
9	v	101	A1EFU	CM4-C9-C8	3.83	124.11	118.08
9	A	103	A1EFU	CM5-C13-C12	3.83	124.11	118.08
9	J	102	A1EFU	CM6-C18-C19	3.83	124.11	118.08
8	s	101	BCL	OBB-CAB-CBB	-3.83	111.56	120.17
9	M	406	A1EFU	C10-C11-C12	-3.83	111.28	123.22
8	E	101	BCL	OBB-CAB-CBB	-3.82	111.56	120.17
8	I	103	BCL	OBB-CAB-CBB	-3.82	111.57	120.17
16	C	403	HEC	CBD-CAD-C3D	3.82	119.14	112.62
8	P	101	BCL	OBB-CAB-CBB	-3.82	111.57	120.17
8	G	102	BCL	OBB-CAB-CBB	-3.82	111.58	120.17
8	t	101	BCL	CHA-C1A-NA	-3.82	117.66	126.40
9	1	103	A1EFU	CM5-C13-C12	3.82	124.09	118.08
8	M	404	BCL	OBB-CAB-CBB	-3.81	111.58	120.17
8	N	101	BCL	OBB-CAB-CBB	-3.81	111.59	120.17
8	A	101	BCL	OBB-CAB-CBB	-3.81	111.59	120.17
8	f	101	BCL	OBB-CAB-CBB	-3.81	111.60	120.17
9	i	101	A1EFU	CM6-C18-C19	3.81	124.07	118.08
9	G	104	A1EFU	CM3-C5-C4	3.80	124.07	118.08
9	p	101	A1EFU	CM6-C18-C19	3.80	124.06	118.08
9	r	102	A1EFU	C6-C7-C8	-3.80	111.36	123.22
8	B	102	BCL	OBB-CAB-CBB	-3.80	111.62	120.17
8	1	102	BCL	OBB-CAB-CBB	-3.80	111.63	120.17
9	I	101	A1EFU	CM5-C13-C12	3.80	124.06	118.08
9	S	304	A1EFU	CM5-C13-C12	3.79	124.06	118.08
8	M	404	BCL	O2D-CGD-O1D	-3.79	116.42	123.84
9	J	102	A1EFU	CM5-C13-C12	3.79	124.05	118.08
8	b	101	BCL	OBB-CAB-CBB	-3.79	111.64	120.17
8	n	101	BCL	OBB-CAB-CBB	-3.79	111.65	120.17
8	Q	102	BCL	OBB-CAB-CBB	-3.78	111.65	120.17
9	F	102	A1EFU	CM5-C13-C12	3.78	124.04	118.08
8	J	101	BCL	OBB-CAB-CBB	-3.78	111.66	120.17
9	Q	101	A1EFU	CM5-C13-C12	3.78	124.03	118.08
9	K	103	A1EFU	C10-C11-C12	-3.78	111.42	123.22
9	N	102	A1EFU	C23-C22-C21	-3.78	110.54	121.98
9	A	103	A1EFU	CM6-C18-C19	3.78	124.03	118.08
9	S	303	A1EFU	C10-C11-C12	-3.78	111.43	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	E	102	A1EFU	CM5-C13-C12	3.77	124.02	118.08
8	r	101	BCL	OBB-CAB-CBB	-3.77	111.68	120.17
8	D	101	BCL	OBB-CAB-CBB	-3.77	111.69	120.17
9	q	102	A1EFU	CM6-C18-C19	3.77	124.02	118.08
9	G	103	A1EFU	CM5-C13-C12	3.77	124.01	118.08
8	q	101	BCL	CHD-C1D-ND	-3.77	120.99	124.45
9	J	103	A1EFU	CM6-C18-C19	3.76	124.01	118.08
9	A	103	A1EFU	CM3-C5-C4	3.76	124.01	118.08
9	G	103	A1EFU	C6-C7-C8	-3.76	111.48	123.22
8	P	102	BCL	OBB-CAB-CBB	-3.76	111.71	120.17
9	p	101	A1EFU	C23-C22-C21	-3.76	110.61	121.98
9	T	101	A1EFU	C23-C22-C21	-3.75	110.61	121.98
9	i	101	A1EFU	C10-C11-C12	-3.75	111.50	123.22
9	n	102	A1EFU	CM4-C9-C8	3.75	123.98	118.08
9	K	104	A1EFU	CM6-C18-C19	3.75	123.98	118.08
9	J	103	A1EFU	C6-C7-C8	-3.74	111.53	123.22
9	p	101	A1EFU	CM5-C13-C12	3.74	123.98	118.08
9	S	303	A1EFU	C23-C22-C21	-3.74	110.65	121.98
9	1	103	A1EFU	C10-C11-C12	-3.74	111.54	123.22
9	r	102	A1EFU	CM6-C18-C19	3.74	123.97	118.08
8	R	101	BCL	C2C-C3C-C4C	-3.74	95.74	101.34
8	F	101	BCL	OBB-CAB-CBB	-3.73	111.77	120.17
9	F	102	A1EFU	CM6-C18-C19	3.73	123.96	118.08
9	1	103	A1EFU	C21-C20-C19	-3.73	111.58	123.22
8	J	101	BCL	CHD-C1D-ND	-3.73	121.03	124.45
9	A	102	A1EFU	C21-C20-C19	-3.73	111.58	123.22
16	C	401	HEC	CMB-C2B-C3B	3.73	130.20	125.82
9	n	102	A1EFU	C6-C7-C8	-3.73	111.59	123.22
9	A	103	A1EFU	C6-C7-C8	-3.73	111.59	123.22
9	F	103	A1EFU	CM6-C18-C19	3.72	123.94	118.08
9	p	101	A1EFU	C6-C7-C8	-3.72	111.61	123.22
9	F	103	A1EFU	C23-C22-C21	-3.72	110.72	121.98
9	T	103	A1EFU	C23-C22-C21	-3.72	110.72	121.98
8	b	101	BCL	CAC-C3C-C2C	-3.72	104.97	114.26
8	R	101	BCL	CHD-C1D-ND	-3.72	121.04	124.45
9	Q	101	A1EFU	C23-C22-C21	-3.71	110.74	121.98
9	P	103	A1EFU	C23-C22-C21	-3.71	110.75	121.98
9	I	101	A1EFU	CM6-C18-C19	3.71	123.92	118.08
8	L	301	BCL	CHD-C1D-ND	-3.70	121.05	124.45
8	B	102	BCL	O2D-CGD-O1D	-3.70	116.60	123.84
9	D	104	A1EFU	C10-C11-C12	-3.70	111.68	123.22
9	R	102	A1EFU	C10-C11-C12	-3.70	111.68	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	P	102	BCL	CHD-C1D-ND	-3.70	121.06	124.45
8	e	101	BCL	CHD-C1D-ND	-3.69	121.06	124.45
8	B	102	BCL	CHD-C1D-ND	-3.68	121.07	124.45
9	I	101	A1EFU	C23-C22-C21	-3.68	110.83	121.98
9	S	303	A1EFU	CM6-C18-C19	3.68	123.87	118.08
9	D	103	A1EFU	CM5-C13-C12	3.68	123.87	118.08
9	D	104	A1EFU	C21-C20-C19	-3.68	111.74	123.22
9	G	103	A1EFU	CM6-C18-C19	3.67	123.86	118.08
8	I	103	BCL	CHD-C1D-ND	-3.67	121.08	124.45
9	v	101	A1EFU	C10-C11-C12	-3.66	111.78	123.22
9	b	102	A1EFU	C10-C11-C12	-3.66	111.79	123.22
8	A	101	BCL	CHD-C1D-ND	-3.66	121.09	124.45
9	1	104	A1EFU	C21-C20-C19	-3.65	111.82	123.22
9	R	102	A1EFU	C23-C22-C21	-3.65	110.94	121.98
9	K	103	A1EFU	CM6-C18-C19	3.65	123.82	118.08
9	F	102	A1EFU	C10-C11-C12	-3.65	111.84	123.22
9	d	101	A1EFU	C6-C7-C8	-3.64	111.84	123.22
9	A	102	A1EFU	C10-C11-C12	-3.64	111.85	123.22
8	r	101	BCL	CHD-C1D-ND	-3.64	121.11	124.45
9	E	102	A1EFU	C10-C11-C12	-3.64	111.85	123.22
9	J	103	A1EFU	CM5-C13-C12	3.64	123.81	118.08
9	K	104	A1EFU	CM5-C13-C12	3.64	123.81	118.08
8	n	101	BCL	C1C-NC-C4C	-3.64	105.07	106.71
9	G	103	A1EFU	C10-C11-C12	-3.64	111.87	123.22
9	J	102	A1EFU	C10-C11-C12	-3.64	111.87	123.22
9	M	406	A1EFU	CM5-C13-C12	3.63	123.80	118.08
8	K	102	BCL	CHD-C1D-ND	-3.62	121.12	124.45
9	F	103	A1EFU	C10-C11-C12	-3.62	111.92	123.22
9	G	104	A1EFU	C6-C7-C8	-3.62	111.92	123.22
10	B	101	LMT	C3'-C4'-C5'	-3.62	104.98	110.30
9	T	101	A1EFU	C10-C11-C12	-3.62	111.93	123.22
9	q	102	A1EFU	C23-C22-C21	-3.62	111.03	121.98
8	n	101	BCL	CHD-C1D-ND	-3.62	121.13	124.45
9	P	103	A1EFU	CM6-C18-C19	3.61	123.77	118.08
8	F	101	BCL	CHA-C1A-NA	-3.61	118.13	126.40
9	b	102	A1EFU	C21-C20-C19	-3.61	111.95	123.22
9	K	103	A1EFU	C23-C22-C21	-3.61	111.05	121.98
9	A	102	A1EFU	C6-C7-C8	-3.61	111.96	123.22
8	F	101	BCL	C1C-NC-C4C	-3.61	105.08	106.71
9	G	103	A1EFU	CM3-C5-C4	3.60	123.76	118.08
8	j	101	BCL	CHD-C1D-ND	-3.60	121.14	124.45
9	d	101	A1EFU	CM4-C9-C8	3.60	123.75	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	K	104	A1EFU	C23-C22-C21	-3.60	111.08	121.98
8	V	101	BCL	CHD-C1D-ND	-3.59	121.16	124.45
9	a	103	A1EFU	C21-C20-C19	-3.58	112.03	123.22
9	G	104	A1EFU	C23-C22-C21	-3.58	111.13	121.98
8	b	101	BCL	CHD-C1D-ND	-3.58	121.16	124.45
16	C	402	HEC	CMB-C2B-C1B	-3.57	122.98	128.46
9	n	102	A1EFU	C21-C20-C19	-3.57	112.08	123.22
8	t	101	BCL	CMB-C2B-C1B	-3.57	122.98	128.46
9	i	101	A1EFU	CM5-C13-C12	3.56	123.69	118.08
9	T	103	A1EFU	CM5-C13-C12	3.56	123.69	118.08
8	d	102	BCL	OBB-CAB-CBB	-3.56	112.16	120.17
9	M	406	A1EFU	C23-C22-C21	-3.56	111.21	121.98
8	S	302	BCL	CHD-C1D-ND	-3.55	121.19	124.45
8	E	101	BCL	CHD-C1D-ND	-3.55	121.19	124.45
8	P	102	BCL	C4A-NA-C1A	-3.55	105.11	106.71
8	a	102	BCL	CHD-C1D-ND	-3.55	121.19	124.45
9	T	103	A1EFU	C10-C11-C12	-3.55	112.15	123.22
9	E	102	A1EFU	C23-C22-C21	-3.55	111.24	121.98
9	n	102	A1EFU	CM5-C13-C12	3.54	123.66	118.08
8	t	101	BCL	C1C-NC-C4C	-3.54	105.11	106.71
8	T	102	BCL	CHD-C1D-ND	-3.54	121.20	124.45
9	v	101	A1EFU	C6-C7-C8	-3.54	112.18	123.22
9	D	103	A1EFU	C23-C22-C21	-3.54	111.28	121.98
10	L	306	LMT	C3'-C4'-C5'	-3.54	105.10	110.30
9	N	102	A1EFU	CM6-C18-C19	3.54	123.65	118.08
9	r	102	A1EFU	C23-C22-C21	-3.53	111.28	121.98
16	C	401	HEC	CMB-C2B-C1B	-3.53	123.04	128.46
9	G	104	A1EFU	C10-C11-C12	-3.53	112.21	123.22
9	I	101	A1EFU	C10-C11-C12	-3.53	112.21	123.22
9	A	103	A1EFU	C21-C20-C19	-3.52	112.22	123.22
8	N	101	BCL	CHD-C1D-ND	-3.52	121.22	124.45
9	J	102	A1EFU	C23-C22-C21	-3.52	111.33	121.98
9	E	102	A1EFU	CM6-C18-C19	3.52	123.62	118.08
8	P	101	BCL	CHD-C1D-ND	-3.52	121.22	124.45
8	P	102	BCL	C16-C15-C13	-3.51	104.56	115.92
9	i	101	A1EFU	C21-C20-C19	-3.51	112.26	123.22
9	A	102	A1EFU	CM3-C5-C4	3.51	123.61	118.08
9	R	102	A1EFU	CM6-C18-C19	3.51	123.60	118.08
8	D	101	BCL	C4B-CHC-C1C	-3.50	123.18	130.12
9	G	104	A1EFU	C21-C20-C19	-3.50	112.29	123.22
9	F	103	A1EFU	CM5-C13-C12	3.50	123.59	118.08
9	d	101	A1EFU	C23-C22-C21	-3.50	111.39	121.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	G	103	A1EFU	C23-C22-C21	-3.49	111.41	121.98
16	C	401	HEC	CBD-CAD-C3D	3.49	118.57	112.62
9	T	103	A1EFU	C21-C20-C19	-3.47	112.38	123.22
9	p	101	A1EFU	C10-C11-C12	-3.47	112.39	123.22
8	r	101	BCL	C16-C15-C13	-3.47	104.70	115.92
8	b	101	BCL	C2C-C3C-C4C	-3.47	96.15	101.34
8	D	101	BCL	CHA-C1A-NA	-3.47	118.46	126.40
9	n	102	A1EFU	C10-C11-C12	-3.45	112.45	123.22
9	F	102	A1EFU	C23-C22-C21	-3.44	111.55	121.98
8	P	101	BCL	C16-C15-C13	-3.44	104.81	115.92
8	K	101	BCL	C16-C15-C13	-3.44	104.81	115.92
9	r	102	A1EFU	CM5-C13-C12	3.44	123.49	118.08
9	Q	101	A1EFU	C21-C20-C19	-3.43	112.51	123.22
8	T	102	BCL	C16-C15-C13	-3.43	104.84	115.92
9	A	103	A1EFU	C10-C11-C12	-3.43	112.52	123.22
8	t	101	BCL	C4B-CHC-C1C	-3.42	123.34	130.12
9	r	102	A1EFU	C10-C11-C12	-3.42	112.54	123.22
8	Q	102	BCL	CHD-C1D-ND	-3.41	121.32	124.45
8	M	404	BCL	C16-C15-C13	-3.41	104.90	115.92
9	Q	101	A1EFU	C10-C11-C12	-3.41	112.58	123.22
8	v	102	BCL	CHD-C1D-ND	-3.40	121.33	124.45
9	S	303	A1EFU	C21-C20-C19	-3.40	112.61	123.22
8	q	101	BCL	C16-C15-C13	-3.40	104.94	115.92
8	D	101	BCL	CGD-CBD-CAD	-3.39	99.74	110.73
8	D	101	BCL	CHD-C1D-ND	-3.39	121.34	124.45
9	p	101	A1EFU	C21-C20-C19	-3.39	112.64	123.22
9	a	103	A1EFU	C10-C11-C12	-3.39	112.65	123.22
8	F	101	BCL	CGD-CBD-CAD	-3.38	99.77	110.73
8	E	101	BCL	C2C-C3C-C4C	-3.38	96.27	101.34
8	G	102	BCL	CHD-C1D-ND	-3.38	121.35	124.45
8	R	101	BCL	C16-C15-C13	-3.38	105.00	115.92
9	M	406	A1EFU	C21-C20-C19	-3.37	112.70	123.22
8	n	101	BCL	C16-C15-C13	-3.37	105.03	115.92
8	s	101	BCL	C16-C15-C13	-3.37	105.03	115.92
9	d	101	A1EFU	C10-C11-C12	-3.36	112.72	123.22
9	P	103	A1EFU	C21-C20-C19	-3.36	112.73	123.22
8	G	101	BCL	CHD-C1D-ND	-3.35	121.38	124.45
8	1	102	BCL	CHD-C1D-ND	-3.35	121.38	124.45
8	S	302	BCL	C16-C15-C13	-3.35	105.10	115.92
8	1	101	BCL	CHD-C1D-ND	-3.34	121.39	124.45
9	d	101	A1EFU	CM5-C13-C12	3.34	123.34	118.08
8	I	102	BCL	CHD-C1D-ND	-3.33	121.39	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	N	102	A1EFU	C21-C20-C19	-3.33	112.84	123.22
9	G	104	A1EFU	CM5-C13-C12	3.32	123.31	118.08
9	T	101	A1EFU	C21-C20-C19	-3.32	112.87	123.22
9	F	103	A1EFU	C21-C20-C19	-3.30	112.92	123.22
9	D	103	A1EFU	C21-C20-C19	-3.30	112.93	123.22
8	n	101	BCL	CHA-C1A-NA	-3.29	118.87	126.40
8	M	402	BCL	CHA-C1A-NA	-3.29	118.87	126.40
9	I	101	A1EFU	C21-C20-C19	-3.28	112.99	123.22
8	Q	102	BCL	C16-C15-C13	-3.27	105.35	115.92
8	P	102	BCL	CMB-C2B-C3B	3.27	130.79	124.68
8	d	102	BCL	CHD-C1D-ND	-3.27	121.45	124.45
8	q	101	BCL	CHA-C1A-NA	-3.27	118.92	126.40
8	f	101	BCL	C16-C15-C13	-3.26	105.37	115.92
8	L	301	BCL	C1C-NC-C4C	-3.26	105.24	106.71
8	j	101	BCL	CHA-C1A-NA	-3.25	118.95	126.40
9	q	102	A1EFU	C21-C20-C19	-3.25	113.08	123.22
8	B	102	BCL	C4D-CHA-C1A	3.24	125.19	121.25
8	a	102	BCL	C16-C15-C13	-3.23	105.47	115.92
8	I	102	BCL	C1C-NC-C4C	-3.23	105.25	106.71
8	B	102	BCL	C16-C15-C13	-3.22	105.50	115.92
8	e	101	BCL	CHA-C1A-NA	-3.22	119.02	126.40
8	E	101	BCL	CHA-C1A-NA	-3.22	119.03	126.40
9	R	102	A1EFU	C21-C20-C19	-3.22	113.18	123.22
8	I	103	BCL	C4B-CHC-C1C	-3.22	123.75	130.12
8	G	102	BCL	CHA-C1A-NA	-3.22	119.03	126.40
8	v	102	BCL	CHA-C1A-NA	-3.21	119.04	126.40
8	J	101	BCL	CHA-C1A-NA	-3.20	119.06	126.40
9	K	104	A1EFU	C21-C20-C19	-3.20	113.23	123.22
8	G	102	BCL	C2C-C3C-C4C	-3.20	96.55	101.34
8	N	101	BCL	C16-C15-C13	-3.20	105.59	115.92
9	v	101	A1EFU	C21-C20-C19	-3.19	113.25	123.22
8	I	103	BCL	CHA-C1A-NA	-3.19	119.08	126.40
8	K	101	BCL	CHA-C1A-NA	-3.19	119.09	126.40
8	A	101	BCL	CHA-C1A-NA	-3.19	119.10	126.40
9	J	102	A1EFU	C21-C20-C19	-3.18	113.28	123.22
8	J	101	BCL	O2A-CGA-O1A	-3.18	115.56	123.59
8	r	101	BCL	CHA-C1A-NA	-3.18	119.11	126.40
8	N	101	BCL	C2C-C3C-C4C	-3.18	96.57	101.34
16	C	402	HEC	CMB-C2B-C3B	3.18	129.56	125.82
9	r	102	A1EFU	C21-C20-C19	-3.18	113.31	123.22
8	Q	102	BCL	C4B-CHC-C1C	-3.17	123.83	130.12
8	1	102	BCL	CHA-C1A-NA	-3.17	119.14	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	L	301	BCL	O2A-CGA-O1A	-3.17	115.60	123.59
8	J	101	BCL	C4B-CHC-C1C	-3.16	123.85	130.12
8	n	101	BCL	CMB-C2B-C3B	3.16	130.59	124.68
8	F	101	BCL	O2A-CGA-O1A	-3.16	115.61	123.59
8	r	101	BCL	CMB-C2B-C3B	3.16	130.59	124.68
8	I	103	BCL	C16-C15-C13	-3.16	105.71	115.92
8	A	101	BCL	CMB-C2B-C3B	3.15	130.58	124.68
8	F	101	BCL	C2A-C1A-CHA	3.15	129.36	123.86
8	1	101	BCL	C16-C15-C13	-3.14	105.77	115.92
8	L	301	BCL	C4A-NA-C1A	-3.13	105.30	106.71
8	L	304	BCL	C16-C15-C13	-3.13	105.81	115.92
8	a	102	BCL	CHA-C1A-NA	-3.13	119.23	126.40
8	J	101	BCL	C16-C15-C13	-3.13	105.81	115.92
8	n	101	BCL	C11-C10-C8	-3.12	105.84	115.92
8	K	101	BCL	C4D-CHA-C1A	3.11	125.03	121.25
8	P	101	BCL	CHA-C1A-NA	-3.11	119.28	126.40
9	K	103	A1EFU	C21-C20-C19	-3.11	113.52	123.22
8	V	101	BCL	O2A-CGA-O1A	-3.11	115.75	123.59
8	G	102	BCL	C4B-CHC-C1C	-3.11	123.97	130.12
8	J	101	BCL	C11-C10-C8	-3.10	105.90	115.92
8	V	101	BCL	C16-C15-C13	-3.10	105.90	115.92
8	1	102	BCL	C11-C10-C8	-3.09	105.93	115.92
8	1	102	BCL	C4D-CHA-C1A	3.09	125.01	121.25
8	Q	102	BCL	CHA-C1A-NA	-3.09	119.33	126.40
8	D	101	BCL	C4D-CHA-C1A	3.09	125.01	121.25
8	1	102	BCL	C16-C15-C13	-3.08	105.96	115.92
9	S	304	A1EFU	C21-C20-C19	-3.08	113.60	123.22
8	R	101	BCL	CHA-C1A-NA	-3.08	119.34	126.40
8	d	102	BCL	C11-C10-C8	-3.08	105.97	115.92
8	d	102	BCL	CHA-C1A-NA	-3.08	119.35	126.40
8	1	102	BCL	C4B-CHC-C1C	-3.08	124.02	130.12
8	Q	102	BCL	C1C-NC-C4C	-3.08	105.32	106.71
8	N	101	BCL	CHA-C1A-NA	-3.08	119.36	126.40
8	Q	102	BCL	O2A-CGA-O1A	-3.07	115.84	123.59
8	T	102	BCL	CHA-C1A-NA	-3.07	119.37	126.40
8	G	102	BCL	C11-C10-C8	-3.07	106.01	115.92
8	V	101	BCL	CHA-C1A-NA	-3.07	119.38	126.40
16	C	401	HEC	CMC-C2C-C3C	3.06	129.42	125.82
8	A	101	BCL	C4D-CHA-C1A	3.06	124.97	121.25
8	M	402	BCL	C16-C15-C13	-3.06	106.04	115.92
8	V	101	BCL	C7-C6-C5	-3.05	105.06	113.36
8	d	102	BCL	C16-C15-C13	-3.05	106.05	115.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	f	101	BCL	C4B-CHC-C1C	-3.05	124.08	130.12
8	L	304	BCL	CHA-C1A-NA	-3.04	119.42	126.40
8	T	102	BCL	C7-C6-C5	-3.04	105.09	113.36
8	1	101	BCL	C11-C10-C8	-3.04	106.08	115.92
8	P	101	BCL	C7-C6-C5	-3.04	105.11	113.36
8	f	101	BCL	CHA-C1A-NA	-3.03	119.45	126.40
8	1	101	BCL	CHA-C1A-NA	-3.03	119.45	126.40
8	M	402	BCL	CMC-C2C-C3C	-3.03	101.60	113.83
16	C	403	HEC	O1D-CGD-CBD	-3.03	113.34	123.08
9	E	102	A1EFU	C21-C20-C19	-3.03	113.77	123.22
8	F	101	BCL	C7-C6-C5	-3.03	105.14	113.36
8	F	101	BCL	C16-C15-C13	-3.02	106.14	115.92
8	K	102	BCL	C16-C15-C13	-3.02	106.15	115.92
8	P	101	BCL	C4D-CHA-C1A	3.02	124.93	121.25
8	E	101	BCL	C16-C15-C13	-3.02	106.16	115.92
8	a	102	BCL	C11-C10-C8	-3.02	106.16	115.92
8	A	101	BCL	C16-C15-C13	-3.02	106.16	115.92
8	G	102	BCL	C7-C6-C5	-3.02	105.16	113.36
8	K	102	BCL	C4B-CHC-C1C	-3.02	124.14	130.12
8	v	102	BCL	C16-C15-C13	-3.02	106.17	115.92
8	P	101	BCL	C4B-CHC-C1C	-3.02	124.14	130.12
9	F	102	A1EFU	C21-C20-C19	-3.02	113.81	123.22
8	T	102	BCL	C4B-CHC-C1C	-3.01	124.15	130.12
8	j	101	BCL	C16-C15-C13	-3.01	106.18	115.92
8	N	101	BCL	C7-C6-C5	-3.01	105.17	113.36
8	G	102	BCL	C16-C15-C13	-3.01	106.18	115.92
8	S	302	BCL	CHA-C1A-NA	-3.01	119.50	126.40
8	K	101	BCL	C11-C10-C8	-3.01	106.20	115.92
8	I	103	BCL	C7-C6-C5	-3.00	105.20	113.36
9	G	103	A1EFU	C21-C20-C19	-3.00	113.84	123.22
8	a	102	BCL	C4B-CHC-C1C	-3.00	124.17	130.12
8	R	101	BCL	C7-C6-C5	-3.00	105.21	113.36
10	C	404	LMT	C1'-O5'-C5'	-3.00	107.80	113.69
9	a	101	A1EFU	C21-C20-C19	-3.00	113.85	123.22
8	K	102	BCL	C2C-C3C-C4C	-3.00	96.85	101.34
8	G	101	BCL	C16-C15-C13	-3.00	106.22	115.92
8	P	102	BCL	CHA-C1A-NA	-3.00	119.53	126.40
8	L	301	BCL	C4B-CHC-C1C	-3.00	124.18	130.12
8	I	102	BCL	CHA-C1A-NA	-2.99	119.54	126.40
8	d	102	BCL	C4B-CHC-C1C	-2.99	124.19	130.12
8	K	101	BCL	C3D-C2D-C1D	-2.99	101.75	105.83
8	t	101	BCL	C16-C15-C13	-2.99	106.26	115.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	P	102	BCL	O2A-CGA-O1A	-2.99	116.05	123.59
9	J	103	A1EFU	C21-C20-C19	-2.99	113.90	123.22
8	G	101	BCL	C7-C6-C5	-2.98	105.26	113.36
8	L	301	BCL	C3D-C2D-C1D	-2.97	101.77	105.83
8	s	101	BCL	C4B-CHC-C1C	-2.97	124.23	130.12
8	E	101	BCL	C4B-CHC-C1C	-2.97	124.23	130.12
8	J	101	BCL	C7-C6-C5	-2.97	105.30	113.36
8	L	304	BCL	C4A-NA-C1A	-2.96	105.37	106.71
8	I	102	BCL	C16-C15-C13	-2.96	106.34	115.92
8	K	102	BCL	C7-C6-C5	-2.96	105.31	113.36
8	I	103	BCL	C2C-C3C-C4C	-2.96	96.90	101.34
8	d	102	BCL	O2A-CGA-O1A	-2.96	116.12	123.59
8	L	304	BCL	C4B-CHC-C1C	-2.96	124.26	130.12
8	K	101	BCL	CMD-C2D-C1D	2.96	129.92	124.71
8	S	302	BCL	C4D-CHA-C1A	2.95	124.84	121.25
8	L	301	BCL	C11-C10-C8	-2.95	106.37	115.92
8	N	101	BCL	C11-C10-C8	-2.95	106.37	115.92
8	M	402	BCL	C7-C6-C5	-2.95	105.35	113.36
8	b	101	BCL	C4B-CHC-C1C	-2.95	124.28	130.12
8	B	102	BCL	C4B-CHC-C1C	-2.95	124.28	130.12
8	q	101	BCL	C11-C10-C8	-2.94	106.41	115.92
9	d	101	A1EFU	C21-C20-C19	-2.94	114.04	123.22
8	1	101	BCL	O2A-CGA-O1A	-2.94	116.18	123.59
8	S	302	BCL	C4B-CHC-C1C	-2.94	124.30	130.12
8	T	102	BCL	C11-C10-C8	-2.94	106.43	115.92
8	j	101	BCL	C11-C10-C8	-2.94	106.43	115.92
8	1	102	BCL	O2A-CGA-O1A	-2.93	116.19	123.59
8	L	301	BCL	C11-C12-C13	-2.93	106.46	115.92
8	s	101	BCL	C1C-NC-C4C	-2.92	105.39	106.71
8	v	102	BCL	C4B-CHC-C1C	-2.92	124.33	130.12
8	A	101	BCL	C11-C10-C8	-2.92	106.48	115.92
8	1	102	BCL	C7-C6-C5	-2.92	105.43	113.36
8	S	302	BCL	C1C-NC-C4C	-2.92	105.39	106.71
8	G	101	BCL	CHA-C1A-NA	-2.92	119.72	126.40
8	b	101	BCL	CHA-C1A-NA	-2.92	119.72	126.40
8	P	102	BCL	C11-C10-C8	-2.92	106.50	115.92
10	B	101	LMT	C1'-O5'-C5'	-2.91	108.66	113.67
8	a	102	BCL	C1C-NC-C4C	-2.91	105.40	106.71
10	L	306	LMT	C1'-O5'-C5'	-2.91	108.66	113.67
8	G	101	BCL	C4B-CHC-C1C	-2.91	124.35	130.12
8	T	102	BCL	C4D-CHA-C1A	2.91	124.79	121.25
13	M	403	BPH	C1-C2-C3	2.91	131.07	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	M	402	BCL	C11-C10-C8	-2.90	106.53	115.92
8	1	101	BCL	C4B-CHC-C1C	-2.89	124.39	130.12
8	P	101	BCL	C11-C10-C8	-2.89	106.57	115.92
8	A	101	BCL	C7-C6-C5	-2.89	105.50	113.36
8	L	304	BCL	C4D-CHA-C1A	2.89	124.77	121.25
8	J	101	BCL	C4D-CHA-C1A	2.89	124.77	121.25
8	D	101	BCL	O2A-CGA-O1A	-2.89	116.30	123.59
8	Q	102	BCL	C4D-CHA-C1A	2.89	124.76	121.25
8	b	101	BCL	C3D-C2D-C1D	-2.89	101.89	105.83
8	G	101	BCL	C1C-NC-C4C	-2.88	105.41	106.71
8	f	101	BCL	C11-C10-C8	-2.88	106.60	115.92
8	F	101	BCL	C3D-C2D-C1D	-2.88	101.90	105.83
8	M	404	BCL	CHA-C1A-NA	-2.88	119.80	126.40
16	C	403	HEC	CMC-C2C-C3C	2.88	129.21	125.82
8	b	101	BCL	O2A-CGA-O1A	-2.88	116.32	123.59
8	L	304	BCL	C2C-C3C-C4C	-2.88	97.02	101.34
8	K	102	BCL	O2A-CGA-O1A	-2.88	116.32	123.59
8	I	102	BCL	C4B-CHC-C1C	-2.88	124.41	130.12
8	I	102	BCL	C11-C10-C8	-2.88	106.61	115.92
8	B	102	BCL	CHA-C1A-NA	-2.88	119.80	126.40
8	A	101	BCL	C1C-NC-C4C	-2.88	105.41	106.71
8	e	101	BCL	C4B-CHC-C1C	-2.88	124.42	130.12
8	s	101	BCL	C7-C6-C5	-2.88	105.55	113.36
8	r	101	BCL	O2A-CGA-O1A	-2.88	116.34	123.59
8	a	102	BCL	C4D-CHA-C1A	2.87	124.75	121.25
8	J	101	BCL	C3D-C2D-C1D	-2.87	101.91	105.83
8	s	101	BCL	C11-C10-C8	-2.87	106.64	115.92
8	n	101	BCL	C7-C6-C5	-2.87	105.56	113.36
8	K	101	BCL	C4B-CHC-C1C	-2.87	124.43	130.12
8	r	101	BCL	C11-C10-C8	-2.87	106.64	115.92
8	A	101	BCL	C3D-C2D-C1D	-2.87	101.92	105.83
8	I	103	BCL	C3D-C2D-C1D	-2.87	101.92	105.83
8	e	101	BCL	C16-C15-C13	-2.87	106.65	115.92
8	q	101	BCL	C3D-C2D-C1D	-2.87	101.92	105.83
8	P	102	BCL	C4D-CHA-C1A	2.86	124.73	121.25
8	F	101	BCL	C4B-CHC-C1C	-2.86	124.45	130.12
8	a	102	BCL	C7-C6-C5	-2.86	105.60	113.36
8	L	301	BCL	CMC-C2C-C3C	-2.86	102.31	113.83
8	K	102	BCL	C3D-C2D-C1D	-2.85	101.94	105.83
8	N	101	BCL	C4B-CHC-C1C	-2.85	124.47	130.12
8	s	101	BCL	C2A-C3A-C4A	-2.85	97.26	101.87
8	M	404	BCL	C4B-CHC-C1C	-2.85	124.48	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	R	101	BCL	C11-C10-C8	-2.85	106.72	115.92
8	D	101	BCL	C3D-C2D-C1D	-2.85	101.95	105.83
8	P	101	BCL	C1C-NC-C4C	-2.84	105.43	106.71
8	B	102	BCL	O2A-CGA-O1A	-2.84	116.42	123.59
8	f	101	BCL	C7-C6-C5	-2.84	105.64	113.36
8	E	101	BCL	C11-C10-C8	-2.84	106.74	115.92
8	I	103	BCL	C4D-CHA-C1A	2.84	124.70	121.25
8	R	101	BCL	O2A-CGA-O1A	-2.84	116.43	123.59
9	E	102	A1EFU	CM7-C22-C23	-2.84	110.50	115.27
8	1	101	BCL	C1C-NC-C4C	-2.84	105.43	106.71
8	e	101	BCL	C7-C6-C5	-2.83	105.67	113.36
8	D	101	BCL	C7-C6-C5	-2.83	105.67	113.36
8	P	101	BCL	O2A-CGA-O1A	-2.83	116.44	123.59
8	G	101	BCL	C11-C10-C8	-2.83	106.77	115.92
8	F	101	BCL	C11-C12-C13	-2.83	106.77	115.92
8	A	101	BCL	C4B-CHC-C1C	-2.83	124.51	130.12
8	L	301	BCL	CMA-C3A-C4A	-2.83	104.17	111.77
8	t	101	BCL	C7-C6-C5	-2.83	105.68	113.36
8	K	102	BCL	CHA-C1A-NA	-2.83	119.92	126.40
8	s	101	BCL	C4D-CHA-C1A	2.83	124.69	121.25
8	I	103	BCL	O2A-CGA-O1A	-2.83	116.46	123.59
8	Q	102	BCL	C7-C6-C5	-2.83	105.69	113.36
8	v	102	BCL	O2A-CGA-O1A	-2.82	116.47	123.59
8	L	301	BCL	CHA-C1A-NA	-2.82	119.94	126.40
8	L	304	BCL	C11-C10-C8	-2.82	106.81	115.92
8	e	101	BCL	C4D-CHA-C1A	2.82	124.68	121.25
8	I	102	BCL	C7-C6-C5	-2.82	105.71	113.36
8	j	101	BCL	C7-C6-C5	-2.82	105.71	113.36
8	I	103	BCL	C11-C10-C8	-2.81	106.83	115.92
8	s	101	BCL	CHA-C1A-NA	-2.81	119.96	126.40
8	j	101	BCL	C2C-C3C-C4C	-2.81	97.13	101.34
8	f	101	BCL	O2A-CGA-O1A	-2.81	116.50	123.59
8	j	101	BCL	C4B-CHC-C1C	-2.80	124.57	130.12
8	S	302	BCL	C11-C10-C8	-2.80	106.86	115.92
8	T	102	BCL	O2A-CGA-O1A	-2.80	116.52	123.59
8	K	102	BCL	C11-C10-C8	-2.80	106.87	115.92
8	P	102	BCL	C3D-C2D-C1D	-2.80	102.01	105.83
8	M	404	BCL	O2A-CGA-O1A	-2.80	116.53	123.59
8	I	102	BCL	O2A-CGA-O1A	-2.80	116.53	123.59
8	L	304	BCL	CMA-C3A-C4A	-2.80	104.25	111.77
8	N	101	BCL	C4D-CHA-C1A	2.80	124.65	121.25
16	C	403	HEC	CMC-C2C-C1C	-2.80	124.17	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	M	402	BCL	C4D-CHA-C1A	2.80	124.65	121.25
8	R	101	BCL	C4B-CHC-C1C	-2.79	124.59	130.12
8	S	302	BCL	C7-C6-C5	-2.79	105.78	113.36
8	A	101	BCL	O2A-CGA-O1A	-2.79	116.55	123.59
8	j	101	BCL	O2A-CGA-O1A	-2.79	116.56	123.59
8	M	404	BCL	C4D-CHA-C1A	2.79	124.64	121.25
8	R	101	BCL	C3D-C2D-C1D	-2.79	102.03	105.83
8	B	102	BCL	C7-C6-C5	-2.79	105.80	113.36
8	F	101	BCL	C2C-C3C-C4C	-2.78	97.17	101.34
8	S	302	BCL	C3D-C2D-C1D	-2.78	102.03	105.83
8	s	101	BCL	C3D-C2D-C1D	-2.78	102.03	105.83
15	H	303	CDL	OA8-CA7-C31	2.78	120.64	111.91
16	C	402	HEC	O1D-CGD-CBD	-2.78	114.15	123.08
8	q	101	BCL	C1C-NC-C4C	-2.78	105.46	106.71
8	n	101	BCL	C4B-CHC-C1C	-2.78	124.61	130.12
8	M	402	BCL	O2A-CGA-O1A	-2.78	116.58	123.59
8	1	101	BCL	C7-C6-C5	-2.78	105.82	113.36
8	M	402	BCL	C4B-CHC-C1C	-2.78	124.62	130.12
8	1	102	BCL	C3D-C2D-C1D	-2.78	102.04	105.83
8	G	101	BCL	C3D-C2D-C1D	-2.77	102.05	105.83
8	V	101	BCL	C3D-C2D-C1D	-2.77	102.05	105.83
8	e	101	BCL	C3D-C2D-C1D	-2.77	102.05	105.83
8	r	101	BCL	C7-C6-C5	-2.77	105.83	113.36
8	t	101	BCL	O2A-CGA-O1A	-2.77	116.61	123.59
8	N	101	BCL	O2A-CGA-O1A	-2.77	116.61	123.59
8	v	102	BCL	C3D-C2D-C1D	-2.77	102.05	105.83
8	v	102	BCL	C7-C6-C5	-2.77	105.85	113.36
8	q	101	BCL	C7-C6-C5	-2.77	105.85	113.36
8	M	404	BCL	CMA-C3A-C4A	-2.76	104.34	111.77
8	a	102	BCL	O2A-CGA-O1A	-2.76	116.62	123.59
8	d	102	BCL	C4D-CHA-C1A	2.76	124.61	121.25
8	N	101	BCL	C3D-C2D-C1D	-2.76	102.06	105.83
8	G	102	BCL	O2A-CGA-O1A	-2.76	116.62	123.59
8	K	102	BCL	C4D-CHA-C1A	2.76	124.61	121.25
8	G	102	BCL	C4D-CHA-C1A	2.76	124.61	121.25
8	M	404	BCL	C3D-C2D-C1D	-2.76	102.07	105.83
8	P	101	BCL	C3D-C2D-C1D	-2.76	102.07	105.83
8	n	101	BCL	C3D-C2D-C1D	-2.76	102.07	105.83
8	Q	102	BCL	C3D-C2D-C1D	-2.75	102.08	105.83
16	C	401	HEC	O1D-CGD-CBD	-2.75	114.25	123.08
8	e	101	BCL	C11-C10-C8	-2.75	107.03	115.92
8	M	402	BCL	C3D-C2D-C1D	-2.75	102.08	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	L	304	BCL	C7-C6-C5	-2.75	105.89	113.36
8	q	101	BCL	C4B-CHC-C1C	-2.75	124.68	130.12
8	L	304	BCL	O2A-CGA-O1A	-2.75	116.66	123.59
8	r	101	BCL	C3D-C2D-C1D	-2.74	102.09	105.83
8	T	102	BCL	C3D-C2D-C1D	-2.74	102.09	105.83
8	Q	102	BCL	CMC-C2C-C3C	-2.74	102.78	113.83
8	G	102	BCL	C3D-C2D-C1D	-2.74	102.10	105.83
8	n	101	BCL	O2A-CGA-O1A	-2.73	116.69	123.59
16	C	401	HEC	CMC-C2C-C1C	-2.73	124.27	128.46
8	s	101	BCL	C4A-NA-C1A	-2.72	105.48	106.71
8	s	101	BCL	CMC-C2C-C3C	-2.72	102.84	113.83
8	I	102	BCL	C3D-C2D-C1D	-2.72	102.12	105.83
11	L	305	MW9	O1-C17-C16	2.72	120.44	111.91
8	j	101	BCL	C3D-C2D-C1D	-2.72	102.12	105.83
8	E	101	BCL	O2A-CGA-O1A	-2.72	116.73	123.59
8	r	101	BCL	C4B-CHC-C1C	-2.72	124.73	130.12
8	J	101	BCL	C2C-C3C-C4C	-2.72	97.27	101.34
8	D	101	BCL	CMA-C3A-C4A	-2.71	104.49	111.77
8	q	101	BCL	C4D-CHA-C1A	2.71	124.55	121.25
8	b	101	BCL	C4D-CHA-C1A	2.71	124.55	121.25
8	V	101	BCL	C1C-NC-C4C	-2.71	105.49	106.71
8	1	101	BCL	C4A-NA-C1A	-2.71	105.49	106.71
8	E	101	BCL	C3D-C2D-C1D	-2.71	102.14	105.83
8	L	304	BCL	C3D-C2D-C1D	-2.71	102.14	105.83
8	E	101	BCL	C4D-CHA-C1A	2.70	124.54	121.25
8	a	102	BCL	C3D-C2D-C1D	-2.70	102.14	105.83
8	S	302	BCL	CMC-C2C-C3C	-2.70	102.94	113.83
8	V	101	BCL	CMA-C3A-C4A	-2.70	104.52	111.77
8	q	101	BCL	O2A-CGA-O1A	-2.70	116.78	123.59
8	P	101	BCL	CMC-C2C-C3C	-2.70	102.94	113.83
8	M	402	BCL	CMA-C3A-C4A	-2.70	104.53	111.77
8	S	302	BCL	O2A-CGA-O1A	-2.70	116.79	123.59
8	P	102	BCL	C4B-CHC-C1C	-2.69	124.78	130.12
8	t	101	BCL	CHB-C4A-NA	-2.69	120.79	124.51
8	V	101	BCL	CMC-C2C-C3C	-2.69	102.98	113.83
8	G	101	BCL	O2A-CGA-O1A	-2.69	116.81	123.59
8	t	101	BCL	C3D-C2D-C1D	-2.69	102.16	105.83
8	K	101	BCL	O2A-CGA-O1A	-2.69	116.81	123.59
8	K	101	BCL	C7-C6-C5	-2.69	106.07	113.36
9	d	101	A1EFU	CM7-C22-C23	-2.68	110.76	115.27
9	F	102	A1EFU	CM7-C22-C23	-2.68	110.76	115.27
8	s	101	BCL	O2A-CGA-O1A	-2.68	116.82	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	j	101	BCL	CMC-C2C-C3C	-2.68	103.02	113.83
8	e	101	BCL	O2A-CGA-O1A	-2.68	116.83	123.59
8	n	101	BCL	C11-C12-C13	-2.68	107.26	115.92
8	v	102	BCL	CMC-C2C-C3C	-2.68	103.03	113.83
8	P	102	BCL	CMA-C3A-C4A	-2.68	104.58	111.77
8	q	101	BCL	CMC-C2C-C3C	-2.68	103.04	113.83
8	L	301	BCL	C2A-C3A-C4A	-2.67	97.55	101.87
8	r	101	BCL	C4A-NA-C1A	-2.67	105.50	106.71
8	r	101	BCL	CMC-C2C-C3C	-2.67	103.05	113.83
10	E	103	LMT	C1'-O5'-C5'	-2.67	108.44	113.69
8	t	101	BCL	CMC-C2C-C3C	-2.67	103.06	113.83
8	n	101	BCL	CMA-C3A-C4A	-2.67	104.60	111.77
8	K	102	BCL	C11-C12-C13	-2.67	107.30	115.92
8	G	102	BCL	C11-C12-C13	-2.66	107.31	115.92
8	G	102	BCL	CMC-C2C-C3C	-2.66	103.09	113.83
8	1	101	BCL	C3D-C2D-C1D	-2.66	102.20	105.83
8	T	102	BCL	C11-C12-C13	-2.66	107.33	115.92
8	d	102	BCL	C7-C6-C5	-2.66	106.14	113.36
8	F	101	BCL	CMC-C2C-C3C	-2.66	103.11	113.83
8	M	404	BCL	C1B-CHB-C4A	-2.65	124.86	130.12
8	A	101	BCL	CMC-C2C-C3C	-2.65	103.13	113.83
9	G	103	A1EFU	CM7-C22-C23	-2.65	110.81	115.27
8	Q	102	BCL	C11-C10-C8	-2.65	107.35	115.92
8	P	102	BCL	C1C-NC-C4C	-2.65	105.52	106.71
8	L	301	BCL	C7-C6-C5	-2.65	106.17	113.36
8	j	101	BCL	C11-C12-C13	-2.65	107.37	115.92
8	v	102	BCL	C4D-CHA-C1A	2.64	124.47	121.25
8	1	102	BCL	C11-C12-C13	-2.64	107.38	115.92
10	S	301	LMT	C3'-C4'-C5'	-2.64	104.87	110.93
8	b	101	BCL	C7-C6-C5	-2.64	106.19	113.36
10	H	304	LMT	C1'-O5'-C5'	-2.64	108.51	113.69
8	N	101	BCL	CMA-C3A-C4A	-2.64	104.68	111.77
8	M	404	BCL	C7-C6-C5	-2.64	106.19	113.36
8	1	101	BCL	C4D-CHA-C1A	2.64	124.46	121.25
8	T	102	BCL	CMC-C2C-C3C	-2.64	103.19	113.83
8	J	101	BCL	CMC-C2C-C3C	-2.64	103.19	113.83
8	f	101	BCL	CMA-C3A-C4A	-2.64	104.69	111.77
8	R	101	BCL	C11-C12-C13	-2.63	107.40	115.92
8	e	101	BCL	CMC-C2C-C3C	-2.63	103.21	113.83
8	n	101	BCL	C4D-CHA-C1A	2.63	124.45	121.25
8	n	101	BCL	CMC-C2C-C3C	-2.63	103.21	113.83
8	a	102	BCL	CMC-C2C-C3C	-2.63	103.21	113.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	G	101	BCL	CMC-C2C-C3C	-2.63	103.21	113.83
8	M	404	BCL	CMC-C2C-C3C	-2.63	103.22	113.83
8	K	102	BCL	CMC-C2C-C3C	-2.63	103.23	113.83
11	H	301	MW9	O1-C17-C16	2.63	120.15	111.91
8	n	101	BCL	C2C-C3C-C4C	-2.62	97.41	101.34
8	J	101	BCL	C11-C12-C13	-2.62	107.44	115.92
8	e	101	BCL	CMA-C3A-C4A	-2.62	104.73	111.77
8	G	102	BCL	CMA-C3A-C4A	-2.62	104.73	111.77
8	L	304	BCL	CMC-C2C-C3C	-2.62	103.27	113.83
8	B	102	BCL	CMC-C2C-C3C	-2.62	103.28	113.83
15	M	408	CDL	OA8-CA7-C31	2.61	120.11	111.91
9	J	102	A1EFU	CM7-C22-C23	-2.61	110.87	115.27
8	M	404	BCL	C11-C10-C8	-2.61	107.47	115.92
8	d	102	BCL	C3D-C2D-C1D	-2.61	102.27	105.83
10	G	107	LMT	C3'-C4'-C5'	-2.61	105.59	110.24
8	E	101	BCL	C11-C12-C13	-2.61	107.49	115.92
11	G	105	MW9	O1-C17-C16	2.61	120.09	111.91
8	I	102	BCL	CMC-C2C-C3C	-2.61	103.31	113.83
8	R	101	BCL	C4D-CHA-C1A	2.61	124.42	121.25
8	P	102	BCL	CMC-C2C-C3C	-2.61	103.31	113.83
8	D	101	BCL	CMC-C2C-C3C	-2.60	103.33	113.83
8	1	101	BCL	CMC-C2C-C3C	-2.60	103.33	113.83
11	F	104	MW9	O1-C17-C16	2.60	120.07	111.91
8	M	402	BCL	C11-C12-C13	-2.60	107.53	115.92
8	E	101	BCL	CMA-C3A-C4A	-2.59	104.81	111.77
8	j	101	BCL	C4D-CHA-C1A	2.59	124.40	121.25
8	f	101	BCL	C2A-C1A-CHA	2.59	128.38	123.86
8	I	102	BCL	CMA-C3A-C4A	-2.59	104.82	111.77
8	a	102	BCL	CMA-C3A-C4A	-2.59	104.82	111.77
8	I	103	BCL	CMC-C2C-C3C	-2.58	103.40	113.83
8	E	101	BCL	CMC-C2C-C3C	-2.58	103.41	113.83
8	j	101	BCL	CMA-C3A-C4A	-2.58	104.84	111.77
8	T	102	BCL	CMA-C3A-C4A	-2.58	104.84	111.77
11	D	102	MW9	O1-C17-C16	2.58	120.00	111.91
8	f	101	BCL	CMC-C2C-C3C	-2.58	103.43	113.83
11	H	302	MW9	O1-C17-C16	2.58	120.00	111.91
16	C	402	HEC	C4C-C3C-C2C	2.58	109.14	106.35
8	e	101	BCL	C2C-C3C-C4C	-2.58	97.48	101.34
15	H	303	CDL	OB8-CB7-C71	2.58	119.99	111.91
8	s	101	BCL	CMA-C3A-C4A	-2.58	104.85	111.77
9	J	103	A1EFU	CM7-C22-C23	-2.58	110.94	115.27
8	t	101	BCL	C11-C10-C8	-2.57	107.60	115.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	M	404	BCL	C11-C12-C13	-2.57	107.60	115.92
8	b	101	BCL	CMC-C2C-C3C	-2.57	103.45	113.83
8	Q	102	BCL	CMA-C3A-C4A	-2.57	104.86	111.77
8	K	101	BCL	CMA-C3A-C4A	-2.57	104.87	111.77
8	1	102	BCL	CGD-CBD-CAD	-2.57	102.41	110.73
8	F	101	BCL	C11-C10-C8	-2.57	107.62	115.92
8	N	101	BCL	CMC-C2C-C3C	-2.57	103.47	113.83
10	G	107	LMT	C1'-O5'-C5'	-2.57	108.65	113.69
8	P	101	BCL	C11-C12-C13	-2.56	107.63	115.92
8	S	302	BCL	C11-C12-C13	-2.56	107.64	115.92
8	B	102	BCL	C3D-C2D-C1D	-2.56	102.33	105.83
8	f	101	BCL	C1C-NC-C4C	-2.56	105.56	106.71
8	b	101	BCL	CGD-CBD-CAD	-2.56	102.44	110.73
8	F	101	BCL	CMA-C3A-C4A	-2.56	104.89	111.77
8	R	101	BCL	CMC-C2C-C3C	-2.56	103.51	113.83
8	V	101	BCL	C11-C12-C13	-2.55	107.66	115.92
8	P	102	BCL	C7-C6-C5	-2.55	106.42	113.36
9	G	104	A1EFU	CM7-C22-C23	-2.55	110.97	115.27
8	V	101	BCL	C2A-C1A-CHA	2.55	128.32	123.86
11	R	103	MW9	O1-C17-C16	2.55	119.90	111.91
8	M	404	BCL	C4A-NA-C1A	-2.54	105.56	106.71
8	G	101	BCL	C4D-CHA-C1A	2.54	124.34	121.25
11	G	106	MW9	C31-C32-C33	-2.54	109.55	126.84
8	N	101	BCL	C11-C12-C13	-2.54	107.70	115.92
8	B	102	BCL	CMA-C3A-C4A	-2.54	104.94	111.77
8	I	103	BCL	CGD-CBD-CAD	-2.54	102.50	110.73
8	1	102	BCL	CMC-C2C-C3C	-2.54	103.58	113.83
15	M	408	CDL	OB8-CB7-C71	2.54	119.88	111.91
11	M	407	MW9	O1-C17-C16	2.54	119.88	111.91
8	E	101	BCL	C7-C6-C5	-2.54	106.47	113.36
8	M	404	BCL	CMD-C2D-C1D	2.53	129.18	124.71
8	K	101	BCL	CMC-C2C-C3C	-2.53	103.62	113.83
8	V	101	BCL	C11-C10-C8	-2.53	107.76	115.92
8	r	101	BCL	C2A-C1A-CHA	2.52	128.27	123.86
8	R	101	BCL	CMA-C3A-C4A	-2.52	105.00	111.77
8	Q	102	BCL	C11-C12-C13	-2.52	107.77	115.92
8	1	101	BCL	CMA-C3A-C4A	-2.52	105.01	111.77
8	q	101	BCL	CMA-C3A-C4A	-2.52	105.01	111.77
9	a	101	A1EFU	CM7-C22-C23	-2.51	111.04	115.27
8	P	101	BCL	CMA-C3A-C4A	-2.51	105.02	111.77
8	G	101	BCL	CMA-C3A-C4A	-2.51	105.02	111.77
8	t	101	BCL	C4D-CHA-C1A	2.51	124.31	121.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	G	106	MW9	O1-C17-C16	2.51	119.78	111.91
8	I	103	BCL	CMA-C3A-C4A	-2.51	105.04	111.77
8	I	102	BCL	C4D-CHA-C1A	2.50	124.30	121.25
8	G	102	BCL	CGD-CBD-CAD	-2.50	102.63	110.73
8	I	103	BCL	C11-C12-C13	-2.50	107.83	115.92
8	I	102	BCL	C4A-NA-C1A	-2.50	105.58	106.71
11	N	103	MW9	O1-C17-C16	2.50	119.76	111.91
8	E	101	BCL	C2A-C1A-CHA	2.50	128.22	123.86
8	r	101	BCL	CMA-C3A-C4A	-2.49	105.08	111.77
8	J	101	BCL	CMA-C3A-C4A	-2.49	105.08	111.77
8	T	102	BCL	C2C-C3C-C4C	-2.48	97.62	101.34
8	b	101	BCL	C11-C10-C8	-2.48	107.89	115.92
8	b	101	BCL	CMA-C3A-C4A	-2.47	105.13	111.77
8	D	101	BCL	C16-C15-C13	-2.47	107.93	115.92
8	1	102	BCL	CMA-C3A-C4A	-2.47	105.14	111.77
9	M	406	A1EFU	CM7-C22-C23	-2.47	111.12	115.27
8	B	102	BCL	C11-C10-C8	-2.47	107.95	115.92
8	f	101	BCL	C2C-C3C-C4C	-2.46	97.65	101.34
8	d	102	BCL	CMC-C2C-C3C	-2.46	103.89	113.83
8	K	101	BCL	C11-C12-C13	-2.46	107.97	115.92
16	C	402	HEC	O1A-CGA-CBA	-2.46	115.18	123.08
8	f	101	BCL	C3D-C2D-C1D	-2.46	102.48	105.83
8	a	102	BCL	C11-C12-C13	-2.45	107.98	115.92
8	A	101	BCL	CMA-C3A-C4A	-2.45	105.18	111.77
8	t	101	BCL	C11-C12-C13	-2.45	108.00	115.92
8	J	101	BCL	CGD-CBD-CAD	-2.45	102.81	110.73
8	L	301	BCL	CMD-C2D-C1D	2.44	129.02	124.71
16	C	402	HEC	CMC-C2C-C1C	-2.44	124.71	128.46
8	A	101	BCL	C11-C12-C13	-2.44	108.03	115.92
8	L	304	BCL	C11-C12-C13	-2.44	108.03	115.92
9	v	101	A1EFU	CM7-C22-C23	-2.44	111.17	115.27
8	S	302	BCL	CMA-C3A-C4A	-2.44	105.22	111.77
8	L	301	BCL	C16-C15-C13	-2.44	108.04	115.92
8	Q	102	BCL	CGD-CBD-CAD	-2.43	102.85	110.73
16	C	403	HEC	CMD-C2D-C3D	2.43	129.53	124.94
8	K	102	BCL	CMA-C3A-C4A	-2.43	105.24	111.77
8	K	101	BCL	C1C-NC-C4C	-2.43	105.61	106.71
8	r	101	BCL	C4D-CHA-C1A	2.43	124.20	121.25
9	K	103	A1EFU	CM7-C22-C23	-2.43	111.19	115.27
8	G	102	BCL	C2A-C1A-CHA	2.42	128.10	123.86
8	P	101	BCL	C3C-C2C-C1C	2.42	105.78	101.87
8	b	101	BCL	C11-C12-C13	-2.42	108.11	115.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	A	101	BCL	C3C-C2C-C1C	2.41	105.77	101.87
8	r	101	BCL	C2A-C3A-C4A	-2.41	97.97	101.87
8	S	302	BCL	CMD-C2D-C1D	2.41	128.96	124.71
8	R	101	BCL	CMD-C2D-C1D	2.41	128.96	124.71
10	C	404	LMT	C2'-C3'-C4'	2.41	115.18	109.68
8	P	101	BCL	CGD-CBD-CAD	-2.41	102.94	110.73
8	J	101	BCL	C2A-C1A-CHA	2.40	128.06	123.86
16	C	401	HEC	CMD-C2D-C3D	2.40	129.47	124.94
8	N	101	BCL	CGD-CBD-CAD	-2.40	102.97	110.73
16	C	402	HEC	CMD-C2D-C3D	2.40	129.46	124.94
8	d	102	BCL	CMA-C3A-C4A	-2.39	105.34	111.77
8	q	101	BCL	C11-C12-C13	-2.39	108.20	115.92
8	P	102	BCL	CMD-C2D-C1D	2.39	128.92	124.71
8	J	101	BCL	CMD-C2D-C1D	2.39	128.92	124.71
8	L	304	BCL	C2A-C3A-C4A	-2.39	98.02	101.87
8	R	101	BCL	CGD-CBD-CAD	-2.39	103.01	110.73
8	A	101	BCL	CMD-C2D-C1D	2.38	128.92	124.71
8	1	101	BCL	C11-C12-C13	-2.38	108.21	115.92
8	B	102	BCL	C3C-C2C-C1C	2.38	105.72	101.87
8	I	103	BCL	CMD-C2D-C1D	2.38	128.91	124.71
8	N	101	BCL	CMD-C2D-C1D	2.38	128.91	124.71
9	S	304	A1EFU	CM7-C22-C23	-2.38	111.27	115.27
8	V	101	BCL	C3C-C2C-C1C	2.37	105.70	101.87
9	T	103	A1EFU	CM7-C22-C23	-2.37	111.28	115.27
8	a	102	BCL	C4A-NA-C1A	-2.37	105.64	106.71
9	T	101	A1EFU	CM7-C22-C23	-2.37	111.29	115.27
8	P	102	BCL	C11-C12-C13	-2.37	108.26	115.92
8	K	102	BCL	CMD-C2D-C1D	2.37	128.89	124.71
16	C	403	HEC	O1A-CGA-CBA	-2.36	115.49	123.08
16	C	401	HEC	O1A-CGA-CBA	-2.36	115.50	123.08
8	D	101	BCL	C11-C10-C8	-2.36	108.30	115.92
8	v	102	BCL	CMA-C3A-C4A	-2.36	105.44	111.77
8	V	101	BCL	CMD-C2D-C1D	2.35	128.86	124.71
8	I	102	BCL	C11-C12-C13	-2.35	108.33	115.92
8	A	101	BCL	CGD-CBD-CAD	-2.35	103.13	110.73
8	Q	102	BCL	C12-C11-C10	-2.35	102.45	113.24
14	L	303	U10	C7-C6-C5	-2.34	115.66	118.48
8	v	102	BCL	C11-C10-C8	-2.34	108.35	115.92
8	1	101	BCL	C3C-C2C-C1C	2.34	105.65	101.87
8	r	101	BCL	C1C-NC-C4C	-2.34	105.66	106.71
8	I	102	BCL	C2A-C3A-C4A	-2.33	98.10	101.87
8	M	402	BCL	CMD-C2D-C1D	2.33	128.82	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	s	101	BCL	C11-C12-C13	-2.33	108.39	115.92
8	L	301	BCL	C4D-CHA-C1A	2.33	124.08	121.25
8	P	101	BCL	CMD-C2D-C1D	2.33	128.81	124.71
8	F	101	BCL	CMD-C2D-C1D	2.32	128.81	124.71
8	G	101	BCL	C2A-C1A-CHA	2.32	127.91	123.86
8	G	101	BCL	C4A-NA-C1A	-2.31	105.67	106.71
16	C	402	HEC	CMC-C2C-C3C	2.31	128.53	125.82
8	G	102	BCL	CBB-CAB-C3B	2.30	127.18	120.34
8	M	402	BCL	CBB-CAB-C3B	2.30	127.17	120.34
8	q	101	BCL	CMD-C2D-C1D	2.30	128.76	124.71
9	P	103	A1EFU	CM7-C22-C23	-2.29	111.41	115.27
8	E	101	BCL	CGD-CBD-CAD	-2.29	103.32	110.73
8	V	101	BCL	C4D-CHA-C1A	2.29	124.03	121.25
8	V	101	BCL	CBB-CAB-C3B	2.28	127.12	120.34
8	K	101	BCL	CBB-CAB-C3B	2.28	127.11	120.34
9	n	102	A1EFU	CM7-C22-C23	-2.28	111.44	115.27
8	K	101	BCL	C3C-C2C-C1C	2.28	105.55	101.87
8	T	102	BCL	CMD-C2D-C1D	2.28	128.73	124.71
8	L	301	BCL	CGD-CBD-CAD	-2.28	103.36	110.73
8	e	101	BCL	CBB-CAB-C3B	2.28	127.10	120.34
14	M	405	U10	C7-C6-C5	-2.28	115.74	118.48
8	Q	102	BCL	CMD-C2D-C1D	2.28	128.72	124.71
8	S	302	BCL	C12-C11-C10	-2.27	102.79	113.24
8	1	102	BCL	CBB-CAB-C3B	2.27	127.09	120.34
8	r	101	BCL	C11-C12-C13	-2.27	108.57	115.92
8	R	101	BCL	CBB-CAB-C3B	2.27	127.08	120.34
8	I	103	BCL	CBB-CAB-C3B	2.27	127.07	120.34
8	L	304	BCL	CMD-C2D-C1D	2.27	128.71	124.71
8	Q	102	BCL	CBB-CAB-C3B	2.26	127.06	120.34
8	j	101	BCL	CBB-CAB-C3B	2.26	127.06	120.34
8	S	302	BCL	CBB-CAB-C3B	2.26	127.06	120.34
8	K	102	BCL	CBB-CAB-C3B	2.26	127.06	120.34
8	f	101	BCL	C11-C12-C13	-2.26	108.60	115.92
13	L	302	BPH	CMD-C2D-C3D	2.26	128.91	124.68
8	L	304	BCL	CBB-CAB-C3B	2.26	127.05	120.34
8	1	102	BCL	CMD-C2D-C1D	2.26	128.69	124.71
13	M	403	BPH	CMD-C2D-C3D	2.26	128.90	124.68
8	e	101	BCL	CMD-C2D-C1D	2.26	128.69	124.71
8	N	101	BCL	CBB-CAB-C3B	2.25	127.03	120.34
8	F	101	BCL	CBB-CAB-C3B	2.25	127.03	120.34
8	G	101	BCL	CBB-CAB-C3B	2.25	127.03	120.34
8	M	404	BCL	CBB-CAB-C3B	2.25	127.02	120.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	J	101	BCL	CBB-CAB-C3B	2.25	127.02	120.34
8	D	101	BCL	CBB-CAB-C3B	2.25	127.02	120.34
8	v	102	BCL	CGD-CBD-CAD	-2.25	103.45	110.73
8	E	101	BCL	CBB-CAB-C3B	2.25	127.01	120.34
8	s	101	BCL	CBB-CAB-C3B	2.25	127.01	120.34
8	e	101	BCL	C12-C11-C10	-2.25	102.92	113.24
8	T	102	BCL	CBB-CAB-C3B	2.24	127.00	120.34
9	R	102	A1EFU	CM7-C22-C23	-2.24	111.50	115.27
16	C	402	HEC	C1D-C2D-C3D	2.24	108.56	107.00
8	R	101	BCL	C2A-C1A-CHA	2.24	127.78	123.86
8	b	101	BCL	CBB-CAB-C3B	2.24	126.98	120.34
8	f	101	BCL	CBB-CAB-C3B	2.24	126.98	120.34
8	s	101	BCL	C3C-C2C-C1C	2.24	105.48	101.87
8	I	103	BCL	C2A-C1A-CHA	2.24	127.77	123.86
8	M	402	BCL	C12-C11-C10	-2.24	102.97	113.24
8	V	101	BCL	CGD-CBD-CAD	-2.24	103.49	110.73
8	1	101	BCL	C2A-C1A-CHA	2.24	127.77	123.86
8	G	101	BCL	C11-C12-C13	-2.23	108.70	115.92
8	P	101	BCL	CBB-CAB-C3B	2.23	126.96	120.34
8	G	101	BCL	C12-C11-C10	-2.23	102.99	113.24
8	v	102	BCL	C11-C12-C13	-2.23	108.71	115.92
8	1	101	BCL	CBB-CAB-C3B	2.23	126.96	120.34
8	e	101	BCL	C4A-NA-C1A	-2.23	105.70	106.71
8	I	102	BCL	CBB-CAB-C3B	2.23	126.96	120.34
8	L	301	BCL	CBB-CAB-C3B	2.23	126.95	120.34
9	a	103	A1EFU	CM7-C22-C23	-2.22	111.53	115.27
8	q	101	BCL	CBB-CAB-C3B	2.22	126.93	120.34
8	a	102	BCL	CMD-C2D-C1D	2.22	128.63	124.71
9	I	101	A1EFU	CM7-C22-C23	-2.22	111.54	115.27
9	p	101	A1EFU	CM7-C22-C23	-2.22	111.54	115.27
8	S	302	BCL	C3C-C2C-C1C	2.22	105.45	101.87
8	v	102	BCL	CBB-CAB-C3B	2.21	126.91	120.34
8	a	102	BCL	CBB-CAB-C3B	2.21	126.91	120.34
8	P	102	BCL	C3C-C2C-C1C	2.21	105.44	101.87
9	Q	101	A1EFU	CM7-C22-C23	-2.21	111.55	115.27
16	C	403	HEC	C1D-C2D-C3D	2.21	108.53	107.00
8	r	101	BCL	CMD-C2D-C1D	2.21	128.61	124.71
9	1	104	A1EFU	CM7-C22-C23	-2.21	111.56	115.27
9	i	101	A1EFU	CM7-C22-C23	-2.21	111.56	115.27
8	L	301	BCL	C2A-C1A-CHA	2.21	127.72	123.86
8	f	101	BCL	CGD-CBD-CAD	-2.21	103.58	110.73
8	I	103	BCL	C12-C11-C10	-2.20	103.11	113.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	C	401	HEC	C4C-C3C-C2C	2.20	108.73	106.35
10	S	301	LMT	C1'-O5'-C5'	-2.20	109.36	113.69
9	r	102	A1EFU	CM7-C22-C23	-2.20	111.57	115.27
8	j	101	BCL	CGD-CBD-CAD	-2.19	103.63	110.73
8	M	404	BCL	CHC-C1C-NC	2.19	127.54	124.51
8	D	101	BCL	C11-C12-C13	-2.19	108.84	115.92
8	T	102	BCL	C2A-C1A-CHA	2.19	127.69	123.86
8	B	102	BCL	CBB-CAB-C3B	2.19	126.84	120.34
8	t	101	BCL	C12-C11-C10	-2.19	103.18	113.24
8	j	101	BCL	C12-C11-C10	-2.19	103.18	113.24
16	C	401	HEC	C2B-C3B-C4B	2.19	108.71	106.35
8	j	101	BCL	C2A-C3A-C4A	-2.18	98.35	101.87
16	C	403	HEC	CMA-C3A-C2A	2.18	129.05	124.94
8	b	101	BCL	C16-C15-C13	-2.18	108.88	115.92
8	V	101	BCL	C12-C11-C10	-2.18	103.24	113.24
8	P	101	BCL	C12-C11-C10	-2.17	103.25	113.24
8	I	102	BCL	C12-C11-C10	-2.17	103.25	113.24
8	q	101	BCL	C12-C11-C10	-2.17	103.26	113.24
8	G	102	BCL	CMD-C2D-C1D	2.17	128.53	124.71
8	t	101	BCL	C2C-C3C-C4C	-2.16	98.10	101.34
8	S	302	BCL	CGD-CBD-CAD	-2.16	103.73	110.73
8	n	101	BCL	CMD-C2D-C1D	2.16	128.52	124.71
8	T	102	BCL	CGD-CBD-CAD	-2.16	103.74	110.73
8	K	101	BCL	C4A-NA-C1A	-2.16	105.74	106.71
8	D	101	BCL	C3C-C2C-C1C	2.15	105.35	101.87
8	j	101	BCL	C2A-C1A-CHA	2.15	127.62	123.86
8	a	102	BCL	C12-C11-C10	-2.15	103.36	113.24
8	B	102	BCL	C1C-NC-C4C	-2.15	105.74	106.71
8	F	101	BCL	C4D-CHA-C1A	2.14	123.86	121.25
8	s	101	BCL	C12-C11-C10	-2.14	103.39	113.24
9	K	104	A1EFU	CM7-C22-C23	-2.14	111.67	115.27
8	L	301	BCL	C3C-C2C-C1C	2.14	105.33	101.87
8	v	102	BCL	CHC-C1C-NC	2.14	127.47	124.51
8	T	102	BCL	C12-C11-C10	-2.14	103.42	113.24
8	1	102	BCL	C12-C11-C10	-2.14	103.42	113.24
9	A	103	A1EFU	CM7-C22-C23	-2.13	111.68	115.27
8	P	102	BCL	C12-C11-C10	-2.13	103.43	113.24
16	C	403	HEC	O2A-CGA-O1A	2.13	128.62	123.30
8	t	101	BCL	OBB-CAB-C3B	2.13	123.77	119.99
8	K	102	BCL	C12-C11-C10	-2.13	103.45	113.24
8	G	102	BCL	C12-C11-C10	-2.13	103.45	113.24
9	F	103	A1EFU	CM7-C22-C23	-2.13	111.70	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	E	101	BCL	CMD-C2D-C1D	2.12	128.45	124.71
8	J	101	BCL	C12-C11-C10	-2.12	103.49	113.24
8	N	101	BCL	C12-C11-C10	-2.12	103.50	113.24
8	L	304	BCL	CHC-C1C-NC	2.12	127.44	124.51
8	Q	102	BCL	C3C-C2C-C1C	2.12	105.29	101.87
8	G	101	BCL	CMD-C2D-C1D	2.12	128.44	124.71
9	1	103	A1EFU	CM7-C22-C23	-2.11	111.72	115.27
8	a	102	BCL	C2A-C1A-CHA	2.11	127.55	123.86
8	f	101	BCL	C12-C11-C10	-2.11	103.55	113.24
9	b	102	A1EFU	CM7-C22-C23	-2.11	111.73	115.27
8	K	101	BCL	C12-C11-C10	-2.10	103.57	113.24
8	v	102	BCL	C12-C11-C10	-2.10	103.58	113.24
8	r	101	BCL	C3C-C2C-C1C	2.10	105.26	101.87
11	H	302	MW9	C31-C32-C33	-2.10	108.64	124.73
8	D	101	BCL	CMD-C2D-C1D	2.09	128.40	124.71
9	N	102	A1EFU	CM7-C22-C23	-2.09	111.76	115.27
8	s	101	BCL	CMD-C2D-C1D	2.08	128.39	124.71
8	t	101	BCL	C3C-C2C-C1C	2.08	105.23	101.87
8	B	102	BCL	C1B-CHB-C4A	-2.08	125.99	130.12
8	S	302	BCL	CHC-C1C-NC	2.08	127.39	124.51
8	K	101	BCL	C2A-C1A-CHA	2.08	127.50	123.86
8	1	101	BCL	C12-C11-C10	-2.08	103.69	113.24
16	C	402	HEC	C2B-C3B-C4B	2.08	108.59	106.35
8	G	101	BCL	C3C-C2C-C1C	2.07	105.22	101.87
8	K	101	BCL	CHC-C1C-NC	2.07	127.38	124.51
8	B	102	BCL	CMD-C2D-C1D	2.07	128.36	124.71
8	n	101	BCL	C12-C11-C10	-2.07	103.73	113.24
8	b	101	BCL	C2A-C1A-CHA	2.06	127.47	123.86
8	L	301	BCL	C1B-CHB-C4A	-2.06	126.03	130.12
8	j	101	BCL	CMD-C2D-C1D	2.06	128.35	124.71
11	M	407	MW9	C31-C32-C33	-2.06	108.90	124.73
8	t	101	BCL	CMD-C2D-C1D	2.06	128.35	124.71
11	G	105	MW9	C31-C32-C33	-2.06	108.91	124.73
8	1	101	BCL	CGD-CBD-CAD	-2.06	104.06	110.73
10	H	304	LMT	C3'-C4'-C5'	-2.06	106.56	110.24
9	q	102	A1EFU	CM7-C22-C23	-2.06	111.81	115.27
8	d	102	BCL	C12-C11-C10	-2.06	103.78	113.24
8	r	101	BCL	CGD-CBD-CAD	-2.06	104.07	110.73
8	V	101	BCL	C4B-C3B-CAB	-2.06	123.16	127.13
8	e	101	BCL	C2A-C1A-CHA	2.06	127.45	123.86
8	n	101	BCL	C2A-C1A-CHA	2.05	127.45	123.86
8	L	304	BCL	C1B-CHB-C4A	-2.05	126.05	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	q	101	BCL	C3C-C2C-C1C	2.05	105.18	101.87
9	S	303	A1EFU	CM7-C22-C23	-2.05	111.82	115.27
8	K	101	BCL	C2A-C3A-C4A	-2.05	98.56	101.87
8	K	101	BCL	CGD-CBD-CAD	-2.05	104.10	110.73
8	v	102	BCL	CMD-C2D-C1D	2.05	128.32	124.71
8	R	101	BCL	C12-C11-C10	-2.04	103.84	113.24
8	b	101	BCL	CMD-C2D-C1D	2.04	128.31	124.71
11	M	407	MW9	C34-C33-C32	-2.04	109.09	124.73
9	D	104	A1EFU	CM7-C22-C23	-2.04	111.84	115.27
8	L	304	BCL	C12-C11-C10	-2.04	103.88	113.24
8	F	101	BCL	C12-C11-C10	-2.03	103.92	113.24
8	q	101	BCL	CHC-C1C-NC	2.03	127.32	124.51
8	E	101	BCL	C12-C11-C10	-2.02	103.94	113.24
16	C	401	HEC	O2A-CGA-O1A	2.02	128.33	123.30
8	L	301	BCL	CHC-C1C-NC	2.02	127.30	124.51
8	q	101	BCL	C4A-NA-C1A	-2.01	105.80	106.71
8	B	102	BCL	C11-C12-C13	-2.01	109.42	115.92
8	n	101	BCL	CGD-CBD-CAD	-2.01	104.23	110.73
8	q	101	BCL	C2A-C3A-C4A	-2.00	98.63	101.87
8	I	102	BCL	C2A-C1A-CHA	2.00	127.36	123.86
8	1	101	BCL	C2A-C3A-C4A	-2.00	98.64	101.87
8	f	101	BCL	C2A-C3A-C4A	-2.00	98.64	101.87

