Full wwPDB EM Validation Report (i)

Aug 6, 2026 – 01:20 AM JST

PDB ID	:	9KLM / pdb_00009klm
EMDB ID	:	EMD-62409
Title	:	Cryo-EM structure of the monomeric Rhodobacter sphaeroides G1C LH1-RC core complex
Authors	:	Wu, Y.-L.; Yu, L.-J.
Deposited on	:	2024-11-14
Resolution	:	2.60 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 (i) 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 (i)) were used in the production of this report:

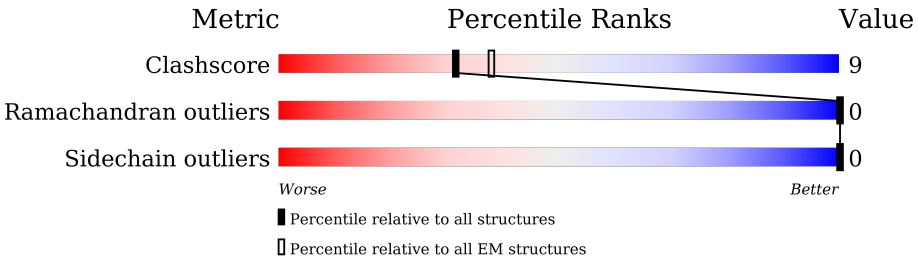
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

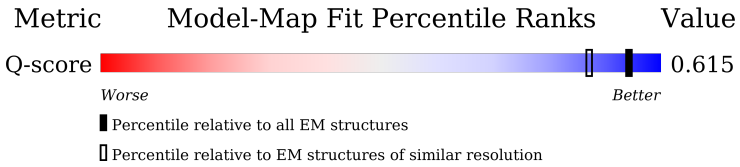
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.





Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	8728 (2.10 - 3.10)

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

Mol	Chain	Length	Quality of chain
1	L	282	83% 17%
2	M	308	85% 14% •
3	H	260	• 82% 14% •
4	A	54	• 63% 20% 17%

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Mol	Chain	Length	Quality of chain
4	B	54	80% 20%
4	C	54	83% 17%
4	D	54	80% 20%
4	E	54	81% 19%
4	F	54	80% 20%
4	G	54	87% 13%
4	I	54	81% 19%
4	J	54	74% 26%
4	K	54	87% 13%
4	N	54	9% 83% 17%
4	O	54	17% 83% 17%
4	P	54	26% 80% 19%
4	Q	54	52% 85% 9% 6%
5	a	49	71% 18% 10%
5	b	49	76% 14% 10%
5	c	49	78% 12% 10%
5	d	49	78% 10% 12%
5	e	49	78% 10% 12%
5	f	49	86% 12%
5	g	49	86% 10%
5	i	49	8% 71% 18% 10%
5	j	49	10% 73% 14% 12%
5	k	49	8% 71% 16% 12%
5	n	49	16% 71% 14% 14%
5	o	49	29% 65% 20% 14%

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Mol	Chain	Length	Quality of chain
5	p	49	41% 71% 14% 14%
5	q	49	61% 76% • 22%
6	U	53	36% 66% 25% 9%
7	X	82	• 52% 12% 35%

2 Entry composition (i)

There are 16 unique types of molecules in this entry. The entry contains 23521 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 Reaction center protein L chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	L	281	2229	1506	352	363	8	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	7	GLN	ARG	conflict	UNP P0C0Y8

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	M	306	2436	1626	398	401	11	0	0

- Molecule 3 is a protein called Reaction center protein H chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	H	250	1897	1215	325	347	10	0	0

- Molecule 4 is a protein called Light-harvesting protein B-875 alpha chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	A	45	386	266	59	58	3	0	0
4	B	54	455	309	73	70	3	0	0
4	C	54	457	311	73	70	3	0	0
4	D	54	457	311	73	70	3	0	0
4	E	54	457	311	73	70	3	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	F	54	457	311	73	70	3	0	0
4	G	54	457	311	73	70	3	0	0
4	I	54	454	309	73	70	2	0	0
4	J	54	457	311	73	70	3	0	0
4	K	54	457	311	73	70	3	0	0
4	N	54	457	311	73	70	3	0	0
4	O	54	457	311	73	70	3	0	0
4	P	53	447	305	72	68	2	0	0
4	Q	51	415	281	68	64	2	0	0

- Molecule 5 is a protein called Antenna pigment protein beta chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	a	44	359	240	56	62	1	0	0
5	b	44	359	240	56	62	1	0	0
5	c	44	359	240	56	62	1	0	0
5	d	43	351	236	55	59	1	0	0
5	e	43	351	236	55	59	1	0	0
5	f	43	351	236	55	59	1	0	0
5	g	44	355	238	56	60	1	0	0
5	i	44	359	240	56	62	1	0	0
5	j	43	347	234	55	57	1	0	0
5	k	43	351	236	55	59	1	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	n	42	343	230	54	58	1	0	0
5	o	42	343	230	54	58	1	0	0
5	p	42	332	222	54	55	1	0	0
5	q	38	296	202	49	44	1	0	0

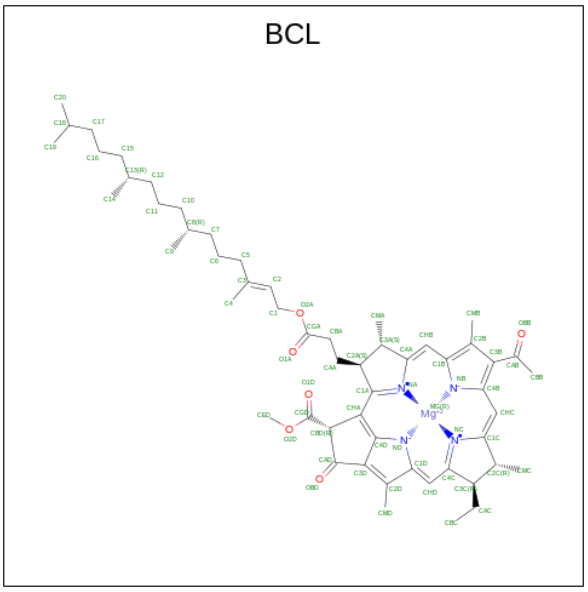
- Molecule 6 is a protein called protein-U.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	U	48	353	242	55	53	3	0	0

- Molecule 7 is a protein called Intrinsic membrane protein PufX.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	X	53	408	270	71	64	3	0	0

- Molecule 8 is BACTERIOCHLOROPHYLL A (CCD ID: BCL) (formula: $C_{55}H_{74}MgN_4O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
8	L	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
8	L	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
8	M	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
8	M	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
8	A	1	61	50	1	4	6	0
			Total	C	Mg	N	O	
8	a	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
8	B	1	61	50	1	4	6	0
			Total	C	Mg	N	O	
8	b	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
8	C	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
8	c	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
8	D	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
8	d	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
8	E	1	57	46	1	4	6	0
			Total	C	Mg	N	O	
8	e	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
8	F	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
8	f	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
8	G	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
8	g	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
8	I	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
8	i	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
8	J	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
8	j	1	66	55	1	4	6	0

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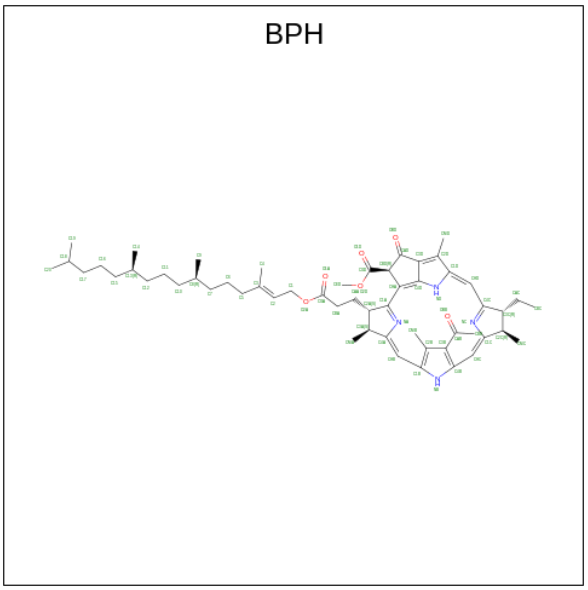
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
8	K	1	66	55	1	4	6	0
8	k	1	66	55	1	4	6	0
8	N	1	66	55	1	4	6	0
8	n	1	66	55	1	4	6	0
8	O	1	57	46	1	4	6	0
8	o	1	66	55	1	4	6	0
8	P	1	61	50	1	4	6	0
8	p	1	66	55	1	4	6	0
8	Q	1	61	50	1	4	6	0
8	q	1	60	49	1	4	6	0

- Molecule 9 is BACTERIOPHEOPHYTIN A (CCD ID: BPH) (formula: $C_{55}H_{76}N_4O_6$) (labeled as "Ligand of Interest" by depositor).



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

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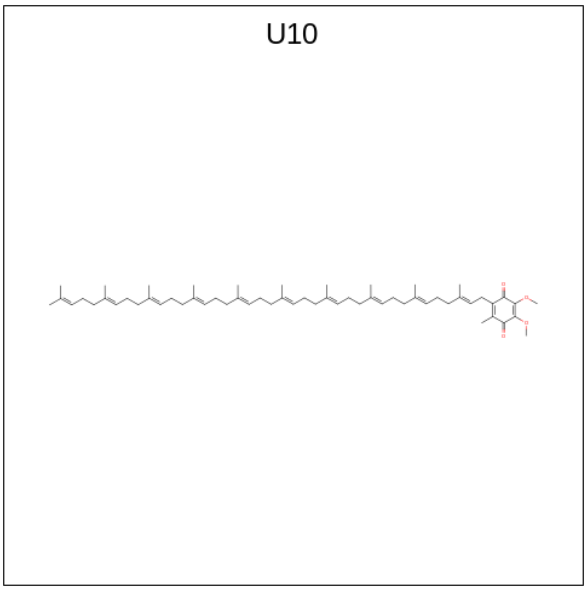
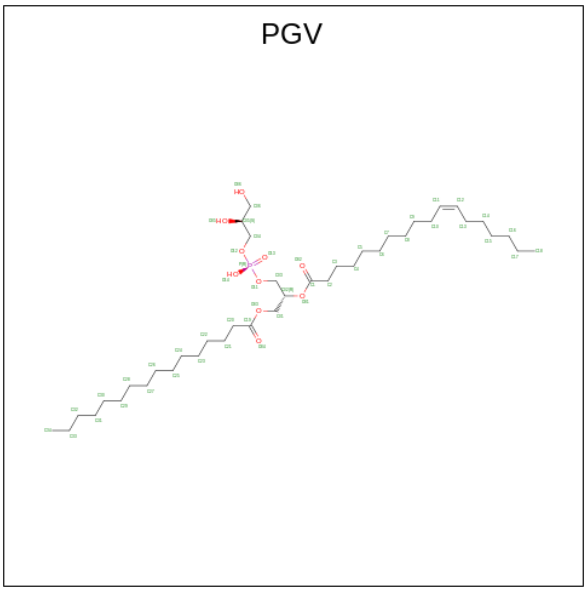
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
9	M	1	65	55	4	6	0

- Molecule 10 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
			Total	C	O		
10	L	1	35	31	4		0
			Total	C	O		
10	L	1	35	31	4		0
			Total	C	O		
10	M	1	48	44	4		0

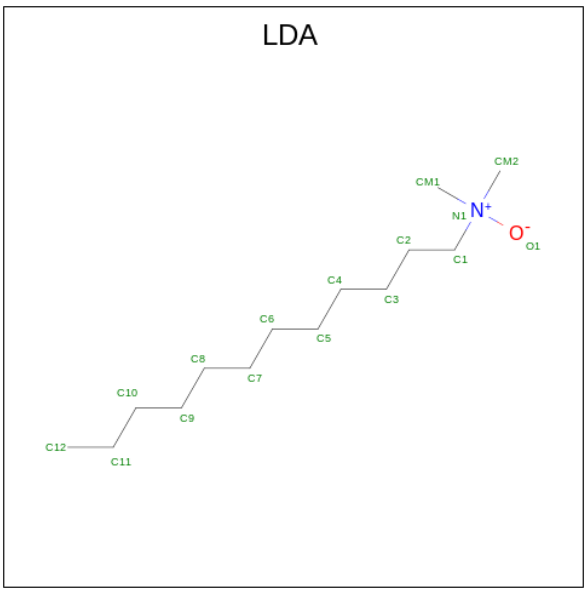
- Molecule 11 is (1R)-2-{[{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (CCD ID: PGV) (formula: $C_{40}H_{77}O_{10}P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
11	L	1	39	28	10	1	0
			Total	C	O	P	
11	L	1	33	22	10	1	0
			Total	C	O	P	
11	L	1	51	40	10	1	0
			Total	C	O	P	
11	L	1	39	28	10	1	0
			Total	C	O	P	
11	M	1	47	36	10	1	0
			Total	C	O	P	
11	M	1	42	31	10	1	0
			Total	C	O	P	
11	H	1	34	25	8	1	0
			Total	C	O	P	
11	H	1	40	29	10	1	0
			Total	C	O	P	
11	C	1	45	36	8	1	0
			Total	C	O	P	
11	C	1	47	36	10	1	0
			Total	C	O	P	
11	E	1	41	34	6	1	0
			Total	C	O	P	
11	G	1	39	28	10	1	0
			Total	C	O	P	
11	K	1	43	32	10	1	0

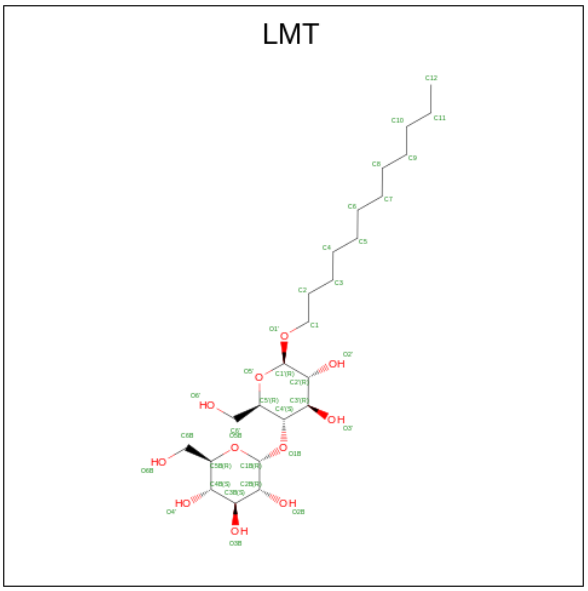
- Molecule 12 is LAURYL DIMETHYLAMINE-N-OXIDE (CCD ID: LDA) (formula:

$C_{14}H_{31}NO$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
12	L	1	Total	C	N	O	0
			16	14	1	1	
12	L	1	Total	C	N	O	0
			16	14	1	1	
12	L	1	Total	C	N	O	0
			16	14	1	1	
12	M	1	Total	C	N	O	0
			16	14	1	1	
12	F	1	Total	C	N	O	0
			16	14	1	1	
12	I	1	Total	C	N	O	0
			16	14	1	1	
12	J	1	Total	C	N	O	0
			16	14	1	1	
12	K	1	Total	C	N	O	0
			12	10	1	1	
12	X	1	Total	C	N	O	0
			13	11	1	1	
12	X	1	Total	C	N	O	0
			16	14	1	1	

- Molecule 13 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
13	L	1	Total 35	C 24	O 11	0
13	L	1	Total 35	C 24	O 11	0
13	L	1	Total 35	C 24	O 11	0
13	M	1	Total 27	C 20	O 7	0
13	M	1	Total 33	C 22	O 11	0
13	H	1	Total 35	C 24	O 11	0
13	H	1	Total 35	C 24	O 11	0
13	A	1	Total 35	C 24	O 11	0
13	a	1	Total 27	C 16	O 11	0
13	B	1	Total 35	C 24	O 11	0
13	b	1	Total 27	C 16	O 11	0
13	c	1	Total 17	C 11	O 6	0
13	c	1	Total 35	C 24	O 11	0
13	D	1	Total 26	C 16	O 10	0

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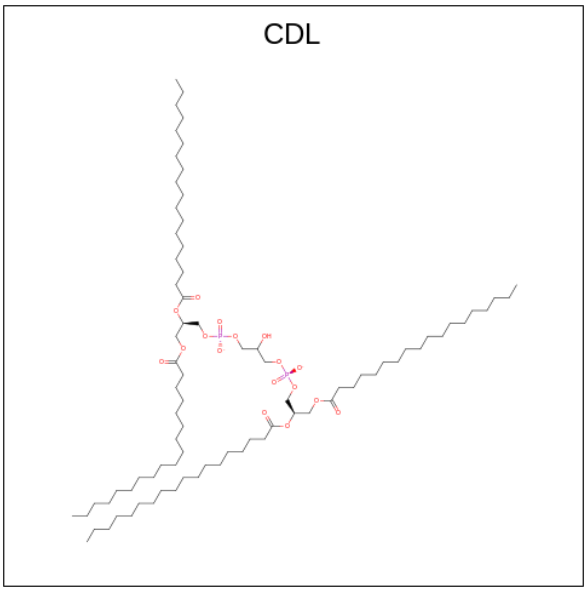
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
13	D	1	27	16	11	0
13	E	1	35	24	11	0
13	F	1	30	19	11	0
13	G	1	24	18	6	0
13	G	1	19	13	6	0
13	I	1	25	19	6	0
13	I	1	30	19	11	0
13	O	1	35	24	11	0
13	P	1	33	22	11	0
13	U	1	35	24	11	0
13	X	1	31	20	11	0

- Molecule 14 is FE (III) ION (CCD ID: FE) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

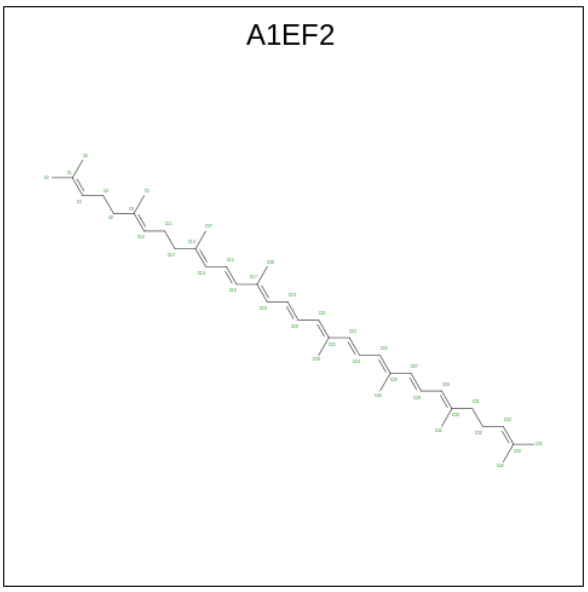
Mol	Chain	Residues	Atoms		AltConf
			Total	Fe	
14	M	1	1	1	0

- Molecule 15 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
15	M	1	Total	C	O	P	0
			79	60	17	2	
15	M	1	Total	C	O	P	0
			48	30	16	2	
15	E	1	Total	C	O	P	0
			57	38	17	2	
15	F	1	Total	C	O	P	0
			37	20	15	2	

- Molecule 16 is (6 {E},8 {E},10 {E},12 {E},14 {E},16 {E},18 {E},20 {E},22 {E},26 {E})-2,6,10,14,19,23,27,31-octamethyldotriaconta-2,6,8,10,12,14,16,18,20,22,26,30-dodecaene (CCD ID: A1EF2) (formula: $C_{40}H_{58}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms		AltConf
			Total	C	
16	M	1	40	40	0
16	a	1	40	40	0
16	B	1	40	40	0
16	b	1	40	40	0
16	C	1	40	40	0
16	c	1	40	40	0
16	D	1	40	40	0
16	D	1	40	40	0
16	d	1	40	40	0
16	E	1	40	40	0
16	e	1	40	40	0
16	f	1	40	40	0
16	g	1	40	40	0
16	g	1	40	40	0
16	I	1	40	40	0
16	J	1	40	40	0
16	J	1	40	40	0
16	J	1	40	40	0
16	J	1	40	40	0
16	k	1	40	40	0
16	N	1	40	40	0
16	N	1	40	40	0

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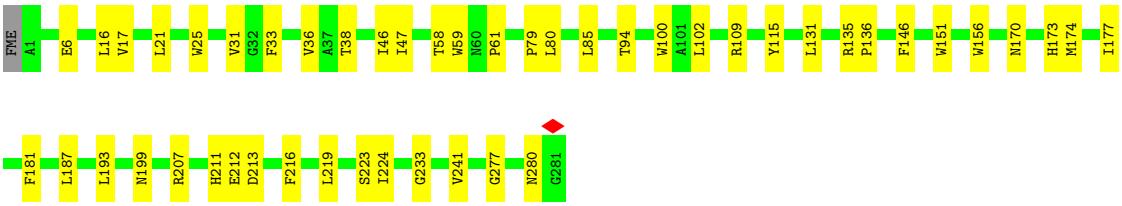
Mol	Chain	Residues	Atoms		AltConf
			Total	C	
16	n	1	40	40	0
			Total	C	
16	O	1	40	40	0
			Total	C	
16	o	1	40	40	0
			Total	C	
16	p	1	40	40	0
			Total	C	
16	q	1	40	40	0

3 Residue-property plots (i)

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

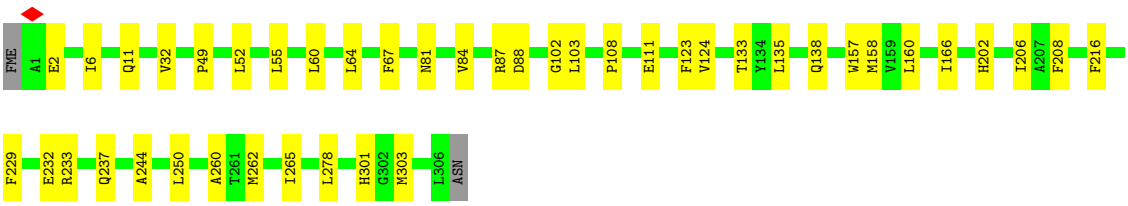
• Molecule 1: Reaction center protein L chain

Chain L: 83% 17%



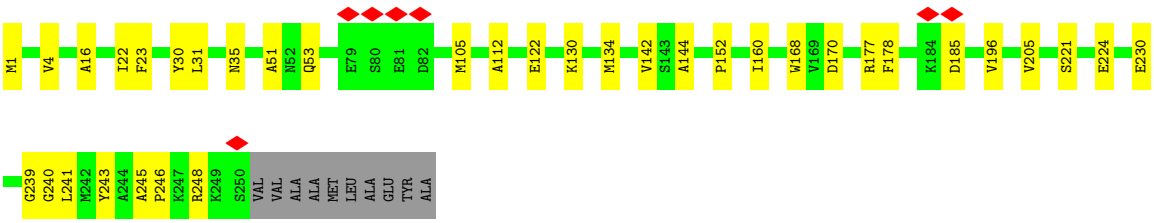
• Molecule 2: Reaction center protein M chain

Chain M: 85% 14%



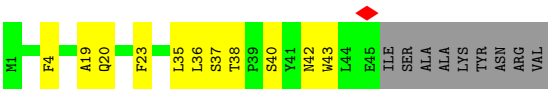
• Molecule 3: Reaction center protein H chain

Chain H: 82% 14%



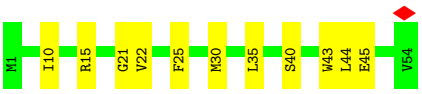
• Molecule 4: Light-harvesting protein B-875 alpha chain

Chain A: 63% 20% 17%



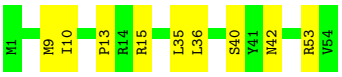
• Molecule 4: Light-harvesting protein B-875 alpha chain

Chain B: 80% 20%



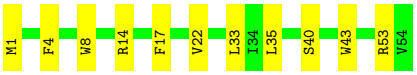
• Molecule 4: Light-harvesting protein B-875 alpha chain