There are no chirality outliers.

All (1680) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	P	101	BCL	C1A-C2A-CAA-CBA
8	P	101	BCL	C3A-C2A-CAA-CBA
8	P	101	BCL	C2C-C3C-CAC-CBC
8	P	101	BCL	C4C-C3C-CAC-CBC
8	V	101	BCL	C4C-C3C-CAC-CBC
8	v	102	BCL	C1A-C2A-CAA-CBA
8	v	102	BCL	C2C-C3C-CAC-CBC
8	v	102	BCL	C4C-C3C-CAC-CBC
8	S	302	BCL	C4C-C3C-CAC-CBC
8	t	101	BCL	C1A-C2A-CAA-CBA
8	t	101	BCL	C3A-C2A-CAA-CBA
8	t	101	BCL	C1-C2-C3-C5
8	T	102	BCL	C2A-CAA-CBA-CGA
8	s	101	BCL	C1A-C2A-CAA-CBA
8	s	101	BCL	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
8	s	101	BCL	C4C-C3C-CAC-CBC
8	Q	102	BCL	C2C-C3C-CAC-CBC
8	Q	102	BCL	C4C-C3C-CAC-CBC
8	r	101	BCL	C2C-C3C-CAC-CBC
8	R	101	BCL	C2A-CAA-CBA-CGA
8	q	101	BCL	C1A-C2A-CAA-CBA
8	q	101	BCL	C2C-C3C-CAC-CBC
8	q	101	BCL	C2-C3-C5-C6
8	1	102	BCL	C1A-C2A-CAA-CBA
8	1	102	BCL	C3A-C2A-CAA-CBA
8	1	102	BCL	C2C-C3C-CAC-CBC
8	1	102	BCL	C4-C3-C5-C6
8	n	101	BCL	C1A-C2A-CAA-CBA
8	n	101	BCL	C3A-C2A-CAA-CBA
8	N	101	BCL	C1A-C2A-CAA-CBA
8	N	101	BCL	C3A-C2A-CAA-CBA
8	K	102	BCL	CHA-CBD-CGD-O1D
8	K	102	BCL	CHA-CBD-CGD-O2D
8	K	102	BCL	CAD-CBD-CGD-O1D
8	I	102	BCL	C2C-C3C-CAC-CBC
8	I	102	BCL	C1-C2-C3-C5
8	G	101	BCL	C2C-C3C-CAC-CBC
8	F	101	BCL	C1-C2-C3-C4
8	e	101	BCL	C1A-C2A-CAA-CBA
8	E	101	BCL	C1-C2-C3-C4
8	E	101	BCL	C1-C2-C3-C5
8	E	101	BCL	C4-C3-C5-C6
8	d	102	BCL	C1-C2-C3-C4
8	d	102	BCL	C1-C2-C3-C5
8	b	101	BCL	C4C-C3C-CAC-CBC
8	b	101	BCL	CAD-CBD-CGD-O1D
8	B	102	BCL	C1A-C2A-CAA-CBA
8	a	102	BCL	C1A-C2A-CAA-CBA
8	a	102	BCL	C3A-C2A-CAA-CBA
8	a	102	BCL	C2C-C3C-CAC-CBC
8	a	102	BCL	C1-C2-C3-C4
8	a	102	BCL	C1-C2-C3-C5
8	A	101	BCL	C1A-C2A-CAA-CBA
8	A	101	BCL	C1-C2-C3-C5
8	A	101	BCL	C2-C3-C5-C6
8	M	402	BCL	CHA-CBD-CGD-O1D
8	M	402	BCL	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
8	M	402	BCL	C6-C7-C8-C9
8	M	404	BCL	C4C-C3C-CAC-CBC
8	M	404	BCL	CHA-CBD-CGD-O1D
8	M	404	BCL	CHA-CBD-CGD-O2D
8	M	404	BCL	C1-C2-C3-C5
8	L	301	BCL	C1A-C2A-CAA-CBA
8	L	301	BCL	C3A-C2A-CAA-CBA
8	L	301	BCL	C2C-C3C-CAC-CBC
8	L	301	BCL	C2-C3-C5-C6
8	L	304	BCL	C3A-C2A-CAA-CBA
8	L	304	BCL	C4C-C3C-CAC-CBC
8	L	304	BCL	O2A-C1-C2-C3
8	L	304	BCL	C1-C2-C3-C4
8	L	304	BCL	C1-C2-C3-C5
8	L	304	BCL	C6-C7-C8-C9
9	P	103	A1EFU	C4-C5-C6-C7
9	P	103	A1EFU	CM3-C5-C6-C7
9	P	103	A1EFU	C6-C7-C8-C9
9	P	103	A1EFU	C10-C11-C12-C13
9	P	103	A1EFU	C18-C19-C20-C21
9	P	103	A1EFU	C11-C10-C9-C8
9	P	103	A1EFU	C11-C10-C9-CM4
9	P	103	A1EFU	C12-C13-C14-C15
9	P	103	A1EFU	CM5-C13-C14-C15
9	P	103	A1EFU	C20-C21-C22-CM7
9	P	103	A1EFU	C25-C26-C27-C28
9	P	103	A1EFU	CM8-C26-C27-C28
9	v	101	A1EFU	C2-C3-C4-C5
9	v	101	A1EFU	C4-C5-C6-C7
9	v	101	A1EFU	CM3-C5-C6-C7
9	v	101	A1EFU	C10-C11-C12-C13
9	v	101	A1EFU	C18-C19-C20-C21
9	v	101	A1EFU	C16-C17-C18-C19
9	v	101	A1EFU	C16-C17-C18-CM6
9	v	101	A1EFU	C11-C10-C9-C8
9	v	101	A1EFU	C11-C10-C9-CM4
9	v	101	A1EFU	C12-C13-C14-C15
9	v	101	A1EFU	CM5-C13-C14-C15
9	v	101	A1EFU	C20-C21-C22-CM7
9	v	101	A1EFU	C22-C23-C24-C25
9	S	303	A1EFU	C4-C5-C6-C7
9	S	303	A1EFU	CM3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
9	S	303	A1EFU	C6-C7-C8-C9
9	S	303	A1EFU	C10-C11-C12-C13
9	S	303	A1EFU	C18-C19-C20-C21
9	S	303	A1EFU	C16-C17-C18-C19
9	S	303	A1EFU	C16-C17-C18-CM6
9	S	303	A1EFU	C11-C10-C9-C8
9	S	303	A1EFU	C11-C10-C9-CM4
9	S	303	A1EFU	C12-C13-C14-C15
9	S	303	A1EFU	CM5-C13-C14-C15
9	S	303	A1EFU	C20-C21-C22-C23
9	S	303	A1EFU	C20-C21-C22-CM7
9	S	303	A1EFU	C26-C27-C28-C29
9	S	304	A1EFU	O1-C1-C2-O2
9	S	304	A1EFU	C2-C3-C4-C5
9	S	304	A1EFU	C4-C5-C6-C7
9	S	304	A1EFU	CM3-C5-C6-C7
9	S	304	A1EFU	C6-C7-C8-C9
9	S	304	A1EFU	C10-C11-C12-C13
9	S	304	A1EFU	C18-C19-C20-C21
9	S	304	A1EFU	C16-C17-C18-C19
9	S	304	A1EFU	C16-C17-C18-CM6
9	S	304	A1EFU	C11-C10-C9-C8
9	S	304	A1EFU	C11-C10-C9-CM4
9	S	304	A1EFU	C12-C13-C14-C15
9	S	304	A1EFU	CM5-C13-C14-C15
9	S	304	A1EFU	C20-C21-C22-CM7
9	T	101	A1EFU	O1-C1-C2-O2
9	T	101	A1EFU	C2-C3-C4-C5
9	T	101	A1EFU	C4-C5-C6-C7
9	T	101	A1EFU	CM3-C5-C6-C7
9	T	101	A1EFU	C6-C7-C8-C9
9	T	101	A1EFU	C10-C11-C12-C13
9	T	101	A1EFU	C18-C19-C20-C21
9	T	101	A1EFU	C16-C17-C18-C19
9	T	101	A1EFU	C16-C17-C18-CM6
9	T	101	A1EFU	C11-C10-C9-C8
9	T	101	A1EFU	C11-C10-C9-CM4
9	T	101	A1EFU	C12-C13-C14-C15
9	T	101	A1EFU	CM5-C13-C14-C15
9	T	101	A1EFU	C20-C21-C22-CM7
9	T	103	A1EFU	C1-C2-C3-C4
9	T	103	A1EFU	O2-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
9	T	103	A1EFU	C2-C3-C4-C5
9	T	103	A1EFU	C4-C5-C6-C7
9	T	103	A1EFU	CM3-C5-C6-C7
9	T	103	A1EFU	C6-C7-C8-C9
9	T	103	A1EFU	C10-C11-C12-C13
9	T	103	A1EFU	C18-C19-C20-C21
9	T	103	A1EFU	C16-C17-C18-C19
9	T	103	A1EFU	C16-C17-C18-CM6
9	T	103	A1EFU	C11-C10-C9-C8
9	T	103	A1EFU	C11-C10-C9-CM4
9	T	103	A1EFU	CM5-C13-C14-C15
9	T	103	A1EFU	C20-C21-C22-CM7
9	Q	101	A1EFU	C4-C5-C6-C7
9	Q	101	A1EFU	CM3-C5-C6-C7
9	Q	101	A1EFU	C6-C7-C8-C9
9	Q	101	A1EFU	C10-C11-C12-C13
9	Q	101	A1EFU	C2-C1-O1-CMA
9	Q	101	A1EFU	C18-C19-C20-C21
9	Q	101	A1EFU	C16-C17-C18-C19
9	Q	101	A1EFU	C16-C17-C18-CM6
9	Q	101	A1EFU	C11-C10-C9-C8
9	Q	101	A1EFU	C11-C10-C9-CM4
9	Q	101	A1EFU	C12-C13-C14-C15
9	Q	101	A1EFU	CM5-C13-C14-C15
9	Q	101	A1EFU	C20-C21-C22-CM7
9	Q	101	A1EFU	CM8-C26-C27-C28
9	r	102	A1EFU	C2-C3-C4-C5
9	r	102	A1EFU	C4-C5-C6-C7
9	r	102	A1EFU	CM3-C5-C6-C7
9	r	102	A1EFU	C10-C11-C12-C13
9	r	102	A1EFU	C16-C17-C18-C19
9	r	102	A1EFU	C16-C17-C18-CM6
9	r	102	A1EFU	C11-C10-C9-C8
9	r	102	A1EFU	C11-C10-C9-CM4
9	r	102	A1EFU	C20-C21-C22-C23
9	r	102	A1EFU	C20-C21-C22-CM7
9	R	102	A1EFU	C4-C5-C6-C7
9	R	102	A1EFU	CM3-C5-C6-C7
9	R	102	A1EFU	C6-C7-C8-C9
9	R	102	A1EFU	C10-C11-C12-C13
9	R	102	A1EFU	C2-C1-O1-CMA
9	R	102	A1EFU	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
9	R	102	A1EFU	C11-C10-C9-C8
9	R	102	A1EFU	C11-C10-C9-CM4
9	R	102	A1EFU	C12-C13-C14-C15
9	R	102	A1EFU	CM5-C13-C14-C15
9	R	102	A1EFU	C20-C21-C22-CM7
9	q	102	A1EFU	C2-C3-C4-C5
9	q	102	A1EFU	C4-C5-C6-C7
9	q	102	A1EFU	CM3-C5-C6-C7
9	q	102	A1EFU	C6-C7-C8-C9
9	q	102	A1EFU	C10-C11-C12-C13
9	q	102	A1EFU	C16-C17-C18-C19
9	q	102	A1EFU	C16-C17-C18-CM6
9	q	102	A1EFU	C11-C10-C9-C8
9	q	102	A1EFU	C11-C10-C9-CM4
9	q	102	A1EFU	C12-C13-C14-C15
9	q	102	A1EFU	CM5-C13-C14-C15
9	q	102	A1EFU	C20-C21-C22-C23
9	q	102	A1EFU	C20-C21-C22-CM7
9	q	102	A1EFU	C25-C26-C27-C28
9	q	102	A1EFU	CM8-C26-C27-C28
9	q	102	A1EFU	C26-C27-C28-C29
9	p	101	A1EFU	C1-C2-C3-C4
9	p	101	A1EFU	O2-C2-C3-C4
9	p	101	A1EFU	C2-C3-C4-C5
9	p	101	A1EFU	C5-C6-C7-C8
9	p	101	A1EFU	C4-C5-C6-C7
9	p	101	A1EFU	CM3-C5-C6-C7
9	p	101	A1EFU	C6-C7-C8-C9
9	p	101	A1EFU	C10-C11-C12-C13
9	p	101	A1EFU	C14-C15-C16-C17
9	p	101	A1EFU	C18-C19-C20-C21
9	p	101	A1EFU	C16-C17-C18-C19
9	p	101	A1EFU	C16-C17-C18-CM6
9	p	101	A1EFU	C11-C10-C9-C8
9	p	101	A1EFU	C11-C10-C9-CM4
9	p	101	A1EFU	C12-C13-C14-C15
9	p	101	A1EFU	CM5-C13-C14-C15
9	p	101	A1EFU	C20-C21-C22-CM7
9	1	103	A1EFU	C4-C5-C6-C7
9	1	103	A1EFU	CM3-C5-C6-C7
9	1	103	A1EFU	C6-C7-C8-C9
9	1	103	A1EFU	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
9	1	103	A1EFU	C18-C19-C20-C21
9	1	103	A1EFU	C16-C17-C18-CM6
9	1	103	A1EFU	C11-C10-C9-C8
9	1	103	A1EFU	C11-C10-C9-CM4
9	1	103	A1EFU	C12-C13-C14-C15
9	1	103	A1EFU	CM5-C13-C14-C15
9	1	103	A1EFU	C20-C21-C22-CM7
9	1	104	A1EFU	O1-C1-C2-O2
9	1	104	A1EFU	C2-C3-C4-C5
9	1	104	A1EFU	C4-C5-C6-C7
9	1	104	A1EFU	CM3-C5-C6-C7
9	1	104	A1EFU	C6-C7-C8-C9
9	1	104	A1EFU	C10-C11-C12-C13
9	1	104	A1EFU	C16-C17-C18-C19
9	1	104	A1EFU	C16-C17-C18-CM6
9	1	104	A1EFU	C11-C10-C9-C8
9	1	104	A1EFU	C11-C10-C9-CM4
9	1	104	A1EFU	C12-C13-C14-C15
9	1	104	A1EFU	CM5-C13-C14-C15
9	1	104	A1EFU	C20-C21-C22-CM7
9	n	102	A1EFU	C2-C3-C4-C5
9	n	102	A1EFU	C4-C5-C6-C7
9	n	102	A1EFU	CM3-C5-C6-C7
9	n	102	A1EFU	C6-C7-C8-C9
9	n	102	A1EFU	C10-C11-C12-C13
9	n	102	A1EFU	C16-C17-C18-C19
9	n	102	A1EFU	C16-C17-C18-CM6
9	n	102	A1EFU	C11-C10-C9-C8
9	n	102	A1EFU	C11-C10-C9-CM4
9	n	102	A1EFU	C12-C13-C14-C15
9	n	102	A1EFU	CM5-C13-C14-C15
9	n	102	A1EFU	C20-C21-C22-CM7
9	n	102	A1EFU	C26-C27-C28-C29
9	N	102	A1EFU	O1-C1-C2-O2
9	N	102	A1EFU	C4-C5-C6-C7
9	N	102	A1EFU	CM3-C5-C6-C7
9	N	102	A1EFU	C6-C7-C8-C9
9	N	102	A1EFU	C10-C11-C12-C13
9	N	102	A1EFU	C11-C10-C9-C8
9	N	102	A1EFU	C11-C10-C9-CM4
9	N	102	A1EFU	C12-C13-C14-C15
9	N	102	A1EFU	CM5-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
9	N	102	A1EFU	C20-C21-C22-CM7
9	K	103	A1EFU	O1-C1-C2-O2
9	K	103	A1EFU	C4-C5-C6-C7
9	K	103	A1EFU	CM3-C5-C6-C7
9	K	103	A1EFU	C6-C7-C8-C9
9	K	103	A1EFU	C10-C11-C12-C13
9	K	103	A1EFU	C18-C19-C20-C21
9	K	103	A1EFU	C16-C17-C18-C19
9	K	103	A1EFU	C16-C17-C18-CM6
9	K	103	A1EFU	C11-C10-C9-C8
9	K	103	A1EFU	C11-C10-C9-CM4
9	K	103	A1EFU	C12-C13-C14-C15
9	K	103	A1EFU	CM5-C13-C14-C15
9	K	103	A1EFU	C20-C21-C22-CM7
9	K	104	A1EFU	O1-C1-C2-O2
9	K	104	A1EFU	C2-C3-C4-C5
9	K	104	A1EFU	C4-C5-C6-C7
9	K	104	A1EFU	CM3-C5-C6-C7
9	K	104	A1EFU	C10-C11-C12-C13
9	K	104	A1EFU	C18-C19-C20-C21
9	K	104	A1EFU	C16-C17-C18-C19
9	K	104	A1EFU	C16-C17-C18-CM6
9	K	104	A1EFU	C11-C10-C9-C8
9	K	104	A1EFU	C11-C10-C9-CM4
9	K	104	A1EFU	C12-C13-C14-C15
9	K	104	A1EFU	CM5-C13-C14-C15
9	K	104	A1EFU	C20-C21-C22-C23
9	K	104	A1EFU	C20-C21-C22-CM7
9	K	104	A1EFU	C25-C26-C27-C28
9	K	104	A1EFU	CM8-C26-C27-C28
9	J	102	A1EFU	C2-C3-C4-C5
9	J	102	A1EFU	C4-C5-C6-C7
9	J	102	A1EFU	CM3-C5-C6-C7
9	J	102	A1EFU	C6-C7-C8-C9
9	J	102	A1EFU	C10-C11-C12-C13
9	J	102	A1EFU	C18-C19-C20-C21
9	J	102	A1EFU	C16-C17-C18-C19
9	J	102	A1EFU	C16-C17-C18-CM6
9	J	102	A1EFU	C11-C10-C9-C8
9	J	102	A1EFU	C11-C10-C9-CM4
9	J	102	A1EFU	C12-C13-C14-C15
9	J	102	A1EFU	CM5-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
9	J	102	A1EFU	C20-C21-C22-CM7
9	J	102	A1EFU	C26-C27-C28-C29
9	J	103	A1EFU	O1-C1-C2-O2
9	J	103	A1EFU	C2-C3-C4-C5
9	J	103	A1EFU	C4-C5-C6-C7
9	J	103	A1EFU	CM3-C5-C6-C7
9	J	103	A1EFU	C10-C11-C12-C13
9	J	103	A1EFU	C18-C19-C20-C21
9	J	103	A1EFU	C16-C17-C18-C19
9	J	103	A1EFU	C16-C17-C18-CM6
9	J	103	A1EFU	C11-C10-C9-C8
9	J	103	A1EFU	C11-C10-C9-CM4
9	J	103	A1EFU	C12-C13-C14-C15
9	J	103	A1EFU	CM5-C13-C14-C15
9	J	103	A1EFU	C20-C21-C22-CM7
9	i	101	A1EFU	C2-C3-C4-C5
9	i	101	A1EFU	C4-C5-C6-C7
9	i	101	A1EFU	CM3-C5-C6-C7
9	i	101	A1EFU	C6-C7-C8-C9
9	i	101	A1EFU	C10-C11-C12-C13
9	i	101	A1EFU	C16-C17-C18-C19
9	i	101	A1EFU	C16-C17-C18-CM6
9	i	101	A1EFU	C11-C10-C9-C8
9	i	101	A1EFU	C11-C10-C9-CM4
9	i	101	A1EFU	C12-C13-C14-C15
9	i	101	A1EFU	CM5-C13-C14-C15
9	i	101	A1EFU	C20-C21-C22-CM7
9	I	101	A1EFU	CM3-C5-C6-C7
9	I	101	A1EFU	C6-C7-C8-C9
9	I	101	A1EFU	C10-C11-C12-C13
9	I	101	A1EFU	C16-C17-C18-C19
9	I	101	A1EFU	C16-C17-C18-CM6
9	I	101	A1EFU	C11-C10-C9-C8
9	I	101	A1EFU	C11-C10-C9-CM4
9	I	101	A1EFU	C12-C13-C14-C15
9	I	101	A1EFU	CM5-C13-C14-C15
9	I	101	A1EFU	C20-C21-C22-CM7
9	I	101	A1EFU	C25-C26-C27-C28
9	I	101	A1EFU	CM8-C26-C27-C28
9	G	103	A1EFU	C2-C3-C4-C5
9	G	103	A1EFU	C6-C7-C8-C9
9	G	103	A1EFU	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
9	G	103	A1EFU	C18-C19-C20-C21
9	G	103	A1EFU	C11-C10-C9-C8
9	G	103	A1EFU	C11-C10-C9-CM4
9	G	103	A1EFU	C12-C13-C14-C15
9	G	103	A1EFU	CM5-C13-C14-C15
9	G	103	A1EFU	C20-C21-C22-CM7
9	G	103	A1EFU	C26-C27-C28-C29
9	G	104	A1EFU	C1-C2-C3-C4
9	G	104	A1EFU	O2-C2-C3-C4
9	G	104	A1EFU	C2-C3-C4-C5
9	G	104	A1EFU	C4-C5-C6-C7
9	G	104	A1EFU	CM3-C5-C6-C7
9	G	104	A1EFU	C18-C19-C20-C21
9	G	104	A1EFU	C16-C17-C18-C19
9	G	104	A1EFU	C16-C17-C18-CM6
9	G	104	A1EFU	C11-C10-C9-C8
9	G	104	A1EFU	C11-C10-C9-CM4
9	G	104	A1EFU	CM5-C13-C14-C15
9	G	104	A1EFU	C20-C21-C22-CM7
9	G	104	A1EFU	C25-C26-C27-C28
9	G	104	A1EFU	CM8-C26-C27-C28
9	F	102	A1EFU	C4-C5-C6-C7
9	F	102	A1EFU	CM3-C5-C6-C7
9	F	102	A1EFU	C6-C7-C8-C9
9	F	102	A1EFU	C10-C11-C12-C13
9	F	102	A1EFU	C2-C1-O1-CMA
9	F	102	A1EFU	CM1-C1-O1-CMA
9	F	102	A1EFU	C18-C19-C20-C21
9	F	102	A1EFU	C16-C17-C18-C19
9	F	102	A1EFU	C16-C17-C18-CM6
9	F	102	A1EFU	C11-C10-C9-C8
9	F	102	A1EFU	C11-C10-C9-CM4
9	F	102	A1EFU	C12-C13-C14-C15
9	F	102	A1EFU	CM5-C13-C14-C15
9	F	102	A1EFU	C20-C21-C22-CM7
9	F	102	A1EFU	C26-C27-C28-C29
9	F	103	A1EFU	C2-C3-C4-C5
9	F	103	A1EFU	C4-C5-C6-C7
9	F	103	A1EFU	CM3-C5-C6-C7
9	F	103	A1EFU	C10-C11-C12-C13
9	F	103	A1EFU	C16-C17-C18-C19
9	F	103	A1EFU	C16-C17-C18-CM6

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Mol	Chain	Res	Type	Atoms
9	F	103	A1EFU	C11-C10-C9-C8
9	F	103	A1EFU	C11-C10-C9-CM4
9	F	103	A1EFU	C12-C13-C14-C15
9	F	103	A1EFU	CM5-C13-C14-C15
9	F	103	A1EFU	C20-C21-C22-CM7
9	F	103	A1EFU	C26-C27-C28-C29
9	E	102	A1EFU	C4-C5-C6-C7
9	E	102	A1EFU	CM3-C5-C6-C7
9	E	102	A1EFU	C6-C7-C8-C9
9	E	102	A1EFU	C10-C11-C12-C13
9	E	102	A1EFU	C2-C1-O1-CMA
9	E	102	A1EFU	CM1-C1-O1-CMA
9	E	102	A1EFU	C18-C19-C20-C21
9	E	102	A1EFU	C11-C10-C9-C8
9	E	102	A1EFU	C11-C10-C9-CM4
9	E	102	A1EFU	C12-C13-C14-C15
9	E	102	A1EFU	CM5-C13-C14-C15
9	E	102	A1EFU	C20-C21-C22-CM7
9	E	102	A1EFU	C26-C27-C28-C29
9	d	101	A1EFU	O1-C1-C2-O2
9	d	101	A1EFU	C2-C3-C4-C5
9	d	101	A1EFU	C4-C5-C6-C7
9	d	101	A1EFU	CM3-C5-C6-C7
9	d	101	A1EFU	C10-C11-C12-C13
9	d	101	A1EFU	C18-C19-C20-C21
9	d	101	A1EFU	C16-C17-C18-C19
9	d	101	A1EFU	C16-C17-C18-CM6
9	d	101	A1EFU	C11-C10-C9-C8
9	d	101	A1EFU	C11-C10-C9-CM4
9	d	101	A1EFU	C20-C21-C22-CM7
9	D	103	A1EFU	C2-C3-C4-C5
9	D	103	A1EFU	C4-C5-C6-C7
9	D	103	A1EFU	CM3-C5-C6-C7
9	D	103	A1EFU	C6-C7-C8-C9
9	D	103	A1EFU	C10-C11-C12-C13
9	D	103	A1EFU	C16-C17-C18-C19
9	D	103	A1EFU	C16-C17-C18-CM6
9	D	103	A1EFU	C11-C10-C9-C8
9	D	103	A1EFU	C11-C10-C9-CM4
9	D	103	A1EFU	C12-C13-C14-C15
9	D	103	A1EFU	CM5-C13-C14-C15
9	D	103	A1EFU	C20-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
9	D	103	A1EFU	C20-C21-C22-CM7
9	D	103	A1EFU	CM7-C22-C23-C24
9	D	104	A1EFU	C2-C3-C4-C5
9	D	104	A1EFU	C4-C5-C6-C7
9	D	104	A1EFU	CM3-C5-C6-C7
9	D	104	A1EFU	C10-C11-C12-C13
9	D	104	A1EFU	C2-C1-O1-CMA
9	D	104	A1EFU	CM1-C1-O1-CMA
9	D	104	A1EFU	CM2-C1-O1-CMA
9	D	104	A1EFU	C18-C19-C20-C21
9	D	104	A1EFU	C16-C17-C18-C19
9	D	104	A1EFU	C16-C17-C18-CM6
9	D	104	A1EFU	C11-C10-C9-C8
9	D	104	A1EFU	C11-C10-C9-CM4
9	D	104	A1EFU	C12-C13-C14-C15
9	D	104	A1EFU	CM5-C13-C14-C15
9	D	104	A1EFU	C20-C21-C22-C23
9	D	104	A1EFU	C20-C21-C22-CM7
9	b	102	A1EFU	C4-C5-C6-C7
9	b	102	A1EFU	CM3-C5-C6-C7
9	b	102	A1EFU	C6-C7-C8-C9
9	b	102	A1EFU	C10-C11-C12-C13
9	b	102	A1EFU	C18-C19-C20-C21
9	b	102	A1EFU	C16-C17-C18-C19
9	b	102	A1EFU	C16-C17-C18-CM6
9	b	102	A1EFU	C11-C10-C9-C8
9	b	102	A1EFU	C11-C10-C9-CM4
9	b	102	A1EFU	C12-C13-C14-C15
9	b	102	A1EFU	CM5-C13-C14-C15
9	b	102	A1EFU	C20-C21-C22-CM7
9	a	101	A1EFU	C2-C3-C4-C5
9	a	101	A1EFU	C4-C5-C6-C7
9	a	101	A1EFU	CM3-C5-C6-C7
9	a	101	A1EFU	C6-C7-C8-C9
9	a	101	A1EFU	C10-C11-C12-C13
9	a	101	A1EFU	C18-C19-C20-C21
9	a	101	A1EFU	C16-C17-C18-C19
9	a	101	A1EFU	C16-C17-C18-CM6
9	a	101	A1EFU	C11-C10-C9-C8
9	a	101	A1EFU	C11-C10-C9-CM4
9	a	101	A1EFU	C12-C13-C14-C15
9	a	101	A1EFU	CM5-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
9	a	101	A1EFU	C20-C21-C22-CM7
9	a	103	A1EFU	C1-C2-C3-C4
9	a	103	A1EFU	O2-C2-C3-C4
9	a	103	A1EFU	O1-C1-C2-O2
9	a	103	A1EFU	C2-C3-C4-C5
9	a	103	A1EFU	C4-C5-C6-C7
9	a	103	A1EFU	CM3-C5-C6-C7
9	a	103	A1EFU	C10-C11-C12-C13
9	a	103	A1EFU	C18-C19-C20-C21
9	a	103	A1EFU	C16-C17-C18-C19
9	a	103	A1EFU	C16-C17-C18-CM6
9	a	103	A1EFU	C11-C10-C9-C8
9	a	103	A1EFU	C11-C10-C9-CM4
9	a	103	A1EFU	C12-C13-C14-C15
9	a	103	A1EFU	CM5-C13-C14-C15
9	a	103	A1EFU	C20-C21-C22-CM7
9	a	103	A1EFU	C21-C22-C23-C24
9	a	103	A1EFU	C26-C27-C28-C29
9	A	102	A1EFU	C2-C3-C4-C5
9	A	102	A1EFU	C10-C11-C12-C13
9	A	102	A1EFU	C16-C17-C18-C19
9	A	102	A1EFU	C16-C17-C18-CM6
9	A	102	A1EFU	C11-C10-C9-C8
9	A	102	A1EFU	C11-C10-C9-CM4
9	A	102	A1EFU	C12-C13-C14-C15
9	A	102	A1EFU	CM5-C13-C14-C15
9	A	102	A1EFU	C20-C21-C22-CM7
9	A	102	A1EFU	CM7-C22-C23-C24
9	A	102	A1EFU	C22-C23-C24-C25
9	A	103	A1EFU	C1-C2-C3-C4
9	A	103	A1EFU	O2-C2-C3-C4
9	A	103	A1EFU	C10-C11-C12-C13
9	A	103	A1EFU	C18-C19-C20-C21
9	A	103	A1EFU	C16-C17-C18-C19
9	A	103	A1EFU	C16-C17-C18-CM6
9	A	103	A1EFU	C11-C10-C9-C8
9	A	103	A1EFU	C11-C10-C9-CM4
9	A	103	A1EFU	C12-C13-C14-C15
9	A	103	A1EFU	CM5-C13-C14-C15
9	A	103	A1EFU	C20-C21-C22-CM7
9	A	103	A1EFU	C25-C26-C27-C28
9	A	103	A1EFU	CM8-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
9	M	406	A1EFU	C2-C3-C4-C5
9	M	406	A1EFU	C4-C5-C6-C7
9	M	406	A1EFU	CM3-C5-C6-C7
9	M	406	A1EFU	C6-C7-C8-C9
9	M	406	A1EFU	C10-C11-C12-C13
9	M	406	A1EFU	C14-C15-C16-C17
9	M	406	A1EFU	C16-C17-C18-C19
9	M	406	A1EFU	C16-C17-C18-CM6
9	M	406	A1EFU	C11-C10-C9-C8
9	M	406	A1EFU	C11-C10-C9-CM4
9	M	406	A1EFU	C20-C21-C22-CM7
10	S	301	LMT	C2'-C1'-O1'-C1
10	S	301	LMT	O5'-C1'-O1'-C1
10	G	107	LMT	C2'-C1'-O1'-C1
10	G	107	LMT	O5'-C1'-O1'-C1
10	E	103	LMT	C2'-C1'-O1'-C1
10	E	103	LMT	O5'-C1'-O1'-C1
10	E	103	LMT	C2-C1-O1'-C1'
10	B	101	LMT	C2'-C1'-O1'-C1
10	B	101	LMT	O5'-C1'-O1'-C1
10	B	101	LMT	C2-C1-O1'-C1'
10	L	306	LMT	C2'-C1'-O1'-C1
10	L	306	LMT	O5'-C1'-O1'-C1
10	L	306	LMT	C2-C1-O1'-C1'
10	H	304	LMT	O5'-C1'-O1'-C1
10	C	404	LMT	O5'-C1'-O1'-C1
11	R	103	MW9	C33-C34-C35-C36
11	R	103	MW9	C20-O2-P-O3
11	R	103	MW9	C20-O2-P-O4
11	N	103	MW9	C20-O2-P-O4
11	G	105	MW9	C21-C22-C23-O6
11	G	105	MW9	C25-C24-O8-C19
11	G	105	MW9	O9-C24-O8-C19
11	G	105	MW9	C20-O2-P-O3
11	G	105	MW9	C21-O5-P-O4
11	G	106	MW9	O5-C21-C22-C23
11	G	106	MW9	C21-C22-C23-O6
11	G	106	MW9	C25-C24-O8-C19
11	G	106	MW9	O9-C24-O8-C19
11	G	106	MW9	C20-O2-P-O4
11	G	106	MW9	C21-O5-P-O4
11	F	104	MW9	C21-C22-C23-O6

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Mol	Chain	Res	Type	Atoms
11	F	104	MW9	C25-C24-O8-C19
11	M	407	MW9	C21-C22-C23-O6
11	M	407	MW9	C33-C34-C35-C36
11	L	305	MW9	C21-C22-C23-O6
11	L	305	MW9	C20-O2-P-O4
11	H	302	MW9	C20-O2-P-O3
11	H	302	MW9	C20-O2-P-O5
13	M	403	BPH	CBA-CGA-O2A-C1
13	M	403	BPH	O1A-CGA-O2A-C1
13	M	403	BPH	O2A-C1-C2-C3
14	M	405	U10	C44-C46-C47-C48
14	M	405	U10	C49-C51-C52-C53
14	L	303	U10	C14-C16-C17-C18
15	M	408	CDL	CA2-OA2-PA1-OA3
15	M	408	CDL	CA2-OA2-PA1-OA4
15	M	408	CDL	CA3-OA5-PA1-OA2
15	M	408	CDL	CA3-OA5-PA1-OA3
15	M	408	CDL	CA3-OA5-PA1-OA4
15	M	408	CDL	CB3-OB5-PB2-OB3
15	M	408	CDL	CB3-OB5-PB2-OB4
15	H	303	CDL	CA2-C1-CB2-OB2
15	H	303	CDL	CA2-OA2-PA1-OA3
15	H	303	CDL	CA2-OA2-PA1-OA4
15	H	303	CDL	CA3-OA5-PA1-OA4
15	H	303	CDL	OA9-CA7-OA8-CA6
15	H	303	CDL	C31-CA7-OA8-CA6
10	C	404	LMT	C5'-C4'-O1B-C1B
8	n	101	BCL	O1A-CGA-O2A-C1
8	E	101	BCL	O1A-CGA-O2A-C1
11	N	103	MW9	O-C17-O1-C18
15	M	408	CDL	OA9-CA7-OA8-CA6
8	F	101	BCL	CBA-CGA-O2A-C1
8	E	101	BCL	CBA-CGA-O2A-C1
11	N	103	MW9	C16-C17-O1-C18
15	M	408	CDL	C31-CA7-OA8-CA6
8	F	101	BCL	O1A-CGA-O2A-C1
8	a	102	BCL	O1A-CGA-O2A-C1
8	L	301	BCL	O1A-CGA-O2A-C1
11	F	104	MW9	O-C17-O1-C18
10	E	103	LMT	C3'-C4'-O1B-C1B
10	S	301	LMT	C3'-C4'-O1B-C1B
11	F	104	MW9	O9-C24-O8-C19

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Mol	Chain	Res	Type	Atoms
15	H	303	CDL	OA7-CA5-OA6-CA4
10	C	404	LMT	C4'-C5'-C6'-O6'
8	P	102	BCL	CBA-CGA-O2A-C1
8	n	101	BCL	CBA-CGA-O2A-C1
8	L	301	BCL	CBA-CGA-O2A-C1
15	H	303	CDL	C11-CA5-OA6-CA4
8	v	102	BCL	C2-C3-C5-C6
8	s	101	BCL	C2-C3-C5-C6
8	Q	102	BCL	C2-C3-C5-C6
9	Q	101	A1EFU	C25-C26-C27-C28
8	S	302	BCL	C2A-CAA-CBA-CGA
8	K	102	BCL	C2A-CAA-CBA-CGA
8	G	102	BCL	C2A-CAA-CBA-CGA
8	D	101	BCL	C2A-CAA-CBA-CGA
11	G	105	MW9	C5-C6-C7-C8
11	H	301	MW9	C5-C6-C7-C8
8	d	102	BCL	C3-C5-C6-C7
8	A	101	BCL	C3-C5-C6-C7
8	M	402	BCL	C3-C5-C6-C7
8	a	102	BCL	CBA-CGA-O2A-C1
11	F	104	MW9	C16-C17-O1-C18
10	E	103	LMT	O5'-C5'-C6'-O6'
10	C	404	LMT	O5'-C5'-C6'-O6'
11	M	407	MW9	C31-C32-C33-C34
11	H	301	MW9	C31-C32-C33-C34
8	B	102	BCL	C1-C2-C3-C5
8	P	102	BCL	O1A-CGA-O2A-C1
11	R	103	MW9	O-C17-O1-C18
11	L	305	MW9	O-C17-O1-C18
9	J	103	A1EFU	C19-C20-C21-C22
11	F	104	MW9	O5-C21-C22-O7
15	M	408	CDL	O1-C1-CB2-OB2
15	H	303	CDL	O1-C1-CB2-OB2
8	1	101	BCL	C3-C5-C6-C7
8	I	102	BCL	C3-C5-C6-C7
11	L	305	MW9	C16-C17-O1-C18
11	N	103	MW9	C25-C24-O8-C19
15	M	408	CDL	C11-CA5-OA6-CA4
10	H	304	LMT	O5'-C5'-C6'-O6'
9	N	102	A1EFU	C14-C15-C16-C17
11	R	103	MW9	C16-C17-O1-C18
15	M	408	CDL	OA7-CA5-OA6-CA4

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Mol	Chain	Res	Type	Atoms
10	E	103	LMT	C4'-C5'-C6'-O6'
10	C	404	LMT	C4B-C5B-C6B-O6B
8	v	102	BCL	O1A-CGA-O2A-C1
8	A	101	BCL	O1A-CGA-O2A-C1
8	S	302	BCL	C4-C3-C5-C6
9	R	102	A1EFU	CM8-C26-C27-C28
9	F	103	A1EFU	CM8-C26-C27-C28
8	S	302	BCL	C2-C3-C5-C6
8	1	102	BCL	C2-C3-C5-C6
8	E	101	BCL	C2-C3-C5-C6
9	T	103	A1EFU	C21-C22-C23-C24
9	R	102	A1EFU	C25-C26-C27-C28
9	p	101	A1EFU	C21-C22-C23-C24
9	1	104	A1EFU	C21-C22-C23-C24
9	n	102	A1EFU	C21-C22-C23-C24
9	i	101	A1EFU	C21-C22-C23-C24
9	G	104	A1EFU	C21-C22-C23-C24
9	F	103	A1EFU	C25-C26-C27-C28
9	M	406	A1EFU	C21-C22-C23-C24
9	P	103	A1EFU	C26-C27-C28-C29
9	Q	101	A1EFU	C26-C27-C28-C29
9	r	102	A1EFU	C26-C27-C28-C29
9	q	102	A1EFU	C22-C23-C24-C25
9	n	102	A1EFU	C22-C23-C24-C25
9	K	104	A1EFU	C26-C27-C28-C29
9	J	102	A1EFU	C22-C23-C24-C25
9	I	101	A1EFU	C26-C27-C28-C29
9	G	103	A1EFU	C22-C23-C24-C25
9	F	102	A1EFU	C22-C23-C24-C25
9	F	103	A1EFU	C22-C23-C24-C25
9	E	102	A1EFU	C22-C23-C24-C25
9	D	103	A1EFU	C26-C27-C28-C29
9	D	104	A1EFU	C26-C27-C28-C29
9	a	103	A1EFU	C22-C23-C24-C25
9	A	102	A1EFU	C26-C27-C28-C29
14	M	405	U10	C24-C26-C27-C28
14	M	405	U10	C34-C36-C37-C38
14	L	303	U10	C9-C11-C12-C13
14	L	303	U10	C19-C21-C22-C23
14	L	303	U10	C24-C26-C27-C28
14	L	303	U10	C34-C36-C37-C38
8	j	101	BCL	C1-C2-C3-C5

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Mol	Chain	Res	Type	Atoms
11	F	104	MW9	O5-C21-C22-C23
15	M	408	CDL	CB2-C1-CA2-OA2
15	M	408	CDL	CA2-C1-CB2-OB2
11	N	103	MW9	O9-C24-O8-C19
8	Q	102	BCL	O1A-CGA-O2A-C1
8	t	101	BCL	C3-C5-C6-C7
8	v	102	BCL	CBA-CGA-O2A-C1
8	D	101	BCL	CBA-CGA-O2A-C1
8	A	101	BCL	CBA-CGA-O2A-C1
11	H	301	MW9	C16-C17-O1-C18
8	I	102	BCL	C8-C10-C11-C12
8	f	101	BCL	C10-C11-C12-C13
8	n	101	BCL	C10-C11-C12-C13
8	e	101	BCL	C8-C10-C11-C12
10	H	304	LMT	C2'-C1'-O1'-C1
8	1	101	BCL	C6-C7-C8-C9
8	n	101	BCL	C6-C7-C8-C9
8	j	101	BCL	C6-C7-C8-C9
8	I	102	BCL	C6-C7-C8-C9
8	b	101	BCL	C6-C7-C8-C9
8	b	101	BCL	C14-C13-C15-C16
13	M	403	BPH	C6-C7-C8-C9
10	C	404	LMT	O5B-C5B-C6B-O6B
15	H	303	CDL	C77-C78-C79-C80
10	S	301	LMT	C4'-C5'-C6'-O6'
8	s	101	BCL	C13-C15-C16-C17
8	n	101	BCL	C5-C6-C7-C8
8	K	101	BCL	C10-C11-C12-C13
8	G	101	BCL	C5-C6-C7-C8
11	D	102	MW9	C18-C19-C20-O2
8	S	302	BCL	C3-C5-C6-C7
16	C	401	HEC	C3D-CAD-CBD-CGD
8	I	102	BCL	C15-C16-C17-C18
8	E	101	BCL	C5-C6-C7-C8
8	D	101	BCL	C5-C6-C7-C8
8	b	101	BCL	C15-C16-C17-C18
8	s	101	BCL	C5-C6-C7-C8
8	e	101	BCL	C15-C16-C17-C18
8	D	101	BCL	C15-C16-C17-C18
11	G	106	MW9	C24-C25-C26-C27
11	M	407	MW9	C14-C15-C16-C17
15	M	408	CDL	CA5-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
11	D	102	MW9	C16-C17-O1-C18
15	H	303	CDL	CA5-C11-C12-C13
15	H	303	CDL	CB7-C71-C72-C73
8	N	101	BCL	C6-C7-C8-C10
8	F	101	BCL	C6-C7-C8-C10
9	S	304	A1EFU	C19-C20-C21-C22
13	M	403	BPH	C2A-CAA-CBA-CGA
8	T	102	BCL	C13-C15-C16-C17
8	e	101	BCL	C10-C11-C12-C13
8	L	301	BCL	C15-C16-C17-C18
11	H	301	MW9	O-C17-O1-C18
9	r	102	A1EFU	C22-C23-C24-C25
9	p	101	A1EFU	C22-C23-C24-C25
9	1	103	A1EFU	C26-C27-C28-C29
9	1	104	A1EFU	C22-C23-C24-C25
9	K	103	A1EFU	C22-C23-C24-C25
9	K	104	A1EFU	C22-C23-C24-C25
9	i	101	A1EFU	C22-C23-C24-C25
9	d	101	A1EFU	C22-C23-C24-C25
9	D	103	A1EFU	C22-C23-C24-C25
9	v	101	A1EFU	C6-C7-C8-C9
9	r	102	A1EFU	C6-C7-C8-C9
9	r	102	A1EFU	C18-C19-C20-C21
9	q	102	A1EFU	C18-C19-C20-C21
9	i	101	A1EFU	C18-C19-C20-C21
9	I	101	A1EFU	C18-C19-C20-C21
9	G	104	A1EFU	C6-C7-C8-C9
9	F	103	A1EFU	C6-C7-C8-C9
9	d	101	A1EFU	C6-C7-C8-C9
9	D	104	A1EFU	C6-C7-C8-C9
9	a	103	A1EFU	C6-C7-C8-C9
9	A	102	A1EFU	C6-C7-C8-C9
9	A	102	A1EFU	C18-C19-C20-C21
11	G	106	MW9	C5-C6-C7-C8
11	F	104	MW9	C5-C6-C7-C8
15	M	408	CDL	O1-C1-CA2-OA2
8	I	102	BCL	C10-C11-C12-C13
8	f	101	BCL	C5-C6-C7-C8
8	L	301	BCL	C13-C15-C16-C17
8	V	101	BCL	O1A-CGA-O2A-C1
8	r	101	BCL	O1A-CGA-O2A-C1
8	J	101	BCL	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
8	q	101	BCL	C15-C16-C17-C18
8	1	102	BCL	C10-C11-C12-C13
8	d	102	BCL	C15-C16-C17-C18
8	A	101	BCL	C15-C16-C17-C18
13	M	403	BPH	C5-C6-C7-C8
8	K	102	BCL	O1A-CGA-O2A-C1
11	H	301	MW9	C12-C13-C14-C15
8	v	102	BCL	C10-C11-C12-C13
8	s	101	BCL	C10-C11-C12-C13
8	j	101	BCL	C5-C6-C7-C8
8	J	101	BCL	C5-C6-C7-C8
8	D	101	BCL	C8-C10-C11-C12
8	s	101	BCL	C1-C2-C3-C5
11	R	103	MW9	C20-O2-P-O5
11	G	105	MW9	C20-O2-P-O5
11	D	102	MW9	C20-O2-P-O5
11	M	407	MW9	C20-O2-P-O5
11	H	301	MW9	C21-O5-P-O2
15	M	408	CDL	CA2-OA2-PA1-OA5
15	M	408	CDL	CB3-OB5-PB2-OB2
15	H	303	CDL	CA2-OA2-PA1-OA5
8	Q	102	BCL	CBA-CGA-O2A-C1
8	J	101	BCL	C10-C11-C12-C13
11	R	103	MW9	C14-C15-C16-C17
8	L	304	BCL	C4-C3-C5-C6
10	H	304	LMT	C4'-C5'-C6'-O6'
8	v	102	BCL	C8-C10-C11-C12
8	G	102	BCL	C10-C11-C12-C13
8	d	102	BCL	C10-C11-C12-C13
8	b	101	BCL	C13-C15-C16-C17
11	N	103	MW9	C24-C25-C26-C27
11	G	105	MW9	C27-C28-C29-C30
11	H	302	MW9	C10-C11-C12-C13
11	M	407	MW9	C25-C24-O8-C19
8	1	101	BCL	C5-C6-C7-C8
8	1	102	BCL	C8-C10-C11-C12
9	P	103	A1EFU	C16-C17-C18-CM6
9	r	102	A1EFU	CM5-C13-C14-C15
9	R	102	A1EFU	C16-C17-C18-CM6
9	N	102	A1EFU	C16-C17-C18-CM6
9	G	103	A1EFU	CM3-C5-C6-C7
9	G	103	A1EFU	C16-C17-C18-CM6

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Mol	Chain	Res	Type	Atoms
9	E	102	A1EFU	C16-C17-C18-CM6
9	d	101	A1EFU	CM5-C13-C14-C15
9	M	406	A1EFU	CM5-C13-C14-C15
11	F	104	MW9	C11-C12-C13-C14
11	D	102	MW9	C13-C14-C15-C16
15	M	408	CDL	C11-C12-C13-C14
15	H	303	CDL	C72-C73-C74-C75
15	H	303	CDL	C75-C76-C77-C78
8	T	102	BCL	C16-C17-C18-C19
8	L	304	BCL	CBA-CGA-O2A-C1
11	G	106	MW9	C6-C7-C8-C9
11	F	104	MW9	C13-C14-C15-C16
11	M	407	MW9	C13-C14-C15-C16
11	M	407	MW9	C6-C7-C8-C9
11	M	407	MW9	O9-C24-O8-C19
8	j	101	BCL	C15-C16-C17-C18
11	R	103	MW9	C27-C28-C29-C30
11	F	104	MW9	C10-C11-C12-C13
15	H	303	CDL	C15-C16-C17-C18
11	D	102	MW9	O-C17-O1-C18
11	G	105	MW9	C9-C10-C11-C12
11	H	302	MW9	C13-C14-C15-C16
11	G	106	MW9	O5-C21-C22-O7
9	P	103	A1EFU	C16-C17-C18-C19
9	T	103	A1EFU	C12-C13-C14-C15
9	Q	101	A1EFU	CM1-C1-O1-CMA
9	Q	101	A1EFU	CM2-C1-O1-CMA
9	r	102	A1EFU	C12-C13-C14-C15
9	R	102	A1EFU	CM1-C1-O1-CMA
9	R	102	A1EFU	CM2-C1-O1-CMA
9	R	102	A1EFU	C16-C17-C18-C19
9	1	103	A1EFU	C16-C17-C18-C19
9	N	102	A1EFU	C16-C17-C18-C19
9	K	104	A1EFU	CM2-C1-O1-CMA
9	I	101	A1EFU	C4-C5-C6-C7
9	G	103	A1EFU	C4-C5-C6-C7
9	G	103	A1EFU	C16-C17-C18-C19
9	G	104	A1EFU	C12-C13-C14-C15
9	F	102	A1EFU	CM2-C1-O1-CMA
9	E	102	A1EFU	CM2-C1-O1-CMA
9	E	102	A1EFU	C16-C17-C18-C19
9	d	101	A1EFU	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
9	M	406	A1EFU	C12-C13-C14-C15
11	R	103	MW9	C12-C13-C14-C15
11	F	104	MW9	C28-C29-C30-C31
11	D	102	MW9	C10-C11-C12-C13
15	M	408	CDL	C52-C53-C54-C55
8	F	101	BCL	C8-C10-C11-C12
8	s	101	BCL	C16-C17-C18-C19
8	I	103	BCL	C16-C17-C18-C20
8	V	101	BCL	C4-C3-C5-C6
8	d	102	BCL	C4-C3-C5-C6
9	d	101	A1EFU	CM7-C22-C23-C24
11	L	305	MW9	C13-C14-C15-C16
15	M	408	CDL	C13-C14-C15-C16
8	1	101	BCL	C11-C10-C8-C9
8	N	101	BCL	C6-C7-C8-C9
8	G	102	BCL	C6-C7-C8-C9
8	F	101	BCL	C6-C7-C8-C9
11	N	103	MW9	C12-C13-C14-C15
11	F	104	MW9	C7-C8-C9-C10
11	M	407	MW9	C27-C28-C29-C30
11	H	301	MW9	C4-C5-C6-C7
11	H	301	MW9	C6-C7-C8-C9
15	M	408	CDL	C14-C15-C16-C17
15	M	408	CDL	C16-C17-C18-C19
15	H	303	CDL	C11-C12-C13-C14
15	H	303	CDL	C34-C35-C36-C37
11	H	301	MW9	C10-C11-C12-C13
11	H	302	MW9	C7-C8-C9-C10
15	H	303	CDL	C21-C22-C23-C24
15	H	303	CDL	C58-C59-C60-C61
15	H	303	CDL	C74-C75-C76-C77
11	N	103	MW9	C21-C22-C23-O6
11	H	301	MW9	O9-C24-O8-C19
8	L	304	BCL	C10-C11-C12-C13
11	H	301	MW9	C25-C24-O8-C19
11	G	106	MW9	C13-C14-C15-C16
11	G	106	MW9	C25-C26-C27-C28
15	H	303	CDL	C63-C64-C65-C66
11	G	105	MW9	C14-C15-C16-C17
11	G	106	MW9	C14-C15-C16-C17
11	G	106	MW9	C10-C11-C12-C13
11	H	301	MW9	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
11	H	301	MW9	C26-C27-C28-C29
8	T	102	BCL	C16-C17-C18-C20
8	Q	102	BCL	C16-C17-C18-C20
8	I	103	BCL	C16-C17-C18-C19
8	G	101	BCL	C10-C11-C12-C13
9	P	103	A1EFU	C22-C23-C24-C25
11	F	104	MW9	C6-C7-C8-C9
11	M	407	MW9	C12-C13-C14-C15
11	H	301	MW9	C2-C3-C4-C5
15	M	408	CDL	C54-C55-C56-C57
11	F	104	MW9	C14-C15-C16-C17
11	H	302	MW9	C24-C25-C26-C27
8	D	101	BCL	O1A-CGA-O2A-C1
11	N	103	MW9	C7-C8-C9-C10
11	G	105	MW9	C10-C11-C12-C13
11	D	102	MW9	C9-C10-C11-C12
8	R	101	BCL	CBA-CGA-O2A-C1
11	N	103	MW9	C10-C11-C12-C13
8	v	102	BCL	C3A-C2A-CAA-CBA
8	S	302	BCL	C3A-C2A-CAA-CBA
8	s	101	BCL	C3A-C2A-CAA-CBA
8	r	101	BCL	C3A-C2A-CAA-CBA
8	q	101	BCL	C3A-C2A-CAA-CBA
8	1	101	BCL	C3A-C2A-CAA-CBA
8	j	101	BCL	C3A-C2A-CAA-CBA
8	G	101	BCL	C3A-C2A-CAA-CBA
8	e	101	BCL	C3A-C2A-CAA-CBA
8	d	102	BCL	C3A-C2A-CAA-CBA
8	B	102	BCL	C3A-C2A-CAA-CBA
8	A	101	BCL	C3A-C2A-CAA-CBA
10	G	107	LMT	C2-C1-O1'-C1'
10	H	304	LMT	C2-C1-O1'-C1'
10	C	404	LMT	C2-C1-O1'-C1'
11	R	103	MW9	C13-C14-C15-C16
11	G	106	MW9	C26-C27-C28-C29
11	G	106	MW9	C27-C28-C29-C30
8	Q	102	BCL	C16-C17-C18-C19
11	R	103	MW9	C10-C11-C12-C13
11	N	103	MW9	C4-C5-C6-C7
11	N	103	MW9	C31-C32-C33-C34
11	M	407	MW9	C9-C10-C11-C12
11	D	102	MW9	O1-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
8	K	102	BCL	CBA-CGA-O2A-C1
11	H	302	MW9	C16-C17-O1-C18
8	D	101	BCL	C2-C3-C5-C6
11	R	103	MW9	C25-C24-O8-C19
8	S	302	BCL	C1-C2-C3-C5
11	F	104	MW9	O7-C22-C23-O6
11	M	407	MW9	O7-C22-C23-O6
11	L	305	MW9	O7-C22-C23-O6
11	N	103	MW9	C9-C10-C11-C12
15	H	303	CDL	C54-C55-C56-C57
11	N	103	MW9	C29-C30-C31-C32
8	s	101	BCL	C16-C17-C18-C20
11	H	302	MW9	C27-C28-C29-C30
11	G	105	MW9	C26-C27-C28-C29
11	L	305	MW9	C26-C27-C28-C29
8	1	102	BCL	O1A-CGA-O2A-C1
8	b	101	BCL	O1A-CGA-O2A-C1
8	b	101	BCL	C5-C6-C7-C8
15	H	303	CDL	C17-C18-C19-C20
11	N	103	MW9	C13-C14-C15-C16
11	M	407	MW9	C24-C25-C26-C27
8	L	304	BCL	C3-C5-C6-C7
15	M	408	CDL	C55-C56-C57-C58
15	H	303	CDL	C76-C77-C78-C79
8	r	101	BCL	CBA-CGA-O2A-C1
8	t	101	BCL	C5-C6-C7-C8
8	G	101	BCL	C8-C10-C11-C12
11	N	103	MW9	C14-C15-C16-C17
11	H	302	MW9	C32-C33-C34-C35
8	a	102	BCL	C15-C16-C17-C18
8	P	101	BCL	C6-C7-C8-C10
8	T	102	BCL	C6-C7-C8-C10
8	T	102	BCL	C11-C12-C13-C15
8	q	101	BCL	C11-C10-C8-C7
8	q	101	BCL	C12-C13-C15-C16
8	1	101	BCL	C11-C10-C8-C7
8	1	102	BCL	C6-C7-C8-C10
8	j	101	BCL	C6-C7-C8-C10
8	G	102	BCL	C6-C7-C8-C10
8	L	301	BCL	C11-C12-C13-C15
13	M	403	BPH	C6-C7-C8-C10
14	L	303	U10	C18-C19-C21-C22