Chain C: 83% 17%



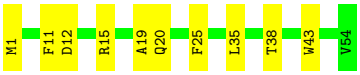
• Molecule 4: Light-harvesting protein B-875 alpha chain

Chain D: 80% 20%



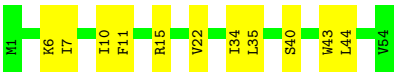
• Molecule 4: Light-harvesting protein B-875 alpha chain

Chain E: 81% 19%



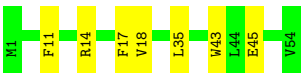
• Molecule 4: Light-harvesting protein B-875 alpha chain

Chain F: 80% 20%



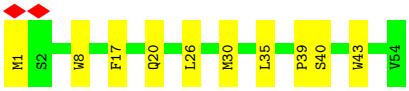
• Molecule 4: Light-harvesting protein B-875 alpha chain

Chain G: 87% 13%



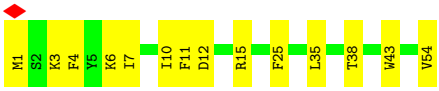
• Molecule 4: Light-harvesting protein B-875 alpha chain

Chain I: 81% 19%



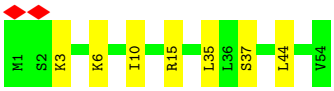
• Molecule 4: Light-harvesting protein B-875 alpha chain

Chain J:



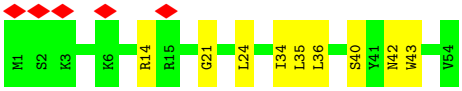
• Molecule 4: Light-harvesting protein B-875 alpha chain

Chain K:



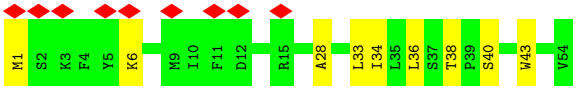
• Molecule 4: Light-harvesting protein B-875 alpha chain

Chain N:



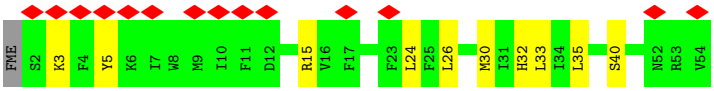
• Molecule 4: Light-harvesting protein B-875 alpha chain

Chain O:



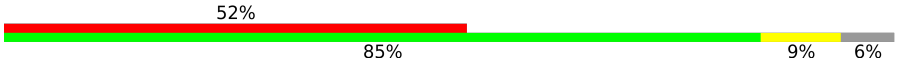
• Molecule 4: Light-harvesting protein B-875 alpha chain

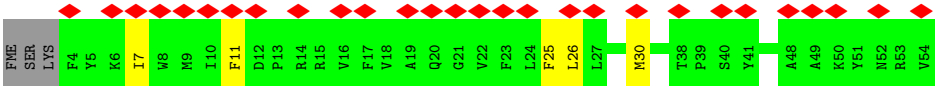
Chain P:



• Molecule 4: Light-harvesting protein B-875 alpha chain

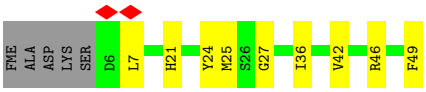
Chain Q:





• Molecule 5: Antenna pigment protein beta chain

Chain a:

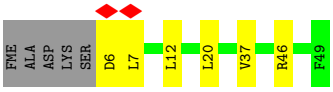


• Molecule 5: Antenna pigment protein beta chain

Chain b:

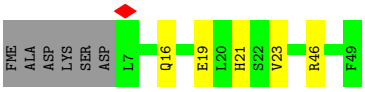
• Molecule 5: Antenna pigment protein beta chain

Chain c:



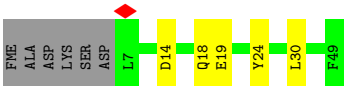
• Molecule 5: Antenna pigment protein beta chain

Chain d:



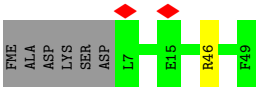
• Molecule 5: Antenna pigment protein beta chain

Chain e:



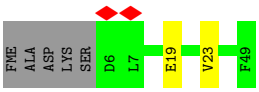
• Molecule 5: Antenna pigment protein beta chain

Chain f:



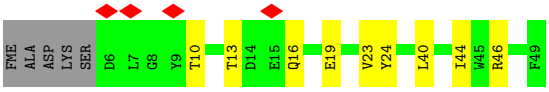
• Molecule 5: Antenna pigment protein beta chain

Chain g:



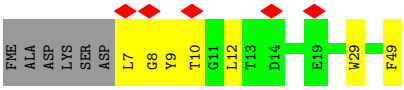
• Molecule 5: Antenna pigment protein beta chain

Chain i:



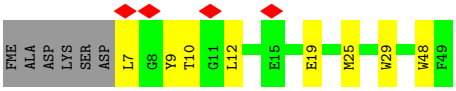
• Molecule 5: Antenna pigment protein beta chain

Chain j:



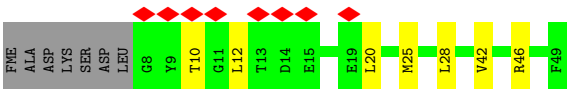
• Molecule 5: Antenna pigment protein beta chain

Chain k:



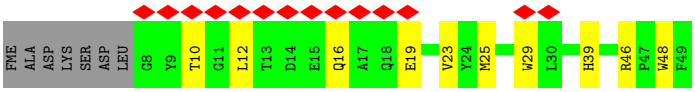
• Molecule 5: Antenna pigment protein beta chain

Chain n:



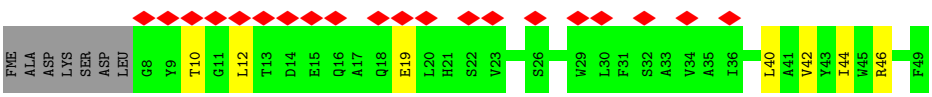
• Molecule 5: Antenna pigment protein beta chain

Chain o:



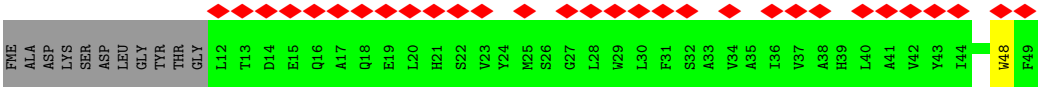
• Molecule 5: Antenna pigment protein beta chain

Chain p:



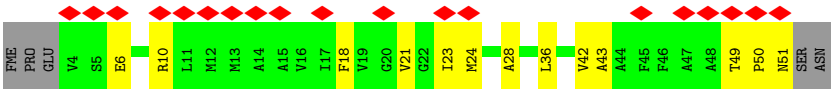
• Molecule 5: Antenna pigment protein beta chain

Chain q:



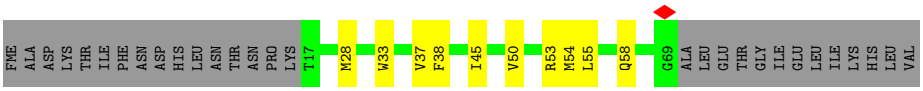
• Molecule 6: protein-U

Chain U:



• Molecule 7: Intrinsic membrane protein PufX

Chain X:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	118603	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50.61	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	2700	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.520	Depositor
Minimum map value	-0.828	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.037	Depositor
Recommended contour level	0.19	Depositor
Map size (Å)	323.2, 323.2, 323.2	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.808, 0.808, 0.808	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: BPH, FME, LDA, LMT, A1EF2, FE, U10, BCL, PGV, CDL

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	L	0.23	0/2317	0.33	0/3171
2	M	0.23	0/2529	0.33	0/3453
3	H	0.19	0/1947	0.30	0/2648
4	A	0.20	0/389	0.28	0/528
4	B	0.22	0/459	0.26	0/622
4	C	0.19	0/461	0.24	0/625
4	D	0.20	0/461	0.26	0/625
4	E	0.20	0/461	0.27	0/625
4	F	0.19	0/461	0.25	0/625
4	G	0.18	0/461	0.23	0/625
4	I	0.20	0/461	0.31	0/625
4	J	0.22	0/461	0.40	0/625
4	K	0.19	0/461	0.29	0/625
4	N	0.17	0/461	0.25	0/625
4	O	0.15	0/461	0.25	0/625
4	P	0.14	0/461	0.29	0/625
4	Q	0.11	0/427	0.24	0/582
5	a	0.20	0/372	0.28	0/510
5	b	0.22	0/372	0.30	0/510
5	c	0.20	0/372	0.32	0/510
5	d	0.21	0/364	0.28	0/499
5	e	0.20	0/364	0.27	0/499
5	f	0.19	0/364	0.32	0/499
5	g	0.19	0/368	0.30	0/505
5	i	0.19	0/372	0.31	0/510
5	j	0.19	0/360	0.30	0/494
5	k	0.20	0/364	0.32	0/499
5	n	0.16	0/356	0.27	0/488
5	o	0.14	0/356	0.22	0/488
5	p	0.14	0/344	0.27	0/472
5	q	0.12	0/308	0.23	0/424
6	U	0.15	0/364	0.28	0/493

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
7	X	0.20	0/419	0.32	0/567
All	All	0.20	0/18958	0.30	0/25846