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Mol	Chain	Res	Type	Atoms
11	H	302	MW9	O-C17-O1-C18
8	G	102	BCL	C5-C6-C7-C8
9	a	101	A1EFU	C19-C20-C21-C22
8	S	302	BCL	C16-C17-C18-C20
11	R	103	MW9	O9-C24-O8-C19
8	S	302	BCL	CBA-CGA-O2A-C1
11	M	407	MW9	C11-C12-C13-C14
8	K	101	BCL	C1-C2-C3-C5
11	D	102	MW9	C12-C13-C14-C15
11	H	301	MW9	C7-C8-C9-C10
11	D	102	MW9	C7-C8-C9-C10
15	H	303	CDL	C12-C13-C14-C15
8	I	103	BCL	C5-C6-C7-C8
9	1	104	A1EFU	C26-C27-C28-C29
9	N	102	A1EFU	C26-C27-C28-C29
11	H	302	MW9	C25-C24-O8-C19
15	H	303	CDL	C51-CB5-OB6-CB4
10	S	301	LMT	O5'-C5'-C6'-O6'
9	M	406	A1EFU	C18-C19-C20-C21
11	H	302	MW9	C6-C7-C8-C9
11	H	302	MW9	O9-C24-O8-C19
15	H	303	CDL	OB7-CB5-OB6-CB4
11	N	103	MW9	C27-C28-C29-C30
10	C	404	LMT	C2'-C1'-O1'-C1
8	b	101	BCL	C4-C3-C5-C6
14	L	303	U10	C20-C19-C21-C22
9	a	103	A1EFU	C25-C26-C27-C28
15	M	408	CDL	C15-C16-C17-C18
8	v	102	BCL	C6-C7-C8-C9
8	T	102	BCL	C6-C7-C8-C9
8	T	102	BCL	C11-C12-C13-C14
8	T	102	BCL	C14-C13-C15-C16
8	1	102	BCL	C6-C7-C8-C9
8	j	101	BCL	C11-C10-C8-C9
8	d	102	BCL	C11-C10-C8-C9
8	L	301	BCL	C11-C12-C13-C14
11	H	301	MW9	C3-C4-C5-C6
8	1	102	BCL	C2A-CAA-CBA-CGA
8	b	101	BCL	C2A-CAA-CBA-CGA
15	H	303	CDL	C13-C14-C15-C16
8	I	102	BCL	C5-C6-C7-C8
11	G	105	MW9	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
8	d	102	BCL	O1A-CGA-O2A-C1
8	S	302	BCL	C1A-C2A-CAA-CBA
8	T	102	BCL	C1A-C2A-CAA-CBA
8	R	101	BCL	C1A-C2A-CAA-CBA
8	1	101	BCL	C1A-C2A-CAA-CBA
8	d	102	BCL	C1A-C2A-CAA-CBA
8	M	404	BCL	C1A-C2A-CAA-CBA
8	L	304	BCL	C1A-C2A-CAA-CBA
8	S	302	BCL	C16-C17-C18-C19
8	1	101	BCL	C16-C17-C18-C20
8	I	102	BCL	C16-C17-C18-C20
10	G	107	LMT	C11-C10-C9-C8
11	G	105	MW9	C21-O5-P-O2
15	H	303	CDL	CA3-OA5-PA1-OA2
15	H	303	CDL	C1-CA2-OA2-PA1
11	F	104	MW9	C12-C13-C14-C15
11	H	301	MW9	C27-C28-C29-C30
8	S	302	BCL	C15-C16-C17-C18
11	N	103	MW9	C18-C19-C20-O2
11	G	105	MW9	C18-C19-C20-O2
11	R	103	MW9	C29-C30-C31-C32
11	H	301	MW9	C29-C30-C31-C32
8	V	101	BCL	C2C-C3C-CAC-CBC
8	S	302	BCL	C2C-C3C-CAC-CBC
8	L	304	BCL	C2C-C3C-CAC-CBC
15	H	303	CDL	C52-C53-C54-C55
8	N	101	BCL	C15-C16-C17-C18
8	L	301	BCL	C8-C10-C11-C12
10	H	304	LMT	C3-C4-C5-C6
8	S	302	BCL	O1A-CGA-O2A-C1
11	R	103	MW9	C9-C10-C11-C12
11	R	103	MW9	O1-C18-C19-C20
11	M	407	MW9	C10-C11-C12-C13
11	M	407	MW9	O1-C18-C19-C20
11	M	407	MW9	C25-C26-C27-C28
11	H	301	MW9	C13-C14-C15-C16
15	M	408	CDL	C34-C35-C36-C37
15	H	303	CDL	C73-C74-C75-C76
15	H	303	CDL	C81-C82-C83-C84
9	v	101	A1EFU	C26-C27-C28-C29
9	p	101	A1EFU	C26-C27-C28-C29
11	M	407	MW9	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
11	G	105	MW9	O7-C22-C23-O6
11	G	106	MW9	O7-C22-C23-O6
11	G	105	MW9	C4-C5-C6-C7
11	N	103	MW9	C6-C7-C8-C9
9	v	101	A1EFU	CM7-C22-C23-C24
9	a	103	A1EFU	CM8-C26-C27-C28
13	L	302	BPH	C4-C3-C5-C6
8	J	101	BCL	CBA-CGA-O2A-C1
15	H	303	CDL	C60-C61-C62-C63
15	M	408	CDL	CA6-CA4-OA6-CA5
8	L	304	BCL	C13-C15-C16-C17
11	G	106	MW9	C12-C13-C14-C15
11	H	302	MW9	C20-O2-P-O4
11	R	103	MW9	C31-C32-C33-C34
8	P	102	BCL	C16-C17-C18-C20
11	H	302	MW9	C12-C13-C14-C15
8	s	101	BCL	C15-C16-C17-C18
8	L	304	BCL	O1A-CGA-O2A-C1
8	d	102	BCL	C5-C6-C7-C8
9	v	101	A1EFU	CM1-C1-O1-CMA
9	v	101	A1EFU	CM2-C1-O1-CMA
9	S	304	A1EFU	CM1-C1-O1-CMA
9	S	304	A1EFU	CM2-C1-O1-CMA
9	1	104	A1EFU	CM1-C1-O1-CMA
9	1	104	A1EFU	CM2-C1-O1-CMA
9	n	102	A1EFU	CM2-C1-O1-CMA
9	K	104	A1EFU	CM1-C1-O1-CMA
9	I	101	A1EFU	CM2-C1-O1-CMA
9	a	101	A1EFU	CM2-C1-O1-CMA
9	a	103	A1EFU	CM1-C1-O1-CMA
9	a	103	A1EFU	CM2-C1-O1-CMA
9	A	102	A1EFU	CM1-C1-O1-CMA
9	A	102	A1EFU	CM2-C1-O1-CMA
15	H	303	CDL	C23-C24-C25-C26
8	v	102	BCL	C6-C7-C8-C10
8	v	102	BCL	C11-C12-C13-C15
8	T	102	BCL	C12-C13-C15-C16
8	j	101	BCL	C11-C10-C8-C7
8	I	102	BCL	C2-C3-C5-C6
8	F	101	BCL	C11-C12-C13-C15
8	d	102	BCL	C11-C10-C8-C7
8	b	101	BCL	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
8	M	402	BCL	C11-C10-C8-C7
13	L	302	BPH	C11-C12-C13-C15
8	P	101	BCL	C6-C7-C8-C9
8	q	101	BCL	C11-C10-C8-C9
8	I	102	BCL	C11-C10-C8-C9
8	F	101	BCL	C11-C12-C13-C14
8	D	101	BCL	C11-C12-C13-C14
8	a	102	BCL	C6-C7-C8-C9
8	M	402	BCL	C11-C10-C8-C9
8	M	404	BCL	C6-C7-C8-C9
8	L	304	BCL	C11-C10-C8-C9
13	M	403	BPH	C11-C10-C8-C9
13	M	403	BPH	C14-C13-C15-C16
11	H	301	MW9	C9-C10-C11-C12
8	Q	102	BCL	C15-C16-C17-C18
8	1	102	BCL	C5-C6-C7-C8
8	V	101	BCL	CBA-CGA-O2A-C1
11	L	305	MW9	C30-C31-C32-C33
8	e	101	BCL	C16-C17-C18-C20
8	I	103	BCL	C8-C10-C11-C12
15	M	408	CDL	OA5-CA3-CA4-CA6
9	T	101	A1EFU	C26-C27-C28-C29
9	K	103	A1EFU	C26-C27-C28-C29
9	J	103	A1EFU	C22-C23-C24-C25
9	i	101	A1EFU	C26-C27-C28-C29
14	M	405	U10	C14-C16-C17-C18
11	G	105	MW9	C12-C13-C14-C15
15	H	303	CDL	C39-C40-C41-C42
8	V	101	BCL	C2-C3-C5-C6
8	M	402	BCL	C2-C3-C5-C6
9	G	103	A1EFU	C21-C22-C23-C24
9	F	102	A1EFU	C21-C22-C23-C24
9	E	102	A1EFU	C21-C22-C23-C24
9	I	101	A1EFU	C2-C3-C4-C5
8	D	101	BCL	C13-C15-C16-C17
8	M	404	BCL	C15-C16-C17-C18
8	N	101	BCL	C2A-CAA-CBA-CGA
8	q	101	BCL	CBA-CGA-O2A-C1
8	1	102	BCL	CBA-CGA-O2A-C1
11	G	106	MW9	C16-C17-O1-C18
11	L	305	MW9	C24-C25-C26-C27
11	F	104	MW9	C27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
11	D	102	MW9	C6-C7-C8-C9
11	N	103	MW9	C19-C20-O2-P
15	M	408	CDL	CA4-CA3-OA5-PA1
8	P	102	BCL	C3A-C2A-CAA-CBA
8	V	101	BCL	C3A-C2A-CAA-CBA
8	T	102	BCL	C3A-C2A-CAA-CBA
8	R	101	BCL	C3A-C2A-CAA-CBA
11	G	106	MW9	C29-C30-C31-C32
8	L	304	BCL	C5-C6-C7-C8
8	b	101	BCL	CBA-CGA-O2A-C1
15	H	303	CDL	C62-C63-C64-C65
15	H	303	CDL	C79-C80-C81-C82
15	M	408	CDL	CB3-CB4-CB6-OB8
11	L	305	MW9	C12-C13-C14-C15
10	S	301	LMT	C5'-C4'-O1B-C1B
8	j	101	BCL	C8-C10-C11-C12
8	q	101	BCL	C4-C3-C5-C6
8	V	101	BCL	C16-C17-C18-C20
15	H	303	CDL	C16-C17-C18-C19
11	G	106	MW9	C20-O2-P-O5
11	G	106	MW9	C21-O5-P-O2
8	1	101	BCL	CAA-CBA-CGA-O2A
8	I	103	BCL	C15-C16-C17-C18
10	S	301	LMT	C3-C4-C5-C6
11	N	103	MW9	C34-C35-C36-C37
11	G	105	MW9	O8-C19-C20-O2
10	C	404	LMT	C1-C2-C3-C4
11	F	104	MW9	C29-C30-C31-C32
8	j	101	BCL	O1A-CGA-O2A-C1
11	R	103	MW9	O1-C18-C19-O8
11	M	407	MW9	O1-C18-C19-O8
11	G	105	MW9	C32-C33-C34-C35
15	H	303	CDL	C33-C34-C35-C36
8	T	102	BCL	C15-C16-C17-C18
9	R	102	A1EFU	C26-C27-C28-C29
9	b	102	A1EFU	C26-C27-C28-C29
14	M	405	U10	C19-C21-C22-C23
11	G	105	MW9	C35-C36-C37-C38
8	L	301	BCL	C3-C5-C6-C7
8	f	101	BCL	C2-C1-O2A-CGA
8	b	101	BCL	C2-C3-C5-C6
9	T	101	A1EFU	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
11	R	103	MW9	C11-C12-C13-C14
8	K	101	BCL	C11-C10-C8-C9
8	J	101	BCL	C6-C7-C8-C9
8	I	103	BCL	C11-C12-C13-C14
8	G	101	BCL	C11-C10-C8-C9
8	d	102	BCL	C6-C7-C8-C9
8	D	101	BCL	C14-C13-C15-C16
11	F	104	MW9	C22-C21-O5-P
15	M	408	CDL	C56-C57-C58-C59
8	I	102	BCL	C16-C17-C18-C19
8	v	102	BCL	C3-C5-C6-C7
10	S	301	LMT	O1'-C1-C2-C3
8	r	101	BCL	C4C-C3C-CAC-CBC
8	q	101	BCL	C4C-C3C-CAC-CBC
8	j	101	BCL	C4C-C3C-CAC-CBC
8	a	102	BCL	C4C-C3C-CAC-CBC
8	N	101	BCL	C5-C6-C7-C8
9	D	103	A1EFU	C14-C15-C16-C17
8	t	101	BCL	C16-C17-C18-C20
8	n	101	BCL	C11-C12-C13-C15
8	I	102	BCL	C6-C7-C8-C10
8	I	102	BCL	C11-C10-C8-C7
8	I	103	BCL	C11-C12-C13-C15
8	G	101	BCL	C11-C10-C8-C7
8	D	101	BCL	C11-C12-C13-C15
8	b	101	BCL	C12-C13-C15-C16
8	a	102	BCL	C6-C7-C8-C10
8	L	304	BCL	C6-C7-C8-C10
8	L	304	BCL	C11-C10-C8-C7
9	J	102	A1EFU	C21-C22-C23-C24
13	M	403	BPH	C11-C10-C8-C7
13	L	302	BPH	C2-C3-C5-C6
8	t	101	BCL	C1-C2-C3-C4
9	n	102	A1EFU	O2-C2-C3-C4
8	P	101	BCL	C5-C6-C7-C8
8	T	102	BCL	CBA-CGA-O2A-C1
11	H	302	MW9	C9-C10-C11-C12
8	M	402	BCL	C5-C6-C7-C8
8	A	101	BCL	C2A-CAA-CBA-CGA
10	C	404	LMT	O1'-C1-C2-C3
8	K	102	BCL	CAD-CBD-CGD-O2D
8	L	304	BCL	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
11	N	103	MW9	C18-C19-O8-C24
13	M	403	BPH	CAD-CBD-CGD-O2D
15	H	303	CDL	CA6-CA4-OA6-CA5
10	B	101	LMT	C1-C2-C3-C4
11	N	103	MW9	C11-C12-C13-C14
11	G	105	MW9	C6-C7-C8-C9
8	A	101	BCL	C4-C3-C5-C6
9	K	103	A1EFU	C21-C22-C23-C24
9	S	303	A1EFU	C22-C23-C24-C25
11	G	105	MW9	O1-C18-C19-C20
11	H	302	MW9	C19-C20-O2-P
11	N	103	MW9	O8-C19-C20-O2
8	E	101	BCL	C10-C11-C12-C13
11	H	302	MW9	C11-C12-C13-C14
8	P	102	BCL	CHA-CBD-CGD-O1D
8	P	102	BCL	CHA-CBD-CGD-O2D
8	G	101	BCL	CHA-CBD-CGD-O1D
8	G	101	BCL	CHA-CBD-CGD-O2D
8	d	102	BCL	CHA-CBD-CGD-O1D
8	d	102	BCL	CHA-CBD-CGD-O2D
8	b	101	BCL	CHA-CBD-CGD-O1D
8	b	101	BCL	CHA-CBD-CGD-O2D
8	K	102	BCL	C5-C6-C7-C8
8	P	101	BCL	O1A-CGA-O2A-C1
11	G	106	MW9	O-C17-O1-C18
9	G	104	A1EFU	CM2-C1-O1-CMA
11	H	301	MW9	O1-C18-C19-O8
8	s	101	BCL	O1A-CGA-O2A-C1
8	R	101	BCL	O1A-CGA-O2A-C1
8	N	101	BCL	O1A-CGA-O2A-C1
11	H	302	MW9	C19-C18-O1-C17
8	J	101	BCL	C4-C3-C5-C6
8	G	102	BCL	C4-C3-C5-C6
8	d	102	BCL	C2-C3-C5-C6
8	v	102	BCL	C15-C16-C17-C18
8	b	101	BCL	C11-C12-C13-C14
11	F	104	MW9	C26-C27-C28-C29
9	r	102	A1EFU	O1-C1-C2-O2
10	E	103	LMT	C5'-C4'-O1B-C1B
8	r	101	BCL	C1A-C2A-CAA-CBA
8	j	101	BCL	C1A-C2A-CAA-CBA
8	I	103	BCL	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
8	G	101	BCL	C1A-C2A-CAA-CBA
8	G	102	BCL	C1A-C2A-CAA-CBA
10	E	103	LMT	C4-C5-C6-C7
9	R	102	A1EFU	C15-C16-C17-C18
11	N	103	MW9	C20-O2-P-O5
11	F	104	MW9	C21-O5-P-O2
11	L	305	MW9	C20-O2-P-O5
11	G	106	MW9	C19-C20-O2-P
15	M	408	CDL	C1-CB2-OB2-PB2
9	A	102	A1EFU	C21-C22-C23-C24
11	G	105	MW9	C21-O5-P-O3
11	G	106	MW9	C20-O2-P-O3
11	D	102	MW9	C20-O2-P-O4
11	M	407	MW9	C20-O2-P-O3
11	L	305	MW9	C21-O5-P-O3
11	H	301	MW9	C21-O5-P-O4
15	H	303	CDL	CA3-OA5-PA1-OA3
8	P	102	BCL	C16-C17-C18-C19
8	1	101	BCL	C16-C17-C18-C19
11	H	301	MW9	C14-C15-C16-C17
10	S	301	LMT	C2-C3-C4-C5
8	f	101	BCL	C13-C15-C16-C17
8	s	101	BCL	CBA-CGA-O2A-C1
11	F	104	MW9	C18-C19-C20-O2
8	r	101	BCL	C3-C5-C6-C7
15	H	303	CDL	C32-C33-C34-C35
8	J	101	BCL	CAD-CBD-CGD-O1D
8	F	101	BCL	CAD-CBD-CGD-O1D
8	F	101	BCL	C5-C6-C7-C8
10	E	103	LMT	C2-C3-C4-C5
8	n	101	BCL	C6-C7-C8-C10
8	K	101	BCL	C11-C10-C8-C7
8	J	101	BCL	C6-C7-C8-C10
8	J	101	BCL	C11-C10-C8-C7
8	d	102	BCL	C6-C7-C8-C10
8	M	402	BCL	C6-C7-C8-C10
9	1	103	A1EFU	C20-C21-C22-C23
9	b	102	A1EFU	C20-C21-C22-C23
11	F	104	MW9	O8-C19-C20-O2
15	M	408	CDL	OA5-CA3-CA4-OA6
9	F	103	A1EFU	C19-C20-C21-C22
8	A	101	BCL	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
8	L	301	BCL	C16-C17-C18-C20
11	H	301	MW9	O1-C18-C19-C20
15	M	408	CDL	OB6-CB4-CB6-OB8
15	H	303	CDL	OA6-CA4-CA6-OA8
10	B	101	LMT	C5-C6-C7-C8
8	L	304	BCL	C8-C10-C11-C12
8	R	101	BCL	C3-C5-C6-C7
11	H	302	MW9	C28-C29-C30-C31
11	N	103	MW9	C22-C21-O5-P
8	M	402	BCL	C4-C3-C5-C6
8	1	101	BCL	CBA-CGA-O2A-C1
15	H	303	CDL	C71-CB7-OB8-CB6
8	v	102	BCL	C11-C12-C13-C14
8	q	101	BCL	C14-C13-C15-C16
8	n	101	BCL	C11-C12-C13-C14
8	e	101	BCL	C1-C2-C3-C5
8	e	101	BCL	C16-C17-C18-C19
15	H	303	CDL	C24-C25-C26-C27
9	S	303	A1EFU	CM1-C1-C2-C3
9	q	102	A1EFU	CM1-C1-C2-C3
15	H	303	CDL	OB9-CB7-OB8-CB6
8	P	101	BCL	C2-C3-C5-C6
8	N	101	BCL	C2-C3-C5-C6
8	s	101	BCL	C2-C1-O2A-CGA
8	N	101	BCL	C2-C1-O2A-CGA
8	J	101	BCL	C2-C1-O2A-CGA
8	I	102	BCL	C2-C1-O2A-CGA
8	e	101	BCL	C2-C1-O2A-CGA
8	d	102	BCL	C2-C1-O2A-CGA
8	B	102	BCL	C2-C1-O2A-CGA
8	M	402	BCL	C2-C1-O2A-CGA
13	M	403	BPH	C2-C1-O2A-CGA
8	d	102	BCL	CBA-CGA-O2A-C1
8	1	101	BCL	C4-C3-C5-C6
9	K	104	A1EFU	CM2-C1-C2-O2
8	V	101	BCL	C16-C17-C18-C19
16	C	403	HEC	C3D-CAD-CBD-CGD
11	H	302	MW9	C26-C27-C28-C29
11	R	103	MW9	C21-O5-P-O2
15	M	408	CDL	CB2-OB2-PB2-OB5
8	I	102	BCL	C4-C3-C5-C6
9	F	103	A1EFU	CM7-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
8	1	101	BCL	C10-C11-C12-C13
8	1	101	BCL	C2-C3-C5-C6
8	b	101	BCL	C11-C12-C13-C15
8	J	101	BCL	C11-C10-C8-C9
8	G	101	BCL	C6-C7-C8-C9
9	P	103	A1EFU	C15-C16-C17-C18
9	r	102	A1EFU	C19-C20-C21-C22
8	q	101	BCL	O1A-CGA-O2A-C1
11	G	106	MW9	C9-C10-C11-C12
11	H	302	MW9	C30-C31-C32-C33
9	q	102	A1EFU	CM7-C22-C23-C24
8	E	101	BCL	C16-C17-C18-C19
8	A	101	BCL	C16-C17-C18-C20
9	d	101	A1EFU	C9-C10-C11-C12
9	A	103	A1EFU	C5-C6-C7-C8
9	N	102	A1EFU	C22-C23-C24-C25
9	G	104	A1EFU	C26-C27-C28-C29
14	M	405	U10	C39-C41-C42-C43
8	T	102	BCL	C5-C6-C7-C8
10	B	101	LMT	C11-C10-C9-C8
11	M	407	MW9	C7-C8-C9-C10
9	1	104	A1EFU	C18-C19-C20-C21
9	D	103	A1EFU	CM8-C26-C27-C28
14	M	405	U10	C35-C34-C36-C37
9	D	103	A1EFU	C25-C26-C27-C28
9	P	103	A1EFU	CM2-C1-C2-C3
9	R	102	A1EFU	CM1-C1-C2-C3
9	F	102	A1EFU	CM1-C1-C2-C3
9	a	103	A1EFU	CM1-C1-C2-C3
11	F	104	MW9	C30-C31-C32-C33
8	P	101	BCL	C2-C1-O2A-CGA
8	E	101	BCL	C2-C1-O2A-CGA
8	I	103	BCL	C2A-CAA-CBA-CGA
8	L	301	BCL	C5-C6-C7-C8
15	H	303	CDL	CA4-CA3-OA5-PA1
14	M	405	U10	C5-C4-O4-C4M
8	G	102	BCL	CBA-CGA-O2A-C1
11	N	103	MW9	C28-C29-C30-C31
9	S	303	A1EFU	CM1-C1-C2-O2
9	F	102	A1EFU	CM1-C1-C2-O2
9	E	102	A1EFU	CM1-C1-C2-O2
8	v	102	BCL	C1-C2-C3-C5

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Mol	Chain	Res	Type	Atoms
8	s	101	BCL	C6-C7-C8-C9
8	f	101	BCL	C6-C7-C8-C9
8	d	102	BCL	C11-C12-C13-C14
8	v	102	BCL	C16-C17-C18-C20
8	D	101	BCL	C10-C11-C12-C13
10	E	103	LMT	O5B-C5B-C6B-O6B
8	P	101	BCL	C2A-CAA-CBA-CGA
13	L	302	BPH	O2A-C1-C2-C3
16	C	403	HEC	CAD-CBD-CGD-O1D
9	S	304	A1EFU	C22-C23-C24-C25
11	G	105	MW9	C34-C35-C36-C37
11	G	105	MW9	C37-C38-C39-C40
11	R	103	MW9	C20-C19-O8-C24
11	G	105	MW9	C18-C19-O8-C24
11	G	105	MW9	C20-C19-O8-C24
8	P	102	BCL	C1A-C2A-CAA-CBA
8	V	101	BCL	C1A-C2A-CAA-CBA
8	K	101	BCL	C1A-C2A-CAA-CBA
8	I	102	BCL	C1A-C2A-CAA-CBA
8	f	101	BCL	C1A-C2A-CAA-CBA
8	P	102	BCL	C12-C13-C15-C16
8	q	101	BCL	C6-C7-C8-C10
15	M	408	CDL	C53-C54-C55-C56
11	F	104	MW9	C32-C33-C34-C35
16	C	402	HEC	CAA-CBA-CGA-O2A
9	n	102	A1EFU	C9-C10-C11-C12
8	E	101	BCL	C2A-CAA-CBA-CGA
11	L	305	MW9	C32-C33-C34-C35
11	N	103	MW9	C3-C4-C5-C6
8	I	103	BCL	C4-C3-C5-C6
14	L	303	U10	C15-C14-C16-C17
14	M	405	U10	C33-C34-C36-C37
15	H	303	CDL	C43-C44-C45-C46
8	j	101	BCL	CBA-CGA-O2A-C1
11	L	305	MW9	O9-C24-O8-C19
9	r	102	A1EFU	CM2-C1-O1-CMA
10	L	306	LMT	C5-C6-C7-C8
9	A	102	A1EFU	C14-C15-C16-C17
9	G	104	A1EFU	C9-C10-C11-C12
11	F	104	MW9	C31-C32-C33-C34
8	M	402	BCL	C15-C16-C17-C18
8	G	101	BCL	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
8	G	101	BCL	C2-C1-O2A-CGA
8	K	102	BCL	C2-C3-C5-C6
8	J	101	BCL	C2-C3-C5-C6
8	G	102	BCL	C2-C3-C5-C6
8	L	301	BCL	C6-C7-C8-C9
9	1	104	A1EFU	CM1-C1-C2-C3
9	K	104	A1EFU	CM2-C1-C2-C3
9	E	102	A1EFU	CM1-C1-C2-C3
9	M	406	A1EFU	CM2-C1-C2-C3
11	G	105	MW9	C7-C8-C9-C10
8	b	101	BCL	C16-C17-C18-C20
11	G	106	MW9	C30-C31-C32-C33
9	P	103	A1EFU	CM1-C1-C2-O2
9	q	102	A1EFU	CM1-C1-C2-O2
9	1	104	A1EFU	CM1-C1-C2-O2
8	q	101	BCL	C5-C6-C7-C8
8	N	101	BCL	C4-C3-C5-C6
8	K	102	BCL	C4-C3-C5-C6
8	t	101	BCL	C4C-C3C-CAC-CBC
8	n	101	BCL	C4C-C3C-CAC-CBC
8	d	102	BCL	C16-C17-C18-C20
8	V	101	BCL	C5-C6-C7-C8
8	G	101	BCL	C15-C16-C17-C18
8	D	101	BCL	C16-C17-C18-C20
10	L	306	LMT	C6-C7-C8-C9
11	M	407	MW9	C34-C35-C36-C37
11	R	103	MW9	C32-C33-C34-C35
11	H	301	MW9	C32-C33-C34-C35
16	C	401	HEC	CAA-CBA-CGA-O2A
16	C	403	HEC	CAD-CBD-CGD-O2D
8	B	102	BCL	C10-C11-C12-C13
8	Q	102	BCL	C4-C3-C5-C6
9	a	101	A1EFU	CM7-C22-C23-C24
8	I	103	BCL	C2-C3-C5-C6
16	C	402	HEC	CAA-CBA-CGA-O1A
8	P	102	BCL	C1-C2-C3-C4
8	I	102	BCL	C1-C2-C3-C4
8	D	101	BCL	C1-C2-C3-C4
8	A	101	BCL	C1-C2-C3-C4
8	M	404	BCL	C1-C2-C3-C4
9	E	102	A1EFU	C15-C16-C17-C18
8	d	102	BCL	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
8	t	101	BCL	C16-C17-C18-C19
8	P	101	BCL	C4-C3-C5-C6
8	f	101	BCL	C4-C3-C5-C6
8	L	301	BCL	C4-C3-C5-C6
14	M	405	U10	C45-C44-C46-C47
14	L	303	U10	C35-C34-C36-C37
8	t	101	BCL	C2-C3-C5-C6
8	T	102	BCL	C2-C3-C5-C6
9	S	304	A1EFU	C21-C22-C23-C24
9	A	103	A1EFU	C21-C22-C23-C24
14	L	303	U10	C13-C14-C16-C17
8	P	102	BCL	C14-C13-C15-C16
8	S	302	BCL	C11-C12-C13-C14
8	r	101	BCL	C6-C7-C8-C9
8	q	101	BCL	C6-C7-C8-C9
8	1	102	BCL	C11-C10-C8-C9
8	n	101	BCL	C14-C13-C15-C16
8	K	101	BCL	C3A-C2A-CAA-CBA
8	I	102	BCL	C3A-C2A-CAA-CBA
8	I	103	BCL	C3A-C2A-CAA-CBA
8	G	102	BCL	C3A-C2A-CAA-CBA
8	f	101	BCL	C3A-C2A-CAA-CBA
11	N	103	MW9	C30-C31-C32-C33
11	N	103	MW9	C32-C33-C34-C35
8	f	101	BCL	CAD-CBD-CGD-O2D
8	D	101	BCL	CAD-CBD-CGD-O2D
8	b	101	BCL	CAD-CBD-CGD-O2D
11	R	103	MW9	C18-C19-O8-C24
8	G	102	BCL	C16-C17-C18-C19
11	M	407	MW9	C26-C27-C28-C29
11	L	305	MW9	C27-C28-C29-C30
9	i	101	A1EFU	C13-C14-C15-C16
8	b	101	BCL	C2-C1-O2A-CGA
8	L	301	BCL	C2-C1-O2A-CGA
11	R	103	MW9	C24-C25-C26-C27
8	I	102	BCL	CAA-CBA-CGA-O2A
8	d	102	BCL	CAA-CBA-CGA-O2A
8	T	102	BCL	C4-C3-C5-C6
8	F	101	BCL	C4-C3-C5-C6
8	M	404	BCL	C4-C3-C5-C6
9	A	102	A1EFU	CM8-C26-C27-C28
16	C	401	HEC	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
8	F	101	BCL	C2-C3-C5-C6
8	j	101	BCL	CAA-CBA-CGA-O2A
9	J	103	A1EFU	C26-C27-C28-C29
11	R	103	MW9	C30-C31-C32-C33
11	M	407	MW9	C29-C30-C31-C32
15	H	303	CDL	CA3-CA4-CA6-OA8
8	r	101	BCL	CAA-CBA-CGA-O2A
8	M	402	BCL	CAA-CBA-CGA-O2A
11	F	104	MW9	O8-C24-C25-C26
8	A	101	BCL	O2A-C1-C2-C3
9	P	103	A1EFU	CM2-C1-C2-O2
9	S	303	A1EFU	CM2-C1-C2-O2
9	S	304	A1EFU	CM1-C1-C2-O2
9	S	304	A1EFU	CM2-C1-C2-O2
9	Q	101	A1EFU	CM1-C1-C2-O2
9	R	102	A1EFU	CM1-C1-C2-O2
9	p	101	A1EFU	CM1-C1-C2-O2
9	1	103	A1EFU	CM2-C1-C2-O2
9	1	104	A1EFU	CM2-C1-C2-O2
9	K	104	A1EFU	CM1-C1-C2-O2
9	F	102	A1EFU	CM2-C1-C2-O2
9	E	102	A1EFU	CM2-C1-C2-O2
9	D	104	A1EFU	CM1-C1-C2-O2
9	D	104	A1EFU	CM2-C1-C2-O2
9	b	102	A1EFU	CM1-C1-C2-O2
9	b	102	A1EFU	CM2-C1-C2-O2
9	a	103	A1EFU	CM1-C1-C2-O2
9	a	103	A1EFU	CM2-C1-C2-O2
9	A	102	A1EFU	CM1-C1-C2-O2
9	M	406	A1EFU	CM2-C1-C2-O2
9	P	103	A1EFU	CM1-C1-C2-C3
9	S	304	A1EFU	CM1-C1-C2-C3
9	q	102	A1EFU	CM2-C1-C2-C3
9	1	103	A1EFU	CM1-C1-C2-C3
9	1	103	A1EFU	CM2-C1-C2-C3
9	K	104	A1EFU	CM1-C1-C2-C3
9	E	102	A1EFU	CM2-C1-C2-C3
9	D	104	A1EFU	CM1-C1-C2-C3
9	D	104	A1EFU	CM2-C1-C2-C3
9	A	102	A1EFU	CM1-C1-C2-C3
9	M	406	A1EFU	CM1-C1-C2-C3
8	q	101	BCL	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
8	1	101	BCL	CHA-CBD-CGD-O1D
8	1	101	BCL	CHA-CBD-CGD-O2D
8	j	101	BCL	CHA-CBD-CGD-O1D
8	j	101	BCL	CHA-CBD-CGD-O2D
8	I	102	BCL	CHA-CBD-CGD-O2D
8	B	102	BCL	CHA-CBD-CGD-O2D
8	A	101	BCL	CHA-CBD-CGD-O1D
8	L	304	BCL	CHA-CBD-CGD-O2D
9	N	102	A1EFU	C15-C16-C17-C18
8	M	404	BCL	CAA-CBA-CGA-O2A
11	R	103	MW9	C15-C16-C17-O1
9	I	101	A1EFU	C21-C22-C23-C24
15	H	303	CDL	OB6-CB4-CB6-OB8
16	C	402	HEC	CAD-CBD-CGD-O1D
8	e	101	BCL	O1A-CGA-O2A-C1
8	r	101	BCL	C2A-CAA-CBA-CGA
9	1	104	A1EFU	C2-C1-O1-CMA
9	K	104	A1EFU	C2-C1-O1-CMA
9	a	103	A1EFU	C2-C1-O1-CMA
13	M	403	BPH	CHA-CBD-CGD-O1D
15	H	303	CDL	C41-C42-C43-C44
8	v	102	BCL	CAA-CBA-CGA-O2A
11	G	106	MW9	O8-C24-C25-C26
11	M	407	MW9	O8-C24-C25-C26
11	D	102	MW9	C11-C12-C13-C14
8	1	101	BCL	C6-C7-C8-C10
8	1	102	BCL	C11-C10-C8-C7
9	Q	101	A1EFU	C21-C22-C23-C24
8	F	101	BCL	C16-C17-C18-C19
11	R	103	MW9	C19-C20-O2-P
11	G	105	MW9	C19-C20-O2-P
8	j	101	BCL	C11-C12-C13-C14
9	a	101	A1EFU	C22-C23-C24-C25
9	K	104	A1EFU	C19-C20-C21-C22
9	G	104	A1EFU	C5-C6-C7-C8
8	s	101	BCL	C3-C5-C6-C7
11	L	305	MW9	C25-C24-O8-C19
11	M	407	MW9	C30-C31-C32-C33
9	R	102	A1EFU	C21-C22-C23-C24
9	1	103	A1EFU	C25-C26-C27-C28
11	N	103	MW9	O8-C24-C25-C26
15	H	303	CDL	CA7-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
8	N	101	BCL	CBA-CGA-O2A-C1
8	e	101	BCL	CBA-CGA-O2A-C1
8	F	101	BCL	C1A-C2A-CAA-CBA
8	P	102	BCL	CAA-CBA-CGA-O1A
8	I	102	BCL	CAA-CBA-CGA-O1A
11	R	103	MW9	C15-C16-C17-O
8	K	101	BCL	C2-C1-O2A-CGA
8	r	101	BCL	CAA-CBA-CGA-O1A
8	M	404	BCL	CAA-CBA-CGA-O1A
11	F	104	MW9	O9-C24-C25-C26
11	R	103	MW9	C36-C37-C38-C39
9	n	102	A1EFU	C1-C2-C3-C4
11	R	103	MW9	C21-O5-P-O4
11	F	104	MW9	C21-O5-P-O4
11	L	305	MW9	O8-C24-C25-C26
15	H	303	CDL	OB5-CB3-CB4-CB6
9	d	101	A1EFU	C26-C27-C28-C29
9	r	102	A1EFU	CM1-C1-C2-O2
9	p	101	A1EFU	CM2-C1-C2-O2
8	s	101	BCL	CAA-CBA-CGA-O2A
11	R	103	MW9	O8-C24-C25-C26
16	C	402	HEC	CAD-CBD-CGD-O2D
11	M	407	MW9	O9-C24-C25-C26
8	v	102	BCL	C5-C6-C7-C8
15	M	408	CDL	C72-C73-C74-C75
9	J	103	A1EFU	CM7-C22-C23-C24
8	K	101	BCL	CAD-CBD-CGD-O1D
8	I	103	BCL	CAD-CBD-CGD-O1D
9	S	303	A1EFU	CM2-C1-C2-C3
9	S	304	A1EFU	CM2-C1-C2-C3
9	Q	101	A1EFU	CM1-C1-C2-C3
9	p	101	A1EFU	CM1-C1-C2-C3
9	1	104	A1EFU	CM2-C1-C2-C3
9	F	102	A1EFU	CM2-C1-C2-C3
9	D	103	A1EFU	CM1-C1-C2-C3
9	b	102	A1EFU	CM1-C1-C2-C3
9	a	103	A1EFU	CM2-C1-C2-C3
8	I	103	BCL	O1A-CGA-O2A-C1
8	M	402	BCL	CAA-CBA-CGA-O1A
11	N	103	MW9	O9-C24-C25-C26
8	j	101	BCL	C10-C11-C12-C13
8	L	301	BCL	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
13	M	403	BPH	C11-C12-C13-C14
8	b	101	BCL	C16-C17-C18-C19
10	E	103	LMT	C1-C2-C3-C4
11	N	103	MW9	C25-C26-C27-C28
13	M	403	BPH	CAA-CBA-CGA-O2A
11	N	103	MW9	C35-C36-C37-C38
8	t	101	BCL	C13-C15-C16-C17
8	J	101	BCL	C8-C10-C11-C12
8	S	302	BCL	C11-C12-C13-C15
8	r	101	BCL	C6-C7-C8-C10
8	n	101	BCL	C12-C13-C15-C16
8	M	404	BCL	C2C-C3C-CAC-CBC
8	M	404	BCL	C6-C7-C8-C10
9	M	406	A1EFU	C20-C21-C22-C23
10	H	304	LMT	C5-C6-C7-C8
11	N	103	MW9	C2-C3-C4-C5
10	B	101	LMT	C4-C5-C6-C7
11	F	104	MW9	C9-C10-C11-C12
13	M	403	BPH	CAA-CBA-CGA-O1A
9	G	104	A1EFU	C15-C16-C17-C18
8	1	102	BCL	C16-C17-C18-C19
8	M	404	BCL	C8-C10-C11-C12
8	b	101	BCL	C10-C11-C12-C13
11	G	106	MW9	O9-C24-C25-C26
9	S	303	A1EFU	CM7-C22-C23-C24
9	1	103	A1EFU	CM8-C26-C27-C28
8	P	102	BCL	CAA-CBA-CGA-O2A

There are no ring outliers.

56 monomers are involved in 204 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	j	101	BCL	8	0
8	1	102	BCL	2	0
8	d	102	BCL	9	0
11	R	103	MW9	1	0
8	D	101	BCL	6	0
10	B	101	LMT	1	0
8	J	101	BCL	5	0
14	M	405	U10	12	0
10	E	103	LMT	3	0
8	a	102	BCL	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	t	101	BCL	9	0
8	r	101	BCL	6	0
15	H	303	CDL	13	0
8	V	101	BCL	6	0
8	L	304	BCL	8	0
8	E	101	BCL	6	0
13	M	403	BPH	3	0
8	P	102	BCL	1	0
13	L	302	BPH	1	0
10	L	306	LMT	1	0
8	B	102	BCL	3	0
16	C	403	HEC	1	0
8	P	101	BCL	2	0
8	M	402	BCL	6	0
10	C	404	LMT	2	0
16	C	401	HEC	5	0
8	N	101	BCL	3	0
8	n	101	BCL	6	0
8	G	101	BCL	2	0
9	J	102	A1EFU	1	0
8	s	101	BCL	5	0
16	C	402	HEC	4	0
8	A	101	BCL	5	0
8	q	101	BCL	4	0
8	Q	102	BCL	2	0
8	T	102	BCL	4	0
8	e	101	BCL	10	0
11	H	302	MW9	1	0
8	G	102	BCL	4	0
8	K	102	BCL	3	0
8	I	102	BCL	2	0
8	f	101	BCL	4	0
8	I	103	BCL	3	0
8	K	101	BCL	3	0
8	v	102	BCL	5	0
14	L	303	U10	5	0
8	b	101	BCL	4	0
15	M	408	CDL	5	0
8	R	101	BCL	4	0
8	M	404	BCL	7	0
8	S	302	BCL	3	0
8	L	301	BCL	6	0

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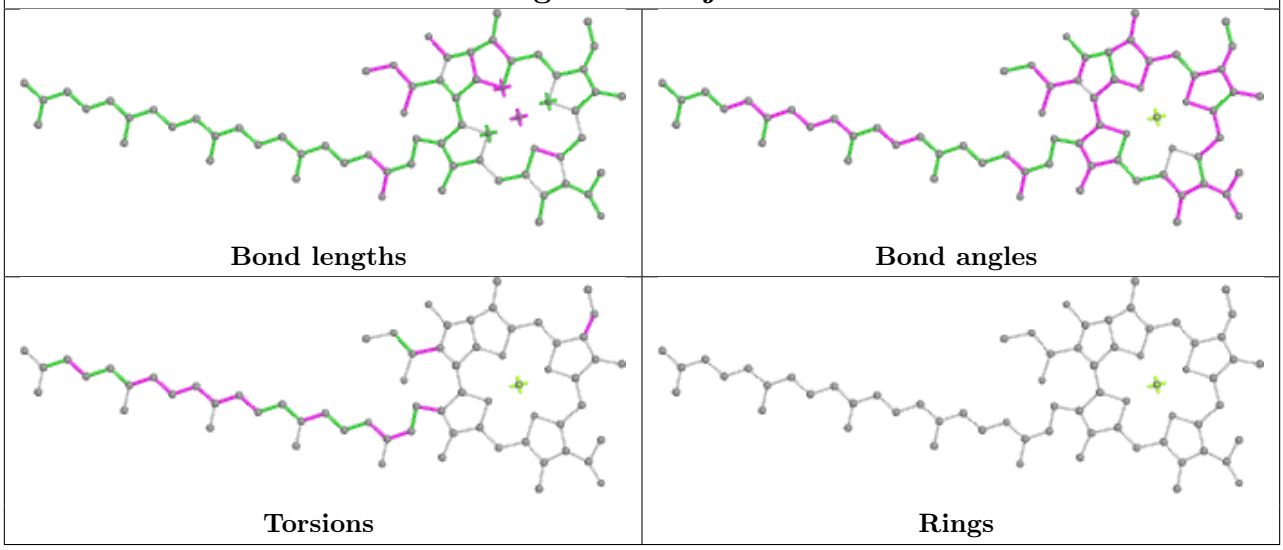
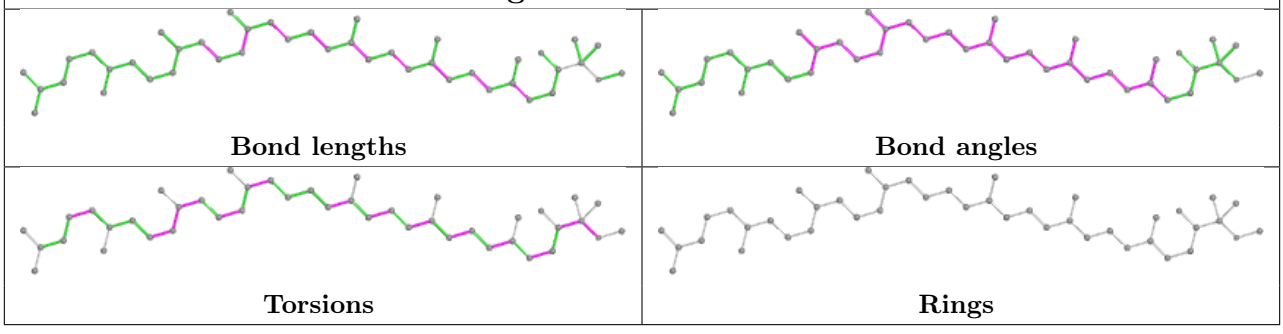
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	F	101	BCL	3	0
10	G	107	LMT	1	0
8	1	101	BCL	2	0
10	S	301	LMT	1	0

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

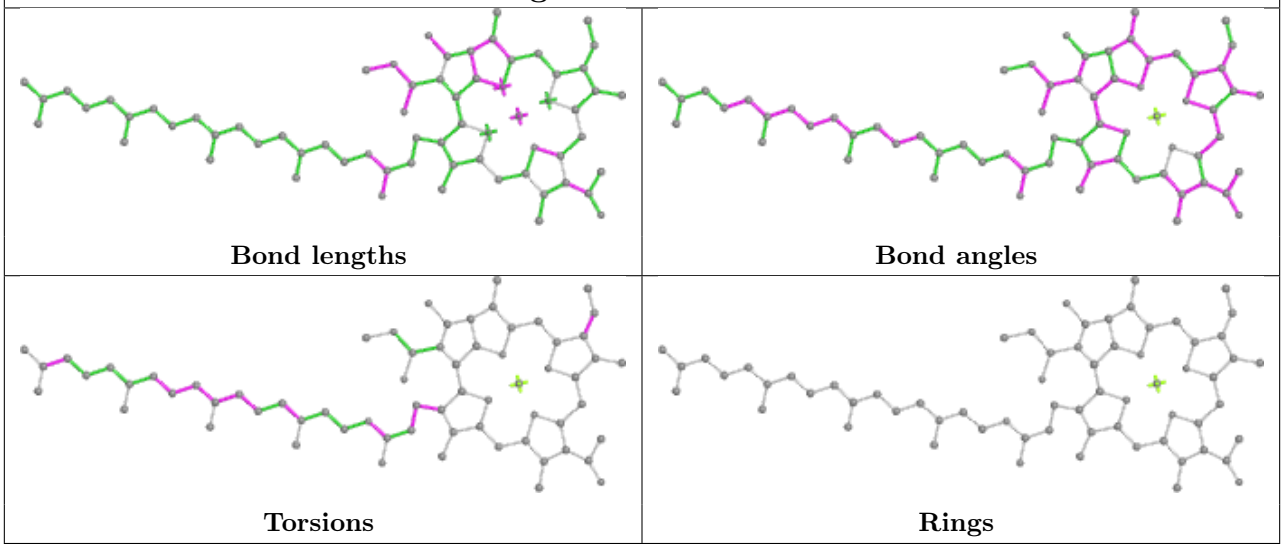
Ligand BCL j 101



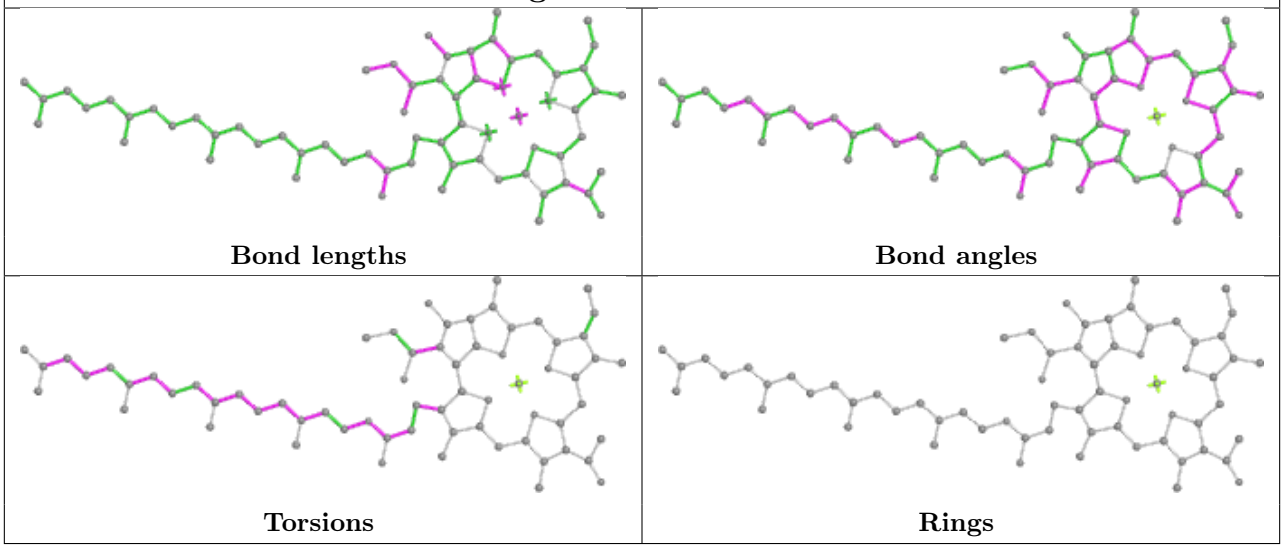
Ligand A1EFU 1 104



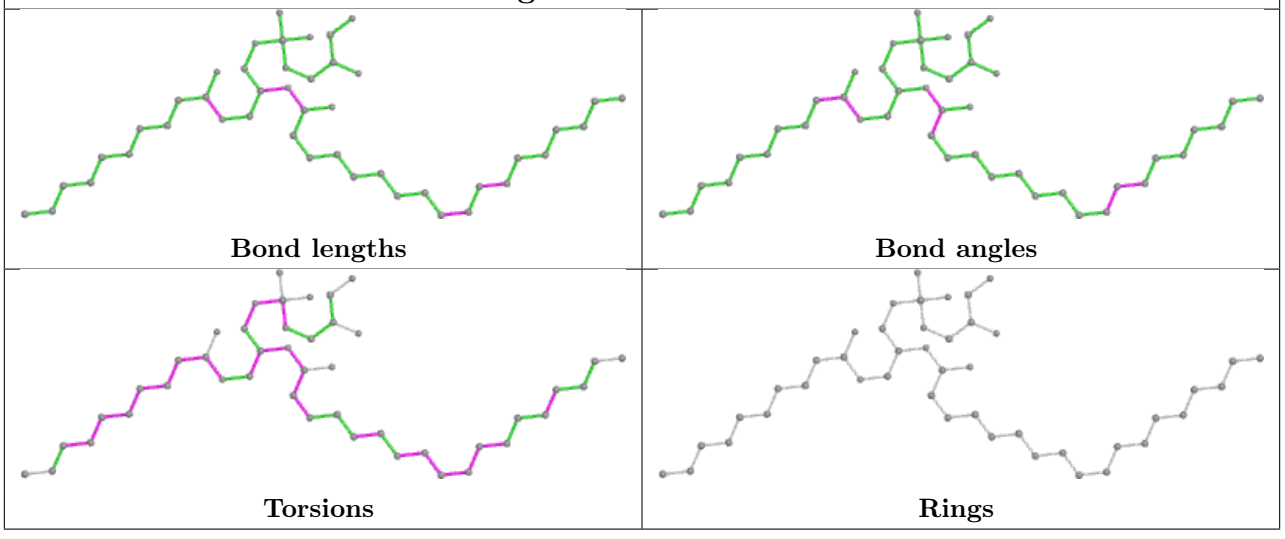
Ligand BCL 1 102



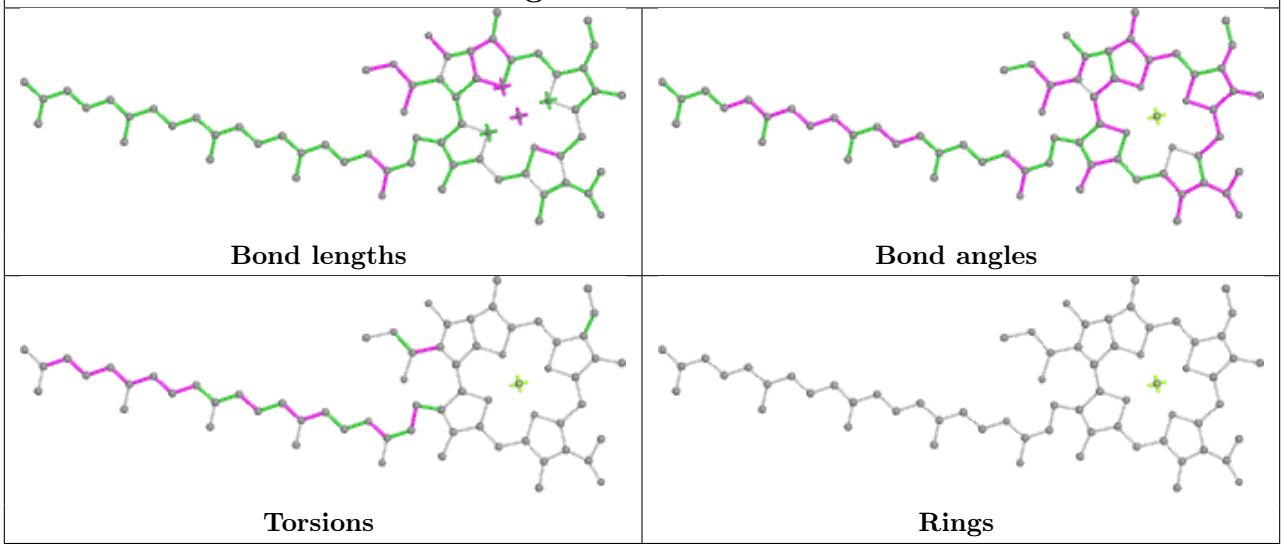
Ligand BCL d 102



Ligand MW9 R 103



Ligand BCL D 101



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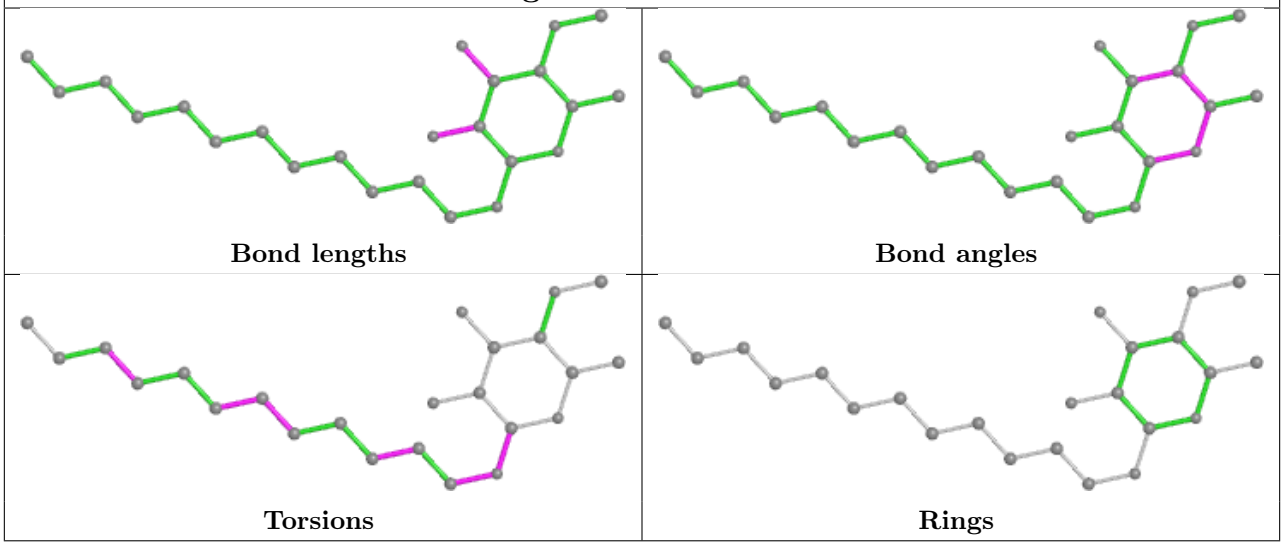
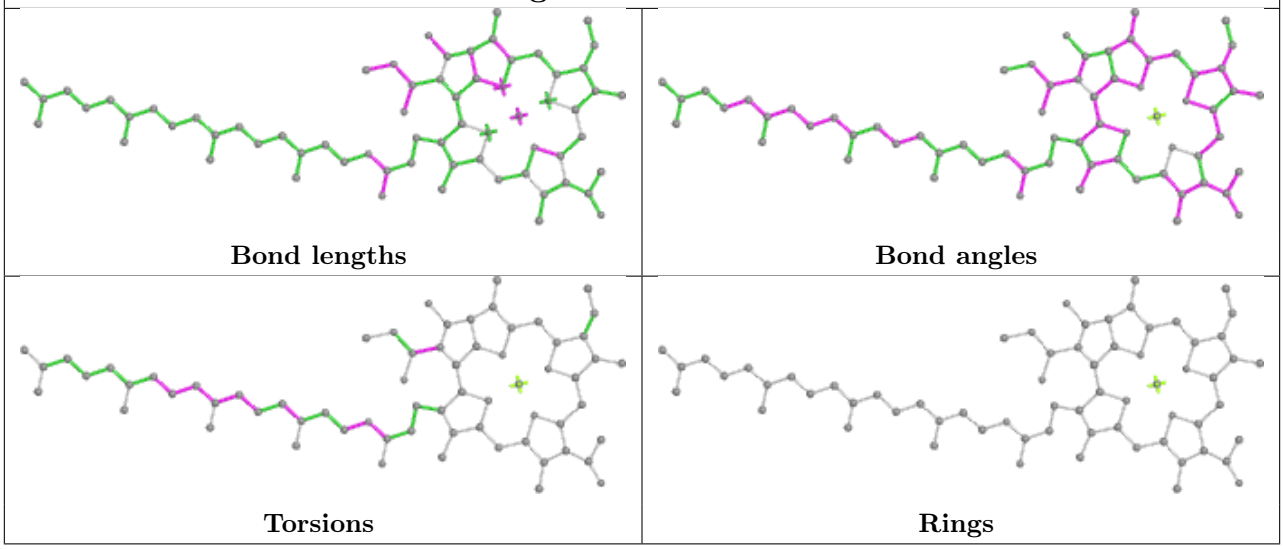
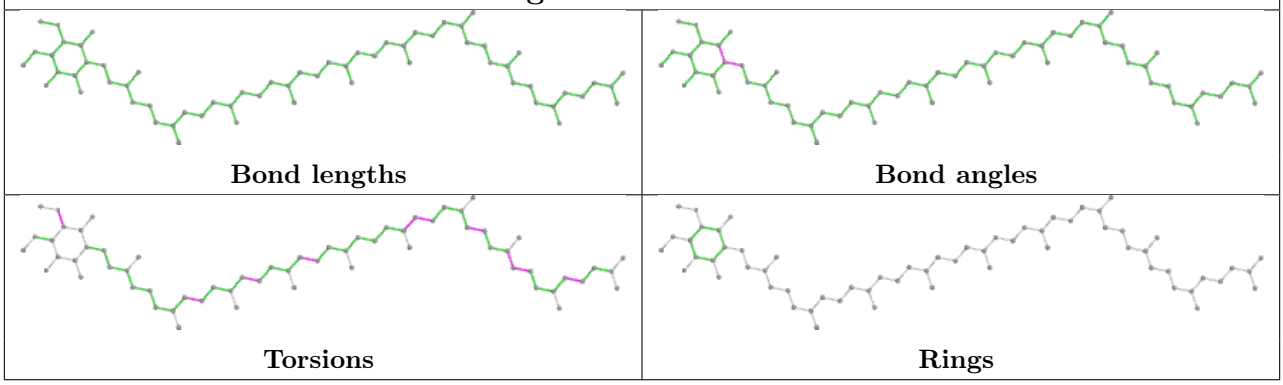


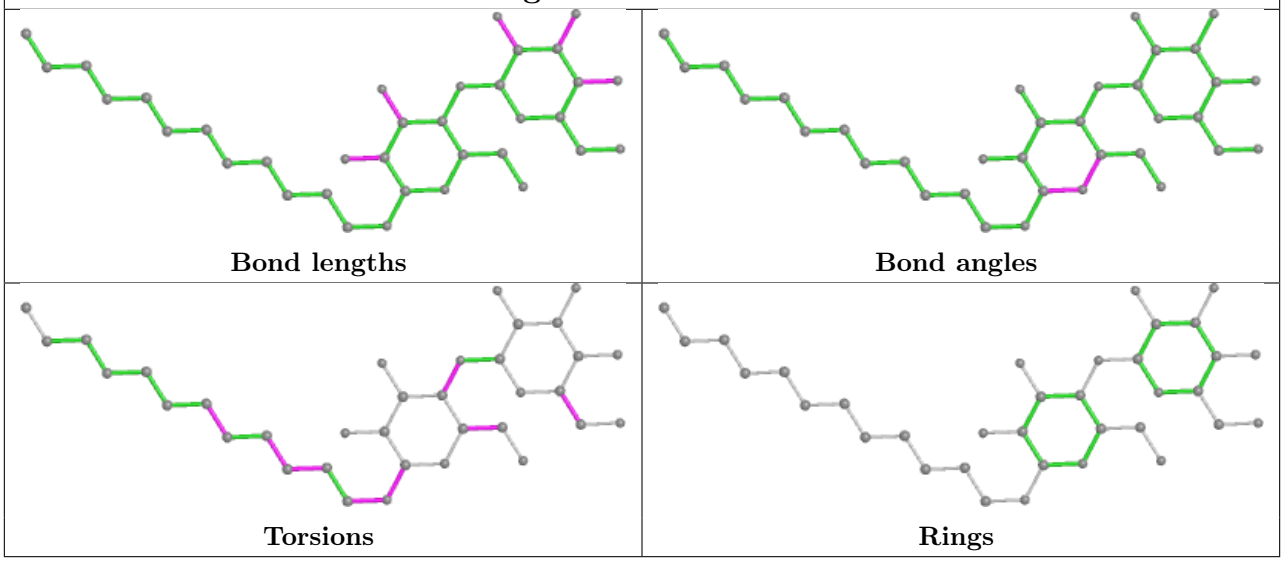
Ligand BCL J 101



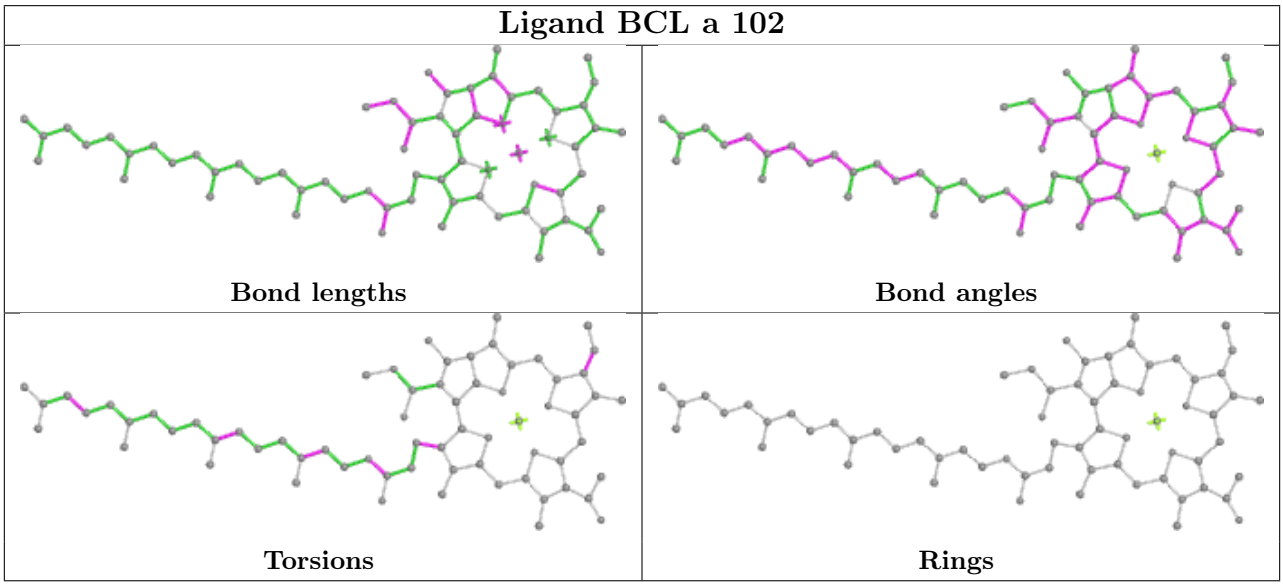
Ligand U10 M 405



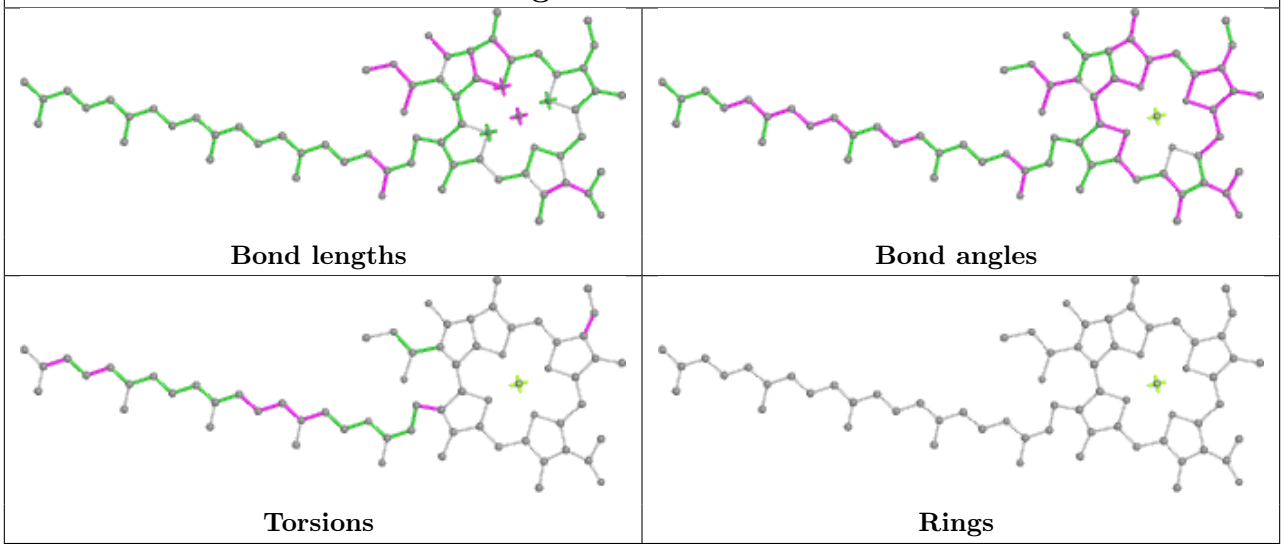
Ligand LMT E 103



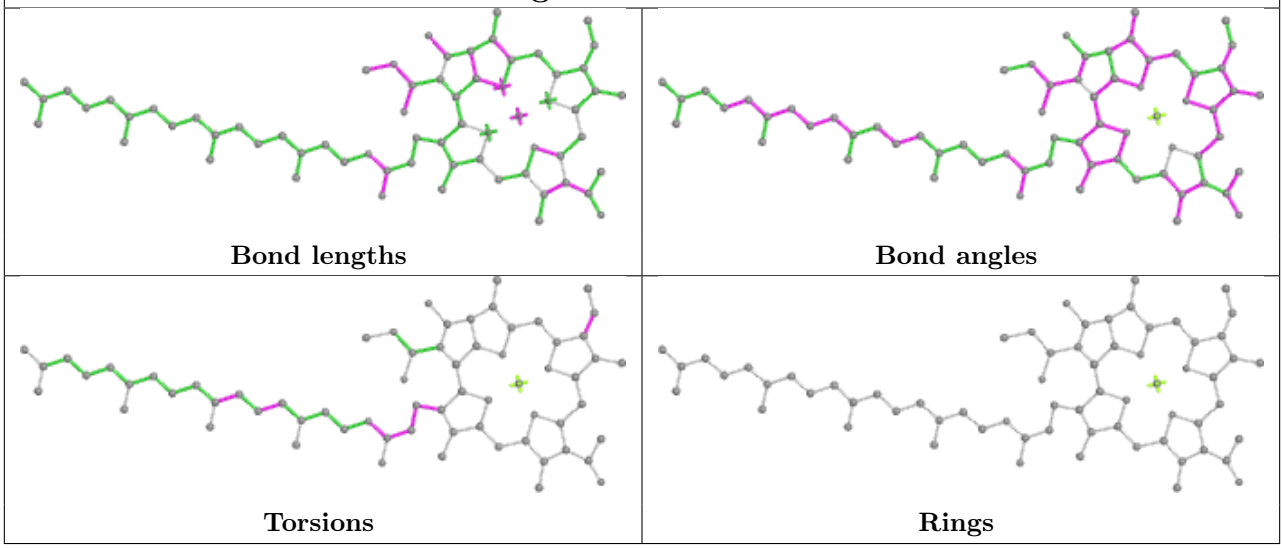
Ligand BCL a 102



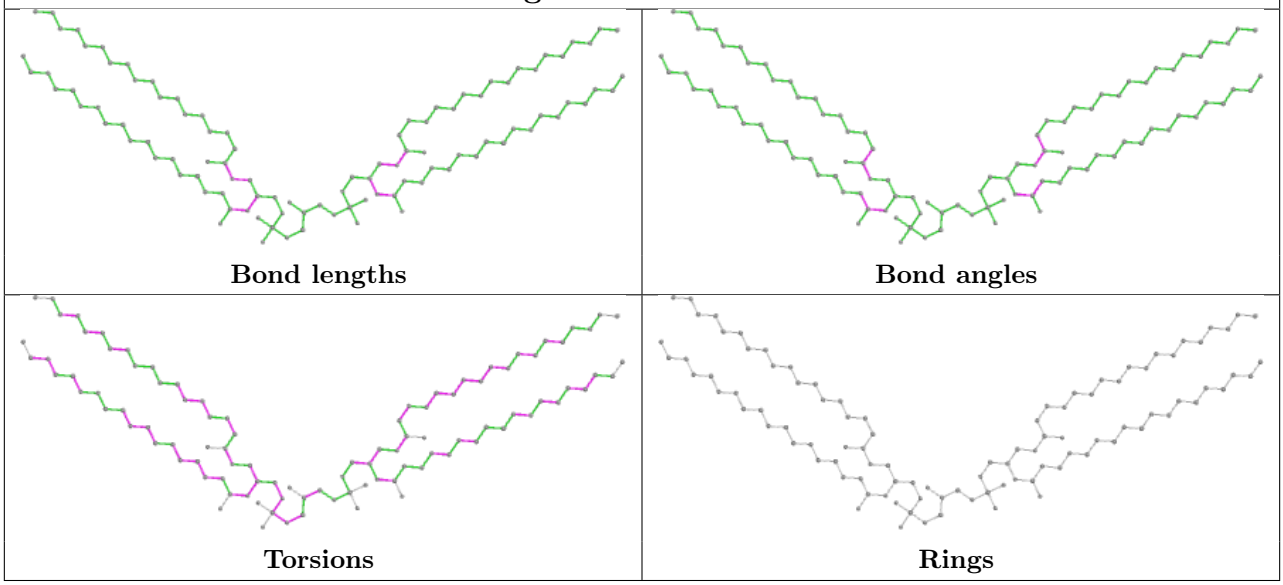
Ligand BCL t 101



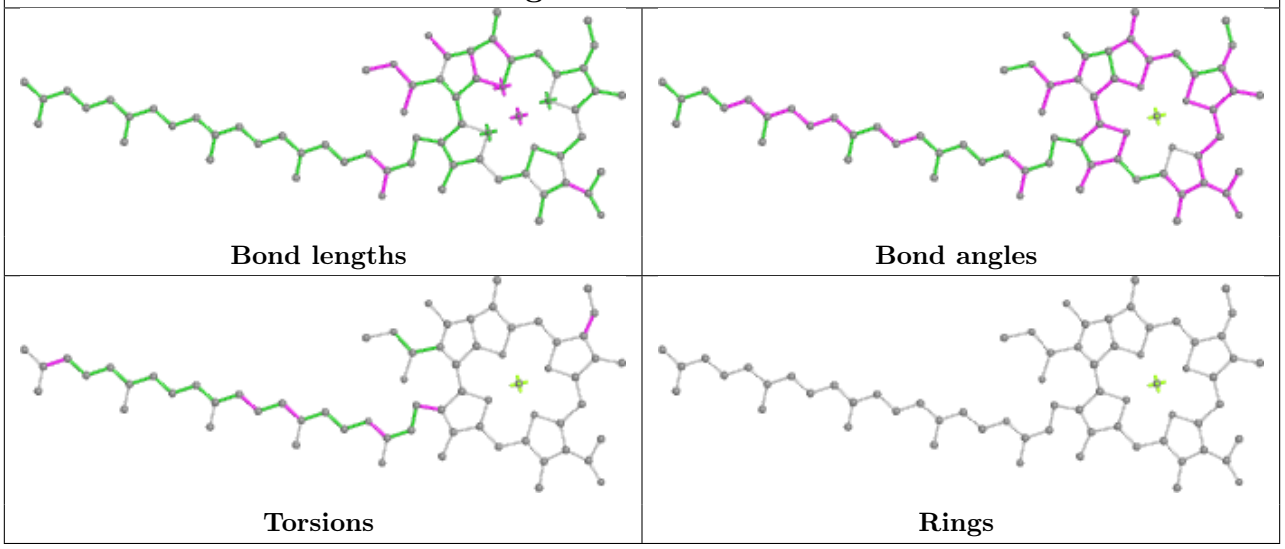
Ligand BCL r 101



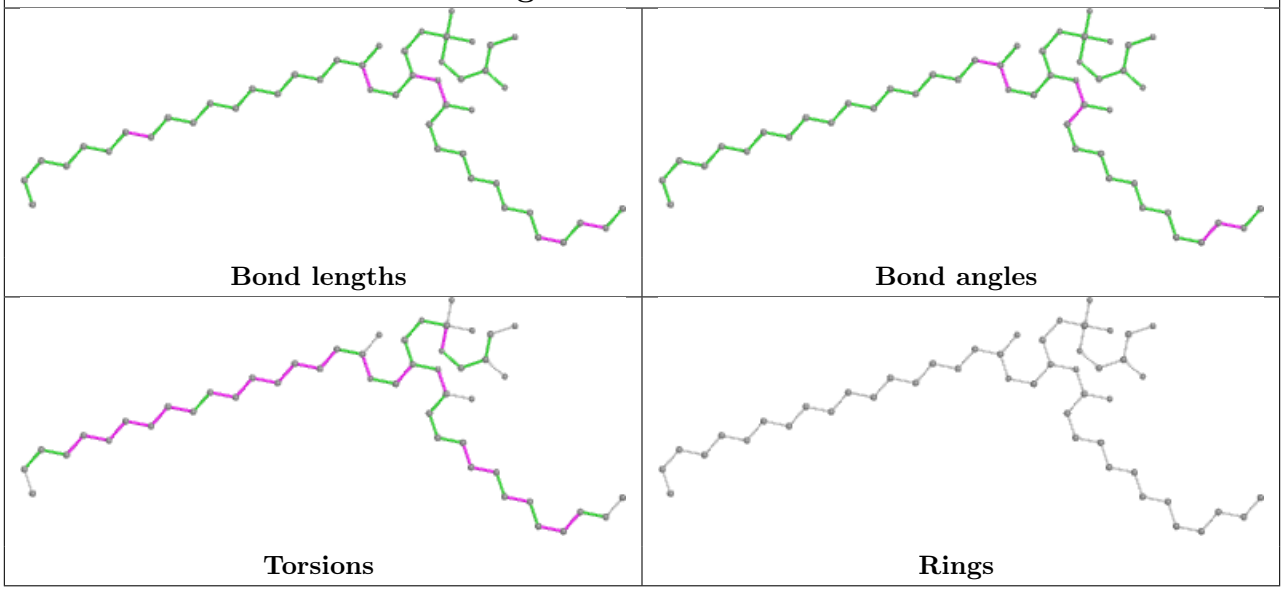
Ligand CDL H 303



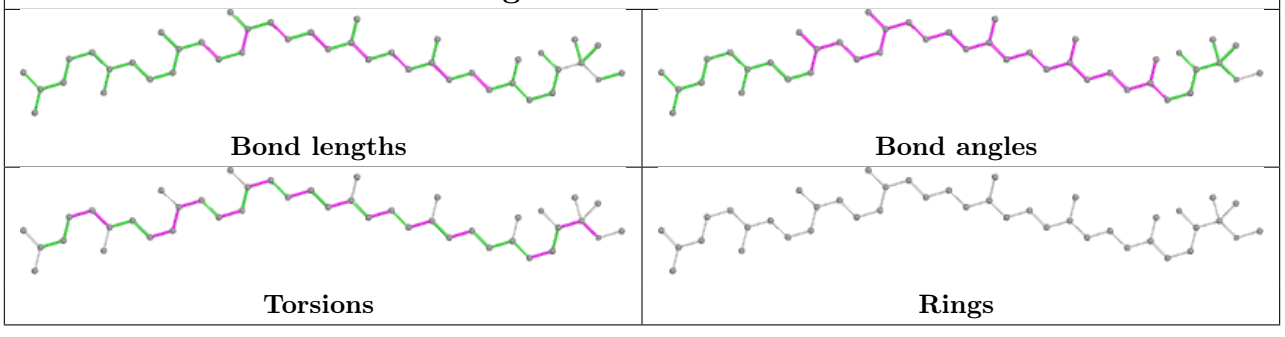
Ligand BCL V 101



Ligand MW9 H 301



Ligand A1EFU A 102



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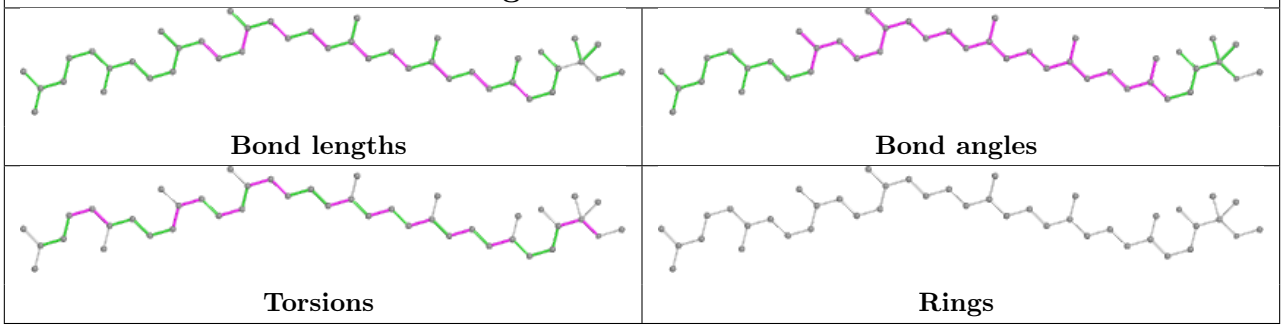

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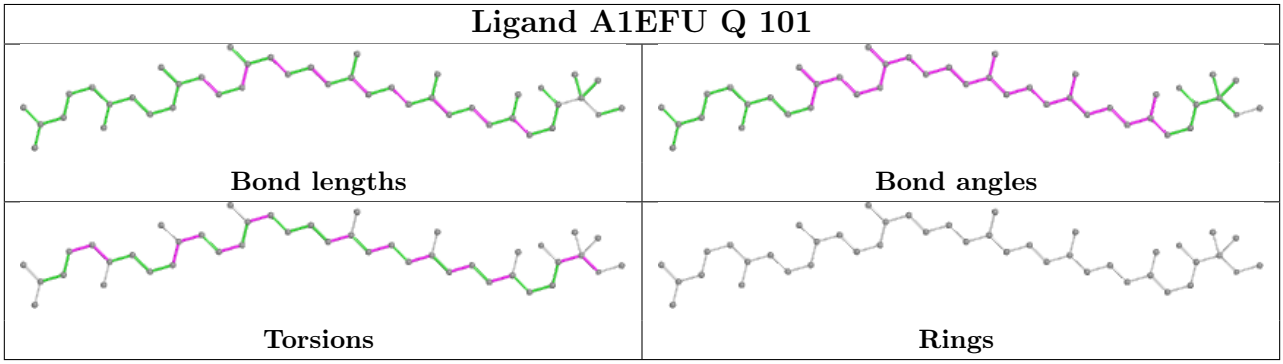
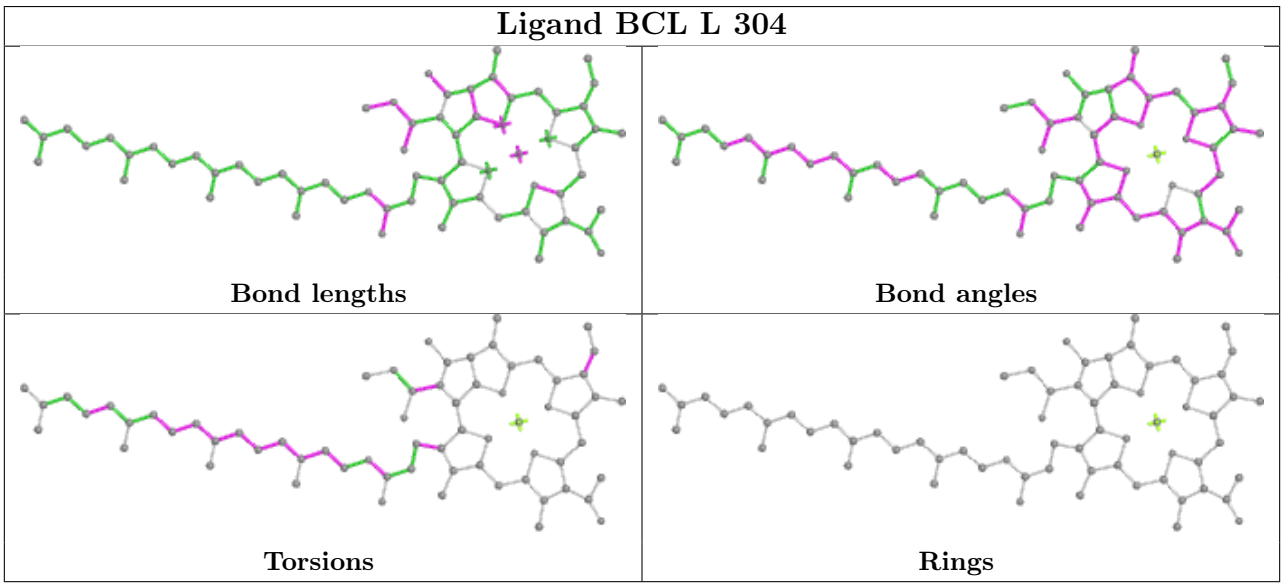


Ligand BCL L 304



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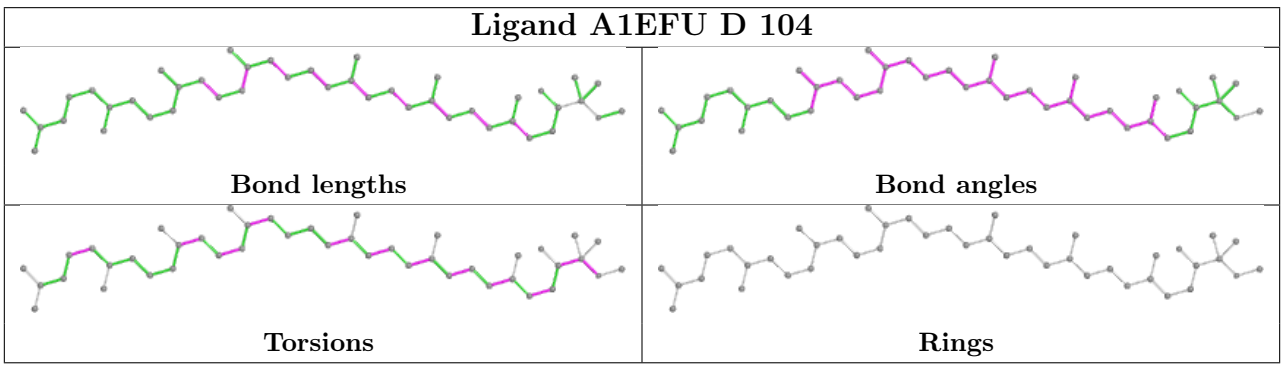

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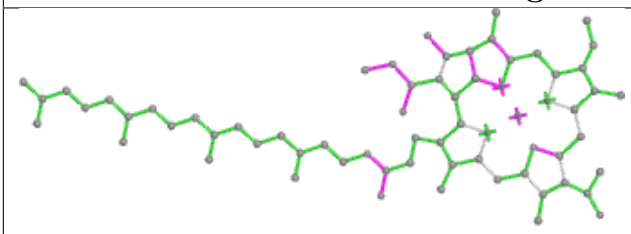
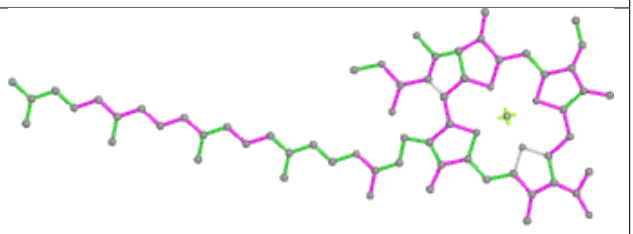
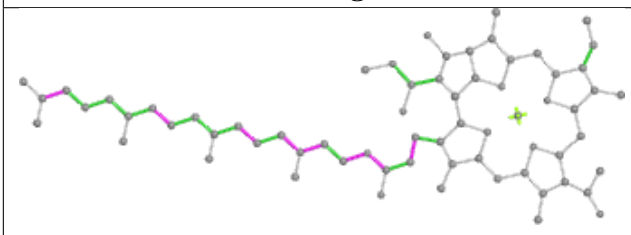


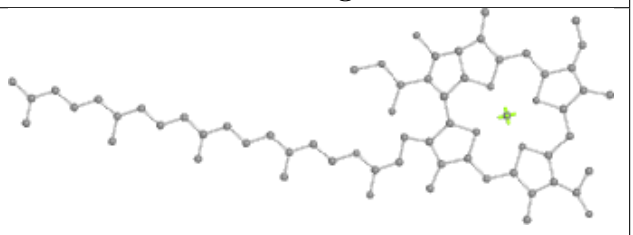
Bond lengths



Bond angles

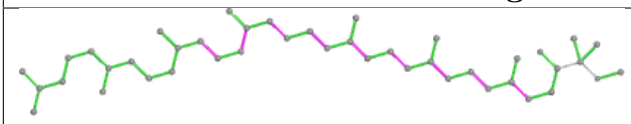


Torsions



Rings

Ligand A1EFU J 103



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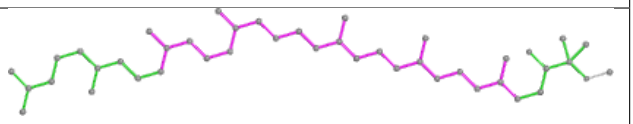
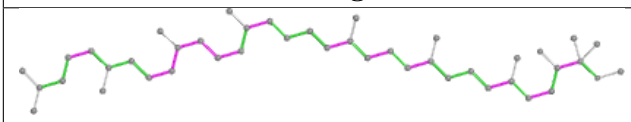


Bond angles



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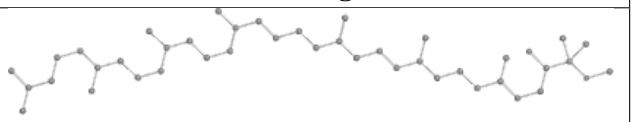
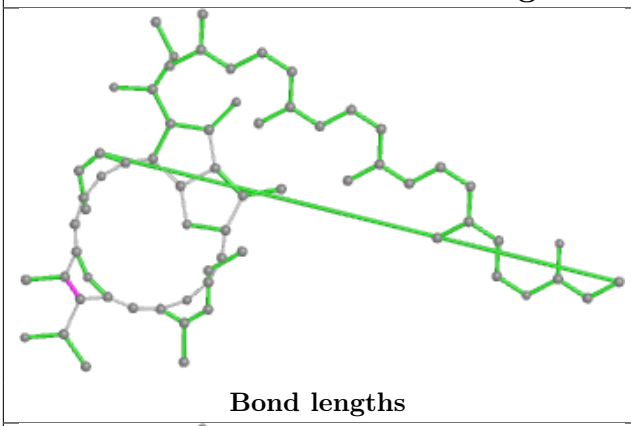


Rings

Ligand BPH M 403



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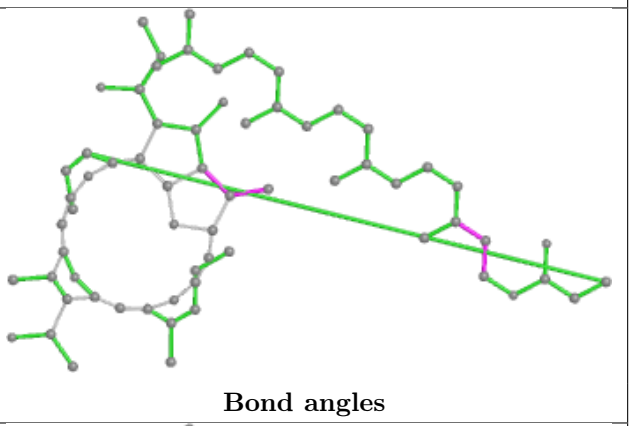
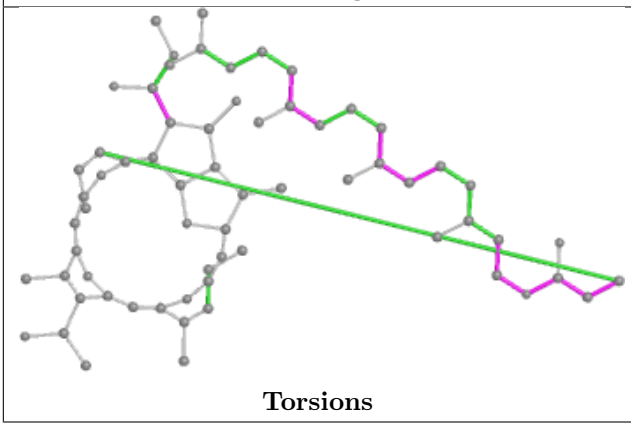


Bond angles



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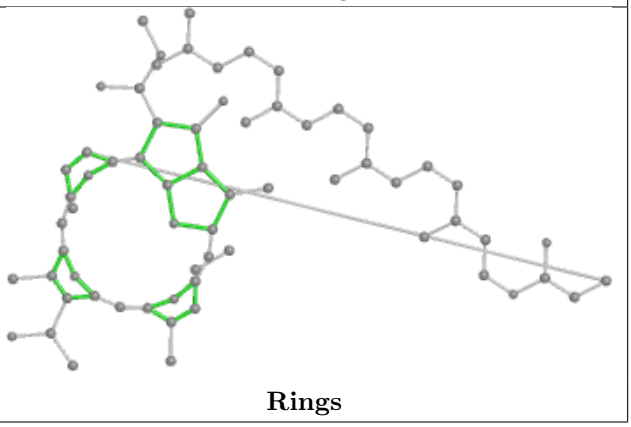
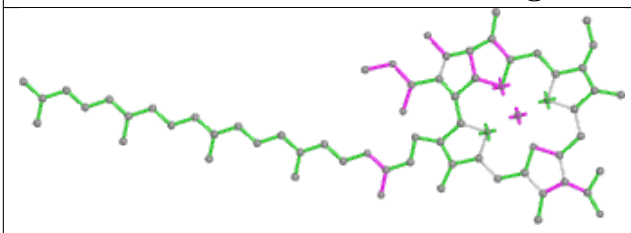
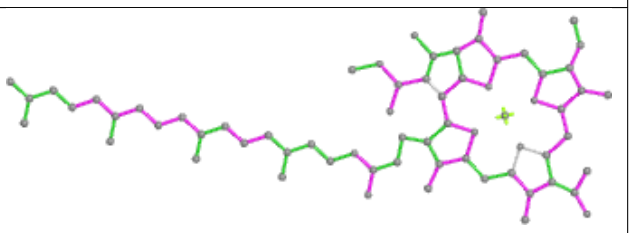


Rings

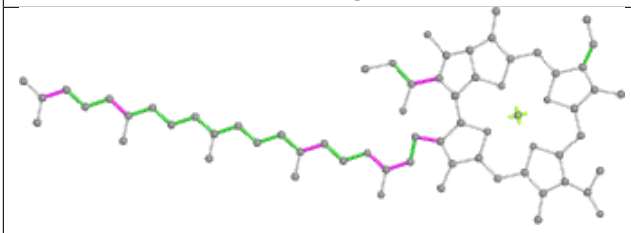
Ligand BCL P 102



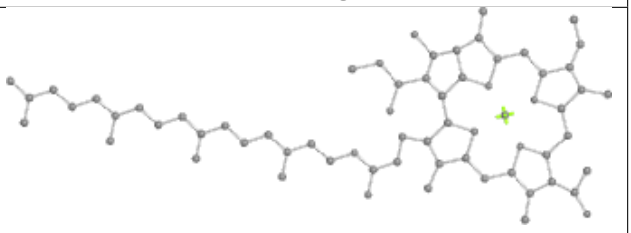
Bond lengths



Bond angles

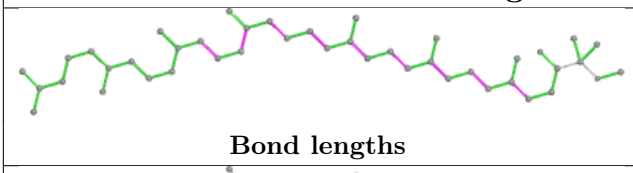


Torsions



Rings

Ligand A1EFU q 102



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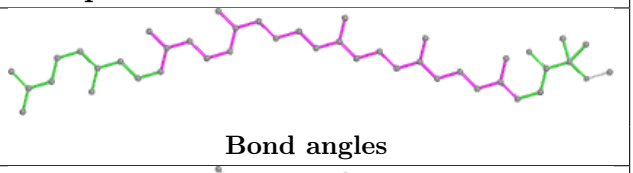
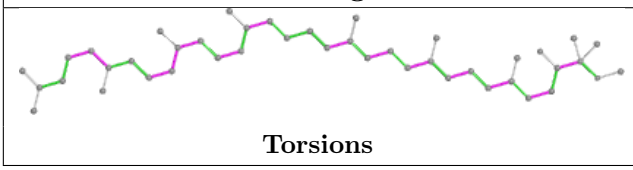
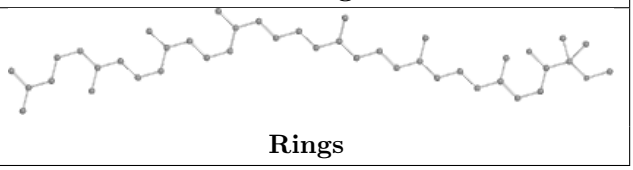