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	L	2229	0	2175	47	0
2	M	2436	0	2353	43	0
3	H	1897	0	1904	28	0
4	A	386	0	400	12	0
4	B	455	0	469	11	0
4	C	457	0	476	9	0
4	D	457	0	476	12	0
4	E	457	0	476	11	0
4	F	457	0	476	12	0
4	G	457	0	476	7	0
4	I	454	0	469	13	0
4	J	457	0	476	15	0
4	K	457	0	476	6	0
4	N	457	0	476	10	0
4	O	457	0	476	7	0
4	P	447	0	465	9	0
4	Q	415	0	422	3	0
5	a	359	0	340	9	0
5	b	359	0	340	7	0
5	c	359	0	340	7	0
5	d	351	0	336	4	0
5	e	351	0	336	4	0
5	f	351	0	336	1	0
5	g	355	0	336	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	i	359	0	340	6	0
5	j	347	0	332	6	0
5	k	351	0	336	10	0
5	n	343	0	325	5	0
5	o	343	0	325	7	0
5	p	332	0	314	5	0
5	q	296	0	273	1	0
6	U	353	0	352	10	0
7	X	408	0	417	12	0
8	A	61	0	59	5	0
8	B	61	0	59	1	0
8	C	66	0	72	2	0
8	D	66	0	72	4	0
8	E	57	0	51	2	0
8	F	66	0	72	2	0
8	G	66	0	72	1	0
8	I	66	0	72	2	0
8	J	66	0	72	4	0
8	K	66	0	72	2	0
8	L	132	0	144	4	0
8	M	132	0	144	9	0
8	N	66	0	72	5	0
8	O	57	0	51	2	0
8	P	61	0	59	2	0
8	Q	61	0	59	1	0
8	a	66	0	72	6	0
8	b	66	0	72	2	0
8	c	66	0	72	4	0
8	d	66	0	72	6	0
8	e	66	0	72	3	0
8	f	66	0	72	4	0
8	g	66	0	72	5	0
8	i	66	0	72	5	0
8	j	66	0	72	3	0
8	k	66	0	72	3	0
8	n	66	0	72	4	0
8	o	66	0	72	8	0
8	p	66	0	72	5	0
8	q	60	0	56	2	0
9	L	65	0	76	6	0
9	M	65	0	76	15	0
10	L	70	0	86	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	M	48	0	63	7	0
11	C	92	0	126	8	0
11	E	41	0	60	4	0
11	G	39	0	48	0	0
11	H	74	0	87	8	0
11	K	43	0	54	4	0
11	L	162	0	207	12	0
11	M	89	0	120	7	0
12	F	16	0	31	3	0
12	I	16	0	31	6	0
12	J	16	0	31	2	0
12	K	12	0	20	1	0
12	L	48	0	93	9	0
12	M	16	0	31	2	0
12	X	29	0	53	4	0
13	A	35	0	46	1	0
13	B	35	0	46	12	0
13	D	53	0	51	6	0
13	E	35	0	46	0	0
13	F	30	0	33	6	0
13	G	43	0	55	0	0
13	H	70	0	92	3	0
13	I	55	0	68	2	0
13	L	105	0	138	22	0
13	M	60	0	75	2	0
13	O	35	0	46	1	0
13	P	33	0	39	2	0
13	U	35	0	46	2	0
13	X	31	0	35	2	0
13	a	27	0	27	4	0
13	b	27	0	27	0	0
13	c	52	0	62	2	0
14	M	1	0	0	0	0
15	E	57	0	58	2	0
15	F	37	0	26	1	0
15	M	127	0	151	8	0
16	B	40	0	0	0	0
16	C	40	0	0	0	0
16	D	80	0	0	1	0
16	E	40	0	0	0	0
16	I	40	0	0	0	0
16	J	160	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	M	40	0	0	0	0
16	N	80	0	0	0	0
16	O	40	0	0	0	0
16	a	40	0	0	1	0
16	b	40	0	0	0	0
16	c	40	0	0	0	0
16	d	40	0	0	0	0
16	e	40	0	0	0	0
16	f	40	0	0	0	0
16	g	80	0	0	0	0
16	k	40	0	0	0	0
16	n	40	0	0	0	0
16	o	40	0	0	0	0
16	p	40	0	0	0	0
16	q	40	0	0	0	0
All	All	23521	0	22973	406	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 (406) 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)
2:M:67:PHE:CD2	9:M:405:BPH:H7C2	1.87	1.10
2:M:67:PHE:HD2	9:M:405:BPH:H7C2	1.16	1.06
4:B:21:GLY:HA3	13:B:102:LMT:H5B	1.48	0.91
4:K:3:LYS:HD2	4:K:6:LYS:HE2	1.58	0.86
4:I:20:GLN:HE21	8:J:102:BCL:H13	1.44	0.81
1:L:187:LEU:HD13	2:M:216:PHE:HB2	1.64	0.80
1:L:36:VAL:HG12	13:B:102:LMT:H6E	1.67	0.77
3:H:105:MET:HE2	3:H:240:GLY:HA2	1.65	0.77
2:M:67:PHE:CD2	9:M:405:BPH:C7	2.67	0.76
2:M:60:LEU:HD21	15:M:413:CDL:H512	1.69	0.75
3:H:53:GLN:H	11:H:304:PGV:H062	1.53	0.74
8:d:102:BCL:H2	8:d:102:BCL:HAA1	1.71	0.72
4:P:40:SER:O	5:p:46:ARG:NH1	2.22	0.72
2:M:229:PHE:HB2	2:M:244:ALA:HB2	1.71	0.72
5:n:10:THR:HG23	5:n:12:LEU:H	1.54	0.71
4:A:35:LEU:HD11	8:a:102:BCL:HHD	1.71	0.71
7:X:50:VAL:HG22	7:X:53:ARG:HH21	1.54	0.71
4:J:35:LEU:HD11	8:j:101:BCL:HHD	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:4:PHE:HB2	13:D:103:LMT:H6'2	1.73	0.71
4:J:4:PHE:O	4:J:7:ILE:HD12	1.92	0.70
13:L:311:LMT:H61	13:A:701:LMT:H52	1.74	0.70
2:M:67:PHE:CE2	9:M:405:BPH:C7	2.75	0.70
2:M:6:ILE:HD13	13:M:409:LMT:H42	1.74	0.69
4:O:40:SER:O	5:o:46:ARG:NH1	2.26	0.69
15:M:410:CDL:H312	15:M:410:CDL:H122	1.73	0.69
4:N:40:SER:O	5:n:46:ARG:NH1	2.26	0.69
4:P:35:LEU:HD11	8:p:102:BCL:HHD	1.74	0.69
12:L:309:LDA:H112	12:L:310:LDA:H42	1.74	0.69
4:B:35:LEU:HD11	8:b:103:BCL:HHD	1.74	0.69
3:H:31:LEU:O	3:H:35:ASN:ND2	2.26	0.68
9:L:302:BPH:H141	8:L:308:BCL:HBB3	1.75	0.68
4:E:35:LEU:HD11	8:e:102:BCL:HHD	1.76	0.68
2:M:232:GLU:OE2	3:H:177:ARG:NH1	2.27	0.68
2:M:52:LEU:O	4:J:15:ARG:NH2	2.27	0.67
2:M:67:PHE:CE2	9:M:405:BPH:H7C1	2.30	0.67
4:D:35:LEU:HD11	8:d:102:BCL:HHD	1.76	0.67
4:J:7:ILE:HG23	4:J:11:PHE:HD2	1.59	0.67
5:o:10:THR:HG23	5:o:12:LEU:H	1.59	0.65
1:L:31:VAL:HG22	10:M:407:U10:H371	1.78	0.65
8:M:404:BCL:H11	9:M:405:BPH:HBB3	1.76	0.65
3:H:152:PRO:HB2	3:H:160:ILE:HD12	1.79	0.65
2:M:124:VAL:HA	11:M:412:PGV:H22	1.80	0.64
4:O:6:LYS:NZ	5:p:19:GLU:OE2	2.30	0.64
4:I:20:GLN:NE2	5:i:24:TYR:OH	2.31	0.64
4:F:40:SER:O	5:f:46:ARG:NH1	2.30	0.63
4:N:35:LEU:HD11	8:n:102:BCL:HHD	1.79	0.63
4:J:38:THR:HG21	4:K:44:LEU:HD13	1.79	0.63
4:K:37:SER:HB3	12:K:101:LDA:H62	1.80	0.63
4:P:30:MET:HG3	6:U:28:ALA:HB2	1.81	0.62
13:L:311:LMT:H6'1	4:B:45:GLU:HG2	1.80	0.62
2:M:67:PHE:CE2	9:M:405:BPH:H7C2	2.34	0.61
1:L:199:ASN:HB3	15:M:410:CDL:HA22	1.81	0.61
4:A:36:LEU:O	4:A:42:ASN:ND2	2.34	0.61
4:C:9:MET:HE1	5:c:6:ASP:HB2	1.81	0.61
11:H:303:PGV:H202	11:C:101:PGV:H231	1.81	0.61
9:M:405:BPH:HBB3	9:M:405:BPH:HHC	1.82	0.61
4:E:25:PHE:HB2	8:E:103:BCL:H61	1.82	0.61
5:c:7:LEU:HD22	5:d:16:GLN:HE22	1.66	0.61
13:L:312:LMT:H4'	13:B:102:LMT:H5'	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:702:BCL:H92	7:X:28:MET:HE3	1.82	0.60
4:B:40:SER:O	5:b:46:ARG:NH2	2.33	0.60
5:i:13:THR:HB	5:i:16:GLN:HG3	1.84	0.60
9:M:405:BPH:HBC3	9:M:405:BPH:HHD	1.83	0.60
4:A:40:SER:O	5:a:46:ARG:NH1	2.34	0.60
2:M:64:LEU:HB2	9:M:405:BPH:H112	1.83	0.59
4:G:35:LEU:HD11	8:g:102:BCL:HHD	1.82	0.59
1:L:216:PHE:HD2	10:L:303:U10:H71	1.68	0.59
4:F:15:ARG:NH2	15:F:102:CDL:OB6	2.34	0.59
11:L:313:PGV:H212	4:N:34:ILE:HG12	1.85	0.59
2:M:2:GLU:HG3	12:M:403:LDA:H12	1.84	0.59
13:L:312:LMT:H4B	13:B:102:LMT:H1B	1.85	0.58
2:M:102:GLY:HA3	13:I:101:LMT:H6E	1.86	0.58
11:H:304:PGV:H32	8:D:102:BCL:H121	1.84	0.58
2:M:67:PHE:HE2	9:M:405:BPH:H7C1	1.67	0.58
4:D:40:SER:O	5:d:46:ARG:NH2	2.35	0.58
8:A:702:BCL:HHD	5:a:42:VAL:HG21	1.85	0.58
4:A:4:PHE:HD2	13:a:101:LMT:H3'	1.69	0.58
4:O:28:ALA:HB2	8:o:102:BCL:HED3	1.86	0.58
4:C:35:LEU:HD11	8:c:102:BCL:HHD	1.85	0.58
7:X:58:GLN:CD	7:X:58:GLN:H	2.12	0.58
2:M:278:LEU:HD21	15:M:410:CDL:H382	1.86	0.57
4:P:33:LEU:HD11	13:P:101:LMT:H52	1.86	0.57
2:M:32:VAL:HG22	2:M:49:PRO:HD3	1.87	0.57
5:k:7:LEU:HD11	5:n:20:LEU:HD12	1.86	0.56
3:H:1:MET:HE1	13:F:101:LMT:H41	1.87	0.56
2:M:265:ILE:HG21	10:M:407:U10:H3M3	1.88	0.56
13:L:312:LMT:O2B	4:A:19:ALA:O	2.23	0.56
8:M:404:BCL:H141	9:M:405:BPH:H4C2	1.86	0.56
4:D:1:FME:SD	13:D:103:LMT:O6'	2.63	0.56
1:L:102:LEU:HD21	12:L:310:LDA:H11	1.87	0.55
11:H:304:PGV:H11	4:D:22:VAL:HG22	1.88	0.55
8:o:102:BCL:H152	8:o:102:BCL:HBB2	1.89	0.55
5:p:10:THR:HG23	5:p:12:LEU:H	1.71	0.55
13:D:103:LMT:H5B	5:d:21:HIS:HE2	1.71	0.55
4:K:35:LEU:HD11	8:k:102:BCL:HHD	1.88	0.55
11:M:412:PGV:H062	12:I:104:LDA:HM11	1.88	0.55
5:a:36:ILE:HA	8:a:102:BCL:H92	1.88	0.54
6:U:21:VAL:HA	6:U:24:MET:HG2	1.87	0.54
1:L:280:ASN:ND2	2:M:88:ASP:OD1	2.37	0.54
8:L:301:BCL:H152	9:L:302:BPH:H3A	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:123:PHE:HA	2:M:157:TRP:HH2	1.72	0.54
4:I:40:SER:O	5:i:46:ARG:NH1	2.39	0.54
12:F:104:LDA:H122	4:G:14:ARG:HE	1.73	0.54
4:C:15:ARG:NH2	11:C:101:PGV:O13	2.40	0.54
12:F:104:LDA:HM12	4:G:18:VAL:HA	1.90	0.54
4:P:32:HIS:CE1	8:p:102:BCL:HMD3	2.43	0.54
8:N:101:BCL:HHD	5:n:42:VAL:HG21	1.89	0.53
4:I:39:PRO:HB2	4:J:54:VAL:HG12	1.90	0.53
10:M:407:U10:H303	11:C:101:PGV:H282	1.89	0.53
4:N:36:LEU:O	4:N:42:ASN:ND2	2.41	0.53
9:L:302:BPH:HHC	9:L:302:BPH:HBB3	1.91	0.53
3:H:51:ALA:O	4:D:14:ARG:NH1	2.42	0.52
1:L:17:VAL:HG22	12:X:101:LDA:HM23	1.91	0.52
4:I:26:LEU:HD21	12:I:104:LDA:H82	1.91	0.52
1:L:36:VAL:CG1	13:B:102:LMT:H6E	2.38	0.52
11:L:305:PGV:H22	4:D:33:LEU:HD13	1.92	0.52
3:H:221:SER:HB2	3:H:224:GLU:HB3	1.92	0.52
3:H:22:ILE:HG23	15:E:101:CDL:H161	1.91	0.52
4:Q:7:ILE:HG23	4:Q:11:PHE:HD2	1.75	0.51
5:a:21:HIS:NE2	13:a:101:LMT:O2B	2.40	0.51
4:E:11:PHE:HD1	11:E:104:PGV:H032	1.76	0.51
11:E:104:PGV:H292	4:F:22:VAL:HA	1.92	0.51
8:q:102:BCL:H121	8:q:102:BCL:C4B	2.40	0.51
3:H:196:VAL:HG12	3:H:205:VAL:HG22	1.93	0.51
1:L:80:LEU:HD21	13:L:311:LMT:H22	1.93	0.51
4:J:3:LYS:NZ	5:k:19:GLU:OE2	2.42	0.51
8:M:401:BCL:H93	8:M:401:BCL:HAA2	1.92	0.51
5:k:9:TYR:HB3	4:N:14:ARG:NH2	2.26	0.51
5:o:48:TRP:HZ2	8:o:102:BCL:H13	1.75	0.51
1:L:241:VAL:HG21	9:L:302:BPH:HBC3	1.93	0.51
11:L:313:PGV:H232	4:N:34:ILE:HD11	1.93	0.51
3:H:241:LEU:HA	3:H:248:ARG:HH22	1.75	0.51
13:H:302:LMT:O2B	13:H:302:LMT:O6'	2.28	0.51
4:F:35:LEU:HD11	8:f:102:BCL:HHD	1.92	0.51
8:n:102:BCL:H2	8:n:102:BCL:HAA1	1.93	0.51
1:L:216:PHE:CD2	10:L:303:U10:H71	2.46	0.50
1:L:193:LEU:HD22	1:L:216:PHE:CE2	2.46	0.50
4:P:15:ARG:HH12	6:U:49:THR:HB	1.76	0.50
4:E:20:GLN:NE2	5:e:24:TYR:OH	2.35	0.50
2:M:233:ARG:NH2	3:H:122:GLU:OE1	2.38	0.50
4:P:26:LEU:HD11	6:U:42:VAL:HG21	1.92	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:P:24:LEU:HB2	8:P:102:BCL:H42	1.93	0.49
11:M:412:PGV:H032	4:J:25:PHE:CZ	2.47	0.49
4:F:6:LYS:NZ	5:g:19:GLU:OE2	2.30	0.49
1:L:58:THR:HA	11:L:305:PGV:H05	1.94	0.49
13:L:312:LMT:O3'	4:A:23:PHE:HB2	2.12	0.49
5:c:46:ARG:NH2	4:D:53:ARG:HD3	2.27	0.49
4:Q:26:LEU:O	4:Q:30:MET:HG2	2.12	0.49
2:M:260:ALA:N	10:M:407:U10:O5	2.44	0.49
1:L:33:PHE:CE1	13:L:312:LMT:H5'	2.48	0.49
13:L:312:LMT:H1B	13:B:102:LMT:O1B	2.13	0.49
4:A:38:THR:HG21	4:B:44:LEU:HD13	1.94	0.49
13:L:312:LMT:H4B	13:B:102:LMT:H4B	1.95	0.48
4:I:30:MET:HB2	12:I:104:LDA:HM22	1.93	0.48
8:L:308:BCL:H151	8:L:308:BCL:H18	1.64	0.48
4:I:35:LEU:HD11	8:i:101:BCL:HHD	1.95	0.48
4:F:7:ILE:HA	4:F:10:ILE:HD12	1.95	0.48
8:g:102:BCL:H162	8:g:102:BCL:H202	1.69	0.48
9:L:302:BPH:HHC	9:L:302:BPH:CBB	2.43	0.48
5:a:25:MET:HE2	13:a:101:LMT:H4'	1.93	0.48
5:k:10:THR:HG23	5:k:12:LEU:HB2	1.94	0.48
11:L:313:PGV:H261	11:L:313:PGV:H51	1.96	0.48
12:L:307:LDA:HM21	12:M:403:LDA:H41	1.95	0.48
11:L:313:PGV:H241	11:L:313:PGV:H41	1.96	0.48
3:H:168:TRP:HB2	3:H:178:PHE:HB2	1.96	0.48
4:D:43:TRP:CE3	8:D:102:BCL:HAC2	2.48	0.48
8:i:101:BCL:H141	8:i:101:BCL:H162	1.72	0.48
5:k:9:TYR:HB3	4:N:14:ARG:HH21	1.79	0.48
1:L:94:THR:HG21	12:L:310:LDA:H123	1.95	0.47
4:B:10:ILE:HA	5:b:9:TYR:HB2	1.96	0.47
5:i:19:GLU:O	5:i:23:VAL:HG23	2.14	0.47
1:L:193:LEU:HD21	1:L:212:GLU:HB3	1.97	0.47
2:M:202:HIS:CE1	2:M:206:ILE:HD11	2.49	0.47
4:A:43:TRP:NE1	8:A:702:BCL:OBB	2.46	0.47
12:L:309:LDA:H122	7:X:37:VAL:HG21	1.97	0.47
11:L:313:PGV:H22	4:O:33:LEU:HD22	1.96	0.47
5:a:27:GLY:HA3	16:a:103:A1EF2:C25	2.45	0.47
8:d:102:BCL:HAA1	8:d:102:BCL:C2	2.41	0.47
1:L:61:PRO:HD3	11:L:305:PGV:H32	1.97	0.47
2:M:11:GLN:HB2	3:H:144:ALA:HB3	1.96	0.47
9:L:302:BPH:C14	8:L:308:BCL:HBB3	2.44	0.47
5:p:40:LEU:O	5:p:44:ILE:HD12	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:M:407:U10:H303	11:C:101:PGV:H251	1.97	0.46
8:c:102:BCL:H61	8:c:102:BCL:H41	1.47	0.46
13:L:312:LMT:O6B	13:L:312:LMT:O4'	2.18	0.46
11:C:102:PGV:H92	8:C:103:BCL:H72	1.96	0.46
4:F:11:PHE:HZ	4:G:17:PHE:HB2	1.80	0.46
1:L:61:PRO:HG3	11:L:305:PGV:H51	1.97	0.46
1:L:207:ARG:HD2	1:L:211:HIS:CD2	2.50	0.46
5:n:25:MET:HE1	5:n:28:LEU:HD22	1.97	0.46
3:H:1:MET:SD	13:F:101:LMT:O2'	2.68	0.46
4:B:25:PHE:HE2	13:B:102:LMT:H32	1.81	0.46
8:p:102:BCL:H92	8:p:102:BCL:HAA1	1.96	0.46
4:O:43:TRP:CE3	8:O:102:BCL:HAC2	2.51	0.46
12:L:309:LDA:H123	12:X:101:LDA:H62	1.97	0.46
8:M:404:BCL:C1	9:M:405:BPH:HBB3	2.45	0.46
3:H:130:LYS:HE3	3:H:170:ASP:OD2	2.15	0.46
1:L:181:PHE:HB3	9:M:405:BPH:HBB2	1.98	0.46
5:b:7:LEU:HD13	5:c:12:LEU:HD21	1.96	0.46
13:L:311:LMT:H11	4:A:37:SER:HB2	1.97	0.45
4:E:19:ALA:HA	15:E:101:CDL:H311	1.97	0.45
4:G:43:TRP:CE3	8:G:104:BCL:HAC2	2.51	0.45
4:J:43:TRP:CE3	8:J:102:BCL:HAC2	2.52	0.45
4:B:43:TRP:CE3	8:B:101:BCL:HAC2	2.51	0.45
5:b:25:MET:HE1	5:b:28:LEU:HD22	1.98	0.45
8:d:102:BCL:H141	8:d:102:BCL:H161	1.66	0.45
2:M:108:PRO:HD2	2:M:111:GLU:HB2	1.98	0.45
3:H:4:VAL:HG11	13:F:101:LMT:O2'	2.16	0.45
8:p:102:BCL:H93	8:p:102:BCL:H61	1.78	0.45
2:M:237:GLN:HB2	2:M:262:MET:HG2	1.99	0.45
15:M:410:CDL:H112	3:H:30:TYR:CZ	2.52	0.45
13:D:103:LMT:H6D	5:e:30:LEU:HD21	1.99	0.45
8:e:102:BCL:H91	8:e:102:BCL:H112	1.76	0.45
1:L:100:TRP:CH2	10:M:407:U10:H28	2.52	0.45
13:M:408:LMT:H111	3:H:16:ALA:HB2	1.97	0.45
4:A:20:GLN:NE2	5:a:24:TYR:OH	2.40	0.45
12:L:309:LDA:HM23	12:L:309:LDA:H21	1.75	0.45
4:I:20:GLN:NE2	8:J:102:BCL:H13	2.22	0.45
4:J:6:LYS:NZ	5:k:19:GLU:OE2	2.42	0.45
1:L:213:ASP:OD1	1:L:223:SER:OG	2.34	0.45
5:c:37:VAL:HG12	13:c:103:LMT:H101	1.99	0.45
8:e:102:BCL:H162	8:e:102:BCL:H192	1.78	0.45
10:L:304:U10:H8	10:L:304:U10:H121	1.65	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:55:LEU:HD12	2:M:135:LEU:HD12	1.97	0.45
15:M:410:CDL:H112	3:H:30:TYR:CE2	2.52	0.45
13:L:312:LMT:O3'	13:B:102:LMT:H1'	2.17	0.44
2:M:250:LEU:HD23	2:M:250:LEU:HA	1.78	0.44
4:E:43:TRP:CE3	8:E:103:BCL:HAC2	2.53	0.44
8:g:102:BCL:H141	8:g:102:BCL:H161	1.64	0.44
5:j:10:THR:HG23	5:j:12:LEU:HD13	1.99	0.44
4:J:3:LYS:HE2	4:J:6:LYS:HD2	1.99	0.44
8:K:102:BCL:H143	8:K:102:BCL:H111	1.73	0.44
8:o:102:BCL:H61	8:o:102:BCL:H41	1.68	0.44
1:L:170:ASN:HB3	1:L:173:HIS:HB2	2.00	0.44
2:M:138:GLN:NE2	13:I:103:LMT:H3B	2.33	0.44
4:J:12:ASP:HB3	4:J:15:ARG:HG3	1.99	0.44
5:j:7:LEU:HD21	5:k:12:LEU:HG	1.99	0.44
7:X:33:TRP:CH2	13:X:103:LMT:H6D	2.53	0.44
13:O:101:LMT:H6'1	13:P:101:LMT:H4B	2.00	0.44
8:d:102:BCL:H143	8:d:102:BCL:H111	1.70	0.44
4:F:43:TRP:CE3	8:F:103:BCL:HAC2	2.53	0.44
5:o:25:MET:O	5:o:29:TRP:HD1	1.99	0.44
6:U:10:ARG:HG3	6:U:50:PRO:HB3	1.99	0.44
13:L:315:LMT:H51	13:L:315:LMT:H22	1.72	0.44
5:g:19:GLU:O	5:g:23:VAL:HG23	2.17	0.44
8:D:102:BCL:H192	8:D:102:BCL:H162	1.78	0.44
8:f:102:BCL:H162	8:f:102:BCL:H141	1.74	0.44
1:L:277:GLY:O	2:M:87:ARG:NH2	2.51	0.43
3:H:241:LEU:HA	3:H:248:ARG:NH2	2.33	0.43
4:D:8:TRP:CH2	4:D:17:PHE:HE1	2.36	0.43
1:L:47:ILE:HG21	4:B:30:MET:HG3	1.99	0.43
2:M:81:ASN:HB3	2:M:84:VAL:HB	1.99	0.43
4:B:22:VAL:HG22	13:B:102:LMT:H4'	2.00	0.43
4:C:10:ILE:HG23	4:D:14:ARG:HG2	2.00	0.43
4:N:24:LEU:HB2	8:N:101:BCL:H42	2.01	0.43
7:X:37:VAL:HA	13:X:103:LMT:H51	1.99	0.43
1:L:174:MET:SD	8:M:401:BCL:HED3	2.58	0.43
15:M:410:CDL:H192	3:H:23:PHE:HA	2.01	0.43
11:M:412:PGV:O02	4:I:26:LEU:HD13	2.18	0.43
13:H:301:LMT:H5B	13:H:301:LMT:H6D	2.00	0.43
4:J:4:PHE:O	4:J:6:LYS:N	2.51	0.43
11:K:103:PGV:H211	11:K:103:PGV:H242	1.64	0.43
4:C:13:PRO:HG3	5:c:20:LEU:HD21	1.99	0.43
11:K:103:PGV:H62	4:N:21:GLY:HA3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:N:101:BCL:H102	8:N:101:BCL:H61	1.61	0.43
5:o:39:HIS:HB3	8:o:102:BCL:H121	2.01	0.43
8:f:102:BCL:H41	8:f:102:BCL:H61	1.46	0.43
4:I:8:TRP:O	5:i:10:THR:HG21	2.18	0.43
4:I:43:TRP:CE3	8:I:102:BCL:HAC2	2.53	0.43
12:I:104:LDA:H71	12:I:104:LDA:H102	1.79	0.43
5:i:40:LEU:O	5:i:44:ILE:HG12	2.19	0.43
3:H:112:ALA:HB2	3:H:239:GLY:HA3	2.00	0.43
13:H:302:LMT:O6'	13:H:302:LMT:O1B	2.35	0.43
13:B:102:LMT:H31	13:B:102:LMT:H61	1.73	0.43
5:b:46:ARG:NH2	4:C:53:ARG:HD3	2.34	0.43
4:C:40:SER:O	5:c:46:ARG:NH2	2.49	0.43
8:g:102:BCL:H61	8:g:102:BCL:H41	1.73	0.43
5:k:25:MET:O	5:k:29:TRP:HD1	2.02	0.43
4:C:36:LEU:O	4:C:42:ASN:ND2	2.52	0.43
8:o:102:BCL:H192	8:o:102:BCL:H162	1.71	0.43
6:U:36:LEU:HB2	13:U:101:LMT:H102	1.99	0.43
1:L:59:TRP:CD1	13:D:101:LMT:H2'	2.54	0.43
1:L:79:PRO:HG3	13:L:311:LMT:H1B	2.00	0.43
10:L:304:U10:H122	10:L:304:U10:H161	1.82	0.43
4:F:34:ILE:HG23	13:F:101:LMT:H12	2.01	0.43
1:L:21:LEU:HD21	13:L:312:LMT:H6'2	2.01	0.43
1:L:223:SER:OG	10:L:303:U10:O5	2.29	0.43
11:L:314:PGV:H251	7:X:55:LEU:HD21	2.01	0.43
13:L:315:LMT:H111	7:X:38:PHE:HB2	2.00	0.43
2:M:103:LEU:HD11	2:M:166:ILE:HA	2.00	0.43
8:a:102:BCL:H162	8:a:102:BCL:H141	1.74	0.43
12:J:105:LDA:H42	12:J:105:LDA:H72	1.89	0.43
2:M:208:PHE:HE1	11:H:303:PGV:H12	1.84	0.43
4:F:15:ARG:HD3	12:F:104:LDA:H82	2.01	0.43
4:O:36:LEU:HD13	4:O:43:TRP:CH2	2.53	0.43
5:q:48:TRP:NE1	8:q:102:BCL:HAC2	2.34	0.43
13:L:312:LMT:O2B	4:A:23:PHE:HB2	2.19	0.42
13:F:101:LMT:O6'	4:G:45:GLU:OE2	2.36	0.42
3:H:134:MET:HE1	3:H:142:VAL:HG23	2.00	0.42
8:i:101:BCL:H61	8:i:101:BCL:H41	1.59	0.42
1:L:219:LEU:HD11	2:M:133:THR:HG22	2.01	0.42
2:M:135:LEU:HD21	11:M:412:PGV:H142	2.02	0.42
11:H:304:PGV:H82	11:H:304:PGV:H52	1.87	0.42
8:o:102:BCL:H61	8:o:102:BCL:H93	1.77	0.42
4:P:3:LYS:HA	4:P:5:TYR:CE1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:25:PHE:CE2	6:U:24:MET:HE1	2.53	0.42
6:U:23:ILE:HD13	13:U:101:LMT:H81	2.02	0.42
1:L:46:ILE:HD12	11:C:101:PGV:H322	2.01	0.42
1:L:233:GLY:HA2	2:M:216:PHE:CE2	2.55	0.42
12:L:309:LDA:H102	12:X:101:LDA:H62	2.00	0.42
8:A:702:BCL:H62	8:A:702:BCL:H2	1.55	0.42
4:C:15:ARG:HD3	11:C:102:PGV:H232	2.02	0.42
12:I:104:LDA:H51	12:I:104:LDA:H21	1.87	0.42
12:J:105:LDA:H22	8:K:102:BCL:H71	2.00	0.42
9:M:405:BPH:HBA2	9:M:405:BPH:H3A	1.79	0.42
8:a:102:BCL:H93	8:a:102:BCL:H62	1.71	0.42
8:n:102:BCL:H91	8:n:102:BCL:H112	1.63	0.42
5:o:19:GLU:O	5:o:23:VAL:HG23	2.19	0.42
1:L:16:LEU:HA	12:L:309:LDA:HM21	2.02	0.42
1:L:135:ARG:HB3	1:L:136:PRO:HD3	2.02	0.42
13:L:315:LMT:H62	13:B:102:LMT:H111	2.02	0.42
2:M:123:PHE:HE2	2:M:158:MET:HE1	1.84	0.42
2:M:301:HIS:HB3	11:M:402:PGV:H032	2.00	0.42
8:M:404:BCL:HAA2	8:M:404:BCL:HBD	2.02	0.42
8:b:103:BCL:H162	8:b:103:BCL:H202	1.72	0.42
8:j:101:BCL:H141	8:j:101:BCL:H162	1.75	0.42
4:K:10:ILE:HG12	5:k:7:LEU:HD12	2.02	0.42
8:n:102:BCL:H2	8:n:102:BCL:H61	1.64	0.42
4:O:34:ILE:O	4:O:38:THR:HG23	2.20	0.42
1:L:25:TRP:O	4:B:15:ARG:NH1	2.53	0.42
1:L:173:HIS:CE1	1:L:177:ILE:HD11	2.55	0.42
11:H:304:PGV:H81	8:D:102:BCL:H72	2.02	0.42
11:C:102:PGV:H301	11:C:102:PGV:H272	1.88	0.42
16:D:105:A1EF2:C35	5:e:19:GLU:HG2	2.50	0.42
5:k:48:TRP:CE3	8:k:102:BCL:HAC2	2.55	0.42
8:k:102:BCL:H92	8:k:102:BCL:H61	1.71	0.42
11:L:305:PGV:H202	11:M:402:PGV:H61	2.01	0.41
13:L:315:LMT:H92	7:X:38:PHE:HD1	1.85	0.41
1:L:38:THR:HG21	1:L:100:TRP:HE3	1.85	0.41
8:i:101:BCL:H91	8:i:101:BCL:H112	1.65	0.41
4:K:15:ARG:NE	11:K:103:PGV:O14	2.35	0.41
8:o:102:BCL:H162	8:o:102:BCL:H141	1.80	0.41
7:X:50:VAL:HG12	7:X:54:MET:HE3	2.01	0.41
5:a:49:PHE:HD2	8:a:102:BCL:H202	1.85	0.41
8:a:102:BCL:H91	8:a:102:BCL:H112	1.69	0.41
5:o:12:LEU:HD22	5:o:16:GLN:HB3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:i:101:BCL:H93	8:i:101:BCL:H142	2.02	0.41
8:J:102:BCL:HHC	8:J:102:BCL:OBB	2.20	0.41
1:L:109:ARG:HG3	1:L:115:TYR:HE1	1.85	0.41
1:L:224:ILE:H	10:L:303:U10:H72	1.85	0.41
3:H:105:MET:HE3	3:H:243:TYR:HB2	2.02	0.41
13:a:101:LMT:H11	5:b:30:LEU:HD21	2.03	0.41
5:j:7:LEU:HB3	5:j:8:GLY:H	1.58	0.41
11:K:103:PGV:H81	8:N:101:BCL:H72	2.03	0.41
6:U:18:PHE:HB2	6:U:43:ALA:HB2	2.03	0.41
13:c:103:LMT:H1B	13:c:103:LMT:H3'	1.44	0.41
6:U:6:GLU:HG2	6:U:51:ASN:HB2	2.03	0.41
2:M:160:LEU:HD13	8:M:401:BCL:HMC2	2.02	0.41
13:L:315:LMT:H12	7:X:45:ILE:HD13	2.03	0.41
5:d:19:GLU:O	5:d:23:VAL:HG23	2.21	0.41
4:F:34:ILE:HG12	13:F:101:LMT:H31	2.02	0.41
8:F:103:BCL:OBB	8:F:103:BCL:HHC	2.21	0.41
8:g:102:BCL:H102	8:g:102:BCL:CAB	2.51	0.41
5:j:29:TRP:HA	5:j:29:TRP:CE3	2.55	0.41
1:L:100:TRP:HH2	10:M:407:U10:H28	1.85	0.41
15:M:410:CDL:OA9	15:M:410:CDL:HB62	2.21	0.41
8:A:702:BCL:H62	8:A:702:BCL:H102	1.89	0.41
5:a:7:LEU:HD11	5:b:12:LEU:HG	2.03	0.41
8:d:102:BCL:H102	8:d:102:BCL:CAB	2.50	0.41
8:f:102:BCL:H142	8:f:102:BCL:H112	1.81	0.41
8:I:102:BCL:H202	8:I:102:BCL:H161	1.72	0.41
4:N:43:TRP:CE3	8:N:101:BCL:HAC2	2.56	0.41
7:X:33:TRP:HB3	12:X:101:LDA:H41	2.02	0.41
1:L:85:LEU:HD23	1:L:85:LEU:HA	1.97	0.41
13:L:312:LMT:H122	13:L:312:LMT:H91	1.92	0.41
3:H:245:ALA:N	3:H:246:PRO:HD2	2.37	0.41
11:H:304:PGV:H202	11:H:304:PGV:H231	1.66	0.41
8:c:102:BCL:H141	8:c:102:BCL:H162	1.86	0.41
8:c:102:BCL:H91	8:c:102:BCL:H112	1.74	0.41
4:I:26:LEU:HD11	12:I:104:LDA:H101	2.01	0.41
8:P:102:BCL:HHD	5:p:42:VAL:HG21	2.03	0.41
1:L:131:LEU:HD23	1:L:131:LEU:HA	1.85	0.40
3:H:185:ASP:OD1	3:H:185:ASP:N	2.51	0.40
4:E:38:THR:HG21	4:F:44:LEU:HD13	2.04	0.40
5:j:49:PHE:HE2	8:j:101:BCL:H161	1.85	0.40
8:O:102:BCL:H101	8:O:102:BCL:H61	1.68	0.40
8:M:401:BCL:HBC1	8:M:404:BCL:HAA2	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:33:LEU:HD22	13:D:101:LMT:H11	2.04	0.40
4:E:12:ASP:HB3	4:E:15:ARG:HG3	2.03	0.40
1:L:6:GLU:HA	2:M:250:LEU:HD11	2.03	0.40
8:M:401:BCL:H41	8:M:401:BCL:H61	1.88	0.40
4:E:11:PHE:CD1	11:E:104:PGV:H032	2.54	0.40
5:e:14:ASP:O	5:e:18:GLN:HG3	2.21	0.40
4:J:3:LYS:HG3	4:J:3:LYS:O	2.22	0.40
4:J:10:ILE:HA	5:j:9:TYR:HD1	1.87	0.40
8:p:102:BCL:H202	8:p:102:BCL:H162	1.76	0.40
8:Q:101:BCL:H112	8:Q:101:BCL:H72	1.81	0.40
1:L:146:PHE:HB3	1:L:156:TRP:CD2	2.57	0.40
1:L:151:TRP:CH2	2:M:303:MET:HE3	2.56	0.40
11:L:313:PGV:H61	11:L:313:PGV:H32	1.85	0.40
4:A:36:LEU:HD13	4:A:43:TRP:CH2	2.56	0.40
8:C:103:BCL:H161	8:C:103:BCL:H141	1.82	0.40
4:E:12:ASP:HB2	11:E:104:PGV:P	2.61	0.40
4:G:11:PHE:HZ	4:I:17:PHE:HB2	1.86	0.40
3:H:178:PHE:CZ	3:H:230:GLU:HG2	2.57	0.40
4:E:1:FME:HE2	4:E:1:FME:HB3	1.73	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	L	279/282 (99%)	276 (99%)	3 (1%)	0	100	100
2	M	304/308 (99%)	298 (98%)	6 (2%)	0	100	100
3	H	248/260 (95%)	242 (98%)	6 (2%)	0	100	100
4	A	43/54 (80%)	43 (100%)	0	0	100	100
4	B	52/54 (96%)	52 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	C	52/54 (96%)	51 (98%)	1 (2%)	0	100	100
4	D	52/54 (96%)	51 (98%)	1 (2%)	0	100	100
4	E	52/54 (96%)	51 (98%)	1 (2%)	0	100	100
4	F	52/54 (96%)	52 (100%)	0	0	100	100
4	G	52/54 (96%)	51 (98%)	1 (2%)	0	100	100
4	I	52/54 (96%)	52 (100%)	0	0	100	100
4	J	52/54 (96%)	50 (96%)	2 (4%)	0	100	100
4	K	52/54 (96%)	52 (100%)	0	0	100	100
4	N	52/54 (96%)	51 (98%)	1 (2%)	0	100	100
4	O	52/54 (96%)	52 (100%)	0	0	100	100
4	P	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
4	Q	49/54 (91%)	48 (98%)	1 (2%)	0	100	100
5	a	42/49 (86%)	42 (100%)	0	0	100	100
5	b	42/49 (86%)	40 (95%)	2 (5%)	0	100	100
5	c	42/49 (86%)	42 (100%)	0	0	100	100
5	d	41/49 (84%)	41 (100%)	0	0	100	100
5	e	41/49 (84%)	41 (100%)	0	0	100	100
5	f	41/49 (84%)	40 (98%)	1 (2%)	0	100	100
5	g	42/49 (86%)	42 (100%)	0	0	100	100
5	i	42/49 (86%)	42 (100%)	0	0	100	100
5	j	41/49 (84%)	41 (100%)	0	0	100	100
5	k	41/49 (84%)	41 (100%)	0	0	100	100
5	n	40/49 (82%)	40 (100%)	0	0	100	100
5	o	40/49 (82%)	39 (98%)	1 (2%)	0	100	100
5	p	40/49 (82%)	40 (100%)	0	0	100	100
5	q	36/49 (74%)	36 (100%)	0	0	100	100
6	U	46/53 (87%)	45 (98%)	1 (2%)	0	100	100
7	X	51/82 (62%)	51 (100%)	0	0	100	100
All	All	2214/2427 (91%)	2184 (99%)	30 (1%)	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	L	220/220 (100%)	220 (100%)	0	100	100
2	M	239/240 (100%)	239 (100%)	0	100	100
3	H	201/208 (97%)	201 (100%)	0	100	100
4	A	41/48 (85%)	41 (100%)	0	100	100
4	B	47/48 (98%)	47 (100%)	0	100	100
4	C	48/48 (100%)	48 (100%)	0	100	100
4	D	48/48 (100%)	48 (100%)	0	100	100
4	E	48/48 (100%)	48 (100%)	0	100	100
4	F	48/48 (100%)	48 (100%)	0	100	100
4	G	48/48 (100%)	48 (100%)	0	100	100
4	I	48/48 (100%)	48 (100%)	0	100	100
4	J	48/48 (100%)	48 (100%)	0	100	100
4	K	48/48 (100%)	48 (100%)	0	100	100
4	N	48/48 (100%)	48 (100%)	0	100	100
4	O	48/48 (100%)	48 (100%)	0	100	100
4	P	48/48 (100%)	48 (100%)	0	100	100
4	Q	43/48 (90%)	43 (100%)	0	100	100
5	a	36/39 (92%)	36 (100%)	0	100	100
5	b	36/39 (92%)	36 (100%)	0	100	100
5	c	36/39 (92%)	36 (100%)	0	100	100
5	d	35/39 (90%)	35 (100%)	0	100	100
5	e	35/39 (90%)	35 (100%)	0	100	100
5	f	35/39 (90%)	35 (100%)	0	100	100
5	g	35/39 (90%)	35 (100%)	0	100	100
5	i	36/39 (92%)	36 (100%)	0	100	100
5	j	34/39 (87%)	34 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	k	35/39 (90%)	35 (100%)	0	100	100
5	n	34/39 (87%)	34 (100%)	0	100	100
5	o	34/39 (87%)	34 (100%)	0	100	100
5	p	32/39 (82%)	32 (100%)	0	100	100
5	q	26/39 (67%)	26 (100%)	0	100	100
6	U	32/36 (89%)	32 (100%)	0	100	100
7	X	40/65 (62%)	40 (100%)	0	100	100
All	All	1870/1987 (94%)	1870 (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 (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	258	GLN
2	M	138	GLN
2	M	195	ASN
2	M	293	ASN
3	H	44	ASN
3	H	98	HIS
3	H	126	HIS
3	H	141	HIS
5	a	18	GLN
4	B	42	ASN
4	D	42	ASN
4	E	42	ASN
4	F	20	GLN
4	F	42	ASN
4	I	20	GLN
4	J	20	GLN
4	N	42	ASN
7	X	61	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	FME	N	1	4	8,9,10	0.95	0	7,9,11	0.84	0
4	FME	O	1	4	8,9,10	0.90	0	7,9,11	1.11	1 (14%)
4	FME	A	1	4	8,9,10	0.93	0	7,9,11	0.85	0
4	FME	I	1	4	5,6,10	1.44	1 (20%)	3,6,11	1.84	1 (33%)
4	FME	F	1	4	8,9,10	0.92	0	7,9,11	0.82	0
4	FME	G	1	4	8,9,10	0.96	0	7,9,11	0.88	0
4	FME	J	1	4	8,9,10	0.89	0	7,9,11	1.32	2 (28%)
4	FME	K	1	4	8,9,10	0.92	0	7,9,11	0.87	0
4	FME	E	1	4	8,9,10	0.91	0	7,9,11	0.98	0
4	FME	B	1	4	8,9,10	0.93	0	7,9,11	0.78	0
4	FME	D	1	4	8,9,10	0.93	0	7,9,11	0.80	0
4	FME	C	1	4	8,9,10	0.93	0	7,9,11	0.80	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	FME	N	1	4	-	0/7/9/11	-
4	FME	O	1	4	-	3/7/9/11	-
4	FME	A	1	4	-	2/7/9/11	-
4	FME	I	1	4	-	0/2/5/11	-
4	FME	F	1	4	-	5/7/9/11	-
4	FME	G	1	4	-	4/7/9/11	-
4	FME	J	1	4	-	2/7/9/11	-
4	FME	K	1	4	-	0/7/9/11	-
4	FME	E	1	4	-	3/7/9/11	-
4	FME	B	1	4	-	5/7/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	FME	D	1	4	-	4/7/9/11	-
4	FME	C	1	4	-	2/7/9/11	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	I	1	FME	CA-N	-2.44	1.44	1.46