Bond angles

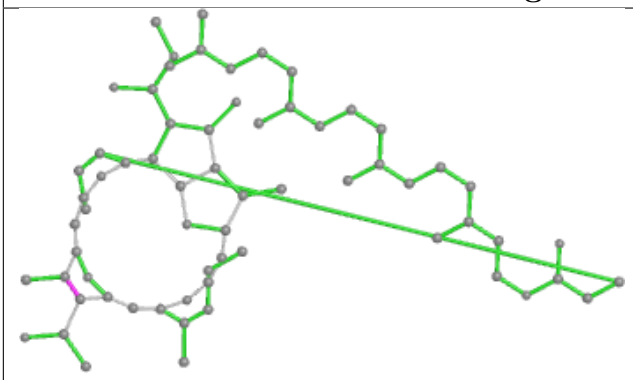


Torsions

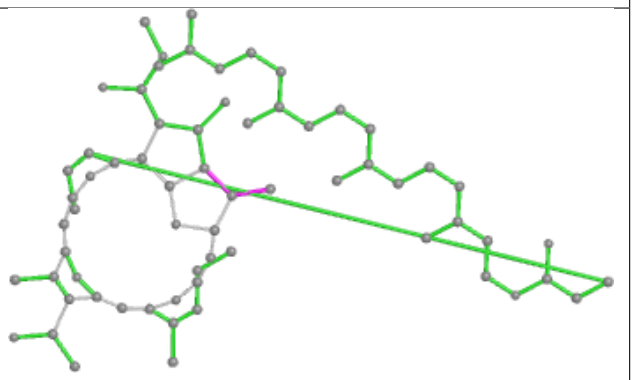


Rings

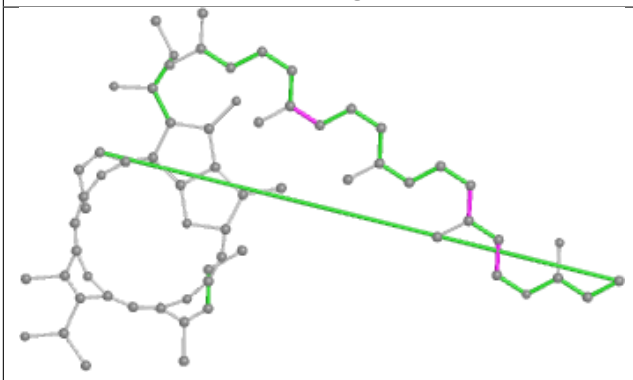
Ligand BPH L 302



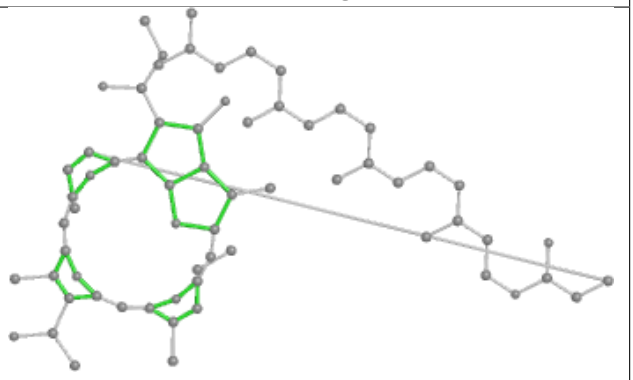
Bond lengths



Bond angles

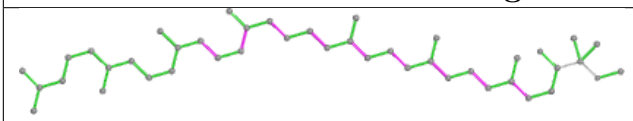


Torsions

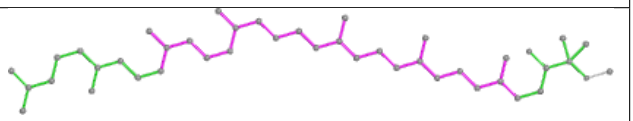


Rings

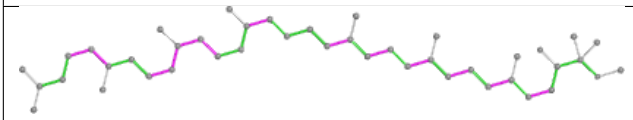
Ligand A1EFU F 103



Bond lengths



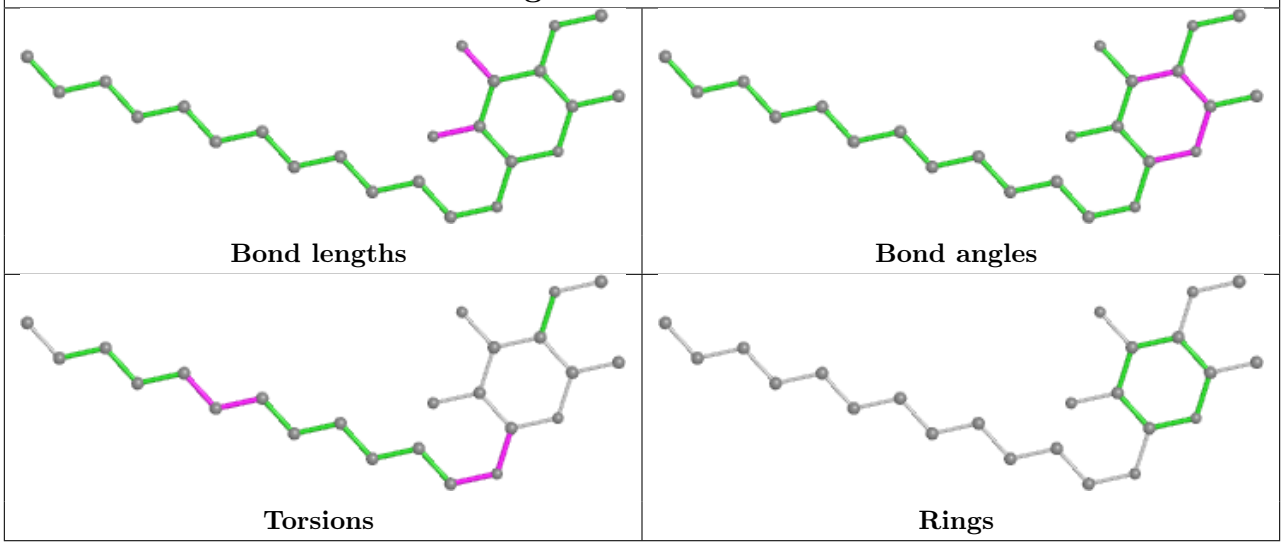
Bond angles



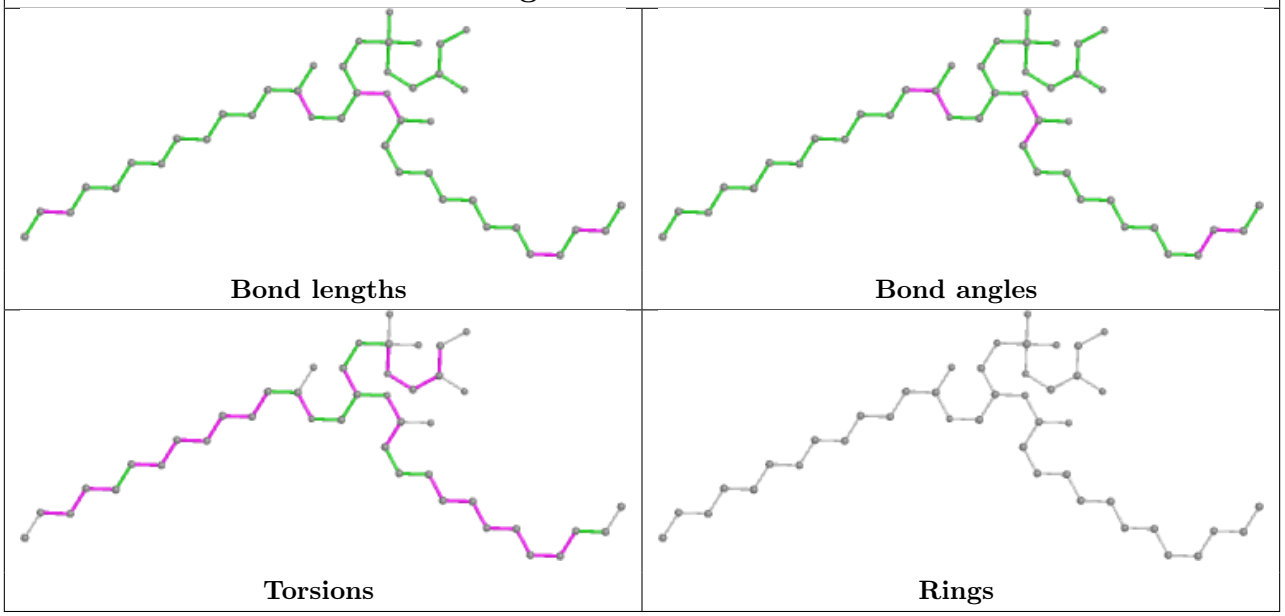
Torsions

Rings

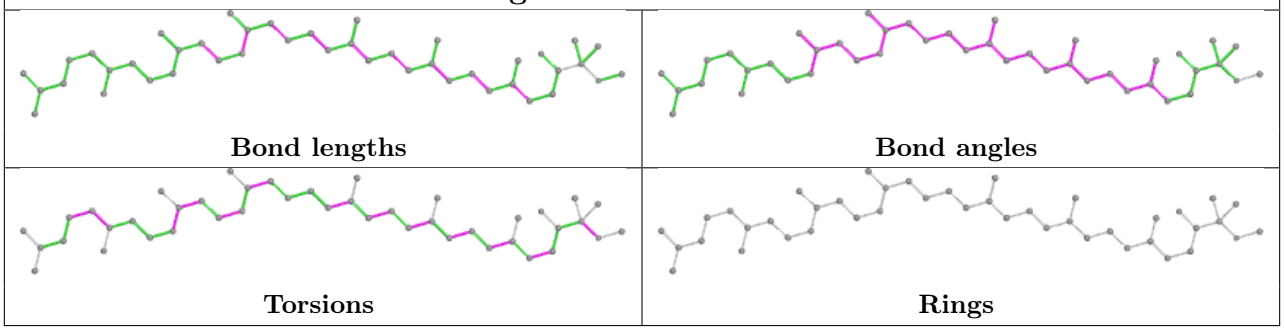
Ligand LMT L 306



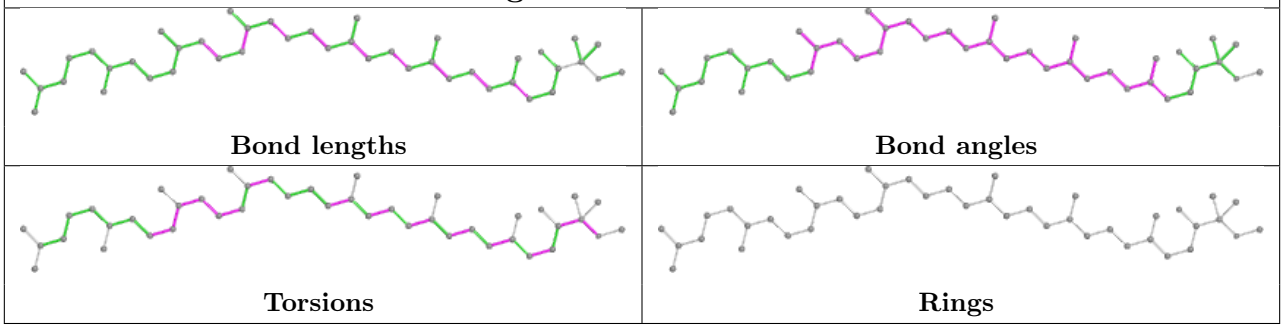
Ligand MW9 F 104



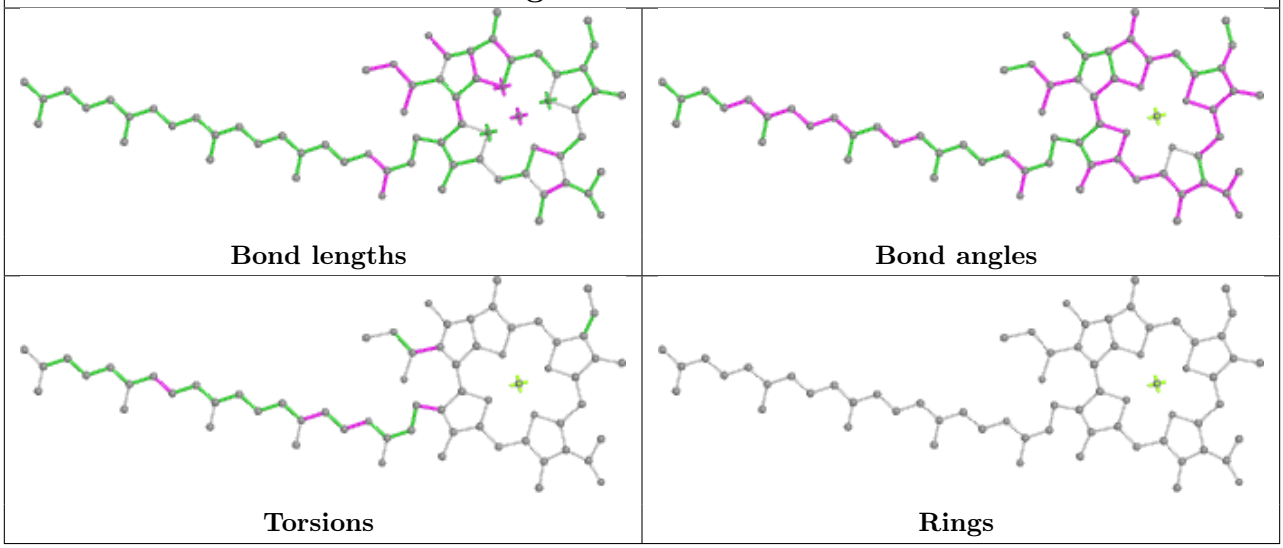
Ligand A1EFU I 101



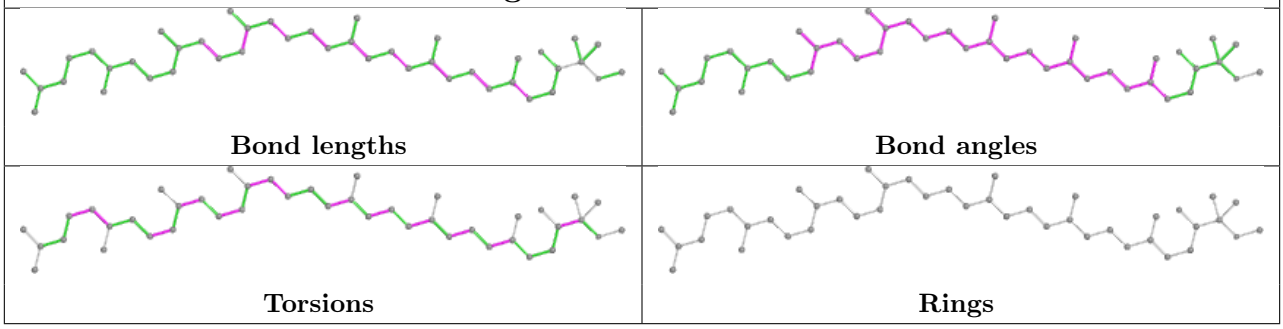
Ligand A1EFU S 304



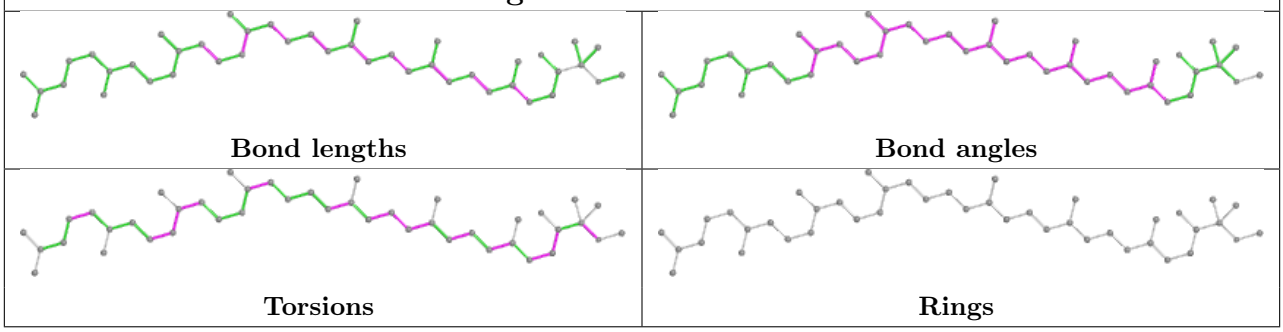
Ligand BCL B 102



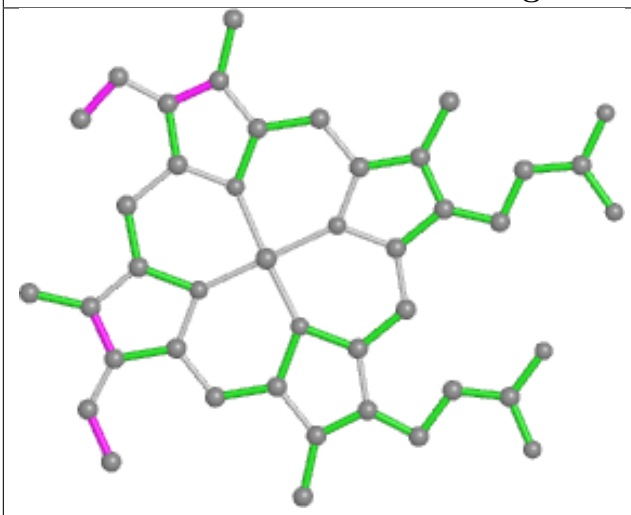
Ligand A1EFU P 103



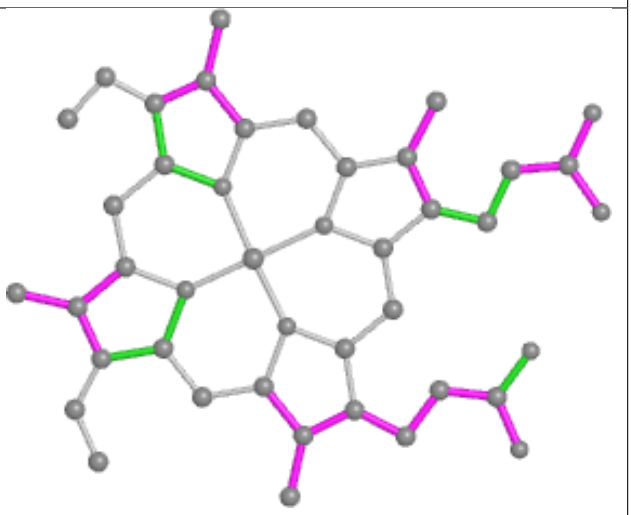
Ligand A1EFU n 102



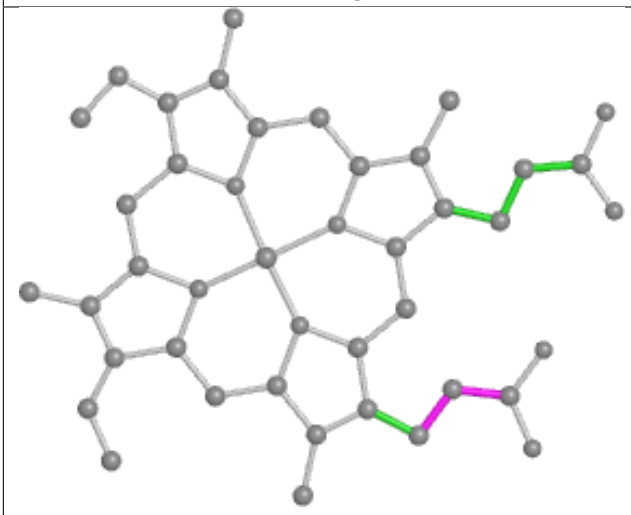
Ligand HEC C 403



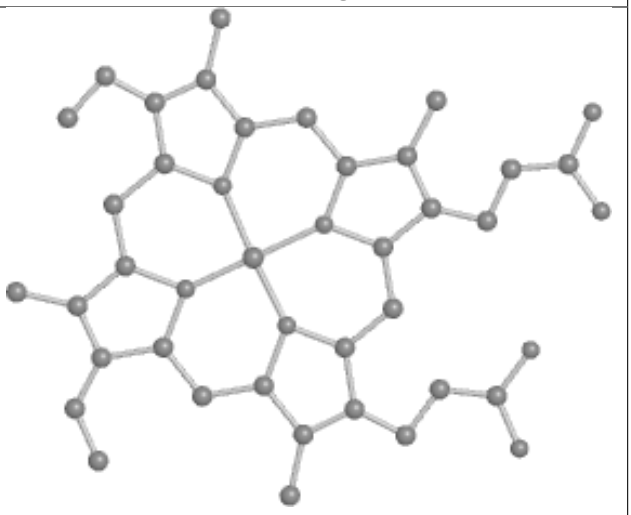
Bond lengths



Bond angles

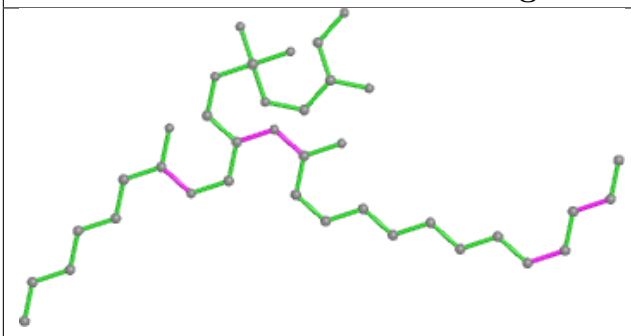


Torsions

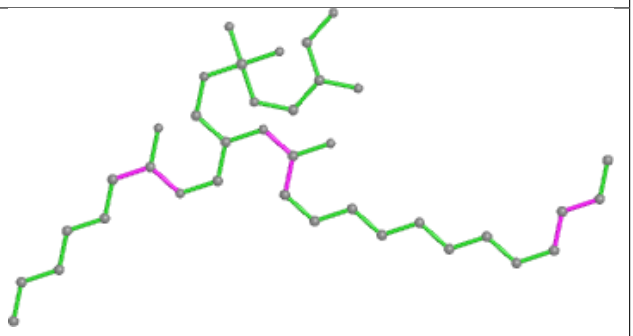


Rings

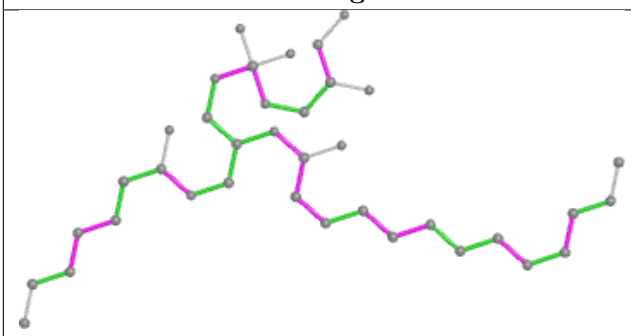
Ligand MW9 L 305



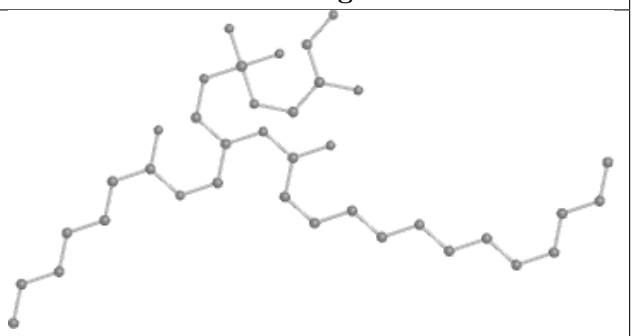
Bond lengths



Bond angles

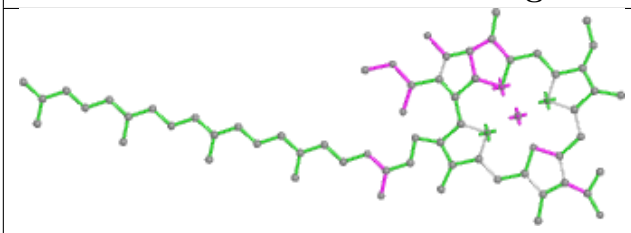


Torsions

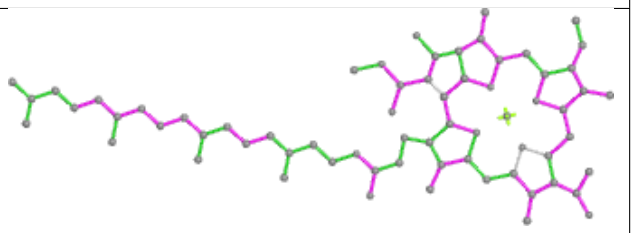


Rings

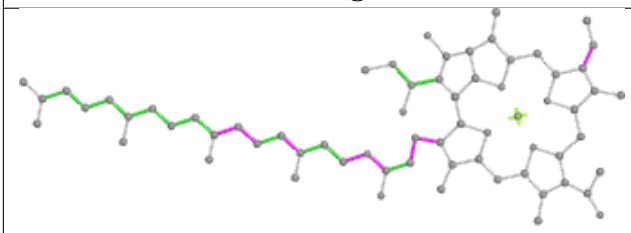
Ligand BCL P 101



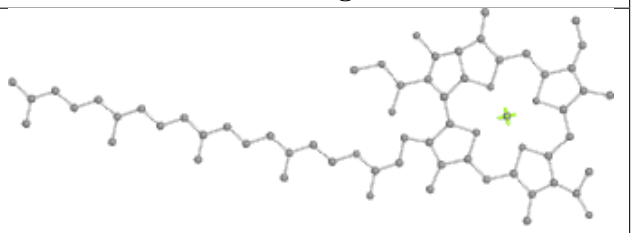
Bond lengths



Bond angles

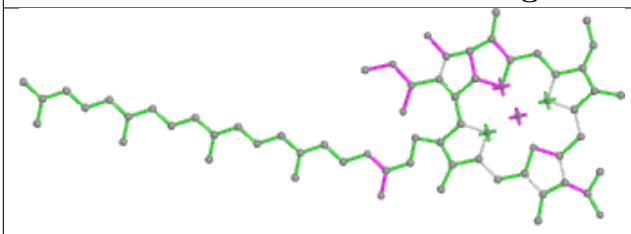


Torsions

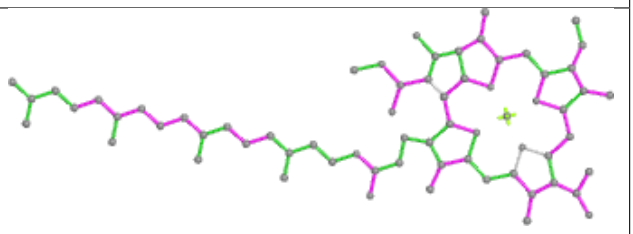


Rings

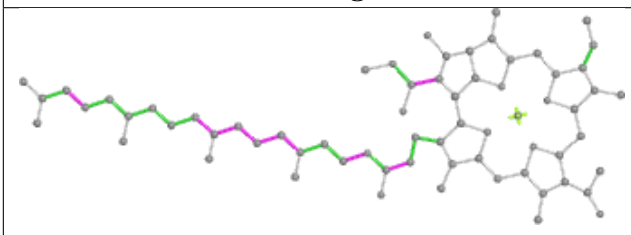
Ligand BCL M 402



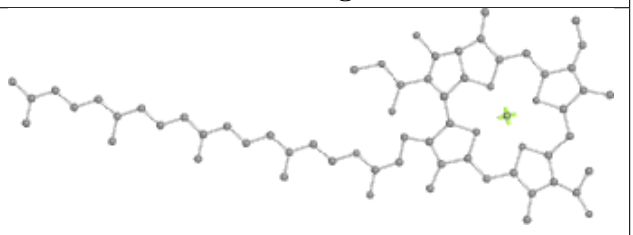
Bond lengths



Bond angles

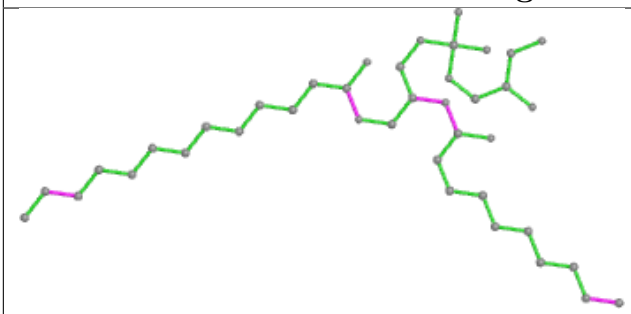


Torsions

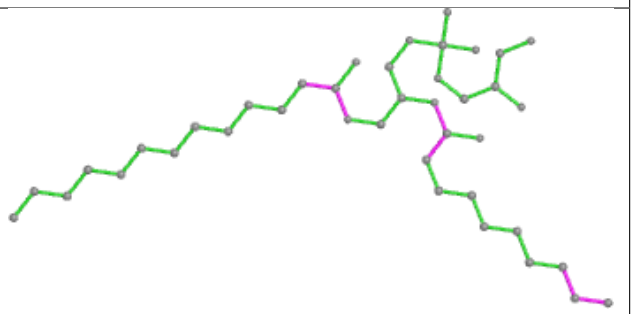


Rings

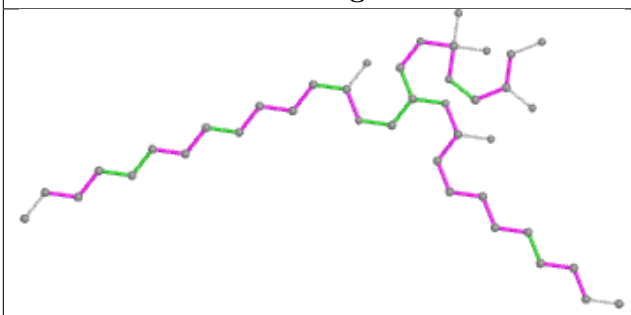
Ligand MW9 G 106



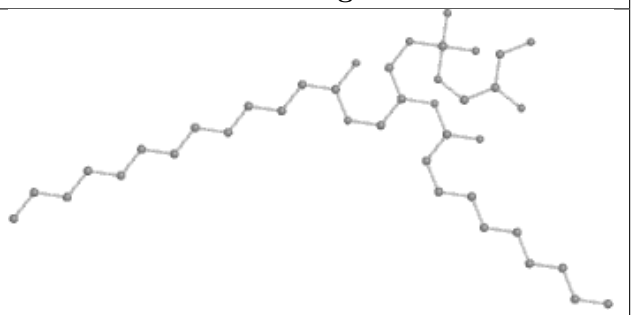
Bond lengths



Bond angles

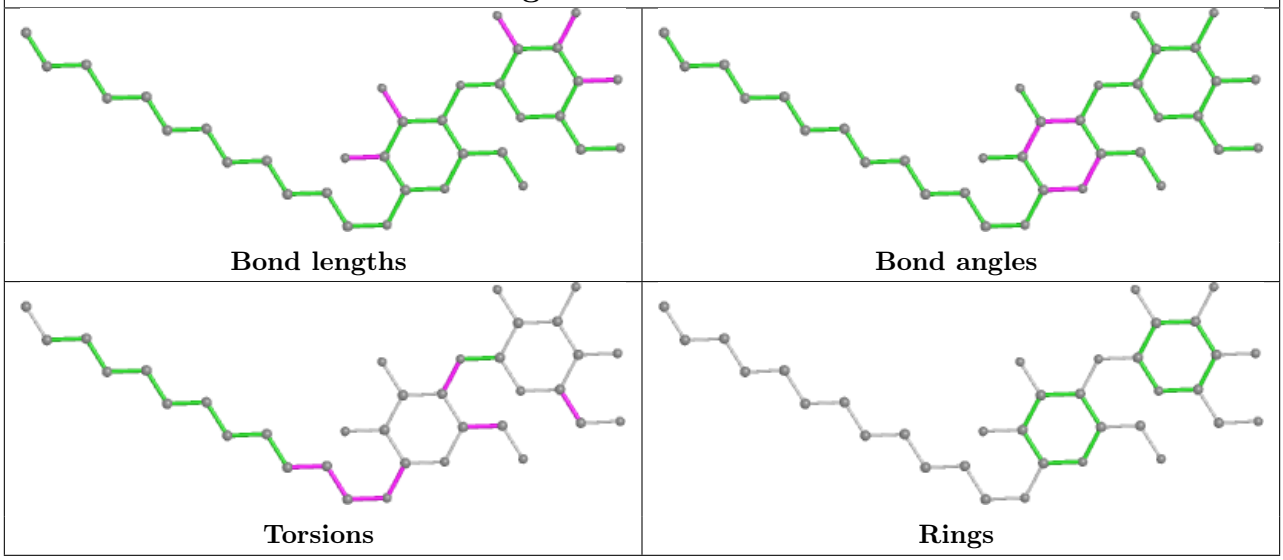


Torsions

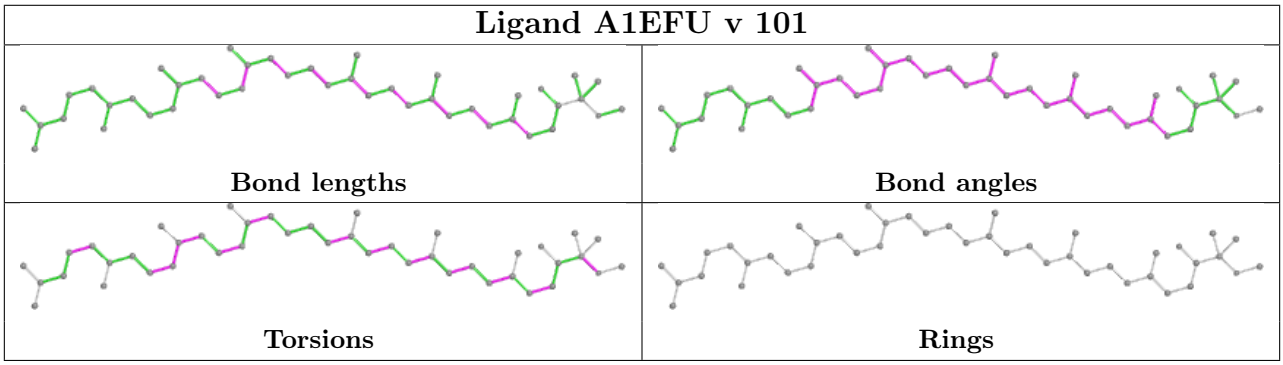


Rings

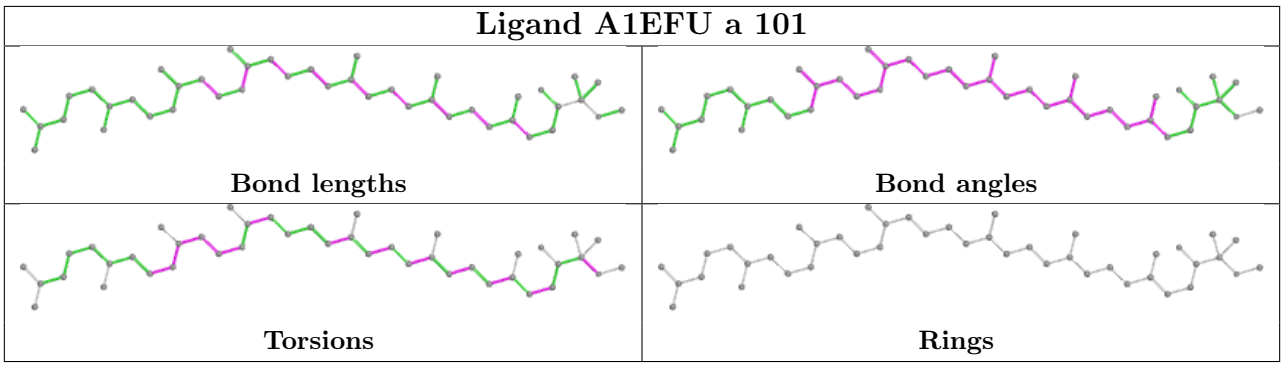
Ligand LMT C 404



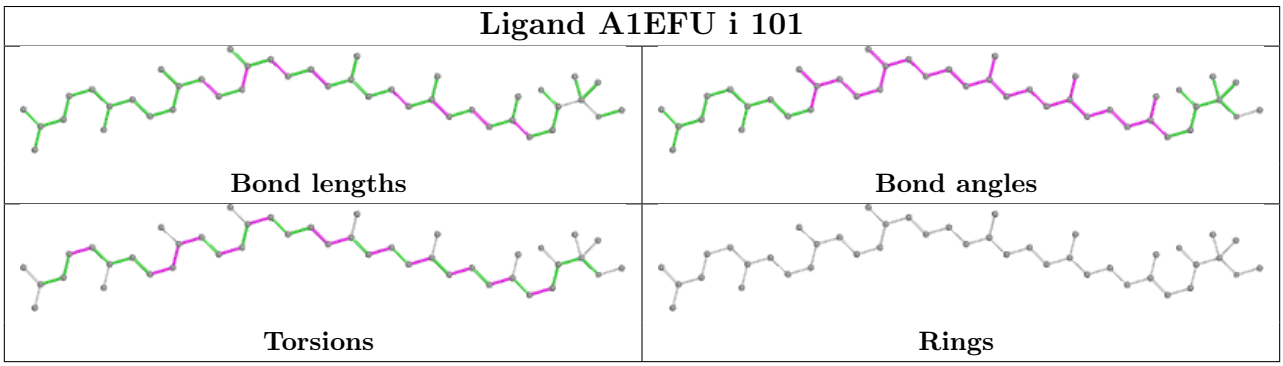
Ligand A1EFU v 101



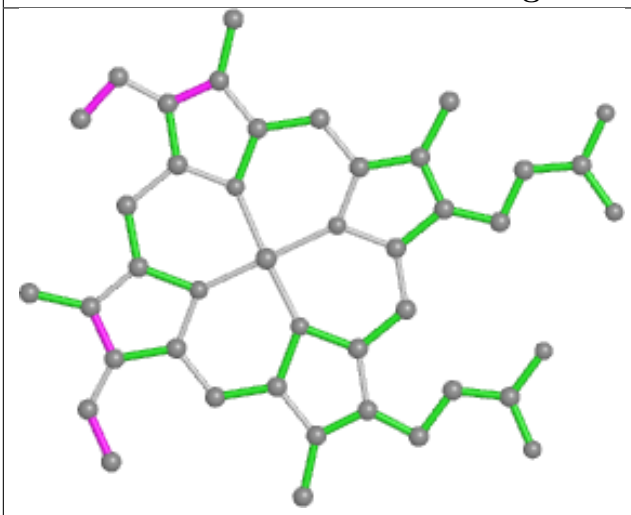
Ligand A1EFU a 101



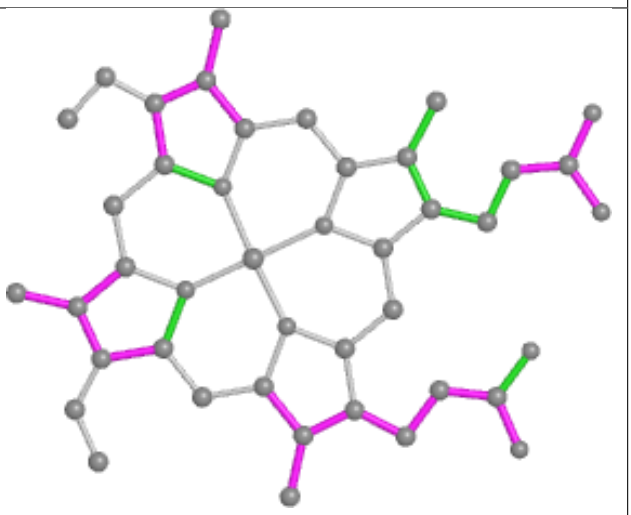
Ligand A1EFU i 101



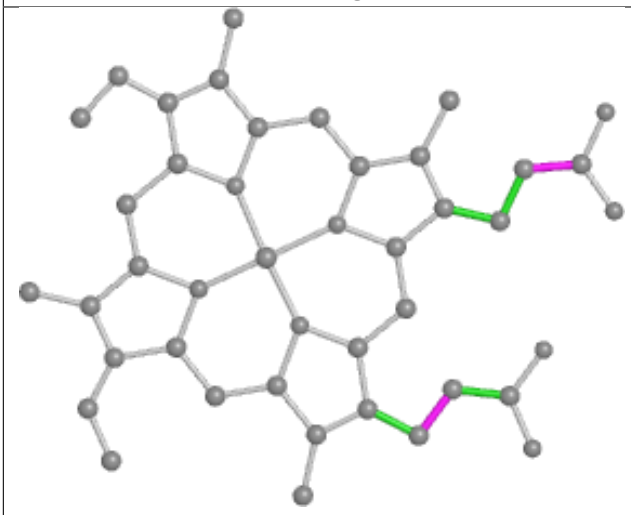
Ligand HEC C 401



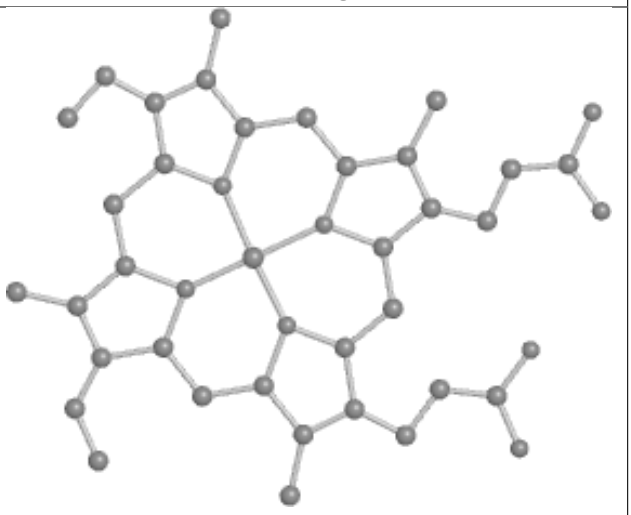
Bond lengths



Bond angles

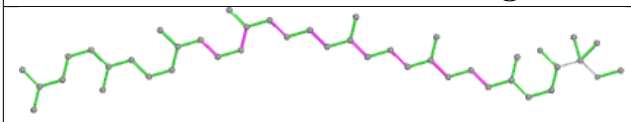


Torsions

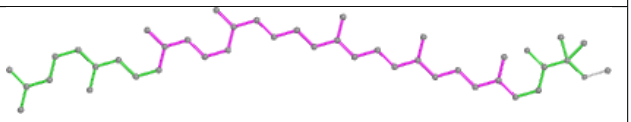


Rings

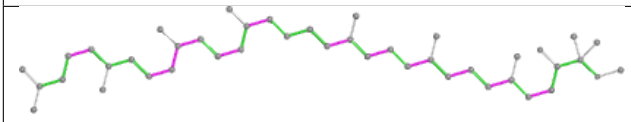
Ligand A1EFU G 103



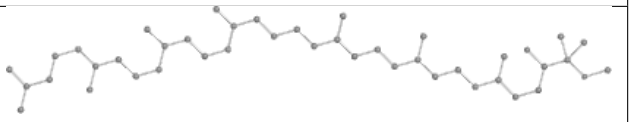
Bond lengths



Bond angles

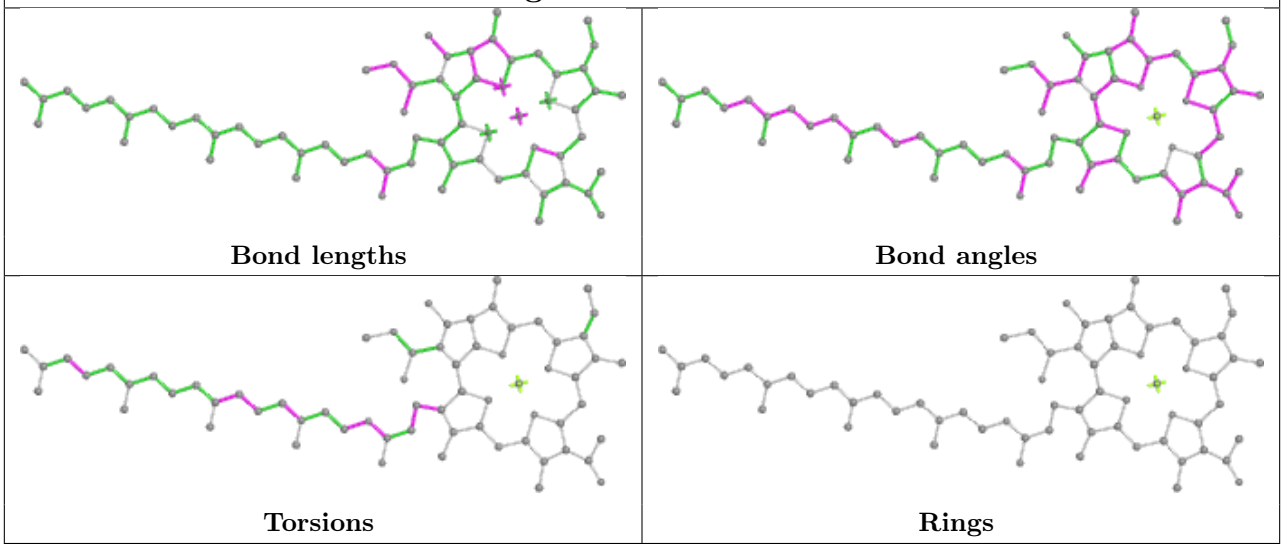


Torsions

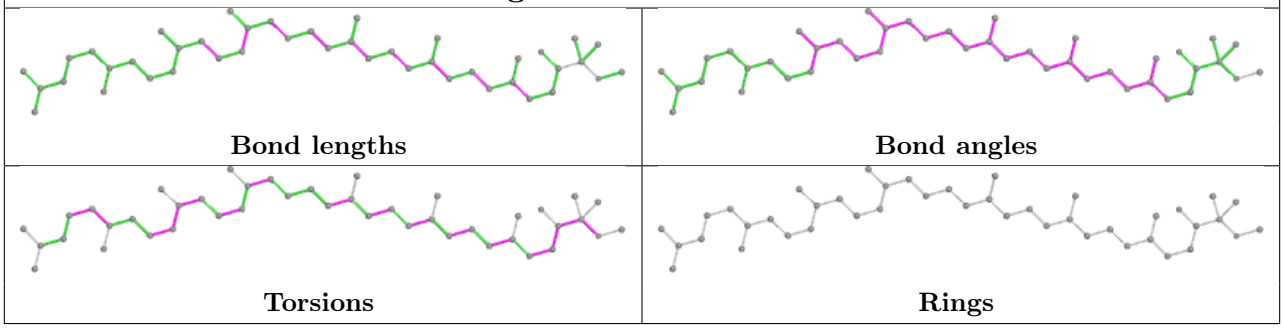


Rings

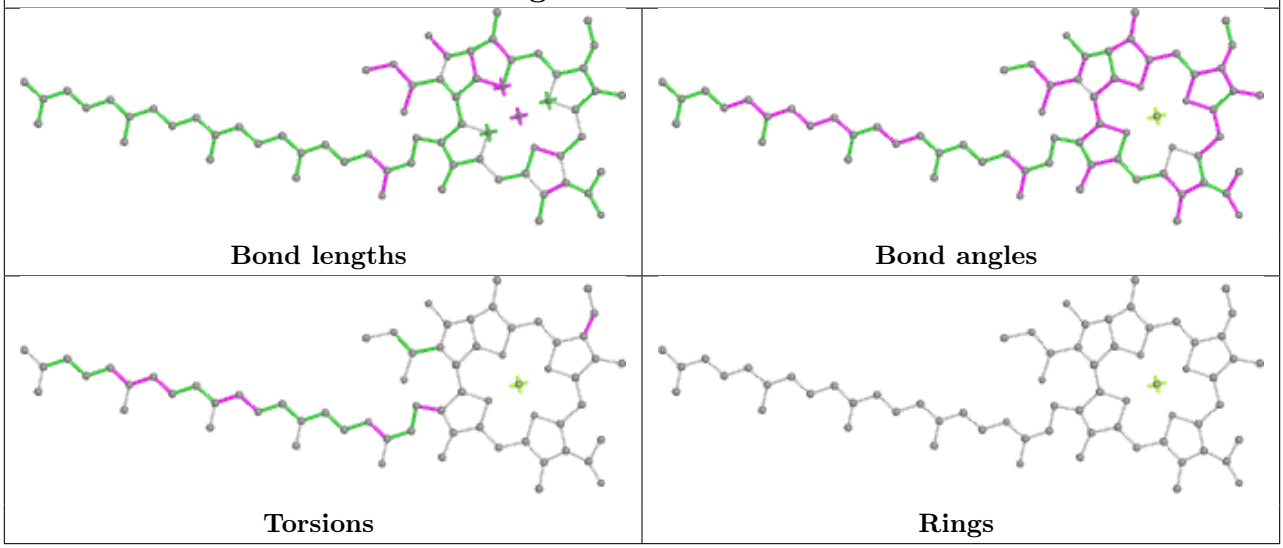
Ligand BCL N 101



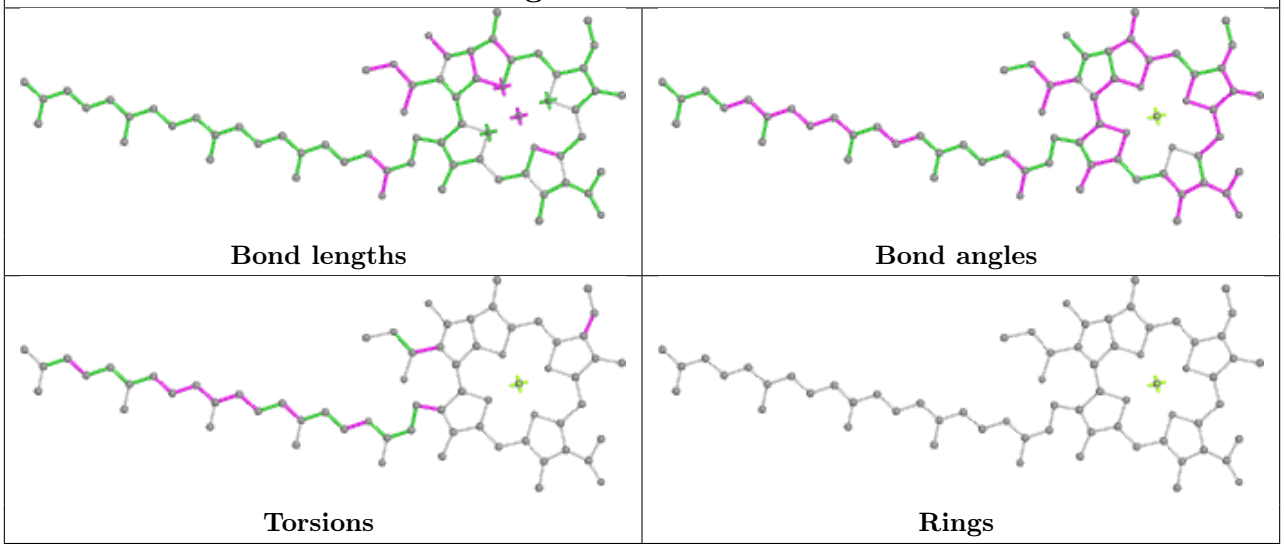
Ligand A1EFU a 103



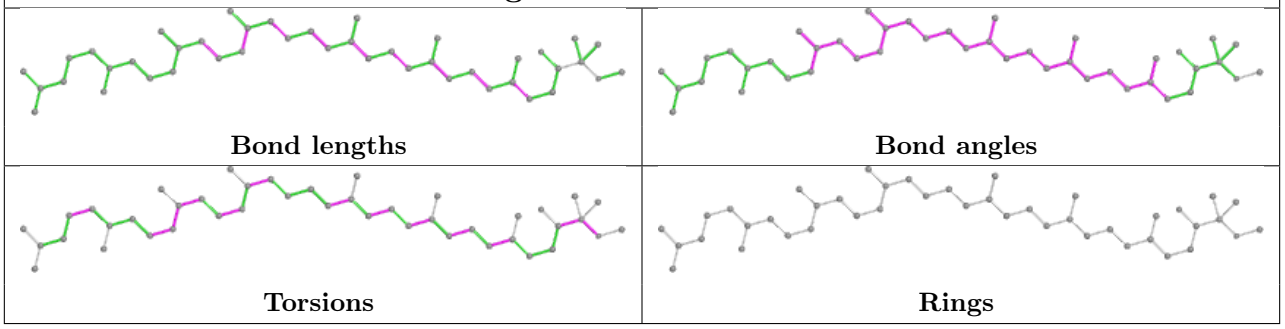
Ligand BCL n 101



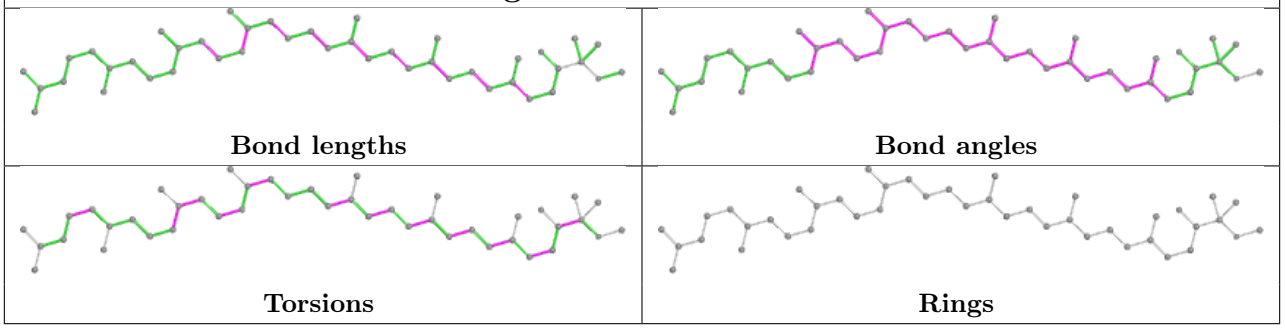
Ligand BCL G 101



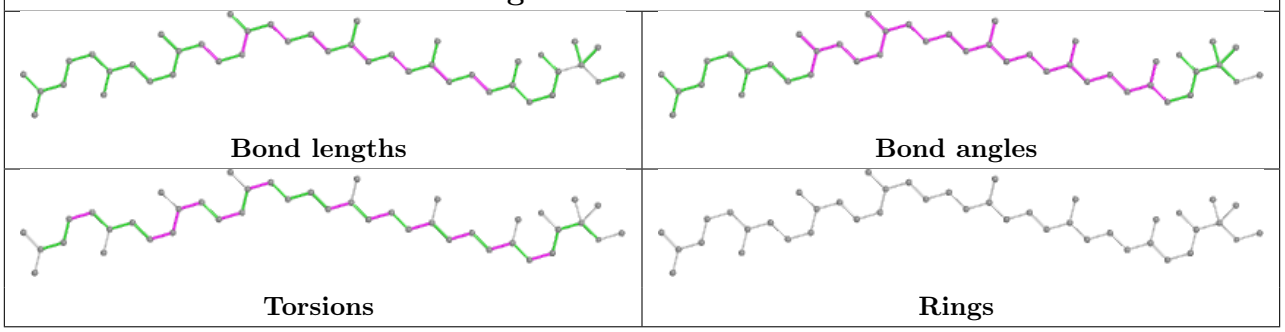
Ligand A1EFU F 102



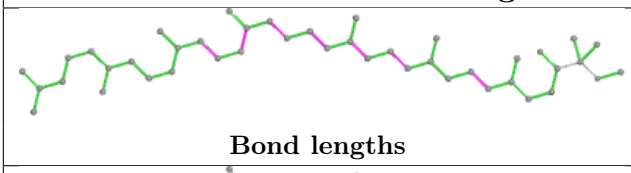
Ligand A1EFU T 101



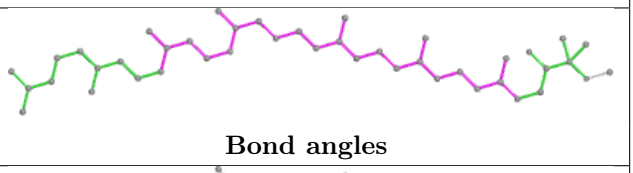
Ligand A1EFU J 102



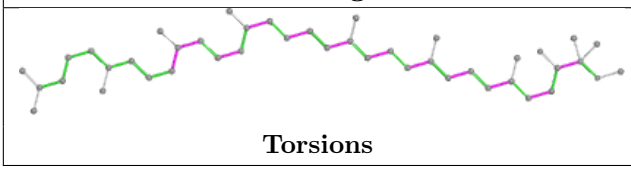
Ligand A1EFU M 406



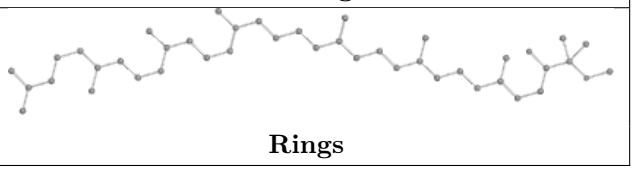
Bond lengths



Bond angles

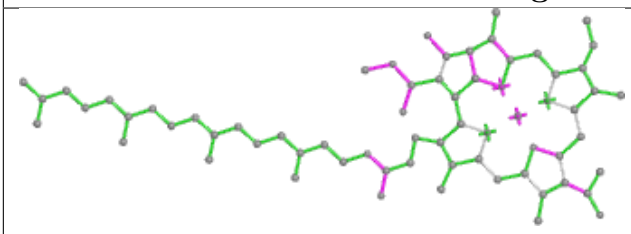


Torsions

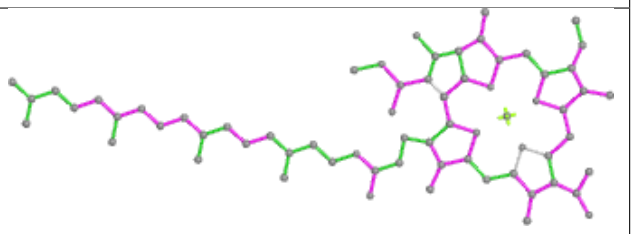


Rings

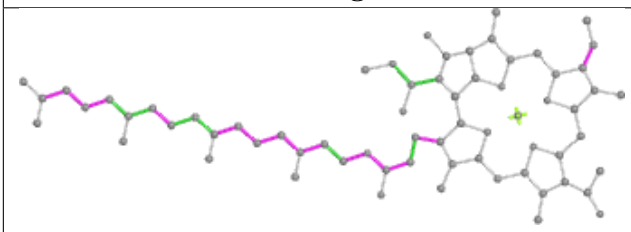
Ligand BCL s 101



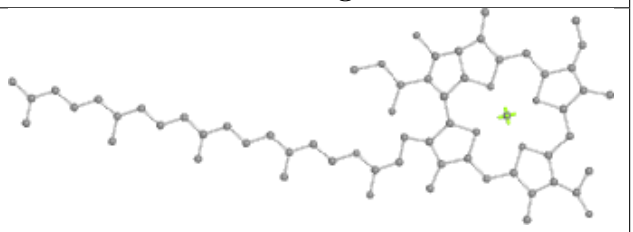
Bond lengths



Bond angles

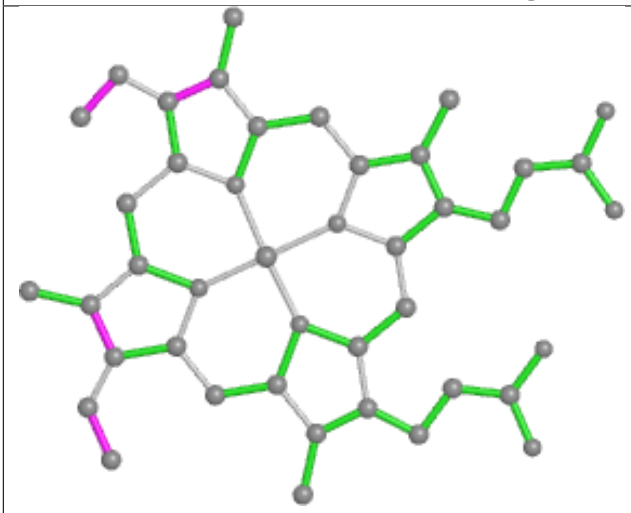


Torsions

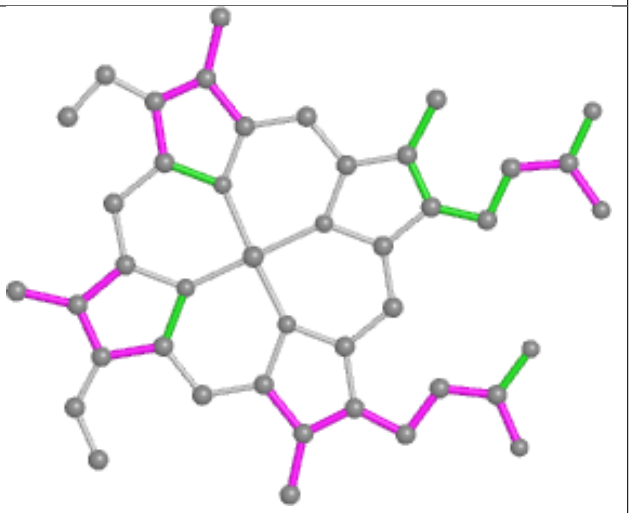


Rings

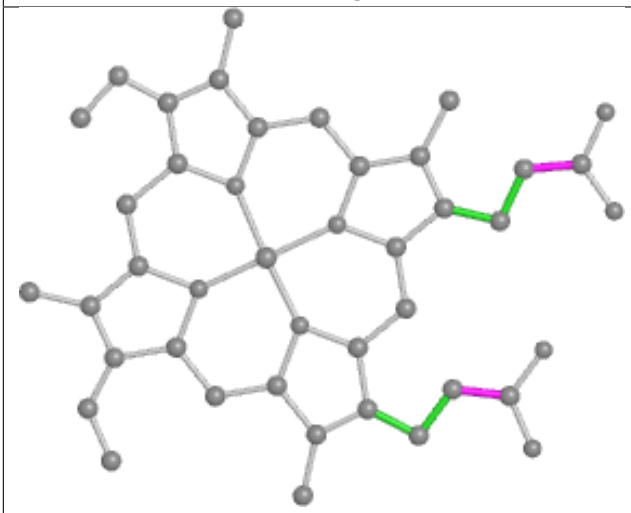
Ligand HEC C 402



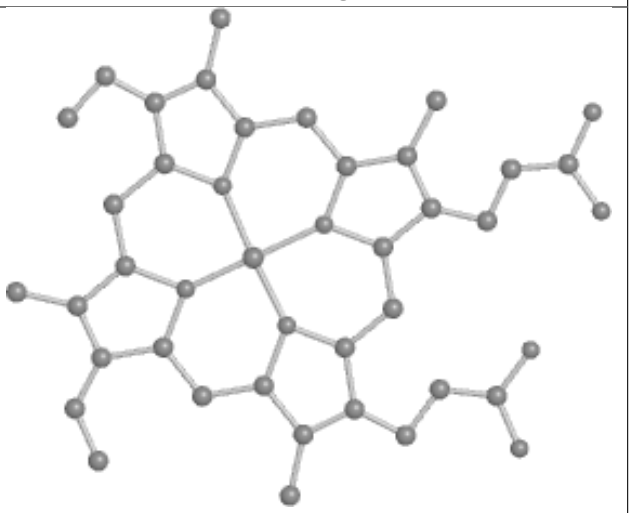
Bond lengths



Bond angles

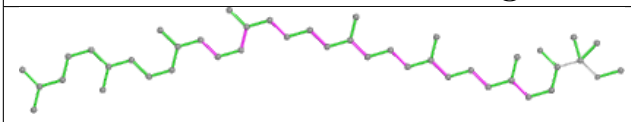


Torsions

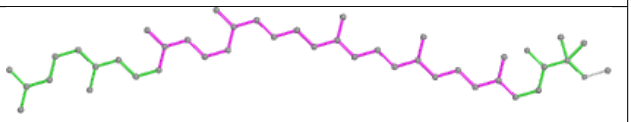


Rings

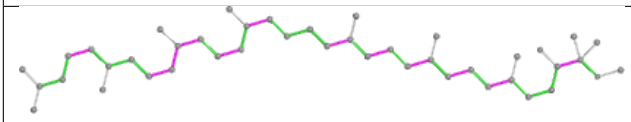
Ligand A1EFU K 103



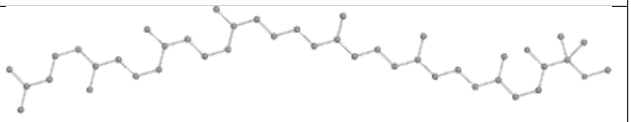
Bond lengths



Bond angles

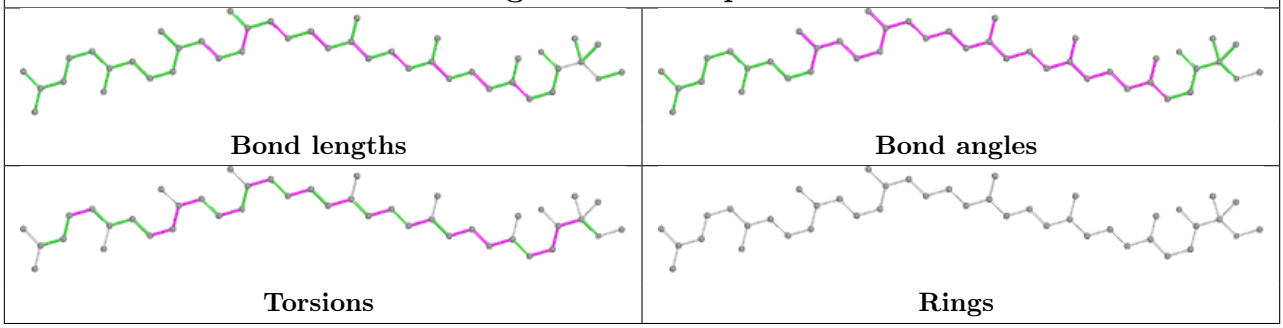


Torsions

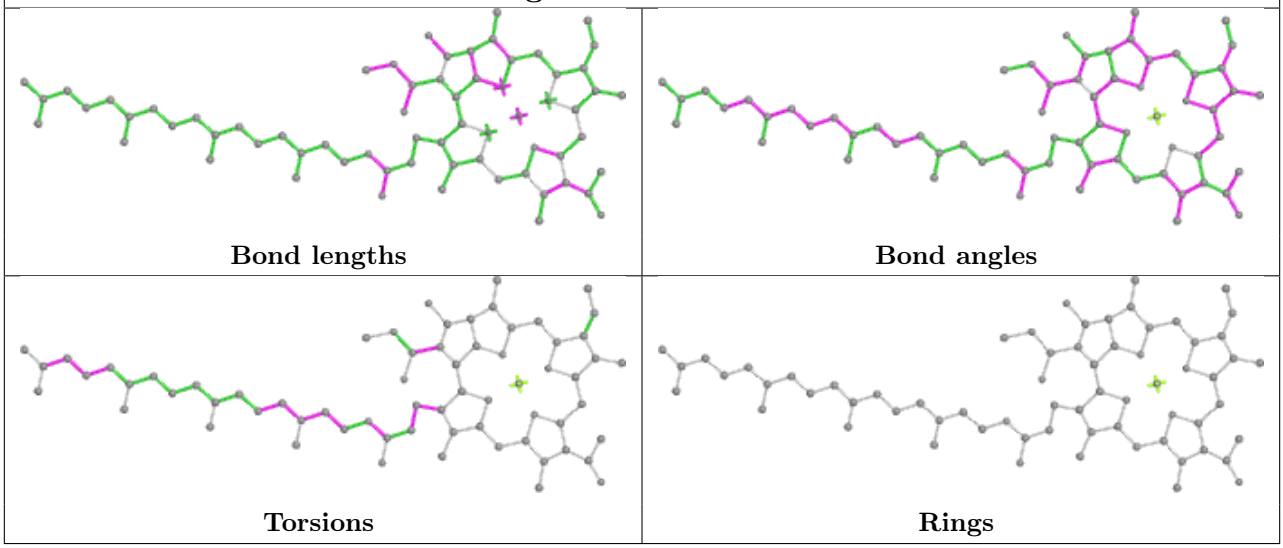


Rings

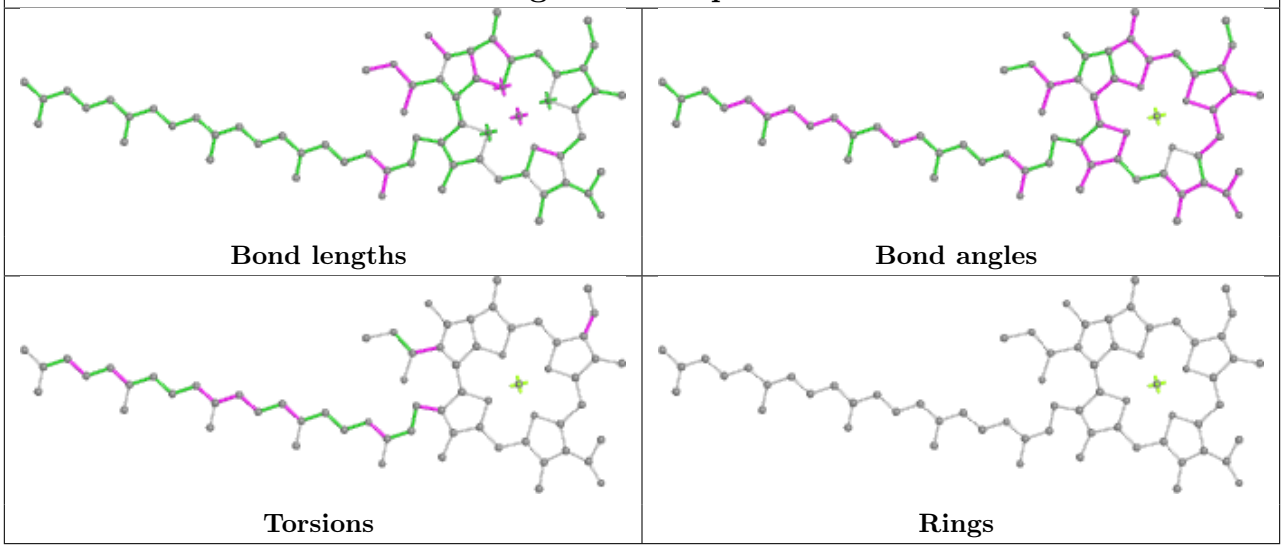
Ligand A1EFU p 101



Ligand BCL A 101

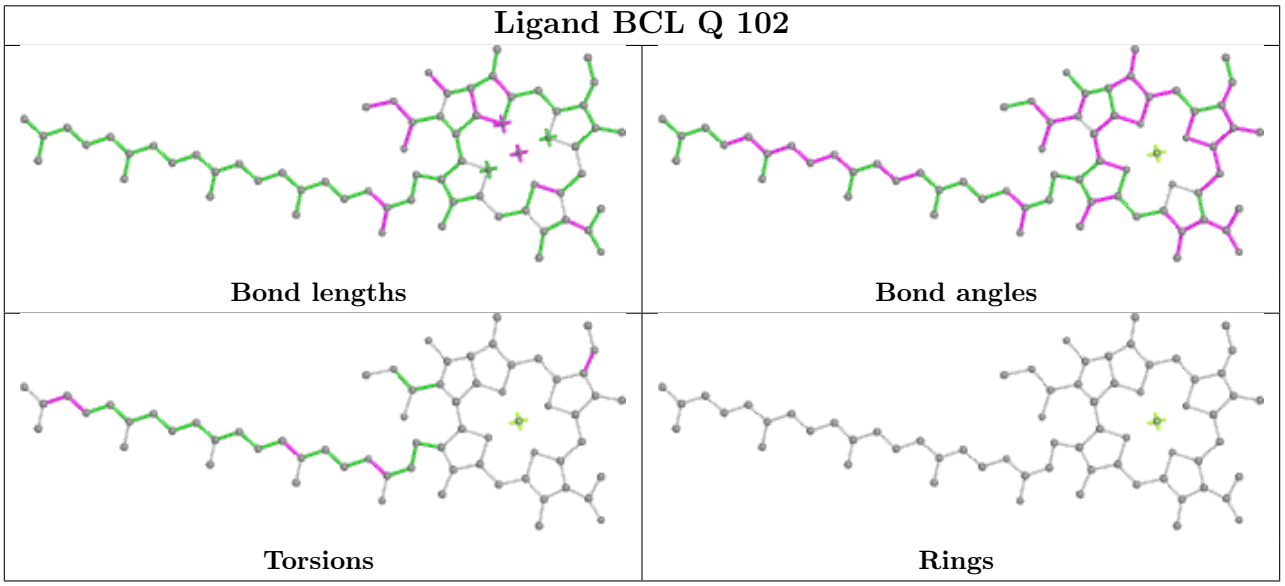


Ligand BCL q 101

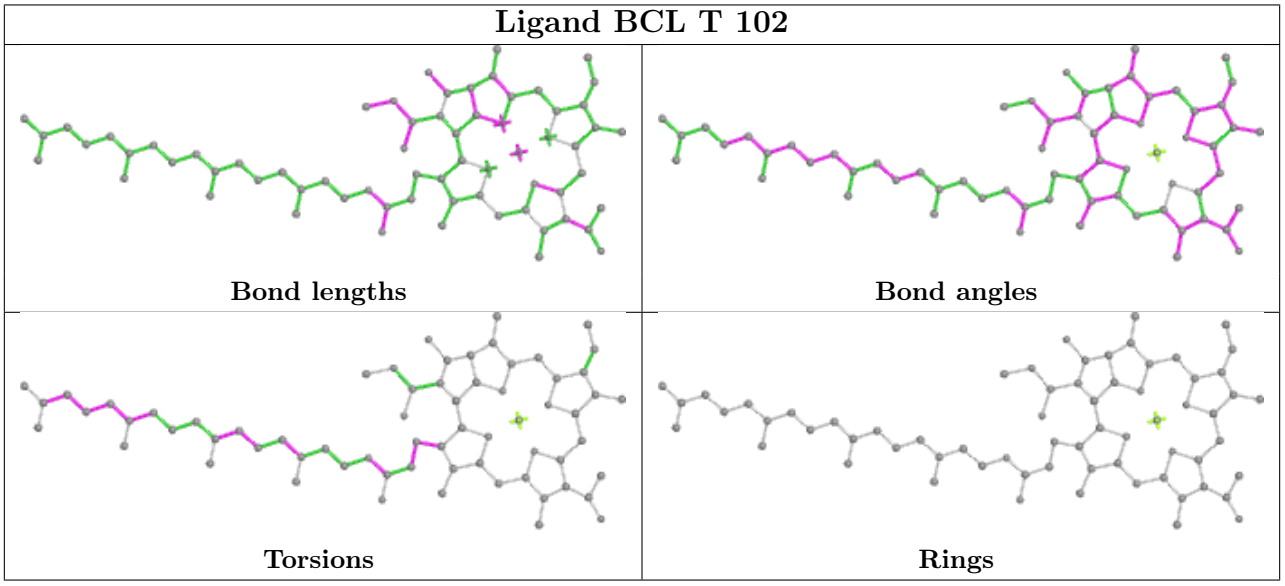


Ligand MW9 D 102

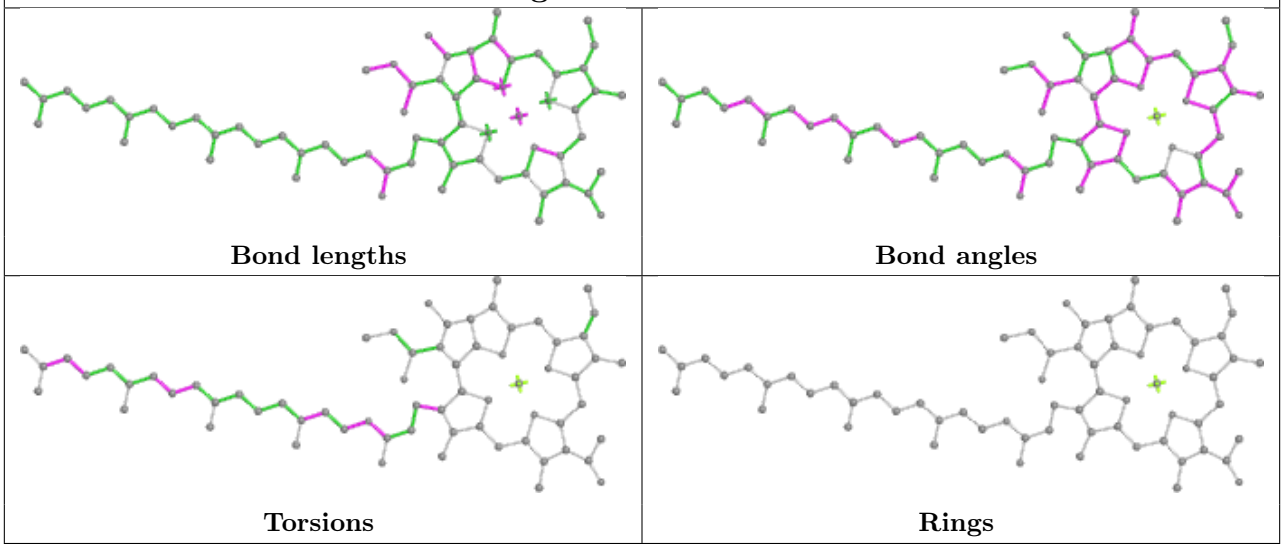
Ligand BCL Q 102



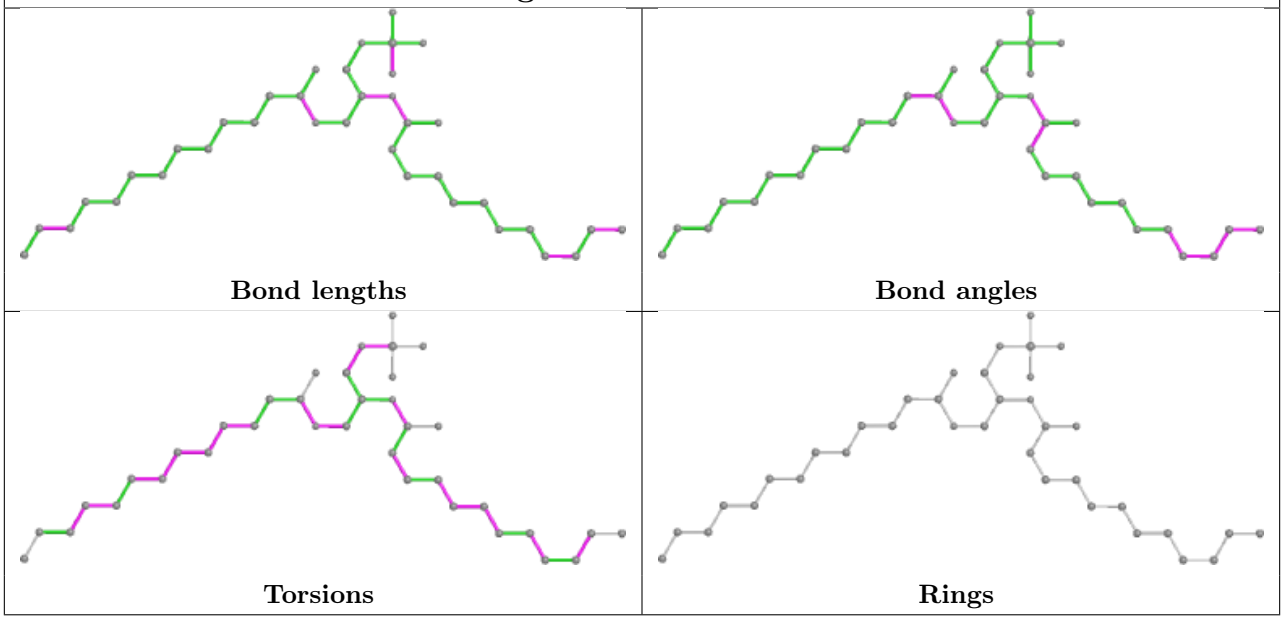
Ligand BCL T 102



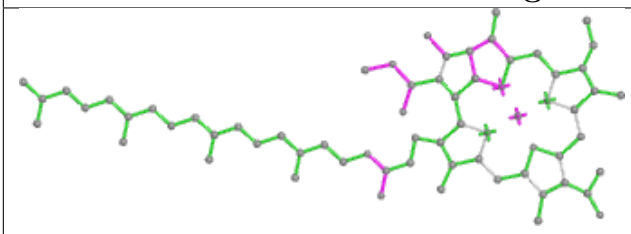
Ligand BCL e 101



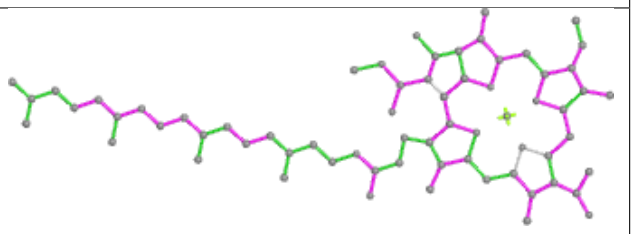
Ligand MW9 H 302



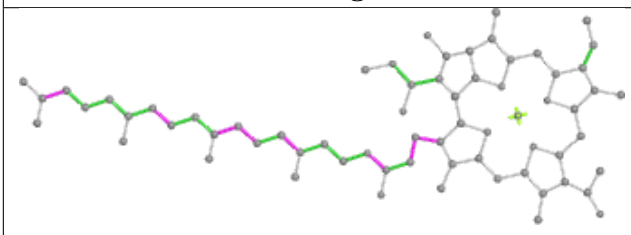
Ligand BCL G 102



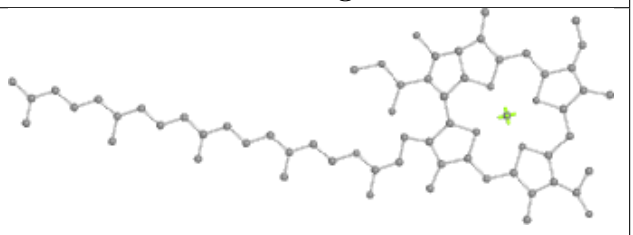
Bond lengths



Bond angles

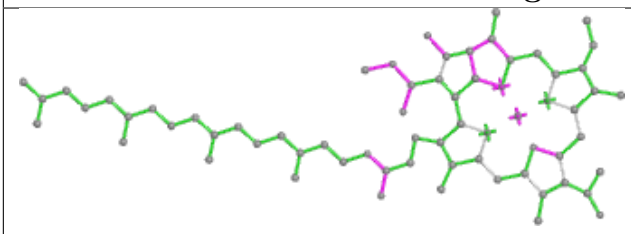


Torsions

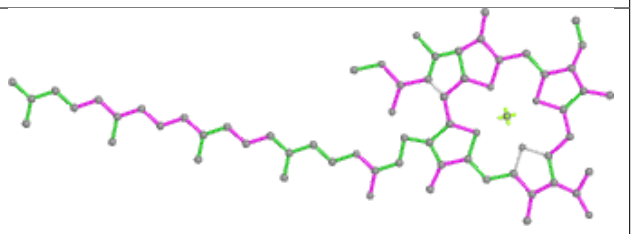


Rings

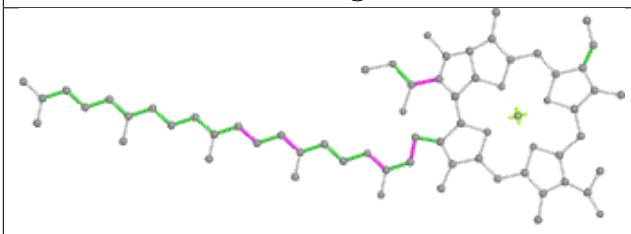
Ligand BCL K 102



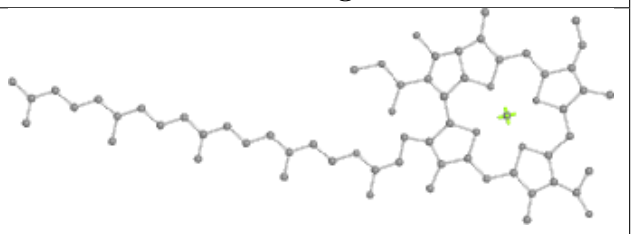
Bond lengths



Bond angles

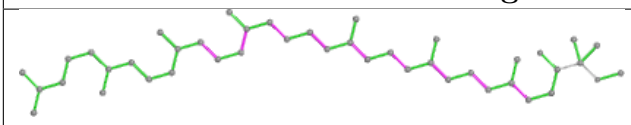


Torsions

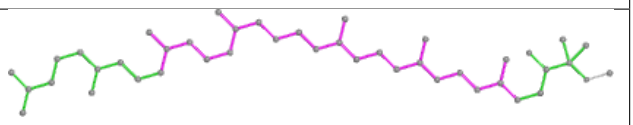


Rings

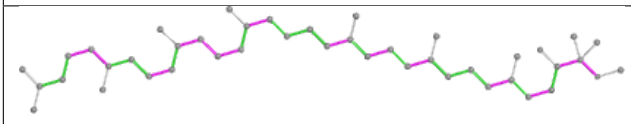
Ligand A1EFU K 104



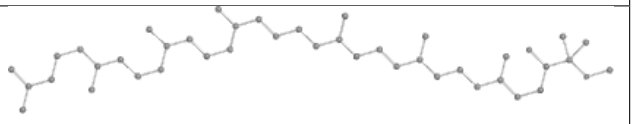
Bond lengths



Bond angles

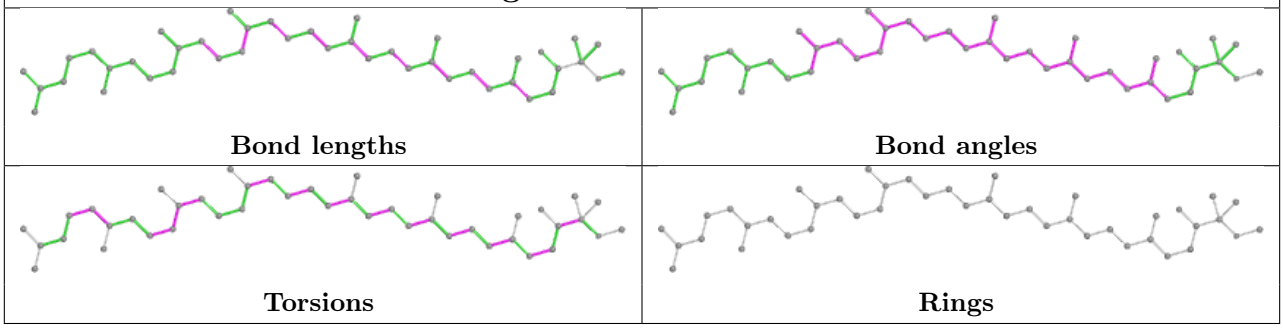


Torsions

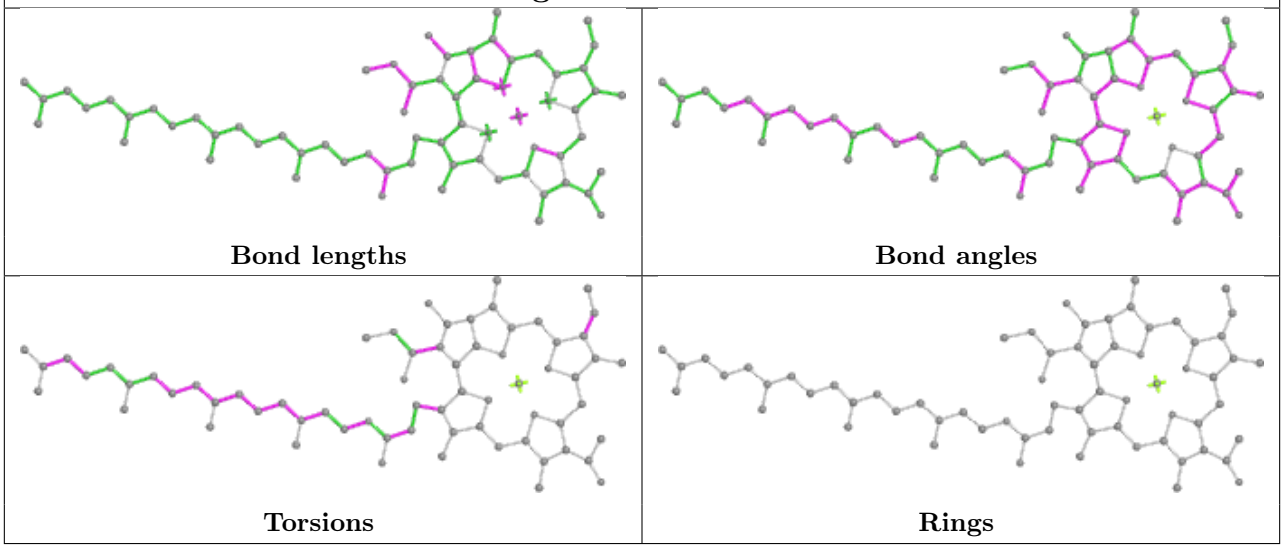


Rings

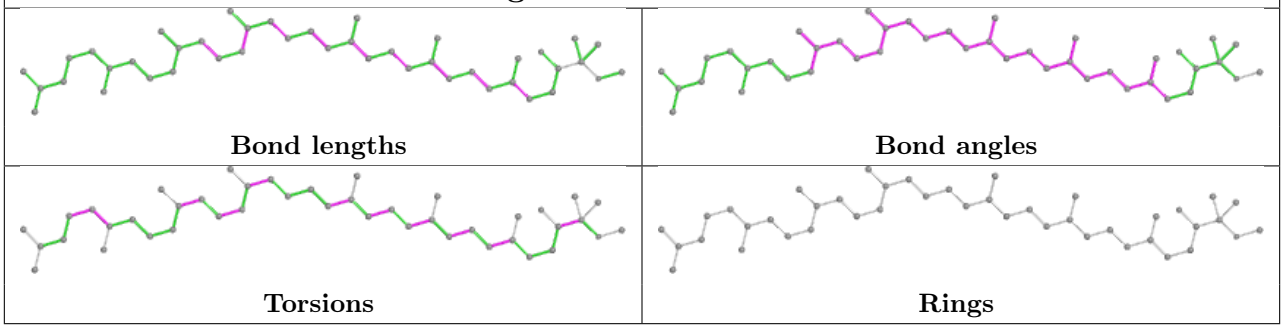
Ligand A1EFU D 103



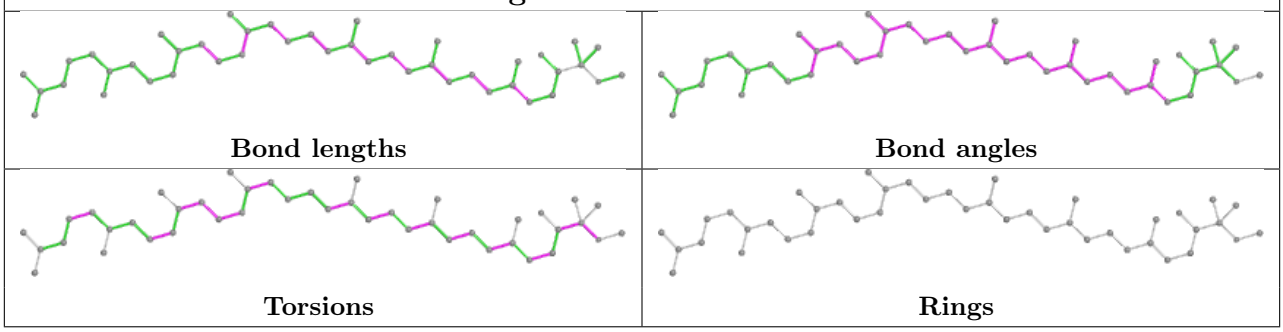
Ligand BCL I 102



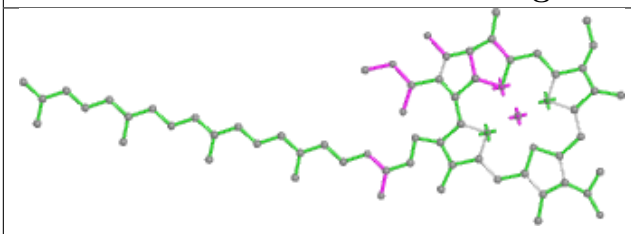
Ligand A1EFU 1 103



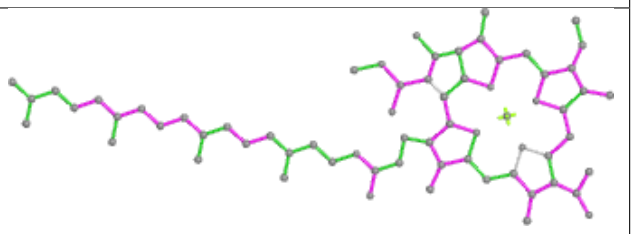
Ligand A1EFU r 102



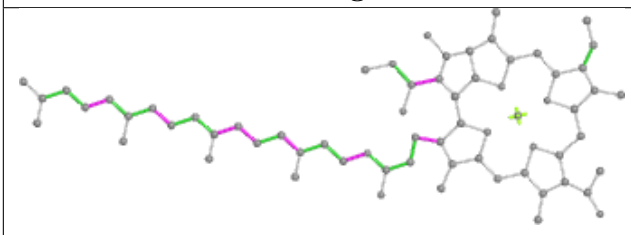
Ligand BCL f 101



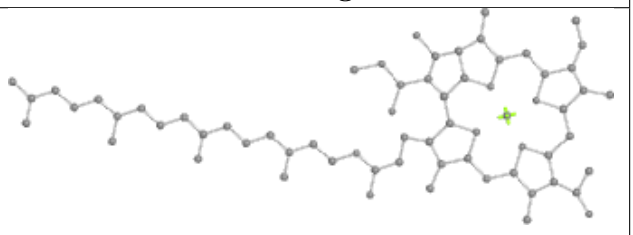
Bond lengths



Bond angles

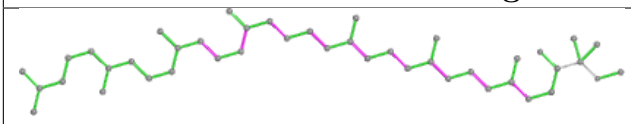


Torsions