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	I	1	FME	CB-CA-N	3.09	113.05	109.61
4	J	1	FME	C-CA-N	2.33	113.94	109.73
4	O	1	FME	C-CA-N	2.20	113.70	109.73
4	J	1	FME	CA-N-CN	2.04	125.96	122.82

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1	FME	O1-CN-N-CA
4	A	1	FME	O-C-CA-CB
4	B	1	FME	O1-CN-N-CA
4	B	1	FME	C-CA-CB-CG
4	B	1	FME	O-C-CA-CB
4	C	1	FME	O1-CN-N-CA
4	D	1	FME	O1-CN-N-CA
4	D	1	FME	O-C-CA-CB
4	D	1	FME	CA-CB-CG-SD
4	E	1	FME	O1-CN-N-CA
4	E	1	FME	N-CA-CB-CG
4	F	1	FME	O1-CN-N-CA
4	F	1	FME	N-CA-CB-CG
4	G	1	FME	O1-CN-N-CA
4	G	1	FME	C-CA-CB-CG
4	G	1	FME	CA-CB-CG-SD
4	J	1	FME	N-CA-CB-CG
4	J	1	FME	C-CA-CB-CG
4	O	1	FME	C-CA-CB-CG
4	O	1	FME	CA-CB-CG-SD
4	D	1	FME	N-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
4	G	1	FME	N-CA-CB-CG
4	O	1	FME	N-CA-CB-CG
4	F	1	FME	C-CA-CB-CG
4	B	1	FME	N-CA-CB-CG
4	C	1	FME	N-CA-CB-CG
4	F	1	FME	CA-CB-CG-SD
4	B	1	FME	CB-CG-SD-CE
4	E	1	FME	C-CA-CB-CG
4	F	1	FME	CB-CA-N-CN

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	1	FME	1	0
4	D	1	FME	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 117 ligands modelled in this entry, 1 is monoatomic - leaving 116 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	$\#\|Z\| > 2$
13	LMT	F	101	-	31,31,36	0.45	0	42,42,47	0.93	1 (2%)
16	A1EF2	B	103	-	39,39,39	2.31	10 (25%)	44,46,46	1.86	11 (25%)
13	LMT	P	101	-	34,34,36	0.42	0	45,45,47	0.66	0
10	U10	L	303	-	35,35,63	1.59	2 (5%)	42,45,79	1.89	11 (26%)
16	A1EF2	p	101	-	39,39,39	2.32	10 (25%)	44,46,46	1.89	12 (27%)
15	CDL	M	413	-	47,47,99	0.36	0	52,58,111	0.43	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
8	BCL	p	102	5	69,74,74	1.79	15 (21%)	83,115,115	2.26	22 (26%)
13	LMT	G	101	-	24,24,36	0.40	0	29,29,47	0.63	0
8	BCL	M	401	2	69,74,74	1.82	16 (23%)	83,115,115	2.36	22 (26%)
13	LMT	b	101	-	28,28,36	0.42	0	39,39,47	0.73	1 (2%)
8	BCL	I	102	4	69,74,74	1.85	16 (23%)	83,115,115	2.33	27 (32%)
12	LDA	I	104	-	12,15,15	2.10	1 (8%)	14,17,17	0.57	0
9	BPH	M	405	-	59,70,70	0.76	2 (3%)	61,101,101	0.94	3 (4%)
8	BCL	n	102	5	69,74,74	1.82	16 (23%)	83,115,115	2.35	26 (31%)
8	BCL	f	102	5	69,74,74	1.81	16 (23%)	83,115,115	2.24	22 (26%)
11	PGV	E	104	-	38,40,50	1.04	2 (5%)	40,42,56	1.10	2 (5%)
13	LMT	L	312	-	36,36,36	0.42	0	47,47,47	1.25	3 (6%)
11	PGV	C	102	-	46,46,50	0.95	2 (4%)	49,52,56	1.02	3 (6%)
16	A1EF2	N	102	-	39,39,39	2.33	11 (28%)	44,46,46	1.90	11 (25%)
16	A1EF2	O	103	-	39,39,39	2.36	10 (25%)	44,46,46	1.90	10 (22%)
13	LMT	B	102	-	36,36,36	0.42	0	47,47,47	1.42	10 (21%)
16	A1EF2	D	104	-	39,39,39	2.36	10 (25%)	44,46,46	1.87	11 (25%)
8	BCL	N	101	4	69,74,74	1.86	16 (23%)	83,115,115	2.30	23 (27%)
13	LMT	A	701	-	36,36,36	0.36	0	47,47,47	0.71	0
16	A1EF2	J	106	-	39,39,39	2.37	10 (25%)	44,46,46	1.97	13 (29%)
11	PGV	C	101	-	44,44,50	1.00	2 (4%)	48,49,56	1.11	3 (6%)
8	BCL	j	101	5	69,74,74	1.82	16 (23%)	83,115,115	2.33	26 (31%)
16	A1EF2	n	101	-	39,39,39	2.31	10 (25%)	44,46,46	1.78	11 (25%)
8	BCL	a	102	5	69,74,74	1.83	16 (23%)	83,115,115	2.28	24 (28%)
8	BCL	o	102	5	69,74,74	1.83	16 (23%)	83,115,115	5.06	28 (33%)
16	A1EF2	I	105	-	39,39,39	2.26	11 (28%)	44,46,46	1.85	10 (22%)
8	BCL	L	308	1	69,74,74	1.82	16 (23%)	83,115,115	2.36	25 (30%)
8	BCL	A	702	4	64,69,74	1.88	15 (23%)	77,109,115	2.49	28 (36%)
8	BCL	F	103	4	69,74,74	1.85	16 (23%)	83,115,115	2.21	24 (28%)
8	BCL	J	102	4	69,74,74	1.83	16 (23%)	83,115,115	2.34	26 (31%)
8	BCL	c	102	5	69,74,74	1.80	16 (23%)	83,115,115	2.30	23 (27%)
13	LMT	L	311	-	36,36,36	0.41	0	47,47,47	0.77	1 (2%)
11	PGV	K	103	-	42,42,50	1.01	2 (4%)	44,48,56	1.00	2 (4%)
16	A1EF2	q	101	-	39,39,39	2.34	10 (25%)	44,46,46	1.91	10 (22%)
16	A1EF2	g	101	-	39,39,39	2.29	10 (25%)	44,46,46	1.94	11 (25%)
8	BCL	B	101	4	64,69,74	1.92	16 (25%)	77,109,115	2.30	24 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
13	LMT	G	102	-	19,19,36	0.45	0	24,24,47	0.71	0
15	CDL	E	101	-	56,56,99	0.35	0	62,68,111	0.48	0
13	LMT	U	101	-	36,36,36	0.39	0	47,47,47	0.71	1 (2%)
15	CDL	M	410	-	78,78,99	0.31	0	84,90,111	0.49	1 (1%)
16	A1EF2	D	105	-	39,39,39	2.31	11 (28%)	44,46,46	1.82	11 (25%)
13	LMT	H	302	-	36,36,36	0.37	0	47,47,47	0.77	1 (2%)
12	LDA	M	403	-	12,15,15	2.08	1 (8%)	14,17,17	0.47	0
8	BCL	P	102	4	64,69,74	1.93	16 (25%)	77,109,115	2.24	21 (27%)
13	LMT	E	102	-	36,36,36	0.43	0	47,47,47	0.96	2 (4%)
12	LDA	J	105	-	12,15,15	2.09	1 (8%)	14,17,17	0.56	0
16	A1EF2	e	101	-	39,39,39	2.30	10 (25%)	44,46,46	1.85	11 (25%)
13	LMT	c	103	-	36,36,36	0.42	0	47,47,47	0.69	0
13	LMT	O	101	-	36,36,36	0.40	0	47,47,47	0.85	1 (2%)
16	A1EF2	M	411	-	39,39,39	2.33	11 (28%)	44,46,46	1.77	10 (22%)
8	BCL	C	103	4	69,74,74	1.84	16 (23%)	83,115,115	2.30	23 (27%)
8	BCL	k	102	5	69,74,74	1.81	16 (23%)	83,115,115	2.26	24 (28%)
11	PGV	M	402	-	46,46,50	0.93	2 (4%)	49,52,56	1.07	3 (6%)
13	LMT	D	101	-	27,27,36	0.47	0	38,38,47	0.98	2 (5%)
13	LMT	L	315	-	36,36,36	0.36	0	47,47,47	0.70	1 (2%)
13	LMT	a	101	-	28,28,36	0.45	0	39,39,47	0.86	2 (5%)
11	PGV	L	306	-	32,32,50	1.11	2 (6%)	35,38,56	1.24	4 (11%)
11	PGV	H	304	-	39,39,50	1.02	2 (5%)	42,45,56	1.17	4 (9%)
8	BCL	K	102	4	69,74,74	1.85	16 (23%)	83,115,115	2.29	25 (30%)
16	A1EF2	N	103	-	39,39,39	2.32	10 (25%)	44,46,46	1.88	11 (25%)
8	BCL	D	102	4	69,74,74	1.82	16 (23%)	83,115,115	2.31	24 (28%)
8	BCL	b	103	5	69,74,74	1.84	16 (23%)	83,115,115	2.31	25 (30%)
8	BCL	e	102	5	69,74,74	1.82	16 (23%)	83,115,115	2.26	22 (26%)
8	BCL	g	102	5	69,74,74	1.84	16 (23%)	83,115,115	2.27	25 (30%)
13	LMT	I	101	-	25,25,36	0.44	0	30,30,47	0.88	0
12	LDA	K	101	-	8,11,15	2.57	1 (12%)	10,13,17	0.43	0
13	LMT	M	409	-	34,34,36	0.48	0	45,45,47	1.08	6 (13%)
8	BCL	O	102	4	60,65,74	2.00	16 (26%)	72,104,115	2.44	27 (37%)
11	PGV	L	305	-	38,38,50	1.06	2 (5%)	41,44,56	1.14	3 (7%)
13	LMT	M	408	-	27,27,36	0.47	0	32,33,47	0.68	0
12	LDA	X	102	-	12,15,15	2.11	1 (8%)	14,17,17	0.59	0
11	PGV	H	303	-	33,33,50	1.15	2 (6%)	36,38,56	1.11	3 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
12	LDA	L	310	-	12,15,15	2.09	1 (8%)	14,17,17	0.55	0
16	A1EF2	f	101	-	39,39,39	2.31	10 (25%)	44,46,46	1.84	10 (22%)
8	BCL	d	102	5	69,74,74	1.83	16 (23%)	83,115,115	2.29	23 (27%)
8	BCL	i	101	5	69,74,74	1.83	16 (23%)	83,115,115	2.31	24 (28%)
8	BCL	Q	101	-	64,69,74	1.85	15 (23%)	77,109,115	2.45	26 (33%)
11	PGV	G	103	-	38,38,50	1.05	2 (5%)	41,44,56	1.10	3 (7%)
13	LMT	D	103	-	28,28,36	0.48	0	39,39,47	0.81	1 (2%)
12	LDA	L	307	-	12,15,15	2.11	1 (8%)	14,17,17	0.52	0
8	BCL	M	404	2	69,74,74	1.86	16 (23%)	83,115,115	2.33	24 (28%)
13	LMT	H	301	-	36,36,36	0.36	0	47,47,47	0.70	0
13	LMT	X	103	-	32,32,36	0.45	0	43,43,47	0.84	1 (2%)
16	A1EF2	J	101	-	39,39,39	2.35	10 (25%)	44,46,46	1.85	11 (25%)
16	A1EF2	o	101	-	39,39,39	2.32	10 (25%)	44,46,46	1.84	11 (25%)
16	A1EF2	J	103	-	39,39,39	2.28	10 (25%)	44,46,46	2.00	11 (25%)
8	BCL	L	301	1	69,74,74	1.81	16 (23%)	83,115,115	2.43	27 (32%)
8	BCL	G	104	4	69,74,74	1.84	16 (23%)	83,115,115	2.32	25 (30%)
16	A1EF2	E	105	-	39,39,39	2.32	10 (25%)	44,46,46	1.89	11 (25%)
10	U10	L	304	-	35,35,63	1.43	2 (5%)	42,45,79	1.74	12 (28%)
12	LDA	X	101	-	9,12,15	2.44	1 (11%)	11,14,17	0.54	0
8	BCL	E	103	4	60,65,74	1.97	16 (26%)	72,104,115	2.43	27 (37%)
16	A1EF2	c	104	-	39,39,39	2.29	10 (25%)	44,46,46	1.94	10 (22%)
12	LDA	F	104	-	12,15,15	2.07	1 (8%)	14,17,17	0.49	0
11	PGV	L	313	-	50,50,50	0.92	2 (4%)	53,56,56	1.02	3 (5%)
11	PGV	M	412	-	41,41,50	1.03	2 (4%)	44,47,56	1.09	2 (4%)
16	A1EF2	k	101	-	39,39,39	2.31	10 (25%)	44,46,46	1.87	11 (25%)
9	BPH	L	302	-	59,70,70	0.81	3 (5%)	61,101,101	0.92	3 (4%)
13	LMT	I	103	-	31,31,36	0.48	1 (3%)	42,42,47	0.84	1 (2%)
13	LMT	c	101	-	17,17,36	0.47	0	22,22,47	0.78	1 (4%)
16	A1EF2	a	103	-	39,39,39	2.30	10 (25%)	44,46,46	1.93	11 (25%)
16	A1EF2	J	104	-	39,39,39	2.34	10 (25%)	44,46,46	1.91	11 (25%)
16	A1EF2	d	101	-	39,39,39	2.32	10 (25%)	44,46,46	1.88	12 (27%)
8	BCL	q	102	5	63,68,74	1.89	16 (25%)	75,107,115	2.36	20 (26%)
12	LDA	L	309	-	12,15,15	2.09	1 (8%)	14,17,17	0.58	0
15	CDL	F	102	-	35,35,99	0.56	0	42,44,111	0.81	2 (4%)
11	PGV	L	314	-	38,38,50	1.03	2 (5%)	41,44,56	1.07	3 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
10	U10	M	407	-	48,48,63	1.29	2 (4%)	58,61,79	1.58	14 (24%)
16	A1EF2	C	104	-	39,39,39	2.34	10 (25%)	44,46,46	1.86	11 (25%)
16	A1EF2	g	103	-	39,39,39	2.31	10 (25%)	44,46,46	2.02	13 (29%)
16	A1EF2	b	102	-	39,39,39	2.33	10 (25%)	44,46,46	1.94	11 (25%)

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
13	LMT	F	101	-	-	6/16/56/61	0/2/2/2
16	A1EF2	B	103	-	-	10/43/43/43	-
13	LMT	P	101	-	-	3/19/59/61	0/2/2/2
10	U10	L	303	-	-	7/30/54/87	0/1/1/1
16	A1EF2	p	101	-	-	4/43/43/43	-
15	CDL	M	413	-	-	11/56/56/110	-
8	BCL	p	102	5	-	15/41/137/137	-
13	LMT	G	101	-	-	5/15/35/61	0/1/1/2
8	BCL	M	401	2	-	13/41/137/137	-
13	LMT	b	101	-	-	1/13/53/61	0/2/2/2
8	BCL	I	102	4	-	15/41/137/137	-
12	LDA	I	104	-	-	3/13/13/13	-
9	BPH	M	405	-	-	6/37/105/105	0/5/6/6
8	BCL	n	102	5	-	18/41/137/137	-
8	BCL	f	102	5	-	16/41/137/137	-
11	PGV	E	104	-	-	6/40/42/55	-
13	LMT	L	312	-	-	10/21/61/61	0/2/2/2
11	PGV	C	102	-	-	19/51/51/55	-
16	A1EF2	N	102	-	-	9/43/43/43	-
16	A1EF2	O	103	-	-	8/43/43/43	-
13	LMT	B	102	-	-	11/21/61/61	0/2/2/2
16	A1EF2	D	104	-	-	11/43/43/43	-
8	BCL	N	101	4	-	17/41/137/137	-
13	LMT	A	701	-	-	5/21/61/61	0/2/2/2
16	A1EF2	J	106	-	-	9/43/43/43	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	PGV	C	101	-	-	13/46/46/55	-
8	BCL	j	101	5	-	13/41/137/137	-
16	A1EF2	n	101	-	-	7/43/43/43	-
8	BCL	a	102	5	-	18/41/137/137	-
8	BCL	o	102	5	-	17/41/137/137	-
16	A1EF2	I	105	-	-	5/43/43/43	-
8	BCL	L	308	1	-	7/41/137/137	-
8	BCL	A	702	4	-	10/35/131/137	-
8	BCL	F	103	4	-	12/41/137/137	-
8	BCL	J	102	4	-	17/41/137/137	-
8	BCL	c	102	5	-	15/41/137/137	-
13	LMT	L	311	-	-	8/21/61/61	0/2/2/2
11	PGV	K	103	-	-	12/47/47/55	-
16	A1EF2	q	101	-	-	6/43/43/43	-
16	A1EF2	g	101	-	-	8/43/43/43	-
8	BCL	B	101	4	-	6/35/131/137	-
13	LMT	G	102	-	-	3/11/31/61	0/1/1/2
15	CDL	E	101	-	-	15/67/67/110	-
13	LMT	U	101	-	-	3/21/61/61	0/2/2/2
15	CDL	M	410	-	-	14/89/89/110	-
16	A1EF2	D	105	-	-	7/43/43/43	-
13	LMT	H	302	-	-	2/21/61/61	0/2/2/2
12	LDA	M	403	-	-	1/13/13/13	-
8	BCL	P	102	4	-	11/35/131/137	-
13	LMT	E	102	-	-	5/21/61/61	0/2/2/2
12	LDA	J	105	-	-	2/13/13/13	-
16	A1EF2	e	101	-	-	7/43/43/43	-
13	LMT	c	103	-	-	5/21/61/61	0/2/2/2
13	LMT	O	101	-	-	7/21/61/61	0/2/2/2
16	A1EF2	M	411	-	-	6/43/43/43	-
8	BCL	C	103	4	-	13/41/137/137	-
8	BCL	k	102	5	-	14/41/137/137	-
11	PGV	M	402	-	-	15/51/51/55	-
13	LMT	D	101	-	-	4/11/51/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	LMT	L	315	-	-	4/21/61/61	0/2/2/2
13	LMT	a	101	-	-	2/13/53/61	0/2/2/2
11	PGV	L	306	-	-	15/37/37/55	-
11	PGV	H	304	-	-	18/44/44/55	-
8	BCL	K	102	4	-	15/41/137/137	-
16	A1EF2	N	103	-	-	8/43/43/43	-
8	BCL	D	102	4	-	8/41/137/137	-
8	BCL	b	103	5	-	18/41/137/137	-
8	BCL	e	102	5	-	16/41/137/137	-
8	BCL	g	102	5	-	19/41/137/137	-
13	LMT	I	101	-	-	6/17/37/61	0/1/1/2
12	LDA	K	101	-	-	0/9/9/13	-
13	LMT	M	409	-	-	8/19/59/61	0/2/2/2
8	BCL	O	102	4	-	9/31/127/137	-
11	PGV	L	305	-	-	14/43/43/55	-
13	LMT	M	408	-	-	5/19/39/61	0/1/1/2
12	LDA	X	102	-	-	5/13/13/13	-
11	PGV	H	303	-	-	9/35/35/55	-
12	LDA	L	310	-	-	4/13/13/13	-
16	A1EF2	f	101	-	-	7/43/43/43	-
8	BCL	d	102	5	-	17/41/137/137	-
8	BCL	i	101	5	-	18/41/137/137	-
8	BCL	Q	101	-	-	11/35/131/137	-
11	PGV	G	103	-	-	16/43/43/55	-
13	LMT	D	103	-	-	8/13/53/61	0/2/2/2
12	LDA	L	307	-	-	2/13/13/13	-
8	BCL	M	404	2	-	7/41/137/137	-
13	LMT	H	301	-	-	1/21/61/61	0/2/2/2
13	LMT	X	103	-	-	1/17/57/61	0/2/2/2
16	A1EF2	J	101	-	-	6/43/43/43	-
16	A1EF2	o	101	-	-	4/43/43/43	-
16	A1EF2	J	103	-	-	7/43/43/43	-
8	BCL	L	301	1	-	8/41/137/137	-
8	BCL	G	104	4	-	17/41/137/137	-
16	A1EF2	E	105	-	-	6/43/43/43	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	U10	L	304	-	-	5/30/54/87	0/1/1/1
12	LDA	X	101	-	-	1/10/10/13	-
8	BCL	E	103	4	-	7/31/127/137	-
16	A1EF2	c	104	-	-	7/43/43/43	-
12	LDA	F	104	-	-	4/13/13/13	-
11	PGV	L	313	-	-	10/55/55/55	-
11	PGV	M	412	-	-	16/46/46/55	-
16	A1EF2	k	101	-	-	8/43/43/43	-
9	BPH	L	302	-	-	3/37/105/105	0/5/6/6
13	LMT	I	103	-	-	2/16/56/61	0/2/2/2
13	LMT	c	101	-	-	1/9/29/61	0/1/1/2
16	A1EF2	a	103	-	-	8/43/43/43	-
16	A1EF2	J	104	-	-	12/43/43/43	-
16	A1EF2	d	101	-	-	8/43/43/43	-
8	BCL	q	102	5	-	12/33/129/137	-
12	LDA	L	309	-	-	1/13/13/13	-
15	CDL	F	102	-	-	11/37/37/110	-
11	PGV	L	314	-	-	10/43/43/55	-
10	U10	M	407	-	-	7/45/69/87	0/1/1/1
16	A1EF2	C	104	-	-	8/43/43/43	-
16	A1EF2	g	103	-	-	11/43/43/43	-
16	A1EF2	b	102	-	-	8/43/43/43	-