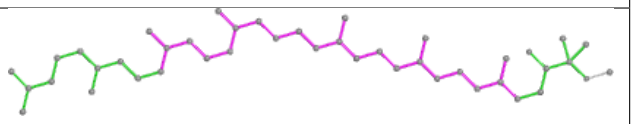


Rings

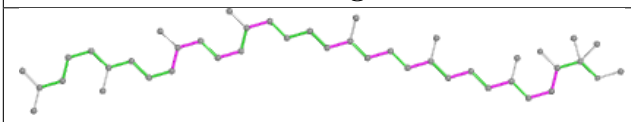
Ligand A1EFU T 103



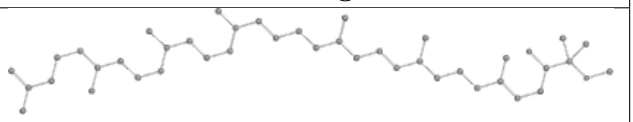
Bond lengths



Bond angles

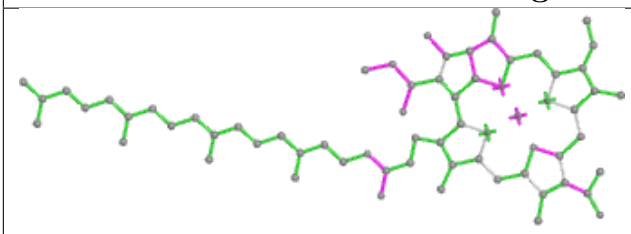


Torsions

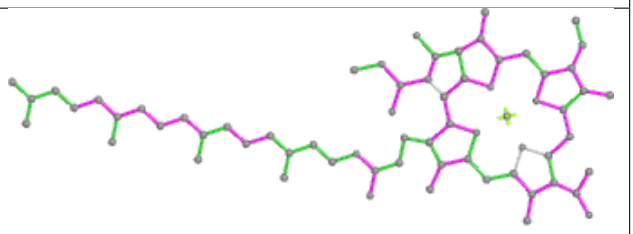


Rings

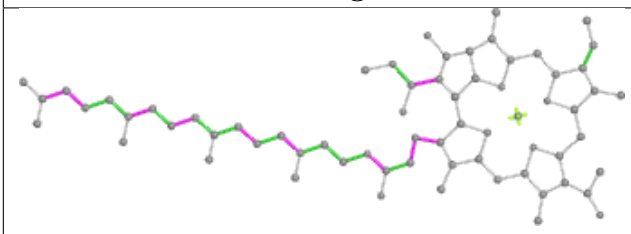
Ligand BCL I 103



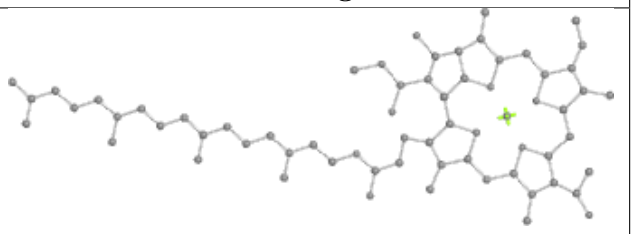
Bond lengths



Bond angles

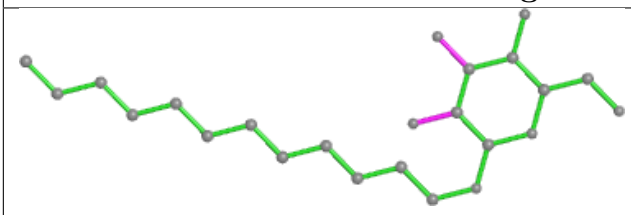


Torsions

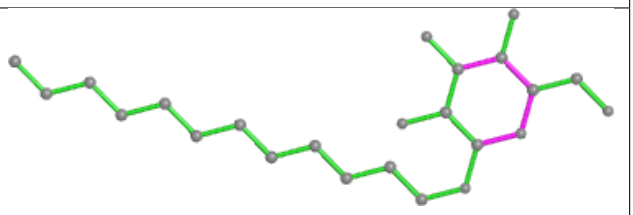


Rings

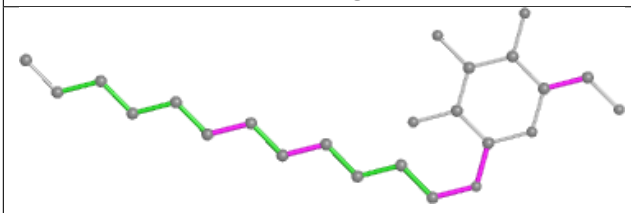
Ligand LMT H 304



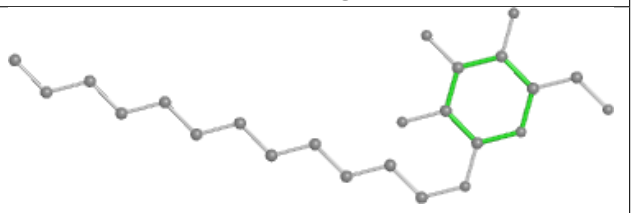
Bond lengths



Bond angles

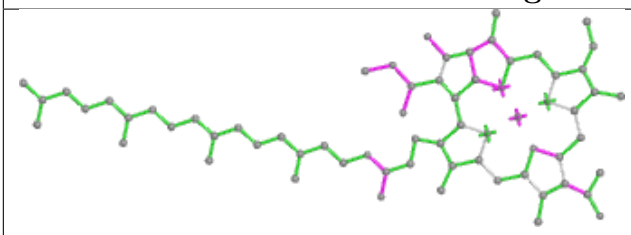


Torsions

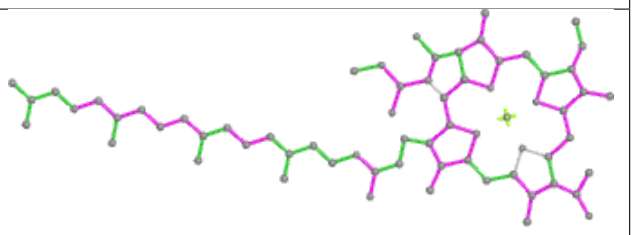


Rings

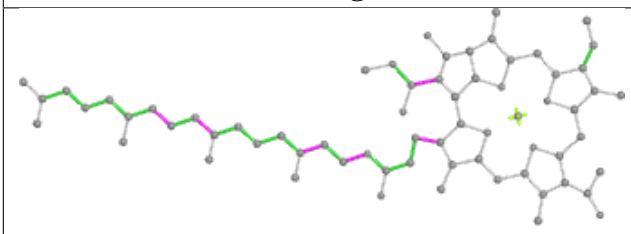
Ligand BCL K 101



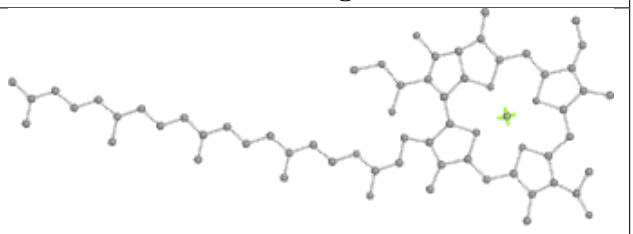
Bond lengths



Bond angles

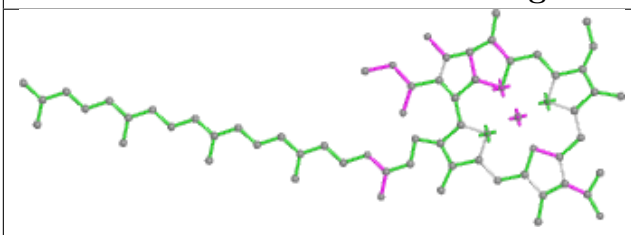


Torsions

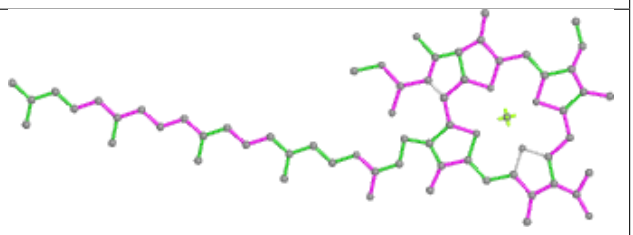


Rings

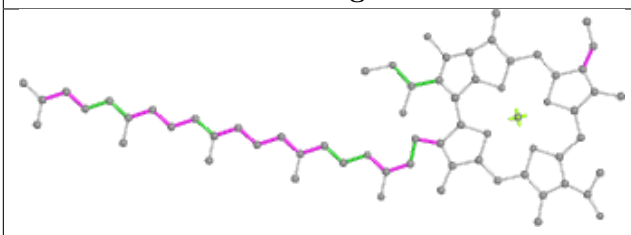
Ligand BCL v 102



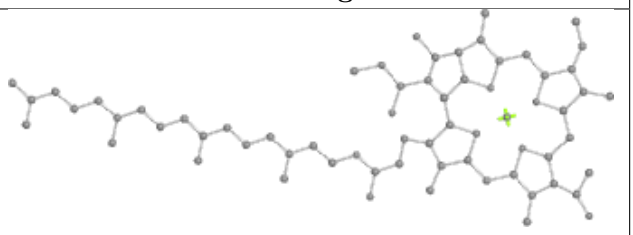
Bond lengths



Bond angles

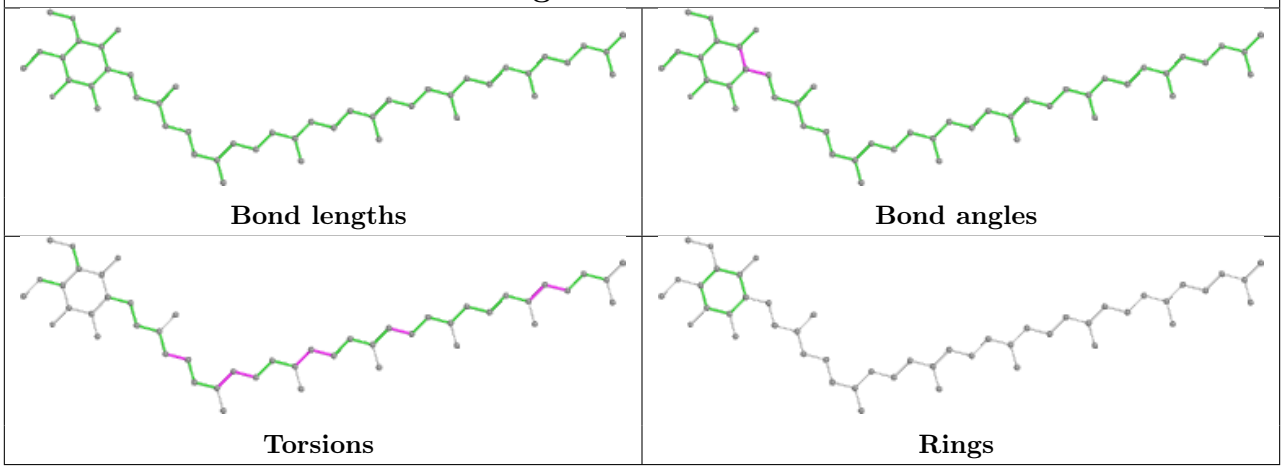


Torsions

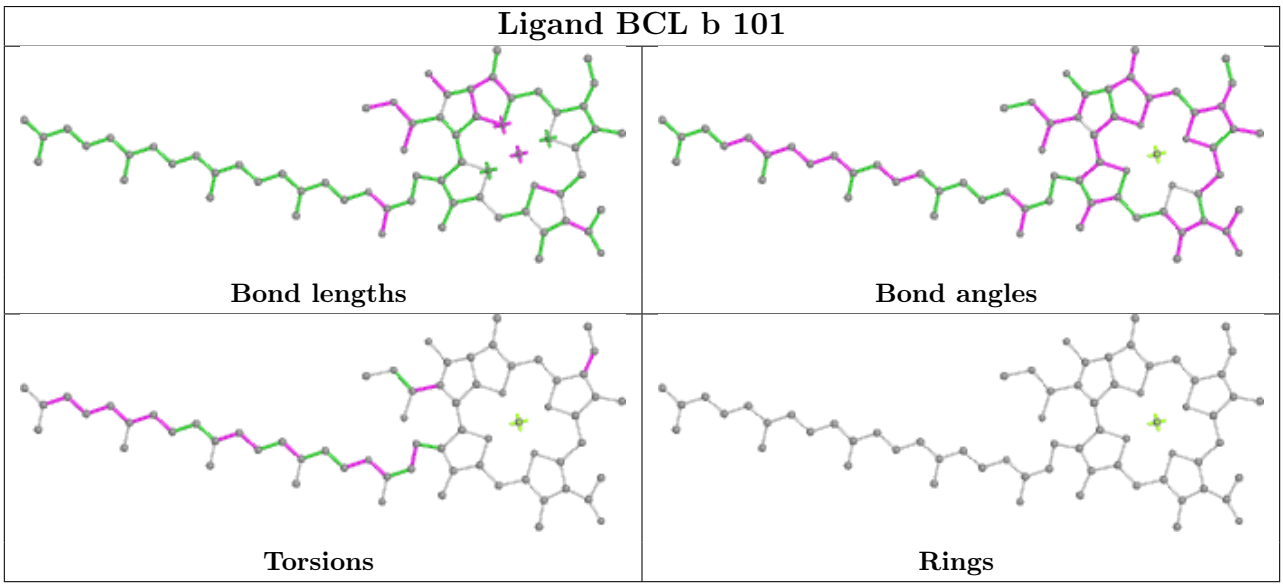


Rings

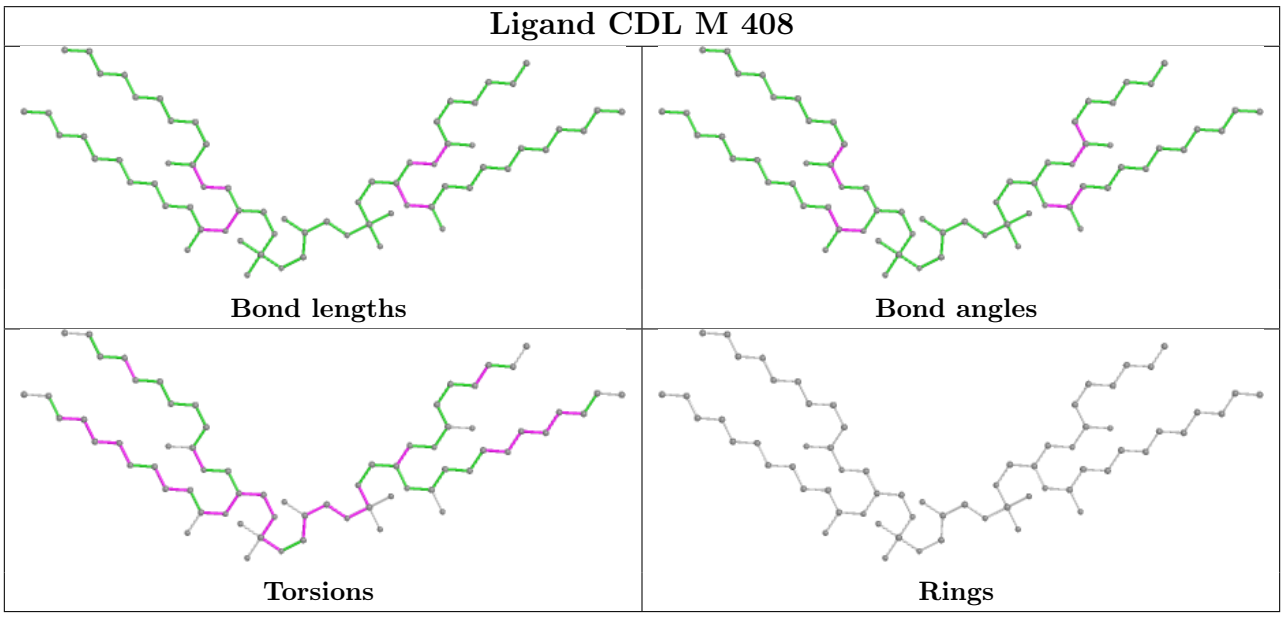
Ligand U10 L 303



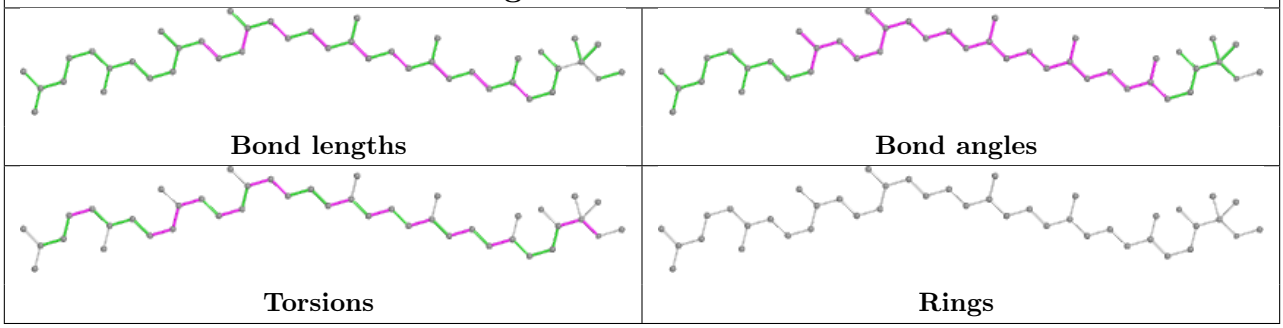
Ligand BCL b 101



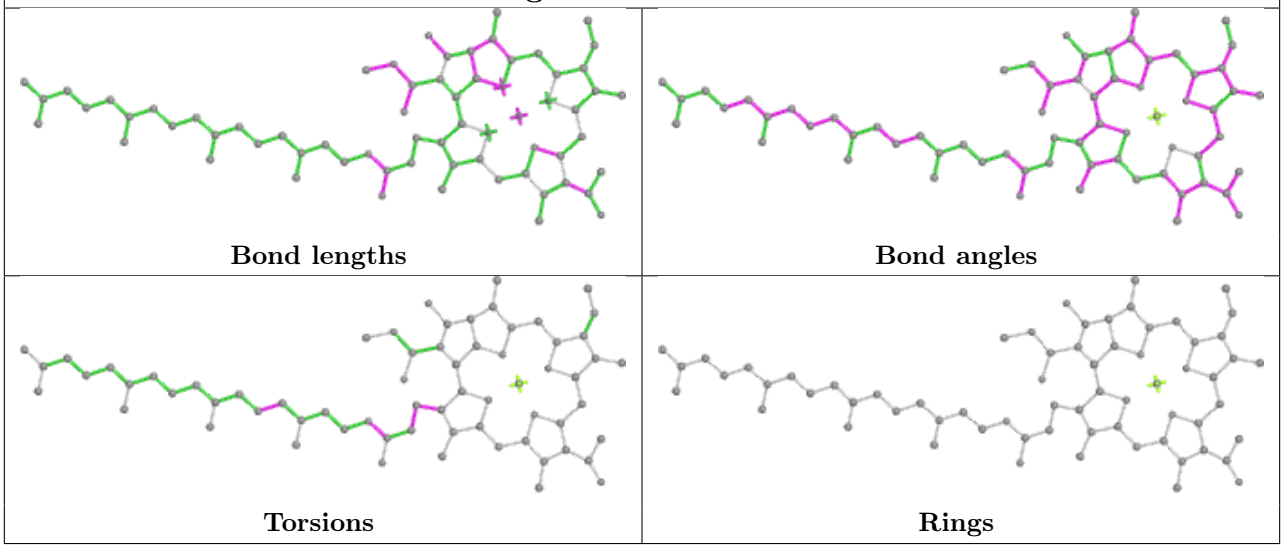
Ligand CDL M 408



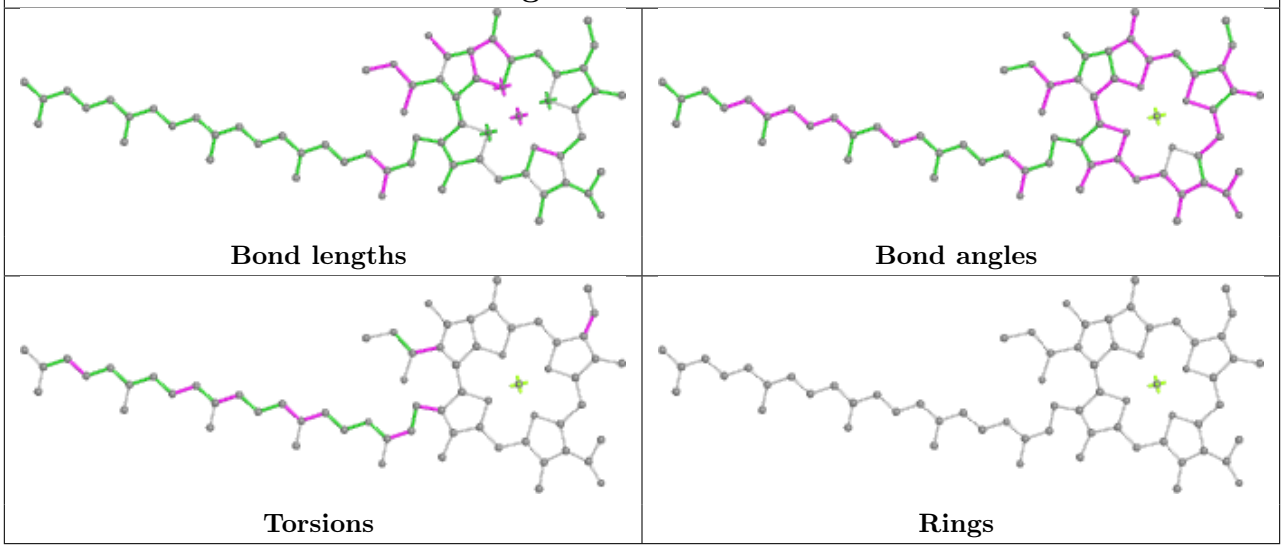
Ligand A1EFU E 102



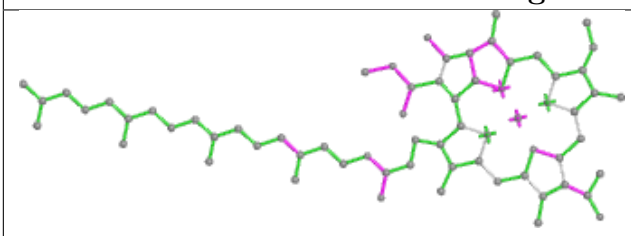
Ligand BCL R 101



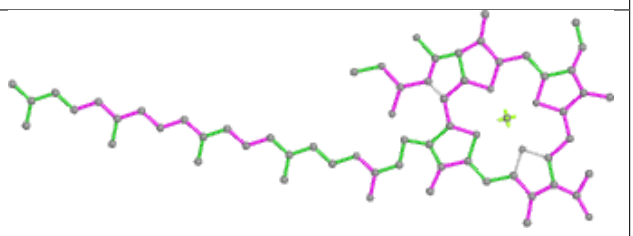
Ligand BCL M 404



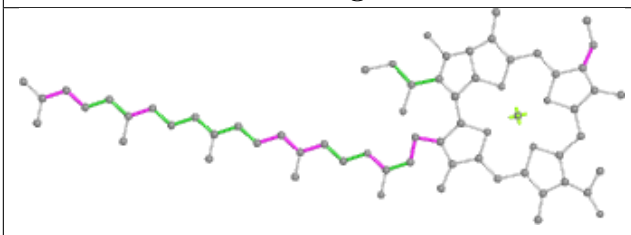
Ligand BCL S 302



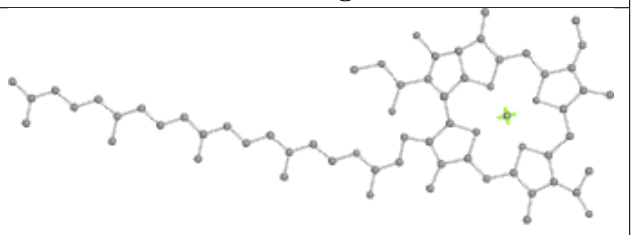
Bond lengths



Bond angles

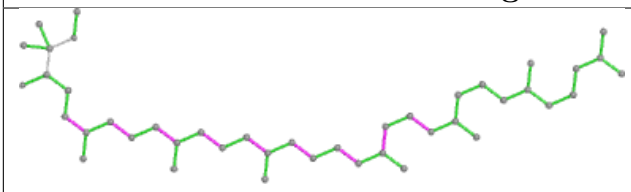


Torsions

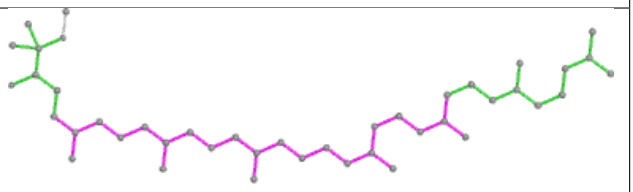


Rings

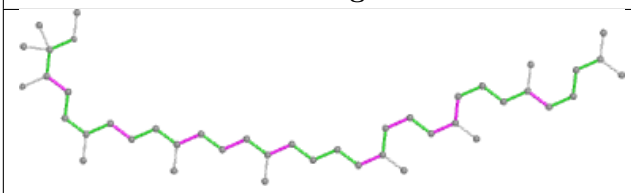
Ligand A1EFU A 103



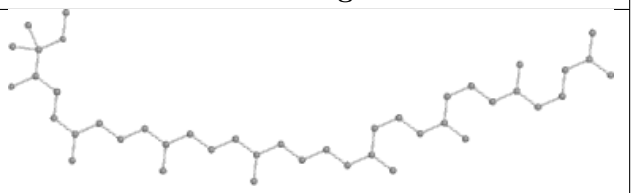
Bond lengths



Bond angles

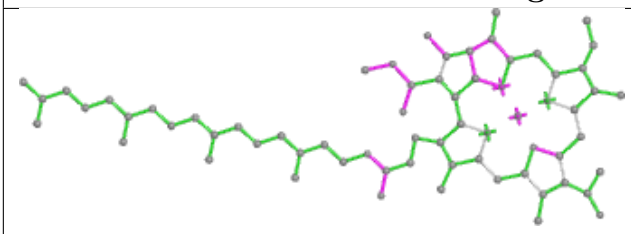


Torsions

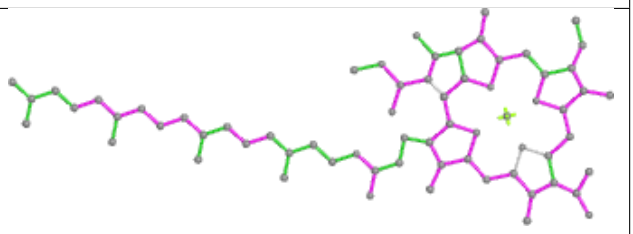


Rings

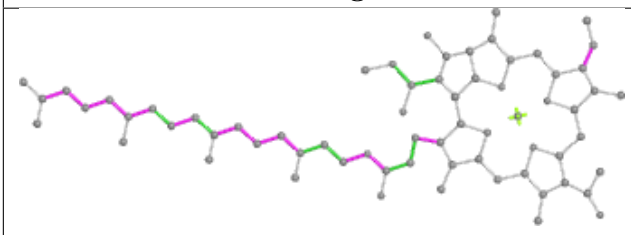
Ligand BCL L 301



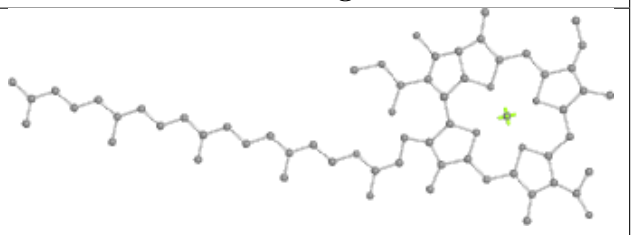
Bond lengths



Bond angles

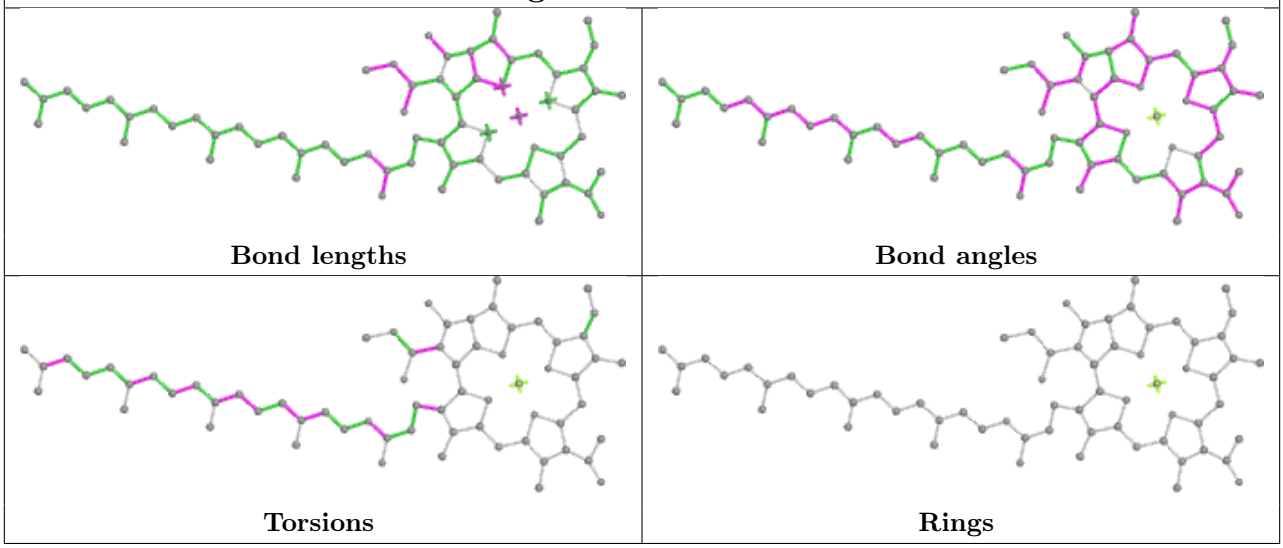


Torsions

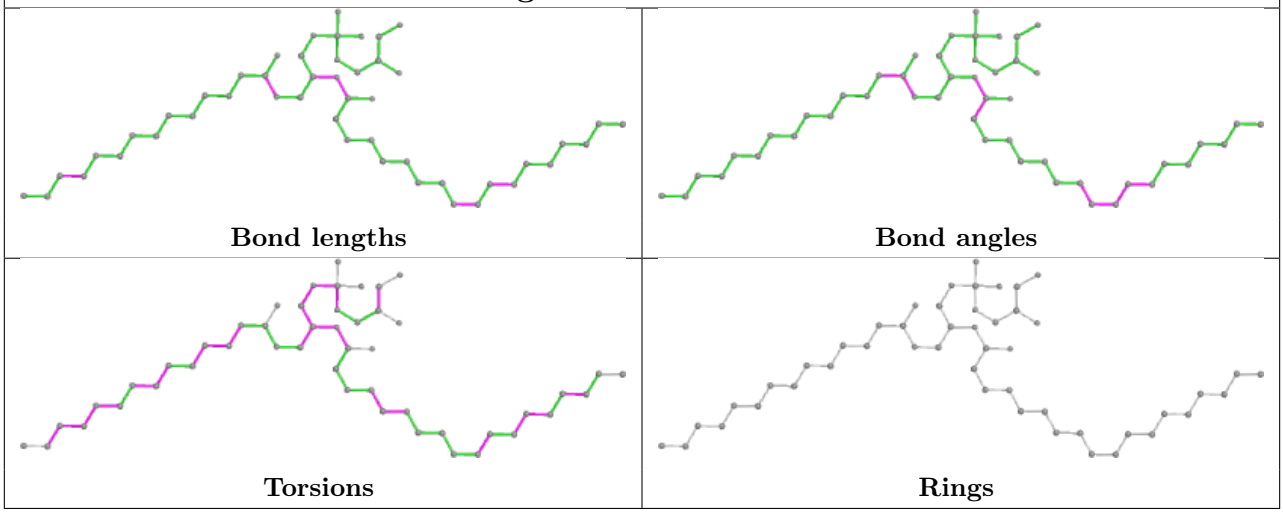


Rings

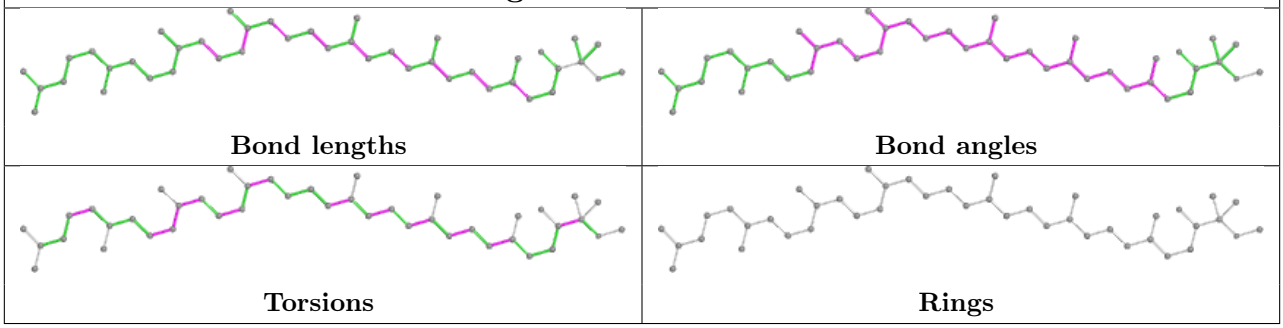
Ligand BCL F 101



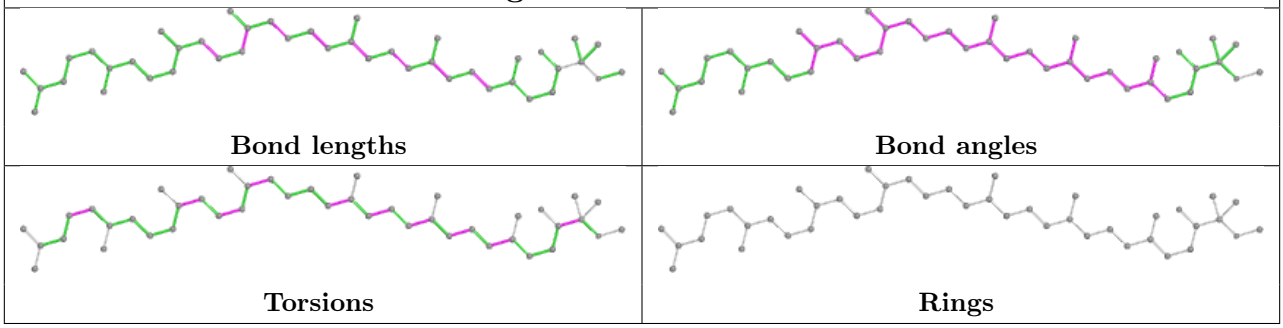
Ligand MW9 G 105



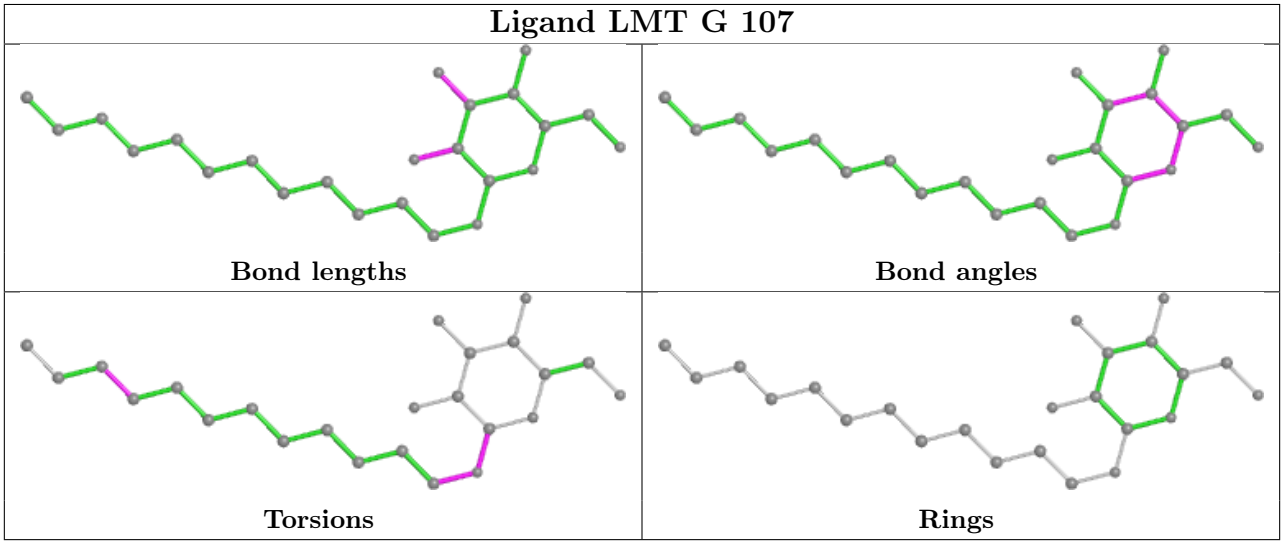
Ligand A1EFU S 303



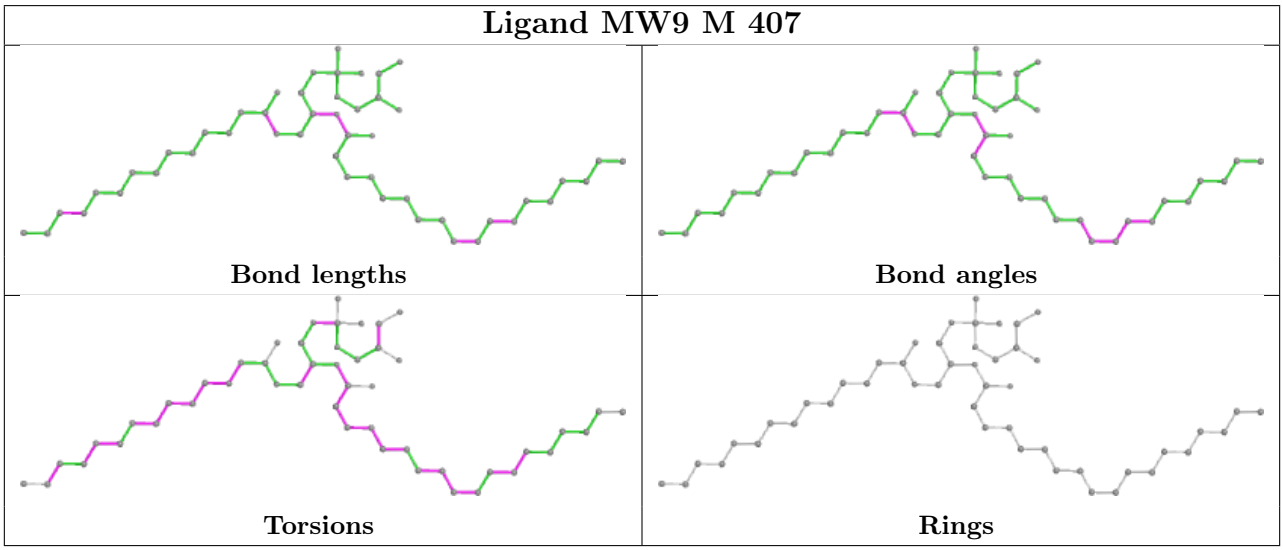
Ligand A1EFU b 102



Ligand LMT G 107



Ligand MW9 M 407



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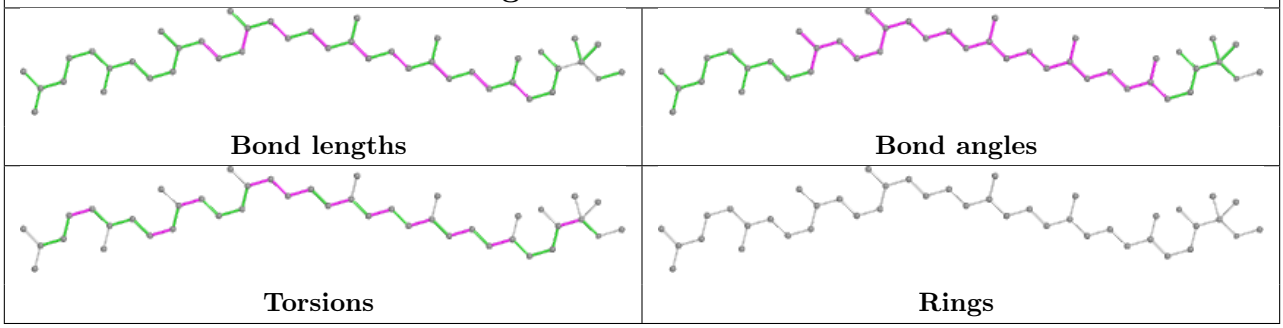
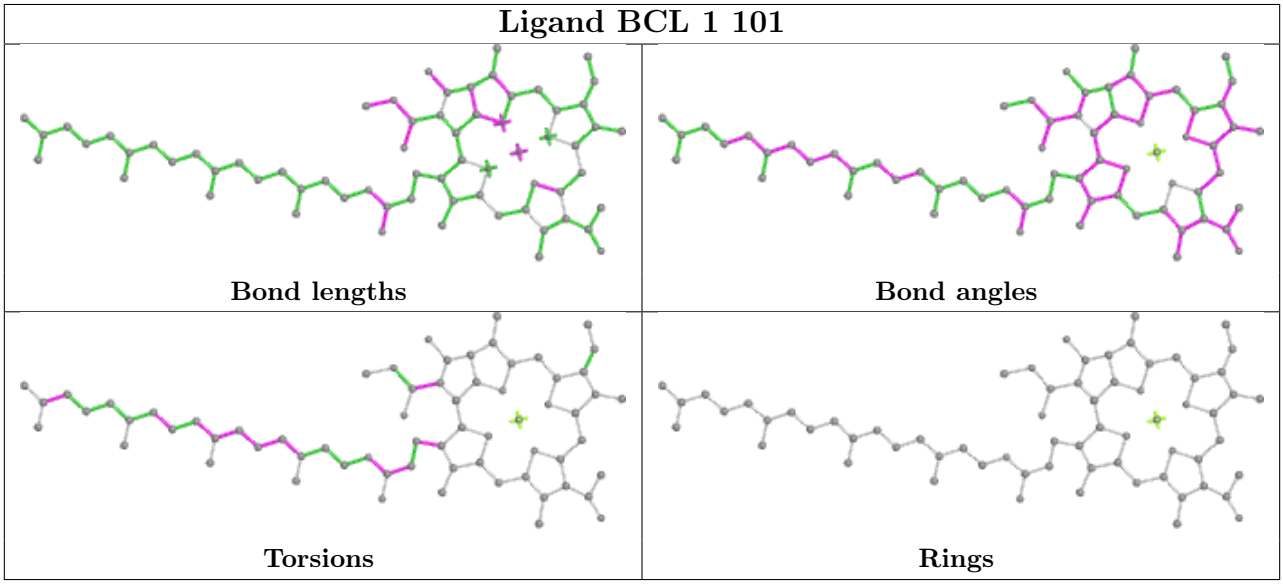


Ligand BCL 1 101



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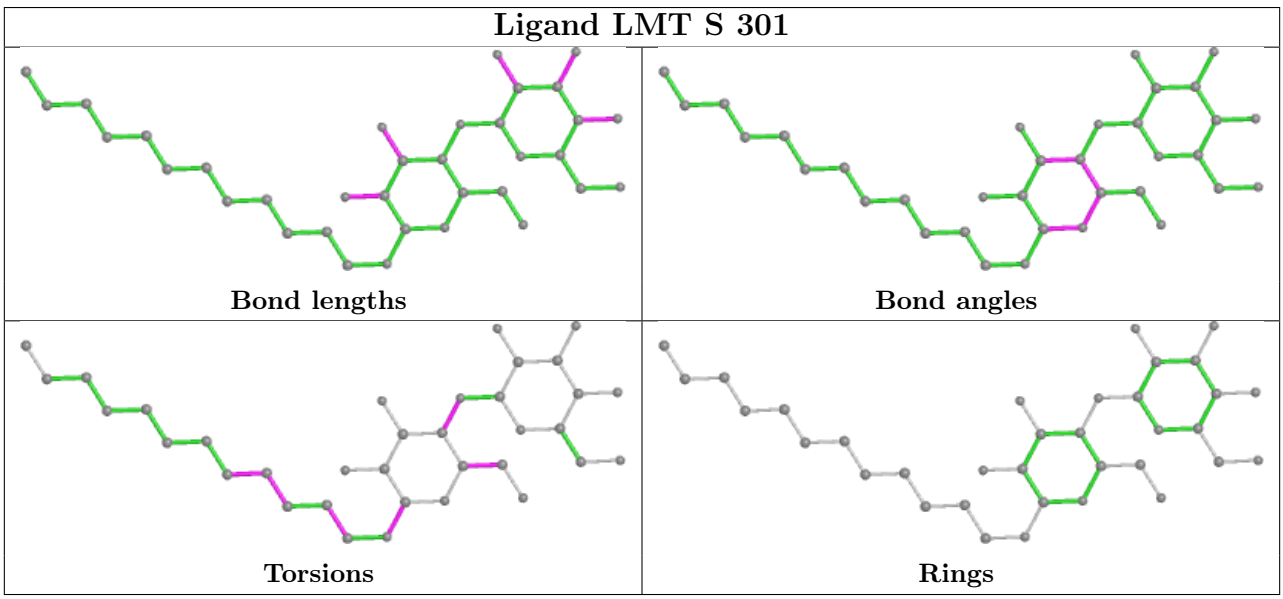

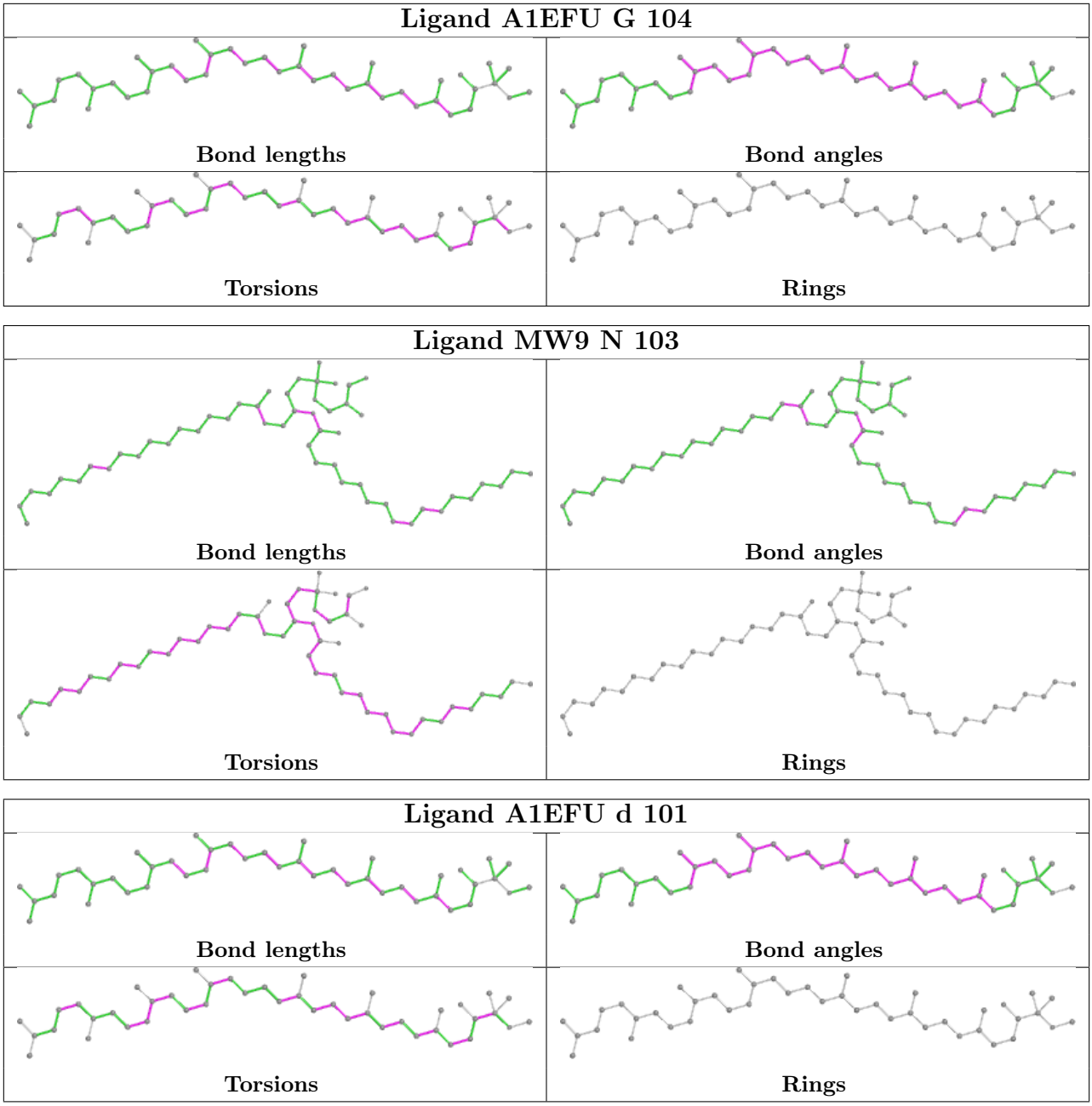

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.