All (831) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	L	303	U10	C6-C1	8.56	1.50	1.35
10	M	407	U10	C6-C1	7.79	1.49	1.35
10	L	304	U10	C6-C1	7.36	1.48	1.35
12	X	101	LDA	O1-N1	-7.31	1.25	1.42
12	L	307	LDA	O1-N1	-7.28	1.25	1.42
12	I	104	LDA	O1-N1	-7.26	1.25	1.42
12	X	102	LDA	O1-N1	-7.26	1.25	1.42
12	K	101	LDA	O1-N1	-7.24	1.25	1.42
12	J	105	LDA	O1-N1	-7.22	1.25	1.42
12	L	310	LDA	O1-N1	-7.20	1.25	1.42
12	L	309	LDA	O1-N1	-7.20	1.25	1.42
12	M	403	LDA	O1-N1	-7.17	1.25	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	F	104	LDA	O1-N1	-7.13	1.25	1.42
16	D	104	A1EF2	C28-C27	6.95	1.52	1.34
16	O	103	A1EF2	C28-C27	6.93	1.52	1.34
16	N	102	A1EF2	C28-C27	6.88	1.52	1.34
16	J	101	A1EF2	C28-C27	6.87	1.52	1.34
16	J	106	A1EF2	C14-C13	6.87	1.41	1.34
16	d	101	A1EF2	C28-C27	6.81	1.52	1.34
16	q	101	A1EF2	C28-C27	6.80	1.52	1.34
16	M	411	A1EF2	C14-C13	6.79	1.41	1.34
16	f	101	A1EF2	C28-C27	6.78	1.52	1.34
16	e	101	A1EF2	C28-C27	6.76	1.52	1.34
16	a	103	A1EF2	C28-C27	6.76	1.52	1.34
16	k	101	A1EF2	C28-C27	6.75	1.52	1.34
16	J	106	A1EF2	C28-C27	6.75	1.52	1.34
16	N	103	A1EF2	C28-C27	6.74	1.51	1.34
16	C	104	A1EF2	C28-C27	6.73	1.51	1.34
16	O	103	A1EF2	C14-C13	6.73	1.41	1.34
16	c	104	A1EF2	C28-C27	6.73	1.51	1.34
16	B	103	A1EF2	C28-C27	6.72	1.51	1.34
16	p	101	A1EF2	C28-C27	6.72	1.51	1.34
16	o	101	A1EF2	C28-C27	6.70	1.51	1.34
16	J	104	A1EF2	C14-C13	6.69	1.41	1.34
16	J	101	A1EF2	C14-C13	6.69	1.41	1.34
16	n	101	A1EF2	C28-C27	6.68	1.51	1.34
16	b	102	A1EF2	C28-C27	6.68	1.51	1.34
16	g	101	A1EF2	C28-C27	6.67	1.51	1.34
16	J	104	A1EF2	C28-C27	6.67	1.51	1.34
16	D	104	A1EF2	C14-C13	6.66	1.41	1.34
16	D	105	A1EF2	C28-C27	6.61	1.51	1.34
16	E	105	A1EF2	C28-C27	6.61	1.51	1.34
16	C	104	A1EF2	C14-C13	6.61	1.41	1.34
16	I	105	A1EF2	C28-C27	6.60	1.51	1.34
16	J	103	A1EF2	C28-C27	6.60	1.51	1.34
16	g	103	A1EF2	C28-C27	6.56	1.51	1.34
16	M	411	A1EF2	C28-C27	6.54	1.51	1.34
16	q	101	A1EF2	C14-C13	6.48	1.40	1.34
16	p	101	A1EF2	C14-C13	6.47	1.40	1.34
16	b	102	A1EF2	C14-C13	6.39	1.40	1.34
16	N	103	A1EF2	C14-C13	6.38	1.40	1.34
16	g	103	A1EF2	C14-C13	6.35	1.40	1.34
16	o	101	A1EF2	C14-C13	6.35	1.40	1.34
16	E	105	A1EF2	C14-C13	6.30	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	B	103	A1EF2	C14-C13	6.25	1.40	1.34
16	a	103	A1EF2	C14-C13	6.24	1.40	1.34
16	N	102	A1EF2	C14-C13	6.22	1.40	1.34
16	D	105	A1EF2	C14-C13	6.20	1.40	1.34
16	n	101	A1EF2	C14-C13	6.11	1.40	1.34
16	d	101	A1EF2	C14-C13	6.11	1.40	1.34
16	k	101	A1EF2	C14-C13	6.06	1.40	1.34
16	g	101	A1EF2	C14-C13	6.06	1.40	1.34
16	J	103	A1EF2	C14-C13	6.00	1.40	1.34
16	e	101	A1EF2	C14-C13	5.99	1.40	1.34
16	f	101	A1EF2	C14-C13	5.96	1.40	1.34
16	c	104	A1EF2	C14-C13	5.90	1.40	1.34
16	I	105	A1EF2	C14-C13	5.85	1.40	1.34
8	o	102	BCL	O2D-CGD	5.43	1.46	1.33
8	M	404	BCL	O2D-CGD	5.23	1.46	1.33
16	E	105	A1EF2	C12-C13	-5.19	1.40	1.51
16	N	102	A1EF2	C12-C13	-5.19	1.40	1.51
16	D	105	A1EF2	C12-C13	-5.17	1.40	1.51
16	M	411	A1EF2	C12-C13	-5.11	1.40	1.51
16	g	103	A1EF2	C12-C13	-5.10	1.40	1.51
8	q	102	BCL	O2D-CGD	5.08	1.45	1.33
16	C	104	A1EF2	C12-C13	-5.08	1.40	1.51
16	D	104	A1EF2	C12-C13	-5.08	1.40	1.51
8	Q	101	BCL	O2D-CGD	5.08	1.45	1.33
8	P	102	BCL	O2D-CGD	5.07	1.45	1.33
16	B	103	A1EF2	C12-C13	-5.05	1.40	1.51
8	p	102	BCL	O2D-CGD	5.03	1.45	1.33
16	J	106	A1EF2	C12-C13	-5.03	1.40	1.51
8	A	702	BCL	O2D-CGD	5.02	1.45	1.33
8	O	102	BCL	O2D-CGD	5.01	1.45	1.33
8	L	301	BCL	O2D-CGD	5.01	1.45	1.33
8	a	102	BCL	O2D-CGD	4.98	1.45	1.33
16	c	104	A1EF2	C12-C13	-4.98	1.40	1.51
16	J	101	A1EF2	C12-C13	-4.97	1.41	1.51
16	f	101	A1EF2	C12-C13	-4.97	1.41	1.51
16	a	103	A1EF2	C12-C13	-4.97	1.41	1.51
8	e	102	BCL	O2D-CGD	4.97	1.45	1.33
16	n	101	A1EF2	C12-C13	-4.97	1.41	1.51
8	d	102	BCL	O2D-CGD	4.96	1.45	1.33
16	N	103	A1EF2	C12-C13	-4.96	1.41	1.51
8	M	401	BCL	O2D-CGD	4.96	1.45	1.33
8	N	101	BCL	O2D-CGD	4.96	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	b	103	BCL	O2D-CGD	4.94	1.45	1.33
16	d	101	A1EF2	C12-C13	-4.93	1.41	1.51
8	n	102	BCL	O2D-CGD	4.92	1.45	1.33
8	c	102	BCL	O2D-CGD	4.92	1.45	1.33
8	C	103	BCL	O2D-CGD	4.92	1.45	1.33
8	k	102	BCL	O2D-CGD	4.91	1.45	1.33
16	b	102	A1EF2	C12-C13	-4.91	1.41	1.51
8	f	102	BCL	O2D-CGD	4.90	1.45	1.33
8	D	102	BCL	O2D-CGD	4.90	1.45	1.33
16	o	101	A1EF2	C12-C13	-4.89	1.41	1.51
8	M	404	BCL	C3B-C4B	4.89	1.50	1.41
8	E	103	BCL	O2D-CGD	4.89	1.45	1.33
8	i	101	BCL	O2D-CGD	4.87	1.45	1.33
8	j	101	BCL	O2D-CGD	4.87	1.45	1.33
8	G	104	BCL	O2D-CGD	4.87	1.45	1.33
16	e	101	A1EF2	C12-C13	-4.87	1.41	1.51
8	L	308	BCL	O2D-CGD	4.87	1.45	1.33
16	k	101	A1EF2	C12-C13	-4.86	1.41	1.51
8	K	102	BCL	O2D-CGD	4.86	1.45	1.33
8	B	101	BCL	O2D-CGD	4.85	1.45	1.33
16	g	101	A1EF2	C12-C13	-4.85	1.41	1.51
16	J	103	A1EF2	C12-C13	-4.84	1.41	1.51
16	I	105	A1EF2	C12-C13	-4.84	1.41	1.51
8	B	101	BCL	C3B-C4B	4.83	1.50	1.41
8	I	102	BCL	C1D-ND	-4.82	1.31	1.37
8	J	102	BCL	O2D-CGD	4.82	1.45	1.33
16	J	104	A1EF2	C12-C13	-4.82	1.41	1.51
16	q	101	A1EF2	C12-C13	-4.81	1.41	1.51
8	J	102	BCL	C3B-C4B	4.81	1.50	1.41
16	O	103	A1EF2	C12-C13	-4.81	1.41	1.51
8	F	103	BCL	O2D-CGD	4.81	1.44	1.33
8	I	102	BCL	O2D-CGD	4.81	1.44	1.33
8	g	102	BCL	O2D-CGD	4.80	1.44	1.33
16	p	101	A1EF2	C12-C13	-4.80	1.41	1.51
8	N	101	BCL	C3B-C4B	4.79	1.50	1.41
8	P	102	BCL	C3B-C4B	4.76	1.50	1.41
8	F	103	BCL	C1D-ND	-4.72	1.32	1.37
8	N	101	BCL	C1D-ND	-4.72	1.32	1.37
8	M	401	BCL	C3B-C4B	4.72	1.49	1.41
8	G	104	BCL	C1D-ND	-4.71	1.32	1.37
8	G	104	BCL	C3B-C4B	4.70	1.49	1.41
16	D	105	A1EF2	C12-C11	-4.68	1.38	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	O	102	BCL	C3B-C4B	4.67	1.49	1.41
8	E	103	BCL	C1D-ND	-4.67	1.32	1.37
8	E	103	BCL	C3B-C4B	4.65	1.49	1.41
16	E	105	A1EF2	C12-C11	-4.65	1.38	1.53
8	L	301	BCL	C3B-C4B	4.64	1.49	1.41
8	K	102	BCL	C1D-ND	-4.63	1.32	1.37
16	B	103	A1EF2	C12-C11	-4.63	1.38	1.53
16	D	104	A1EF2	C12-C11	-4.63	1.38	1.53
8	F	103	BCL	C3B-C4B	4.62	1.49	1.41
8	i	101	BCL	C3B-C4B	4.62	1.49	1.41
16	M	411	A1EF2	C12-C11	-4.62	1.38	1.53
8	D	102	BCL	C3B-C4B	4.59	1.49	1.41
8	C	103	BCL	C3B-C4B	4.58	1.49	1.41
8	I	102	BCL	C3B-C4B	4.58	1.49	1.41
16	N	102	A1EF2	C12-C11	-4.58	1.38	1.53
8	g	102	BCL	C3B-C4B	4.57	1.49	1.41
8	K	102	BCL	C3B-C4B	4.57	1.49	1.41
8	j	101	BCL	C3B-C4B	4.56	1.49	1.41
16	g	103	A1EF2	C12-C11	-4.56	1.38	1.53
8	J	102	BCL	C1D-ND	-4.56	1.32	1.37
16	C	104	A1EF2	C12-C11	-4.56	1.38	1.53
8	Q	101	BCL	C3B-C4B	4.56	1.49	1.41
8	d	102	BCL	C3B-C4B	4.56	1.49	1.41
16	n	101	A1EF2	C12-C11	-4.55	1.38	1.53
16	a	103	A1EF2	C12-C11	-4.54	1.38	1.53
8	M	404	BCL	C1D-ND	-4.54	1.32	1.37
8	L	308	BCL	C3B-C4B	4.52	1.49	1.41
8	k	102	BCL	C3B-C4B	4.52	1.49	1.41
8	O	102	BCL	C1D-ND	-4.52	1.32	1.37
8	b	103	BCL	C3B-C4B	4.51	1.49	1.41
16	f	101	A1EF2	C12-C11	-4.50	1.38	1.53
8	n	102	BCL	C3B-C4B	4.49	1.49	1.41
16	d	101	A1EF2	C12-C11	-4.49	1.38	1.53
16	e	101	A1EF2	C12-C11	-4.49	1.38	1.53
16	N	103	A1EF2	C12-C11	-4.48	1.38	1.53
16	J	101	A1EF2	C12-C11	-4.48	1.38	1.53
8	q	102	BCL	CHD-C1D	4.47	1.47	1.38
16	J	104	A1EF2	C12-C11	-4.47	1.38	1.53
16	g	101	A1EF2	C12-C11	-4.46	1.38	1.53
8	a	102	BCL	C3B-C4B	4.46	1.49	1.41
16	I	105	A1EF2	C12-C11	-4.45	1.38	1.53
8	j	101	BCL	C1D-ND	-4.45	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	J	106	A1EF2	C12-C11	-4.45	1.38	1.53
8	c	102	BCL	C3B-C4B	4.45	1.49	1.41
16	J	103	A1EF2	C12-C11	-4.45	1.38	1.53
16	O	103	A1EF2	C12-C11	-4.45	1.38	1.53
16	o	101	A1EF2	C12-C11	-4.44	1.38	1.53
8	f	102	BCL	C3B-C4B	4.43	1.49	1.41
8	P	102	BCL	CHD-C1D	4.43	1.47	1.38
16	b	102	A1EF2	C12-C11	-4.42	1.38	1.53
16	c	104	A1EF2	C12-C11	-4.42	1.38	1.53
8	o	102	BCL	C3B-C4B	4.42	1.49	1.41
16	k	101	A1EF2	C12-C11	-4.42	1.38	1.53
8	B	101	BCL	C1D-ND	-4.41	1.32	1.37
8	Q	101	BCL	CHD-C1D	4.41	1.46	1.38
8	i	101	BCL	C1D-ND	-4.40	1.32	1.37
16	b	102	A1EF2	C21-C22	4.40	1.41	1.35
16	q	101	A1EF2	C12-C11	-4.38	1.39	1.53
8	p	102	BCL	CHD-C1D	4.38	1.46	1.38
8	g	102	BCL	C1D-ND	-4.37	1.32	1.37
8	e	102	BCL	C3B-C4B	4.37	1.49	1.41
8	d	102	BCL	C1D-ND	-4.36	1.32	1.37
8	D	102	BCL	C1D-ND	-4.35	1.32	1.37
8	A	702	BCL	CHD-C1D	4.35	1.46	1.38
8	f	102	BCL	C1D-ND	-4.35	1.32	1.37
8	A	702	BCL	C3B-C4B	4.34	1.49	1.41
16	p	101	A1EF2	C12-C11	-4.34	1.39	1.53
11	G	103	PGV	O03-C19	4.34	1.46	1.33
8	o	102	BCL	CHD-C1D	4.33	1.46	1.38
8	C	103	BCL	CHD-C1D	4.32	1.46	1.38
8	q	102	BCL	C3B-C4B	4.32	1.49	1.41
8	C	103	BCL	C1D-ND	-4.32	1.32	1.37
16	d	101	A1EF2	C21-C22	4.32	1.41	1.35
8	L	301	BCL	O2A-CGA	4.31	1.45	1.33
8	e	102	BCL	C1D-ND	-4.31	1.32	1.37
16	k	101	A1EF2	C21-C22	4.31	1.41	1.35
11	M	412	PGV	O03-C19	4.31	1.45	1.33
11	K	103	PGV	O03-C19	4.30	1.45	1.33
8	K	102	BCL	CHD-C1D	4.30	1.46	1.38
11	H	304	PGV	O03-C19	4.30	1.45	1.33
8	L	308	BCL	O2A-CGA	4.29	1.45	1.33
11	L	305	PGV	O03-C19	4.29	1.45	1.33
16	q	101	A1EF2	C21-C22	4.28	1.41	1.35
8	a	102	BCL	C1D-ND	-4.28	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	p	101	A1EF2	C21-C22	4.28	1.41	1.35
8	p	102	BCL	O2A-CGA	4.28	1.45	1.33
11	C	101	PGV	O03-C19	4.28	1.45	1.33
8	L	301	BCL	CHD-C1D	4.27	1.46	1.38
16	o	101	A1EF2	C21-C22	4.26	1.41	1.35
8	n	102	BCL	C1D-ND	-4.26	1.32	1.37
8	O	102	BCL	CHD-C1D	4.26	1.46	1.38
8	g	102	BCL	O2A-CGA	4.25	1.45	1.33
8	b	103	BCL	C1D-ND	-4.25	1.32	1.37
11	E	104	PGV	O03-C19	4.25	1.45	1.33
8	L	308	BCL	C1D-ND	-4.25	1.32	1.37
11	L	314	PGV	O03-C19	4.24	1.45	1.33
8	D	102	BCL	CHD-C1D	4.24	1.46	1.38
11	C	102	PGV	O03-C19	4.23	1.45	1.33
8	q	102	BCL	O2A-CGA	4.22	1.45	1.33
16	f	101	A1EF2	C21-C22	4.22	1.41	1.35
8	Q	101	BCL	O2A-CGA	4.21	1.45	1.33
11	M	412	PGV	O01-C1	4.21	1.46	1.34
8	M	401	BCL	O2A-CGA	4.21	1.45	1.33
11	L	313	PGV	O03-C19	4.21	1.45	1.33
8	b	103	BCL	CHD-C1D	4.21	1.46	1.38
11	K	103	PGV	O01-C1	4.20	1.46	1.34
8	d	102	BCL	O2A-CGA	4.20	1.45	1.33
8	J	102	BCL	CHD-C1D	4.19	1.46	1.38
16	n	101	A1EF2	C21-C22	4.19	1.41	1.35
16	e	101	A1EF2	C21-C22	4.19	1.41	1.35
8	o	102	BCL	O2A-CGA	4.19	1.45	1.33
8	M	401	BCL	C1D-ND	-4.18	1.32	1.37
16	J	106	A1EF2	C18-C17	4.18	1.41	1.35
8	P	102	BCL	O2A-CGA	4.18	1.45	1.33
11	E	104	PGV	O01-C1	4.18	1.46	1.34
8	n	102	BCL	O2A-CGA	4.18	1.45	1.33
8	F	103	BCL	O2A-CGA	4.17	1.45	1.33
8	c	102	BCL	CHD-C1D	4.16	1.46	1.38
8	M	404	BCL	CHD-C1D	4.16	1.46	1.38
8	L	308	BCL	CHD-C1D	4.16	1.46	1.38
8	C	103	BCL	O2A-CGA	4.16	1.45	1.33
8	B	101	BCL	O2A-CGA	4.16	1.45	1.33
8	c	102	BCL	O2A-CGA	4.16	1.45	1.33
16	O	103	A1EF2	C21-C22	4.16	1.41	1.35
8	I	102	BCL	O2A-CGA	4.16	1.45	1.33
16	O	103	A1EF2	C18-C17	4.16	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	101	BCL	CHD-C1D	4.15	1.46	1.38
8	a	102	BCL	O2A-CGA	4.15	1.45	1.33
11	L	306	PGV	O03-C19	4.15	1.45	1.33
8	M	401	BCL	CHD-C1D	4.15	1.46	1.38
11	L	313	PGV	O01-C1	4.15	1.46	1.34
8	F	103	BCL	CHD-C1D	4.14	1.46	1.38
8	E	103	BCL	O2A-CGA	4.14	1.45	1.33
8	j	101	BCL	O2A-CGA	4.14	1.45	1.33
16	J	104	A1EF2	C18-C17	4.14	1.41	1.35
8	O	102	BCL	O2A-CGA	4.14	1.45	1.33
8	b	103	BCL	O2A-CGA	4.14	1.45	1.33
8	n	102	BCL	CHD-C1D	4.14	1.46	1.38
16	c	104	A1EF2	C21-C22	4.14	1.41	1.35
11	H	303	PGV	O03-C19	4.13	1.45	1.33
8	I	102	BCL	CHD-C1D	4.13	1.46	1.38
16	q	101	A1EF2	C18-C17	4.12	1.41	1.35
8	i	101	BCL	O2A-CGA	4.12	1.45	1.33
11	C	101	PGV	O01-C1	4.12	1.45	1.34
11	H	303	PGV	O01-C1	4.12	1.45	1.34
11	M	402	PGV	O03-C19	4.12	1.45	1.33
8	a	102	BCL	CHD-C1D	4.12	1.46	1.38
8	d	102	BCL	CHD-C1D	4.11	1.46	1.38
8	k	102	BCL	O2A-CGA	4.11	1.45	1.33
8	E	103	BCL	CHD-C1D	4.11	1.46	1.38
16	J	103	A1EF2	C21-C22	4.10	1.41	1.35
8	e	102	BCL	O2A-CGA	4.10	1.45	1.33
8	g	102	BCL	CHD-C1D	4.10	1.46	1.38
11	L	305	PGV	O01-C1	4.09	1.45	1.34
8	M	404	BCL	O2A-CGA	4.09	1.45	1.33
8	J	102	BCL	O2A-CGA	4.09	1.45	1.33
8	N	101	BCL	O2A-CGA	4.08	1.45	1.33
8	i	101	BCL	CHD-C1D	4.08	1.46	1.38
8	p	102	BCL	C3B-C4B	4.08	1.48	1.41
8	N	101	BCL	CHD-C1D	4.08	1.46	1.38
8	D	102	BCL	O2A-CGA	4.07	1.45	1.33
16	g	101	A1EF2	C21-C22	4.07	1.41	1.35
8	j	101	BCL	CHD-C1D	4.07	1.46	1.38
8	f	102	BCL	O2A-CGA	4.07	1.45	1.33
11	G	103	PGV	O01-C1	4.06	1.45	1.34
8	k	102	BCL	CHD-C1D	4.06	1.46	1.38
8	e	102	BCL	CHD-C1D	4.06	1.46	1.38
16	J	101	A1EF2	C18-C17	4.06	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	J	104	A1EF2	C21-C22	4.04	1.41	1.35
16	J	106	A1EF2	C21-C22	4.04	1.41	1.35
8	G	104	BCL	O2A-CGA	4.04	1.45	1.33
8	M	404	BCL	CHC-C4B	4.03	1.48	1.39
8	N	101	BCL	C1B-NB	-4.03	1.32	1.37
8	k	102	BCL	C1D-ND	-4.03	1.32	1.37
8	f	102	BCL	CHD-C1D	4.02	1.46	1.38
8	K	102	BCL	O2A-CGA	4.02	1.45	1.33
8	G	104	BCL	CHD-C1D	4.01	1.46	1.38
11	C	102	PGV	O01-C1	4.00	1.45	1.34
16	N	103	A1EF2	C18-C17	3.99	1.41	1.35
16	p	101	A1EF2	C18-C17	3.98	1.41	1.35
8	A	702	BCL	O2A-CGA	3.98	1.45	1.33
11	M	402	PGV	O01-C1	3.98	1.45	1.34
16	I	105	A1EF2	C21-C22	3.98	1.41	1.35
8	L	308	BCL	CHC-C4B	3.95	1.48	1.39
16	g	103	A1EF2	C18-C17	3.95	1.41	1.35
16	b	102	A1EF2	C18-C17	3.93	1.41	1.35
11	L	314	PGV	O01-C1	3.93	1.45	1.34
11	L	306	PGV	O01-C1	3.92	1.45	1.34
16	N	103	A1EF2	C21-C22	3.92	1.41	1.35
8	A	702	BCL	C1D-ND	-3.91	1.33	1.37
8	O	102	BCL	C1B-NB	-3.91	1.33	1.37
11	H	304	PGV	O01-C1	3.89	1.45	1.34
16	o	101	A1EF2	C18-C17	3.89	1.40	1.35
16	n	101	A1EF2	C18-C17	3.88	1.40	1.35
8	M	401	BCL	CHC-C4B	3.88	1.48	1.39
8	B	101	BCL	C1B-NB	-3.87	1.33	1.37
8	N	101	BCL	CHC-C4B	3.86	1.48	1.39
16	C	104	A1EF2	C18-C17	3.86	1.40	1.35
8	I	102	BCL	C4B-NB	-3.84	1.33	1.37
16	D	104	A1EF2	C18-C17	3.84	1.40	1.35
8	P	102	BCL	CHC-C4B	3.84	1.48	1.39
8	C	103	BCL	C4B-NB	-3.84	1.33	1.37
16	J	101	A1EF2	C21-C22	3.84	1.40	1.35
16	N	102	A1EF2	C21-C22	3.82	1.40	1.35
8	a	102	BCL	CHC-C4B	3.82	1.48	1.39
8	G	104	BCL	CHC-C4B	3.82	1.48	1.39
16	a	103	A1EF2	C18-C17	3.81	1.40	1.35
16	B	103	A1EF2	C18-C17	3.81	1.40	1.35
16	M	411	A1EF2	C18-C17	3.81	1.40	1.35
8	F	103	BCL	C4B-NB	-3.80	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	K	102	BCL	C1B-NB	-3.80	1.33	1.37
8	i	101	BCL	C4B-NB	-3.80	1.33	1.37
8	d	102	BCL	CHC-C4B	3.79	1.47	1.39
8	G	104	BCL	C4B-NB	-3.79	1.33	1.37
8	E	103	BCL	CHC-C4B	3.78	1.47	1.39
16	k	101	A1EF2	C18-C17	3.78	1.40	1.35
8	J	102	BCL	CHC-C4B	3.78	1.47	1.39
8	E	103	BCL	C1B-NB	-3.78	1.33	1.37
8	b	103	BCL	C4B-NB	-3.77	1.33	1.37
8	C	103	BCL	C1B-NB	-3.77	1.33	1.37
8	B	101	BCL	CHC-C4B	3.77	1.47	1.39
8	c	102	BCL	CHC-C4B	3.77	1.47	1.39
8	N	101	BCL	C4B-NB	-3.77	1.33	1.37
8	D	102	BCL	CHC-C4B	3.77	1.47	1.39
8	q	102	BCL	CHC-C4B	3.77	1.47	1.39
8	L	301	BCL	CHC-C4B	3.77	1.47	1.39
8	P	102	BCL	C1B-NB	-3.76	1.33	1.37
8	b	103	BCL	CHC-C4B	3.76	1.47	1.39
8	K	102	BCL	CHC-C4B	3.76	1.47	1.39
8	o	102	BCL	CHC-C4B	3.76	1.47	1.39
8	M	404	BCL	C1B-NB	-3.76	1.33	1.37
8	c	102	BCL	C1D-ND	-3.75	1.33	1.37
16	d	101	A1EF2	C18-C17	3.75	1.40	1.35
8	n	102	BCL	C4B-NB	-3.75	1.33	1.37
8	k	102	BCL	CHC-C4B	3.74	1.47	1.39
8	P	102	BCL	C4B-NB	-3.74	1.33	1.37
8	C	103	BCL	CHC-C4B	3.74	1.47	1.39
8	F	103	BCL	C1B-NB	-3.74	1.33	1.37
16	N	102	A1EF2	C18-C17	3.74	1.40	1.35
8	p	102	BCL	CHB-C1B	3.73	1.47	1.39
8	i	101	BCL	C1B-NB	-3.73	1.33	1.37
8	A	702	BCL	C4B-NB	-3.72	1.33	1.37
8	f	102	BCL	C4B-NB	-3.72	1.33	1.37
8	f	102	BCL	CHC-C4B	3.72	1.47	1.39
8	n	102	BCL	CHC-C4B	3.71	1.47	1.39
8	e	102	BCL	CHC-C4B	3.71	1.47	1.39
8	J	102	BCL	C1B-NB	-3.71	1.33	1.37
16	D	104	A1EF2	C21-C22	3.71	1.40	1.35
8	q	102	BCL	CHB-C1B	3.71	1.47	1.39
16	g	103	A1EF2	C21-C22	3.71	1.40	1.35
8	F	103	BCL	CHC-C4B	3.71	1.47	1.39
8	K	102	BCL	C4B-NB	-3.70	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	o	102	BCL	C1D-ND	-3.70	1.33	1.37
8	O	102	BCL	C4B-NB	-3.70	1.33	1.37
16	D	105	A1EF2	C18-C17	3.70	1.40	1.35
8	P	102	BCL	C1D-ND	-3.69	1.33	1.37
8	j	101	BCL	CHC-C4B	3.69	1.47	1.39
8	k	102	BCL	C4B-NB	-3.69	1.33	1.37
8	g	102	BCL	C4B-NB	-3.69	1.33	1.37
8	d	102	BCL	C4B-NB	-3.68	1.33	1.37
8	O	102	BCL	CHC-C4B	3.68	1.47	1.39
8	Q	101	BCL	CHB-C1B	3.67	1.47	1.39
8	b	103	BCL	C1B-NB	-3.67	1.33	1.37
8	e	102	BCL	C4B-NB	-3.67	1.33	1.37
8	j	101	BCL	C4B-NB	-3.67	1.33	1.37
8	p	102	BCL	CHC-C4B	3.67	1.47	1.39
8	i	101	BCL	CHC-C4B	3.65	1.47	1.39
8	A	702	BCL	CHC-C4B	3.65	1.47	1.39
16	M	411	A1EF2	C21-C22	3.65	1.40	1.35
8	G	104	BCL	C1B-NB	-3.65	1.33	1.37
8	p	102	BCL	OBD-CAD	3.65	1.28	1.22
16	f	101	A1EF2	C18-C17	3.64	1.40	1.35
16	C	104	A1EF2	C21-C22	3.64	1.40	1.35
8	c	102	BCL	CHB-C1B	3.64	1.47	1.39
16	g	101	A1EF2	C18-C17	3.63	1.40	1.35
8	I	102	BCL	C1B-NB	-3.63	1.33	1.37
8	g	102	BCL	CHC-C4B	3.62	1.47	1.39
8	e	102	BCL	CHB-C1B	3.62	1.47	1.39
8	E	103	BCL	C4B-NB	-3.62	1.33	1.37
8	P	102	BCL	CHB-C1B	3.62	1.47	1.39
8	I	102	BCL	CHC-C4B	3.61	1.47	1.39
8	f	102	BCL	C1B-NB	-3.61	1.33	1.37
8	a	102	BCL	C4B-NB	-3.61	1.33	1.37
16	B	103	A1EF2	C21-C22	3.61	1.40	1.35
16	E	105	A1EF2	C18-C17	3.61	1.40	1.35
16	D	105	A1EF2	C21-C22	3.61	1.40	1.35
8	a	102	BCL	OBD-CAD	3.61	1.28	1.22
16	c	104	A1EF2	C18-C17	3.61	1.40	1.35
8	o	102	BCL	CHB-C1B	3.60	1.47	1.39
8	g	102	BCL	CHB-C1B	3.60	1.47	1.39
8	g	102	BCL	C1B-NB	-3.60	1.33	1.37
8	a	102	BCL	CHB-C1B	3.60	1.47	1.39
8	p	102	BCL	C4B-NB	-3.59	1.33	1.37
8	d	102	BCL	C1B-NB	-3.59	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	q	102	BCL	OBD-CAD	3.59	1.28	1.22
8	D	102	BCL	C1B-NB	-3.58	1.33	1.37
8	k	102	BCL	CHB-C1B	3.58	1.47	1.39
8	A	702	BCL	OBD-CAD	3.57	1.28	1.22
8	Q	101	BCL	CHC-C4B	3.57	1.47	1.39
8	B	101	BCL	C4B-NB	-3.57	1.33	1.37
16	e	101	A1EF2	C18-C17	3.57	1.40	1.35
8	Q	101	BCL	OBD-CAD	3.57	1.28	1.22
16	E	105	A1EF2	C21-C22	3.56	1.40	1.35
8	d	102	BCL	CHB-C1B	3.56	1.47	1.39
8	I	102	BCL	OBD-CAD	3.56	1.28	1.22
8	c	102	BCL	C4B-NB	-3.56	1.33	1.37
8	M	401	BCL	OBD-CAD	3.55	1.28	1.22
8	n	102	BCL	CHB-C1B	3.55	1.47	1.39
8	i	101	BCL	CHB-C1B	3.55	1.47	1.39
8	P	102	BCL	OBD-CAD	3.55	1.28	1.22
8	L	301	BCL	C1B-NB	-3.54	1.33	1.37
8	E	103	BCL	OBD-CAD	3.53	1.28	1.22
8	b	103	BCL	CHB-C1B	3.53	1.47	1.39
8	B	101	BCL	C3D-C2D	3.53	1.48	1.39
8	O	102	BCL	C3D-C2D	3.53	1.48	1.39
8	k	102	BCL	C1B-NB	-3.53	1.33	1.37
8	g	102	BCL	OBD-CAD	3.53	1.28	1.22
8	A	702	BCL	CHB-C1B	3.52	1.47	1.39
8	L	301	BCL	OBD-CAD	3.52	1.28	1.22
8	a	102	BCL	C1B-NB	-3.52	1.33	1.37
8	O	102	BCL	OBD-CAD	3.52	1.28	1.22
8	q	102	BCL	C1D-ND	-3.51	1.33	1.37
8	o	102	BCL	C1B-NB	-3.51	1.33	1.37
8	D	102	BCL	C4B-NB	-3.51	1.33	1.37
8	L	308	BCL	CHB-C1B	3.51	1.47	1.39
16	a	103	A1EF2	C21-C22	3.51	1.40	1.35
8	f	102	BCL	OBD-CAD	3.51	1.28	1.22
8	o	102	BCL	OBD-CAD	3.50	1.28	1.22
8	N	101	BCL	C3D-C2D	3.50	1.48	1.39
8	A	702	BCL	C1B-NB	-3.50	1.33	1.37
8	B	101	BCL	OBD-CAD	3.50	1.28	1.22
8	L	308	BCL	C3D-C2D	3.50	1.48	1.39
8	k	102	BCL	OBD-CAD	3.50	1.28	1.22
8	K	102	BCL	C3D-C2D	3.50	1.48	1.39
8	n	102	BCL	C3D-C2D	3.49	1.48	1.39
8	j	101	BCL	OBD-CAD	3.49	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	L	308	BCL	OBD-CAD	3.49	1.28	1.22
8	J	102	BCL	C4B-NB	-3.49	1.33	1.37
8	d	102	BCL	OBD-CAD	3.49	1.28	1.22
8	f	102	BCL	CHB-C1B	3.49	1.47	1.39
8	L	301	BCL	CHB-C1B	3.48	1.47	1.39
8	D	102	BCL	C3D-C2D	3.48	1.48	1.39
8	b	103	BCL	C3D-C2D	3.48	1.48	1.39
8	F	103	BCL	C3D-C2D	3.48	1.48	1.39
8	F	103	BCL	OBD-CAD	3.47	1.28	1.22
8	G	104	BCL	OBD-CAD	3.47	1.28	1.22
8	n	102	BCL	C1B-NB	-3.47	1.33	1.37
8	O	102	BCL	CHB-C1B	3.46	1.47	1.39
8	E	103	BCL	C3D-C2D	3.46	1.48	1.39
8	e	102	BCL	OBD-CAD	3.46	1.28	1.22
8	g	102	BCL	C3D-C2D	3.46	1.48	1.39
8	I	102	BCL	C3D-C2D	3.45	1.48	1.39
8	M	404	BCL	CHB-C1B	3.45	1.47	1.39
8	C	103	BCL	C3D-C2D	3.45	1.48	1.39
8	n	102	BCL	OBD-CAD	3.45	1.28	1.22
8	N	101	BCL	OBD-CAD	3.45	1.28	1.22
8	e	102	BCL	C1B-NB	-3.45	1.33	1.37
8	o	102	BCL	C4B-NB	-3.45	1.33	1.37
8	G	104	BCL	CHB-C1B	3.44	1.47	1.39
8	M	404	BCL	C3D-C2D	3.44	1.48	1.39
8	M	401	BCL	CHB-C1B	3.44	1.47	1.39
16	I	105	A1EF2	C18-C17	3.44	1.40	1.35
8	A	702	BCL	C3D-C2D	3.44	1.48	1.39
8	G	104	BCL	C3D-C2D	3.44	1.48	1.39
8	L	301	BCL	C1D-ND	-3.44	1.33	1.37
8	M	401	BCL	C4B-NB	-3.43	1.33	1.37
8	p	102	BCL	C1D-ND	-3.43	1.33	1.37
8	f	102	BCL	C3D-C2D	3.43	1.48	1.39
8	j	101	BCL	C1B-NB	-3.43	1.33	1.37
8	J	102	BCL	C3D-C2D	3.43	1.48	1.39
8	j	101	BCL	C3D-C2D	3.43	1.48	1.39
16	J	103	A1EF2	C18-C17	3.43	1.40	1.35
8	i	101	BCL	C3D-C2D	3.42	1.48	1.39
8	i	101	BCL	OBD-CAD	3.42	1.28	1.22
8	c	102	BCL	OBD-CAD	3.42	1.28	1.22
8	q	102	BCL	C3D-C2D	3.42	1.48	1.39
8	M	401	BCL	C3D-C2D	3.42	1.48	1.39
8	d	102	BCL	C3D-C2D	3.41	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	j	101	BCL	CHB-C1B	3.41	1.47	1.39
8	o	102	BCL	C3D-C2D	3.41	1.48	1.39
8	J	102	BCL	OBD-CAD	3.41	1.28	1.22
8	D	102	BCL	OBD-CAD	3.41	1.28	1.22
8	p	102	BCL	C3D-C2D	3.40	1.48	1.39
8	b	103	BCL	OBD-CAD	3.40	1.28	1.22
8	F	103	BCL	CHB-C1B	3.40	1.47	1.39
8	e	102	BCL	C3D-C2D	3.39	1.48	1.39
8	C	103	BCL	OBD-CAD	3.39	1.28	1.22
8	K	102	BCL	OBD-CAD	3.39	1.28	1.22
8	a	102	BCL	C3D-C2D	3.39	1.48	1.39
8	c	102	BCL	C1B-NB	-3.38	1.33	1.37
8	L	308	BCL	C4B-NB	-3.38	1.33	1.37
8	q	102	BCL	C4B-NB	-3.37	1.33	1.37
8	M	404	BCL	OBD-CAD	3.37	1.28	1.22
8	B	101	BCL	CHB-C1B	3.37	1.47	1.39
8	c	102	BCL	C3D-C2D	3.36	1.48	1.39
8	P	102	BCL	C3D-C2D	3.36	1.48	1.39
8	J	102	BCL	CHB-C1B	3.35	1.46	1.39
8	D	102	BCL	CHB-C1B	3.35	1.46	1.39
8	K	102	BCL	CHB-C1B	3.35	1.46	1.39
8	I	102	BCL	CHB-C1B	3.31	1.46	1.39
8	L	301	BCL	C4B-NB	-3.31	1.33	1.37
8	L	308	BCL	C1B-NB	-3.30	1.33	1.37
8	L	301	BCL	C3D-C2D	3.30	1.48	1.39
8	k	102	BCL	C3D-C2D	3.30	1.48	1.39
8	M	401	BCL	C1B-NB	-3.30	1.33	1.37
8	N	101	BCL	CHB-C1B	3.29	1.46	1.39
8	C	103	BCL	CHB-C1B	3.28	1.46	1.39
8	E	103	BCL	CHB-C1B	3.27	1.46	1.39
8	q	102	BCL	C1B-NB	-3.23	1.33	1.37
8	Q	101	BCL	C3D-C2D	3.20	1.47	1.39
10	M	407	U10	C4-C3	3.20	1.49	1.36
8	Q	101	BCL	C4B-NB	-3.19	1.33	1.37
8	M	404	BCL	C4B-NB	-3.14	1.33	1.37
8	Q	101	BCL	C1D-ND	-3.12	1.33	1.37
10	L	304	U10	C4-C3	3.09	1.48	1.36
8	p	102	BCL	C1B-NB	-3.07	1.34	1.37
8	O	102	BCL	CHD-C4C	3.01	1.47	1.39
8	K	102	BCL	CHD-C4C	2.98	1.47	1.39
9	L	302	BPH	C4D-CHA	2.96	1.44	1.39
8	Q	101	BCL	C1B-NB	-2.96	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	D	102	BCL	CHD-C4C	2.93	1.47	1.39
8	F	103	BCL	CHD-C4C	2.92	1.47	1.39
8	C	103	BCL	CHD-C4C	2.92	1.47	1.39
8	P	102	BCL	CHD-C4C	2.91	1.47	1.39
8	M	401	BCL	CHD-C4C	2.90	1.47	1.39
8	A	702	BCL	CHD-C4C	2.90	1.47	1.39
8	B	101	BCL	CHD-C4C	2.90	1.47	1.39
9	M	405	BPH	C4D-CHA	2.89	1.44	1.39
10	L	303	U10	C4-C3	2.88	1.48	1.36
8	E	103	BCL	CHD-C4C	2.86	1.47	1.39
8	G	104	BCL	CHD-C4C	2.86	1.47	1.39
8	I	102	BCL	CHD-C4C	2.86	1.47	1.39
8	Q	101	BCL	CHD-C4C	2.85	1.47	1.39
8	N	101	BCL	CHD-C4C	2.84	1.47	1.39
8	J	102	BCL	CHD-C4C	2.84	1.47	1.39
8	n	102	BCL	CHD-C4C	2.82	1.47	1.39
8	q	102	BCL	CHD-C4C	2.82	1.47	1.39
8	M	404	BCL	CHD-C4C	2.81	1.47	1.39
8	o	102	BCL	CHD-C4C	2.78	1.47	1.39
8	L	301	BCL	CHD-C4C	2.77	1.47	1.39
8	L	308	BCL	CHD-C4C	2.77	1.47	1.39
8	p	102	BCL	CHD-C4C	2.77	1.47	1.39
8	a	102	BCL	CHD-C4C	2.76	1.47	1.39
8	e	102	BCL	CHD-C4C	2.75	1.47	1.39
8	b	103	BCL	CHD-C4C	2.75	1.47	1.39
8	d	102	BCL	CHD-C4C	2.74	1.46	1.39
8	P	102	BCL	C4D-CHA	2.73	1.48	1.38
8	g	102	BCL	CHD-C4C	2.73	1.46	1.39
8	j	101	BCL	CHD-C4C	2.72	1.46	1.39
8	q	102	BCL	C4D-CHA	2.71	1.48	1.38
8	i	101	BCL	CHD-C4C	2.71	1.46	1.39
8	c	102	BCL	CHD-C4C	2.69	1.46	1.39
8	Q	101	BCL	C4D-CHA	2.68	1.47	1.38
9	L	302	BPH	C3A-C2A	-2.66	1.52	1.54
8	f	102	BCL	CHD-C4C	2.66	1.46	1.39
16	E	105	A1EF2	C23-C22	-2.65	1.40	1.45
8	Q	101	BCL	C1B-C2B	2.65	1.49	1.43
8	q	102	BCL	C1B-C2B	2.63	1.49	1.43
8	k	102	BCL	CHD-C4C	2.63	1.46	1.39
8	o	102	BCL	C4D-CHA	2.63	1.47	1.38
16	E	105	A1EF2	C16-C17	-2.62	1.40	1.45
16	c	104	A1EF2	C16-C17	-2.62	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	e	101	A1EF2	C16-C17	-2.61	1.40	1.45
16	k	101	A1EF2	C16-C17	-2.59	1.40	1.45
16	M	411	A1EF2	C23-C22	-2.59	1.40	1.45
8	p	102	BCL	C1B-C2B	2.59	1.49	1.43
16	f	101	A1EF2	C16-C17	-2.59	1.40	1.45
9	M	405	BPH	C3A-C2A	-2.59	1.52	1.54
8	P	102	BCL	C1B-C2B	2.59	1.49	1.43
8	c	102	BCL	C4D-CHA	2.58	1.47	1.38
8	p	102	BCL	C4D-CHA	2.58	1.47	1.38
16	J	106	A1EF2	C27-C26	2.58	1.51	1.45
8	o	102	BCL	C1B-C2B	2.55	1.49	1.43
16	D	104	A1EF2	C27-C26	2.55	1.51	1.45
16	B	103	A1EF2	C16-C17	-2.54	1.40	1.45
8	L	301	BCL	C4D-CHA	2.54	1.47	1.38
16	J	103	A1EF2	C16-C17	-2.54	1.40	1.45
16	O	103	A1EF2	C27-C26	2.53	1.51	1.45
16	e	101	A1EF2	C27-C26	2.53	1.51	1.45
8	O	102	BCL	C4D-CHA	2.53	1.47	1.38
16	q	101	A1EF2	C27-C26	2.53	1.51	1.45
16	k	101	A1EF2	C27-C26	2.52	1.51	1.45
8	g	102	BCL	C4D-CHA	2.52	1.47	1.38
16	d	101	A1EF2	C16-C17	-2.52	1.40	1.45
16	o	101	A1EF2	C27-C26	2.52	1.51	1.45
16	N	102	A1EF2	C27-C26	2.52	1.51	1.45
16	g	101	A1EF2	C27-C26	2.51	1.51	1.45
16	p	101	A1EF2	C27-C26	2.51	1.51	1.45
16	N	102	A1EF2	C16-C17	-2.51	1.40	1.45
16	D	105	A1EF2	C23-C22	-2.51	1.40	1.45
8	e	102	BCL	C4D-CHA	2.51	1.47	1.38
8	k	102	BCL	C4D-CHA	2.51	1.47	1.38
16	f	101	A1EF2	C27-C26	2.51	1.51	1.45
8	f	102	BCL	C4D-CHA	2.51	1.47	1.38
16	N	103	A1EF2	C27-C26	2.50	1.51	1.45
16	J	104	A1EF2	C27-C26	2.50	1.51	1.45
16	a	103	A1EF2	C27-C26	2.50	1.51	1.45
16	I	105	A1EF2	C27-C26	2.50	1.51	1.45
16	J	103	A1EF2	C27-C26	2.50	1.51	1.45
8	g	102	BCL	C1B-C2B	2.50	1.49	1.43
16	b	102	A1EF2	C27-C26	2.50	1.51	1.45
16	I	105	A1EF2	C16-C17	-2.50	1.40	1.45
8	A	702	BCL	C4D-CHA	2.49	1.47	1.38
16	n	101	A1EF2	C16-C17	-2.49	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	b	103	BCL	C4D-CHA	2.49	1.47	1.38
16	c	104	A1EF2	C27-C26	2.48	1.51	1.45
16	d	101	A1EF2	C27-C26	2.48	1.51	1.45
16	J	101	A1EF2	C27-C26	2.48	1.51	1.45
8	j	101	BCL	C4D-CHA	2.48	1.47	1.38
16	D	105	A1EF2	C27-C26	2.47	1.51	1.45
8	D	102	BCL	C4D-CHA	2.47	1.47	1.38
16	C	104	A1EF2	C27-C26	2.47	1.51	1.45
8	a	102	BCL	C4D-CHA	2.47	1.47	1.38
8	N	101	BCL	C4D-CHA	2.47	1.47	1.38
16	D	105	A1EF2	C16-C17	-2.47	1.40	1.45
16	n	101	A1EF2	C27-C26	2.47	1.51	1.45
8	d	102	BCL	C4D-CHA	2.47	1.47	1.38
16	D	104	A1EF2	C16-C17	-2.47	1.40	1.45
8	E	103	BCL	C4D-CHA	2.46	1.47	1.38
16	B	103	A1EF2	C27-C26	2.46	1.51	1.45
16	g	103	A1EF2	C27-C26	2.46	1.51	1.45
8	B	101	BCL	C4D-CHA	2.46	1.47	1.38
16	g	103	A1EF2	C16-C17	-2.46	1.40	1.45
16	b	102	A1EF2	C16-C17	-2.46	1.40	1.45
8	F	103	BCL	C4D-CHA	2.45	1.47	1.38
16	M	411	A1EF2	C27-C26	2.45	1.51	1.45
8	A	702	BCL	C1B-C2B	2.45	1.49	1.43
8	a	102	BCL	C1B-C2B	2.45	1.49	1.43
8	e	102	BCL	C1B-C2B	2.44	1.49	1.43
8	M	404	BCL	C3D-C4D	-2.44	1.38	1.44
8	C	103	BCL	C4D-CHA	2.44	1.47	1.38
8	M	401	BCL	C3D-C4D	-2.44	1.38	1.44
16	g	101	A1EF2	C16-C17	-2.43	1.40	1.45
16	a	103	A1EF2	C16-C17	-2.43	1.40	1.45
16	I	105	A1EF2	C23-C22	-2.43	1.40	1.45
8	K	102	BCL	C4D-CHA	2.42	1.47	1.38
8	n	102	BCL	C1B-C2B	2.42	1.49	1.43
8	L	308	BCL	C1B-C2B	2.42	1.49	1.43
16	E	105	A1EF2	C27-C26	2.42	1.51	1.45
8	J	102	BCL	C4D-CHA	2.41	1.47	1.38
8	I	102	BCL	C4D-CHA	2.41	1.47	1.38
8	L	301	BCL	C1B-C2B	2.41	1.48	1.43
8	n	102	BCL	C4D-CHA	2.41	1.47	1.38
8	d	102	BCL	C1B-C2B	2.41	1.48	1.43
8	i	101	BCL	C4D-CHA	2.40	1.46	1.38
8	O	102	BCL	C1B-C2B	2.40	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	G	104	BCL	C4D-CHA	2.40	1.46	1.38
16	J	104	A1EF2	C16-C17	-2.39	1.40	1.45
16	o	101	A1EF2	C16-C17	-2.39	1.40	1.45
16	a	103	A1EF2	C23-C22	-2.38	1.40	1.45
16	N	103	A1EF2	C16-C17	-2.38	1.40	1.45
8	L	308	BCL	C4D-CHA	2.38	1.46	1.38
8	L	301	BCL	C3D-C4D	-2.37	1.38	1.44
8	b	103	BCL	C1B-C2B	2.37	1.48	1.43
16	C	104	A1EF2	C16-C17	-2.36	1.40	1.45
16	q	101	A1EF2	C16-C17	-2.36	1.40	1.45
16	J	103	A1EF2	C23-C22	-2.36	1.40	1.45
8	f	102	BCL	C1B-C2B	2.35	1.48	1.43
8	c	102	BCL	C1B-C2B	2.34	1.48	1.43
8	I	102	BCL	C1B-C2B	2.34	1.48	1.43
8	k	102	BCL	C1B-C2B	2.33	1.48	1.43
16	g	103	A1EF2	C23-C22	-2.33	1.40	1.45
16	B	103	A1EF2	C23-C22	-2.33	1.40	1.45
8	L	308	BCL	C3D-C4D	-2.32	1.38	1.44
16	c	104	A1EF2	C23-C22	-2.32	1.41	1.45
8	i	101	BCL	C1B-C2B	2.32	1.48	1.43
16	N	103	A1EF2	C23-C22	-2.32	1.41	1.45
16	J	106	A1EF2	C28-C29	2.31	1.50	1.43
8	D	102	BCL	C1B-C2B	2.31	1.48	1.43
8	G	104	BCL	C1B-C2B	2.31	1.48	1.43
16	p	101	A1EF2	C16-C17	-2.31	1.41	1.45
8	K	102	BCL	C1B-C2B	2.31	1.48	1.43
16	C	104	A1EF2	C23-C22	-2.30	1.41	1.45
8	C	103	BCL	C3D-C4D	-2.30	1.39	1.44
8	e	102	BCL	C3D-C4D	-2.30	1.39	1.44
8	d	102	BCL	C3D-C4D	-2.30	1.39	1.44
16	J	101	A1EF2	C16-C17	-2.30	1.41	1.45
8	q	102	BCL	C3D-C4D	-2.30	1.39	1.44
8	j	101	BCL	C1B-C2B	2.29	1.48	1.43
8	A	702	BCL	C3D-C4D	-2.29	1.39	1.44
8	M	401	BCL	C1B-C2B	2.29	1.48	1.43
8	p	102	BCL	C3D-C4D	-2.29	1.39	1.44
8	C	103	BCL	C1B-C2B	2.29	1.48	1.43
8	j	101	BCL	C3D-C4D	-2.28	1.39	1.44
16	J	104	A1EF2	C28-C29	2.28	1.50	1.43
8	k	102	BCL	C3D-C4D	-2.28	1.39	1.44
8	g	102	BCL	C3D-C4D	-2.27	1.39	1.44
8	I	102	BCL	C3D-C4D	-2.27	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	E	103	BCL	C1B-C2B	2.27	1.48	1.43
8	B	101	BCL	C3D-C4D	-2.27	1.39	1.44
16	O	103	A1EF2	C28-C29	2.27	1.50	1.43
16	J	106	A1EF2	C16-C17	-2.27	1.41	1.45
8	M	404	BCL	C4D-CHA	2.27	1.46	1.38
8	a	102	BCL	C3D-C4D	-2.26	1.39	1.44
16	D	104	A1EF2	C23-C22	-2.26	1.41	1.45
16	N	102	A1EF2	C28-C29	2.26	1.50	1.43
16	o	101	A1EF2	C23-C22	-2.26	1.41	1.45
16	J	101	A1EF2	C28-C29	2.26	1.50	1.43
8	B	101	BCL	C1B-C2B	2.26	1.48	1.43
8	M	401	BCL	C4D-CHA	2.25	1.46	1.38
8	c	102	BCL	C3D-C4D	-2.25	1.39	1.44
8	b	103	BCL	C3D-C4D	-2.25	1.39	1.44
16	O	103	A1EF2	C16-C17	-2.24	1.41	1.45
8	P	102	BCL	C3D-C4D	-2.24	1.39	1.44
8	F	103	BCL	C1B-C2B	2.23	1.48	1.43
8	o	102	BCL	C3D-C4D	-2.23	1.39	1.44
8	M	404	BCL	C1B-C2B	2.23	1.48	1.43
16	D	104	A1EF2	C28-C29	2.23	1.50	1.43
8	K	102	BCL	C3D-C4D	-2.23	1.39	1.44
16	q	101	A1EF2	C28-C29	2.23	1.50	1.43
16	N	103	A1EF2	C28-C29	2.23	1.50	1.43
16	q	101	A1EF2	C23-C22	-2.22	1.41	1.45
16	e	101	A1EF2	C28-C29	2.22	1.50	1.43
8	n	102	BCL	C3D-C4D	-2.22	1.39	1.44
8	N	101	BCL	C1B-C2B	2.22	1.48	1.43
16	N	102	A1EF2	C23-C22	-2.22	1.41	1.45
16	g	101	A1EF2	C23-C22	-2.21	1.41	1.45
16	a	103	A1EF2	C28-C29	2.21	1.50	1.43
16	C	104	A1EF2	C28-C29	2.21	1.50	1.43
16	p	101	A1EF2	C28-C29	2.21	1.50	1.43
8	F	103	BCL	C3B-C2B	2.20	1.49	1.42
16	n	101	A1EF2	C23-C22	-2.20	1.41	1.45
16	d	101	A1EF2	C28-C29	2.20	1.50	1.43
16	p	101	A1EF2	C23-C22	-2.20	1.41	1.45
16	g	103	A1EF2	C28-C29	2.20	1.50	1.43
8	J	102	BCL	C3D-C4D	-2.20	1.39	1.44
8	G	104	BCL	C3D-C4D	-2.20	1.39	1.44
16	M	411	A1EF2	C16-C17	-2.20	1.41	1.45
8	I	102	BCL	C3B-C2B	2.20	1.49	1.42
8	P	102	BCL	C3B-C2B	2.19	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	f	102	BCL	C3D-C4D	-2.19	1.39	1.44
16	c	104	A1EF2	C28-C29	2.19	1.50	1.43
16	D	105	A1EF2	C28-C29	2.19	1.50	1.43
16	b	102	A1EF2	C23-C22	-2.19	1.41	1.45
8	Q	101	BCL	C3D-C4D	-2.19	1.39	1.44
8	D	102	BCL	C3D-C4D	-2.18	1.39	1.44
16	g	101	A1EF2	C28-C29	2.18	1.50	1.43
8	B	101	BCL	C3B-C2B	2.18	1.49	1.42
8	L	301	BCL	C3B-C2B	2.18	1.49	1.42
16	f	101	A1EF2	C28-C29	2.18	1.50	1.43
8	C	103	BCL	C3B-C2B	2.18	1.49	1.42
16	o	101	A1EF2	C28-C29	2.17	1.50	1.43
16	k	101	A1EF2	C28-C29	2.17	1.50	1.43
16	n	101	A1EF2	C28-C29	2.17	1.50	1.43
8	D	102	BCL	C3B-C2B	2.17	1.49	1.42
16	b	102	A1EF2	C28-C29	2.17	1.50	1.43
8	F	103	BCL	C3D-C4D	-2.17	1.39	1.44
16	J	101	A1EF2	C23-C22	-2.17	1.41	1.45
8	M	404	BCL	C3B-C2B	2.17	1.49	1.42
8	J	102	BCL	C1B-C2B	2.16	1.48	1.43
8	N	101	BCL	C3D-C4D	-2.16	1.39	1.44
16	B	103	A1EF2	C28-C29	2.16	1.50	1.43
8	N	101	BCL	C3B-C2B	2.16	1.49	1.42
16	I	105	A1EF2	C28-C29	2.15	1.50	1.43
16	e	101	A1EF2	C23-C22	-2.15	1.41	1.45
16	J	104	A1EF2	C23-C22	-2.15	1.41	1.45
16	f	101	A1EF2	C23-C22	-2.15	1.41	1.45
16	J	103	A1EF2	C28-C29	2.14	1.50	1.43
8	g	102	BCL	C3B-C2B	2.14	1.49	1.42
16	E	105	A1EF2	C28-C29	2.14	1.50	1.43
8	E	103	BCL	C3D-C4D	-2.14	1.39	1.44
8	M	401	BCL	C3B-C2B	2.13	1.49	1.42
8	e	102	BCL	C3B-C2B	2.13	1.49	1.42
8	G	104	BCL	C3B-C2B	2.13	1.49	1.42
8	O	102	BCL	C3B-C2B	2.13	1.49	1.42
8	J	102	BCL	C3B-C2B	2.12	1.49	1.42
8	i	101	BCL	C3D-C4D	-2.12	1.39	1.44
8	n	102	BCL	C3B-C2B	2.12	1.49	1.42
8	a	102	BCL	C3B-C2B	2.12	1.49	1.42
16	O	103	A1EF2	C23-C22	-2.11	1.41	1.45
16	M	411	A1EF2	C28-C29	2.11	1.50	1.43
8	k	102	BCL	C3B-C2B	2.11	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	K	102	BCL	C3B-C2B	2.10	1.49	1.42
8	c	102	BCL	C3B-C2B	2.10	1.49	1.42
8	d	102	BCL	C3B-C2B	2.10	1.49	1.42
8	L	308	BCL	C3B-C2B	2.10	1.49	1.42
8	O	102	BCL	C3D-C4D	-2.09	1.39	1.44
8	b	103	BCL	C3B-C2B	2.08	1.49	1.42
16	d	101	A1EF2	C23-C22	-2.08	1.41	1.45
8	j	101	BCL	C3B-C2B	2.08	1.49	1.42
8	i	101	BCL	C3B-C2B	2.08	1.49	1.42
16	J	106	A1EF2	C23-C22	-2.06	1.41	1.45
8	E	103	BCL	C3B-C2B	2.06	1.49	1.42
8	f	102	BCL	C3B-C2B	2.05	1.49	1.42
8	o	102	BCL	C3B-C2B	2.04	1.49	1.42
16	I	105	A1EF2	C25-C26	-2.04	1.33	1.35
16	k	101	A1EF2	C23-C22	-2.04	1.41	1.45
9	L	302	BPH	CBD-CGD	-2.03	1.49	1.52
16	M	411	A1EF2	C25-C26	-2.02	1.33	1.35
16	N	102	A1EF2	C25-C26	-2.00	1.33	1.35
16	D	105	A1EF2	C25-C26	-2.00	1.33	1.35
13	I	103	LMT	O1'-C1'	2.00	1.43	1.40
8	q	102	BCL	C3B-C2B	2.00	1.49	1.42

All (1199) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	o	102	BCL	O2D-CGD-CBD	27.34	159.85	111.27
8	o	102	BCL	O1D-CGD-CBD	-22.50	78.45	124.48
8	o	102	BCL	O2D-CGD-O1D	-21.71	81.40	123.84
8	M	401	BCL	C2B-C1B-NB	9.05	116.30	110.23
8	Q	101	BCL	C2B-C1B-NB	8.85	116.16	110.23
8	L	301	BCL	C2B-C1B-NB	8.82	116.14	110.23
8	D	102	BCL	C2B-C1B-NB	8.80	116.13	110.23
8	I	102	BCL	C2B-C1B-NB	8.77	116.11	110.23
8	c	102	BCL	C2B-C1B-NB	8.76	116.11	110.23
8	q	102	BCL	C2B-C1B-NB	8.71	116.07	110.23
8	L	308	BCL	C2B-C1B-NB	8.69	116.06	110.23
8	j	101	BCL	C2B-C1B-NB	8.63	116.02	110.23
8	g	102	BCL	C2B-C1B-NB	8.57	115.98	110.23
8	G	104	BCL	C2B-C1B-NB	8.57	115.97	110.23
8	b	103	BCL	C2B-C1B-NB	8.46	115.91	110.23
8	O	102	BCL	C2B-C1B-NB	8.40	115.87	110.23
8	f	102	BCL	C2B-C1B-NB	8.40	115.86	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	M	404	BCL	C2B-C1B-NB	8.34	115.83	110.23
8	n	102	BCL	C2B-C1B-NB	8.34	115.82	110.23
8	d	102	BCL	C2B-C1B-NB	8.29	115.79	110.23
8	J	102	BCL	C2B-C1B-NB	8.23	115.75	110.23
8	K	102	BCL	C2B-C1B-NB	8.19	115.72	110.23
8	k	102	BCL	C2B-C1B-NB	8.16	115.70	110.23
8	e	102	BCL	C2B-C1B-NB	8.16	115.70	110.23
8	E	103	BCL	C2B-C1B-NB	8.11	115.67	110.23
8	N	101	BCL	C2B-C1B-NB	8.07	115.64	110.23
8	p	102	BCL	C2B-C1B-NB	8.02	115.61	110.23
8	a	102	BCL	C2B-C1B-NB	7.97	115.57	110.23
8	C	103	BCL	C2B-C1B-NB	7.93	115.55	110.23
8	i	101	BCL	C2B-C1B-NB	7.89	115.52	110.23
8	A	702	BCL	C2B-C1B-NB	7.87	115.51	110.23
8	M	401	BCL	C4A-NA-C1A	-7.85	103.17	106.71
8	i	101	BCL	C4A-NA-C1A	-7.85	103.18	106.71
8	B	101	BCL	C2B-C1B-NB	7.81	115.47	110.23
8	F	103	BCL	C2B-C1B-NB	7.55	115.30	110.23
8	o	102	BCL	C2B-C1B-NB	7.53	115.28	110.23
8	q	102	BCL	CHD-C1D-ND	-7.52	117.54	124.45
8	A	702	BCL	C4A-NA-C1A	-7.47	103.35	106.71
8	n	102	BCL	C4A-NA-C1A	-7.46	103.35	106.71
8	J	102	BCL	C4A-NA-C1A	-7.44	103.36	106.71
8	j	101	BCL	C4A-NA-C1A	-7.43	103.37	106.71
8	I	102	BCL	C4A-NA-C1A	-7.33	103.41	106.71
8	G	104	BCL	C4A-NA-C1A	-7.26	103.44	106.71
8	b	103	BCL	C4A-NA-C1A	-7.18	103.48	106.71
8	L	301	BCL	C4A-NA-C1A	-7.16	103.49	106.71
8	d	102	BCL	C4A-NA-C1A	-7.02	103.55	106.71
8	a	102	BCL	C4A-NA-C1A	-6.72	103.69	106.71
8	L	308	BCL	C4A-NA-C1A	-6.69	103.70	106.71
8	L	308	BCL	CAC-C3C-C4C	6.67	127.38	112.58
8	o	102	BCL	CHD-C1D-ND	-6.65	118.34	124.45
8	Q	101	BCL	CHD-C1D-ND	-6.63	118.36	124.45
8	p	102	BCL	C4A-NA-C1A	-6.63	103.72	106.71
8	Q	101	BCL	CAC-C3C-C4C	6.54	127.11	112.58
8	P	102	BCL	C2B-C1B-NB	6.48	114.57	110.23
8	P	102	BCL	CHD-C1D-ND	-6.47	118.51	124.45
8	e	102	BCL	C4A-NA-C1A	-6.39	103.83	106.71
8	A	702	BCL	CAC-C3C-C4C	6.38	126.75	112.58
8	O	102	BCL	C4A-NA-C1A	-6.37	103.84	106.71
8	g	102	BCL	C4A-NA-C1A	-6.36	103.85	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	E	103	BCL	C4A-NA-C1A	-6.31	103.87	106.71
8	d	102	BCL	CAC-C3C-C4C	6.30	126.58	112.58
8	i	101	BCL	CAC-C3C-C4C	6.27	126.50	112.58
8	c	102	BCL	C4A-NA-C1A	-6.26	103.89	106.71
8	f	102	BCL	C4A-NA-C1A	-6.23	103.91	106.71
8	M	401	BCL	CAC-C3C-C4C	6.22	126.38	112.58
8	p	102	BCL	CAC-C3C-C4C	6.21	126.37	112.58
8	N	101	BCL	CMC-C2C-C1C	6.21	128.46	111.77
8	b	103	BCL	CAC-C3C-C4C	6.16	126.26	112.58
8	k	102	BCL	CAC-C3C-C4C	6.15	126.24	112.58
8	P	102	BCL	CAC-C3C-C4C	6.15	126.23	112.58
8	C	103	BCL	C4A-NA-C1A	-6.15	103.94	106.71
8	n	102	BCL	CAC-C3C-C4C	6.14	126.21	112.58
8	k	102	BCL	C4A-NA-C1A	-6.12	103.95	106.71
8	N	101	BCL	CAC-C3C-C4C	6.12	126.16	112.58
8	M	404	BCL	CMC-C2C-C1C	6.11	128.20	111.77
8	d	102	BCL	CMC-C2C-C1C	6.11	128.19	111.77
8	O	102	BCL	CAC-C3C-C4C	6.10	126.12	112.58
8	k	102	BCL	CMC-C2C-C1C	6.10	128.16	111.77
8	L	301	BCL	CAC-C3C-C4C	6.09	126.09	112.58
8	M	404	BCL	CAC-C3C-C4C	6.05	126.01	112.58
8	K	102	BCL	C4A-NA-C1A	-6.04	103.99	106.71
8	e	102	BCL	CAC-C3C-C4C	6.03	125.97	112.58
8	J	102	BCL	CMC-C2C-C1C	6.03	127.97	111.77
8	p	102	BCL	CMC-C2C-C1C	6.02	127.94	111.77
8	L	301	BCL	CMC-C2C-C1C	6.01	127.93	111.77
8	g	102	BCL	CAC-C3C-C4C	6.01	125.93	112.58
8	L	301	BCL	CHD-C1D-ND	-6.01	118.93	124.45
8	B	101	BCL	O2D-CGD-CBD	6.01	121.94	111.27
8	A	702	BCL	CMC-C2C-C1C	6.00	127.89	111.77
8	C	103	BCL	O2D-CGD-CBD	5.99	121.92	111.27
8	G	104	BCL	CMC-C2C-C1C	5.99	127.87	111.77
8	c	102	BCL	CMC-C2C-C1C	5.99	127.86	111.77
8	b	103	BCL	CMC-C2C-C1C	5.96	127.79	111.77
8	j	101	BCL	CAC-C3C-C4C	5.95	125.78	112.58
8	D	102	BCL	C4A-NA-C1A	-5.94	104.04	106.71
8	o	102	BCL	CMC-C2C-C1C	5.93	127.72	111.77
8	C	103	BCL	CAC-C3C-C4C	5.92	125.73	112.58
8	J	102	BCL	CAC-C3C-C4C	5.91	125.69	112.58
8	c	102	BCL	CAC-C3C-C4C	5.90	125.69	112.58
8	K	102	BCL	CAC-C3C-C4C	5.90	125.69	112.58
8	E	103	BCL	CMC-C2C-C1C	5.90	127.62	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	A	702	BCL	CHD-C1D-ND	-5.88	119.05	124.45
8	P	102	BCL	CMC-C2C-C1C	5.88	127.58	111.77
8	n	102	BCL	CMC-C2C-C1C	5.88	127.57	111.77
8	O	102	BCL	CMC-C2C-C1C	5.87	127.54	111.77
8	g	102	BCL	CMC-C2C-C1C	5.86	127.51	111.77
8	K	102	BCL	CMC-C2C-C1C	5.85	127.50	111.77
8	L	308	BCL	CMC-C2C-C1C	5.85	127.50	111.77
8	F	103	BCL	CAC-C3C-C4C	5.85	125.57	112.58
8	e	102	BCL	CMC-C2C-C1C	5.85	127.50	111.77
8	N	101	BCL	C4A-NA-C1A	-5.84	104.08	106.71
8	o	102	BCL	CAC-C3C-C4C	5.82	125.50	112.58
8	i	101	BCL	CMC-C2C-C1C	5.81	127.40	111.77
8	F	103	BCL	CMC-C2C-C1C	5.80	127.36	111.77
8	j	101	BCL	CMC-C2C-C1C	5.80	127.35	111.77
8	C	103	BCL	CMC-C2C-C1C	5.78	127.32	111.77
8	I	102	BCL	CAC-C3C-C4C	5.78	125.41	112.58
8	a	102	BCL	CAC-C3C-C4C	5.77	125.40	112.58
8	E	103	BCL	O2D-CGD-CBD	5.76	121.51	111.27
8	G	104	BCL	CAC-C3C-C4C	5.76	125.37	112.58
8	B	101	BCL	CMC-C2C-C1C	5.76	127.25	111.77
8	E	103	BCL	CAC-C3C-C4C	5.74	125.33	112.58
8	F	103	BCL	O2D-CGD-CBD	5.74	121.47	111.27
8	I	102	BCL	CMC-C2C-C1C	5.74	127.19	111.77
8	a	102	BCL	CMC-C2C-C1C	5.72	127.14	111.77
8	f	102	BCL	CMC-C2C-C1C	5.71	127.13	111.77
8	D	102	BCL	CMC-C2C-C1C	5.71	127.11	111.77
8	D	102	BCL	O2D-CGD-CBD	5.71	121.41	111.27
8	I	102	BCL	O2D-CGD-CBD	5.69	121.38	111.27
8	J	102	BCL	O2D-CGD-CBD	5.68	121.37	111.27
8	M	401	BCL	CMC-C2C-C1C	5.68	127.05	111.77
8	G	104	BCL	O2D-CGD-CBD	5.64	121.29	111.27
8	q	102	BCL	CMC-C2C-C1C	5.62	126.88	111.77
8	D	102	BCL	CAC-C3C-C4C	5.61	125.03	112.58
8	f	102	BCL	CAC-C3C-C4C	5.60	125.02	112.58
8	O	102	BCL	O2D-CGD-CBD	5.58	121.19	111.27
8	C	103	BCL	CHD-C1D-ND	-5.55	119.36	124.45
8	Q	101	BCL	CMC-C2C-C1C	5.52	126.62	111.77
8	F	103	BCL	C4A-NA-C1A	-5.52	104.22	106.71
8	Q	101	BCL	C4A-NA-C1A	-5.51	104.23	106.71
8	o	102	BCL	C4A-NA-C1A	-5.49	104.24	106.71
8	Q	101	BCL	O2D-CGD-CBD	5.48	121.00	111.27
8	B	101	BCL	CAC-C3C-C4C	5.47	124.72	112.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	g	103	A1EF2	C11-C12-C13	5.46	130.92	112.98
8	K	102	BCL	O2D-CGD-CBD	5.44	120.94	111.27
8	M	401	BCL	CHD-C1D-ND	-5.44	119.46	124.45
8	N	101	BCL	O2D-CGD-CBD	5.41	120.89	111.27
16	J	104	A1EF2	C11-C12-C13	5.40	130.75	112.98
16	E	105	A1EF2	C28-C27-C26	-5.40	111.25	126.42
16	J	101	A1EF2	C11-C12-C13	5.39	130.71	112.98
16	J	103	A1EF2	C19-C20-C21	5.37	134.48	123.47
8	L	301	BCL	O2D-CGD-CBD	5.34	120.76	111.27
16	J	106	A1EF2	C11-C12-C13	5.33	130.52	112.98
16	D	104	A1EF2	C11-C12-C13	5.32	130.48	112.98
16	N	102	A1EF2	C11-C12-C13	5.32	130.46	112.98
8	c	102	BCL	CHD-C1D-ND	-5.31	119.57	124.45
16	e	101	A1EF2	C11-C12-C13	5.27	130.31	112.98
16	E	105	A1EF2	C11-C12-C13	5.24	130.23	112.98
16	c	104	A1EF2	C19-C20-C21	5.24	134.21	123.47
10	L	303	U10	C7-C8-C9	-5.22	118.10	126.79
16	C	104	A1EF2	C11-C12-C13	5.22	130.15	112.98
8	B	101	BCL	C4A-NA-C1A	-5.21	104.36	106.71
16	f	101	A1EF2	C11-C12-C13	5.19	130.05	112.98
16	p	101	A1EF2	C11-C12-C13	5.18	130.01	112.98
16	k	101	A1EF2	C11-C12-C13	5.18	130.00	112.98
16	B	103	A1EF2	C11-C12-C13	5.15	129.93	112.98
16	J	103	A1EF2	C11-C12-C13	5.14	129.90	112.98
16	D	105	A1EF2	C11-C12-C13	5.14	129.90	112.98
16	N	102	A1EF2	C28-C27-C26	-5.14	111.98	126.42
8	c	102	BCL	O2D-CGD-CBD	5.13	120.39	111.27
16	N	103	A1EF2	C11-C12-C13	5.12	129.83	112.98
16	o	101	A1EF2	C11-C12-C13	5.12	129.82	112.98
16	M	411	A1EF2	C11-C12-C13	5.12	129.82	112.98
8	a	102	BCL	CHD-C1D-ND	-5.09	119.77	124.45
8	M	404	BCL	C1C-NC-C4C	-5.09	104.42	106.71
16	n	101	A1EF2	C11-C12-C13	5.07	129.67	112.98
16	c	104	A1EF2	C11-C12-C13	5.07	129.66	112.98
8	j	101	BCL	O2D-CGD-CBD	5.06	120.25	111.27
8	q	102	BCL	O2D-CGD-CBD	5.05	120.25	111.27
8	L	308	BCL	O2D-CGD-CBD	5.05	120.24	111.27
16	d	101	A1EF2	C11-C12-C13	5.02	129.49	112.98
8	A	702	BCL	O2D-CGD-CBD	5.02	120.18	111.27
8	a	102	BCL	O2D-CGD-CBD	5.02	120.18	111.27
16	g	101	A1EF2	C11-C12-C13	5.01	129.45	112.98
16	k	101	A1EF2	C19-C20-C21	5.00	133.71	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	I	105	A1EF2	C11-C12-C13	4.99	129.40	112.98
8	q	102	BCL	CAC-C3C-C4C	4.99	123.65	112.58
8	M	404	BCL	C4A-NA-C1A	-4.98	104.47	106.71
8	e	102	BCL	O2D-CGD-CBD	4.98	120.11	111.27
16	b	102	A1EF2	C29-C28-C27	-4.98	107.69	123.22
8	d	102	BCL	O2D-CGD-CBD	4.97	120.11	111.27
8	P	102	BCL	O2D-CGD-CBD	4.97	120.11	111.27
16	a	103	A1EF2	C11-C12-C13	4.97	129.32	112.98
8	M	401	BCL	O2D-CGD-CBD	4.96	120.09	111.27
16	q	101	A1EF2	C11-C12-C13	4.96	129.29	112.98
16	O	103	A1EF2	C11-C12-C13	4.95	129.25	112.98
16	g	101	A1EF2	C19-C20-C21	4.94	133.60	123.47
8	b	103	BCL	O2D-CGD-CBD	4.92	120.01	111.27
16	b	102	A1EF2	C11-C12-C13	4.91	129.13	112.98
8	p	102	BCL	O2D-CGD-CBD	4.91	119.99	111.27
8	g	102	BCL	O2D-CGD-CBD	4.86	119.90	111.27
8	n	102	BCL	CHD-C1D-ND	-4.85	119.99	124.45
8	f	102	BCL	O2D-CGD-CBD	4.85	119.89	111.27
16	J	103	A1EF2	C29-C28-C27	-4.84	108.10	123.22
8	a	102	BCL	C1D-CHD-C4C	-4.84	114.94	126.62
16	a	103	A1EF2	C12-C11-C10	4.84	127.80	111.88
8	M	404	BCL	C1D-CHD-C4C	-4.83	114.97	126.62
16	b	102	A1EF2	C19-C20-C21	4.83	133.37	123.47
16	I	105	A1EF2	C19-C20-C21	4.81	133.33	123.47
8	n	102	BCL	O2D-CGD-CBD	4.79	119.77	111.27
8	D	102	BCL	CHD-C1D-ND	-4.77	120.07	124.45
8	L	308	BCL	C1D-CHD-C4C	-4.77	115.11	126.62
8	p	102	BCL	CHD-C1D-ND	-4.76	120.08	124.45
8	C	103	BCL	C1D-CHD-C4C	-4.75	115.16	126.62
8	D	102	BCL	C1D-CHD-C4C	-4.73	115.22	126.62
8	M	401	BCL	C1D-CHD-C4C	-4.72	115.23	126.62
8	K	102	BCL	C1D-CHD-C4C	-4.71	115.26	126.62
8	M	404	BCL	CHD-C1D-ND	-4.69	120.14	124.45
8	q	102	BCL	C4A-NA-C1A	-4.69	104.60	106.71
8	Q	101	BCL	C1D-CHD-C4C	-4.66	115.38	126.62
8	i	101	BCL	O2D-CGD-CBD	4.66	119.55	111.27
16	b	102	A1EF2	C12-C11-C10	4.66	127.19	111.88
16	d	101	A1EF2	C19-C20-C21	4.66	133.01	123.47
16	g	103	A1EF2	C28-C27-C26	-4.63	113.42	126.42
16	O	103	A1EF2	C20-C19-C18	4.62	132.93	123.47
16	O	103	A1EF2	C12-C11-C10	4.61	127.03	111.88
8	n	102	BCL	C1D-CHD-C4C	-4.61	115.51	126.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	b	103	BCL	CHD-C1D-ND	-4.58	120.25	124.45
16	I	105	A1EF2	C12-C11-C10	4.57	126.90	111.88
16	a	103	A1EF2	C28-C27-C26	-4.56	113.60	126.42
16	D	105	A1EF2	C28-C27-C26	-4.56	113.61	126.42
10	L	303	U10	C7-C6-C5	-4.56	112.99	118.48
8	b	103	BCL	C1D-CHD-C4C	-4.56	115.63	126.62
8	K	102	BCL	CHD-C1D-ND	-4.51	120.31	124.45
8	c	102	BCL	C1D-CHD-C4C	-4.51	115.75	126.62
8	B	101	BCL	CHD-C1D-ND	-4.47	120.34	124.45
16	g	101	A1EF2	C12-C11-C10	4.47	126.57	111.88
8	B	101	BCL	C1D-CHD-C4C	-4.45	115.89	126.62
8	L	308	BCL	C1C-NC-C4C	-4.45	104.71	106.71
16	q	101	A1EF2	C19-C20-C21	4.44	132.58	123.47
16	C	104	A1EF2	C20-C19-C18	4.44	132.57	123.47
16	c	104	A1EF2	C29-C28-C27	-4.44	109.37	123.22
8	I	102	BCL	C1D-CHD-C4C	-4.44	115.92	126.62
8	A	702	BCL	C1D-CHD-C4C	-4.42	115.95	126.62
16	N	103	A1EF2	C28-C27-C26	-4.42	114.00	126.42
16	g	103	A1EF2	C20-C19-C18	4.42	132.53	123.47
8	e	102	BCL	C1D-CHD-C4C	-4.41	115.99	126.62
16	d	101	A1EF2	C29-C28-C27	-4.40	109.48	123.22
16	e	101	A1EF2	C19-C20-C21	4.39	132.48	123.47
16	d	101	A1EF2	C12-C11-C10	4.39	126.31	111.88
8	d	102	BCL	C1D-CHD-C4C	-4.38	116.05	126.62
11	M	412	PGV	O01-C1-C2	4.38	120.94	111.50
16	J	106	A1EF2	C20-C19-C18	4.37	132.44	123.47
8	g	102	BCL	C1D-CHD-C4C	-4.37	116.08	126.62
16	f	101	A1EF2	C19-C20-C21	4.36	132.41	123.47
16	q	101	A1EF2	C12-C11-C10	4.35	126.19	111.88
8	j	101	BCL	C1D-CHD-C4C	-4.33	116.17	126.62
8	o	102	BCL	C1D-CHD-C4C	-4.33	116.19	126.62
16	g	101	A1EF2	C29-C28-C27	-4.32	109.74	123.22
8	k	102	BCL	O2D-CGD-CBD	4.32	118.94	111.27
11	M	402	PGV	O01-C1-C2	4.31	120.80	111.50
8	N	101	BCL	C1D-CHD-C4C	-4.31	116.23	126.62
13	L	312	LMT	C1B-C2B-C3B	4.30	118.95	110.00
11	L	306	PGV	O01-C1-C2	4.29	120.75	111.50
8	f	102	BCL	C1D-CHD-C4C	-4.29	116.28	126.62
8	i	101	BCL	C1D-CHD-C4C	-4.28	116.29	126.62
16	E	105	A1EF2	C20-C19-C18	4.28	132.25	123.47
8	k	102	BCL	C1C-NC-C4C	-4.28	104.78	106.71
8	G	104	BCL	C1D-CHD-C4C	-4.27	116.32	126.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	F	103	BCL	C1D-CHD-C4C	-4.27	116.33	126.62
16	D	104	A1EF2	C20-C19-C18	4.26	132.21	123.47
16	o	101	A1EF2	C19-C20-C21	4.26	132.19	123.47
16	J	103	A1EF2	C12-C11-C10	4.24	125.82	111.88
8	E	103	BCL	C1D-CHD-C4C	-4.24	116.40	126.62
16	N	103	A1EF2	C12-C11-C10	4.24	125.81	111.88
16	M	411	A1EF2	C12-C11-C10	4.22	125.76	111.88
8	p	102	BCL	C1D-CHD-C4C	-4.22	116.45	126.62
8	k	102	BCL	C1D-CHD-C4C	-4.21	116.45	126.62
16	a	103	A1EF2	C19-C20-C21	4.21	132.09	123.47
16	n	101	A1EF2	C12-C11-C10	4.20	125.69	111.88
16	c	104	A1EF2	C12-C11-C10	4.19	125.65	111.88
16	O	103	A1EF2	C28-C27-C26	-4.18	114.67	126.42
8	P	102	BCL	C1D-CHD-C4C	-4.18	116.54	126.62
16	p	101	A1EF2	C12-C11-C10	4.16	125.56	111.88
16	J	104	A1EF2	C28-C27-C26	-4.16	114.73	126.42
16	k	101	A1EF2	C12-C11-C10	4.16	125.54	111.88
11	L	305	PGV	O01-C1-C2	4.13	120.41	111.50
8	O	102	BCL	C1D-CHD-C4C	-4.12	116.67	126.62
8	f	102	BCL	C1C-NC-C4C	-4.12	104.86	106.71
8	d	102	BCL	CHD-C1D-ND	-4.11	120.68	124.45
16	N	103	A1EF2	C20-C19-C18	4.11	131.88	123.47
8	L	301	BCL	C1C-NC-C4C	-4.10	104.86	106.71
11	G	103	PGV	O01-C1-C2	4.10	120.34	111.50
16	B	103	A1EF2	C29-C28-C27	-4.09	110.44	123.22
11	L	313	PGV	O01-C1-C2	4.09	120.31	111.50
16	D	104	A1EF2	C29-C28-C27	-4.08	110.47	123.22
8	q	102	BCL	C1D-CHD-C4C	-4.08	116.78	126.62
8	k	102	BCL	CHD-C1D-ND	-4.07	120.71	124.45
8	A	702	BCL	C1C-NC-C4C	-4.05	104.89	106.71
16	o	101	A1EF2	C12-C11-C10	4.03	125.13	111.88
9	L	302	BPH	C4D-CHA-CBD	-4.03	106.69	108.52
8	N	101	BCL	C1C-NC-C4C	-4.03	104.90	106.71
16	k	101	A1EF2	C29-C28-C27	-4.02	110.67	123.22
8	J	102	BCL	C1D-CHD-C4C	-4.02	116.92	126.62
16	o	101	A1EF2	C28-C27-C26	-4.02	115.13	126.42
16	f	101	A1EF2	C29-C28-C27	-4.02	110.68	123.22
16	J	101	A1EF2	C28-C27-C26	-4.01	115.14	126.42
16	M	411	A1EF2	C28-C27-C26	-4.01	115.15	126.42
8	g	102	BCL	CHD-C1D-ND	-4.01	120.77	124.45
16	C	104	A1EF2	C28-C27-C26	-4.00	115.17	126.42
8	P	102	BCL	C1D-ND-C4D	4.00	109.17	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	C	102	PGV	O01-C1-C2	4.00	120.11	111.50
16	e	101	A1EF2	C12-C11-C10	3.99	124.98	111.88
11	H	304	PGV	O01-C1-C2	3.98	120.09	111.50
16	f	101	A1EF2	C12-C11-C10	3.95	124.87	111.88
16	p	101	A1EF2	C19-C20-C21	3.95	131.56	123.47
16	I	105	A1EF2	C29-C28-C27	-3.94	110.91	123.22
16	B	103	A1EF2	C20-C19-C18	3.93	131.53	123.47
8	e	102	BCL	C1C-NC-C4C	-3.91	104.95	106.71
16	J	103	A1EF2	C24-C25-C26	3.91	132.89	127.31
8	j	101	BCL	CHD-C1D-ND	-3.91	120.86	124.45
16	p	101	A1EF2	C29-C28-C27	-3.90	111.04	123.22
11	E	104	PGV	O01-C1-C2	3.90	119.90	111.50
16	n	101	A1EF2	C29-C28-C27	-3.88	111.12	123.22
16	J	106	A1EF2	C28-C27-C26	-3.87	115.54	126.42
16	q	101	A1EF2	C28-C27-C26	-3.87	115.54	126.42
11	C	101	PGV	O01-C1-C2	3.86	119.83	111.50
11	L	314	PGV	O01-C1-C2	3.86	119.82	111.50
13	B	102	LMT	O1'-C1'-C2'	3.86	114.33	108.30
16	e	101	A1EF2	C28-C27-C26	-3.85	115.59	126.42
16	J	104	A1EF2	C20-C19-C18	3.84	131.35	123.47
8	e	102	BCL	CHD-C1D-ND	-3.83	120.93	124.45
8	q	102	BCL	C1D-ND-C4D	3.82	109.05	106.33
16	I	105	A1EF2	C28-C27-C26	-3.81	115.71	126.42
8	M	404	BCL	O2D-CGD-CBD	3.81	118.03	111.27
16	B	103	A1EF2	C28-C27-C26	-3.80	115.73	126.42
8	M	404	BCL	C2C-C3C-C4C	-3.78	95.67	101.34
16	N	102	A1EF2	C20-C19-C18	3.76	131.18	123.47
16	n	101	A1EF2	C28-C27-C26	-3.76	115.86	126.42
16	B	103	A1EF2	C12-C11-C10	3.75	124.20	111.88
8	b	103	BCL	C1C-NC-C4C	-3.75	105.02	106.71
9	M	405	BPH	C4D-CHA-CBD	-3.74	106.83	108.52
16	q	101	A1EF2	C29-C28-C27	-3.72	111.62	123.22
16	D	105	A1EF2	C12-C11-C10	3.71	124.07	111.88
8	i	101	BCL	C1C-NC-C4C	-3.70	105.04	106.71
8	E	103	BCL	C3C-C4C-CHD	-3.70	115.50	123.39
16	o	101	A1EF2	C29-C28-C27	-3.69	111.69	123.22
16	C	104	A1EF2	C29-C28-C27	-3.68	111.73	123.22
8	G	104	BCL	C3C-C4C-CHD	-3.68	115.53	123.39
8	J	102	BCL	C3C-C4C-CHD	-3.67	115.54	123.39
10	L	303	U10	C27-C26-C24	-3.64	108.66	114.62
8	I	102	BCL	CHD-C1D-ND	-3.64	121.11	124.45
16	f	101	A1EF2	C28-C27-C26	-3.64	116.20	126.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	O	102	BCL	C3C-C4C-CHD	-3.64	115.62	123.39
16	M	411	A1EF2	C29-C28-C27	-3.63	111.88	123.22
16	a	103	A1EF2	C39-C22-C21	-3.63	117.84	122.92
8	F	103	BCL	C3C-C4C-CHD	-3.63	115.64	123.39
8	L	308	BCL	CHD-C1D-ND	-3.62	121.13	124.45
8	f	102	BCL	C3C-C4C-CHD	-3.61	115.67	123.39
8	j	101	BCL	C1C-NC-C4C	-3.61	105.08	106.71
16	p	101	A1EF2	C28-C27-C26	-3.60	116.31	126.42
16	J	104	A1EF2	C19-C20-C21	3.59	130.84	123.47
8	n	102	BCL	C1C-NC-C4C	-3.57	105.10	106.71
8	i	101	BCL	C3C-C4C-CHD	-3.57	115.77	123.39
16	k	101	A1EF2	C28-C27-C26	-3.56	116.43	126.42
8	A	702	BCL	C4-C3-C5	3.55	121.25	115.27
8	L	301	BCL	C1D-CHD-C4C	-3.55	118.06	126.62
16	J	101	A1EF2	C20-C19-C18	3.54	130.73	123.47
16	e	101	A1EF2	C29-C28-C27	-3.54	112.17	123.22
16	D	104	A1EF2	C28-C27-C26	-3.54	116.47	126.42
11	K	103	PGV	O01-C1-C2	3.52	119.10	111.50
16	J	101	A1EF2	C29-C28-C27	-3.52	112.23	123.22
16	D	105	A1EF2	C29-C28-C27	-3.52	112.23	123.22
16	J	106	A1EF2	C39-C22-C21	-3.51	118.01	122.92
8	f	102	BCL	CHD-C1D-ND	-3.51	121.23	124.45
8	N	101	BCL	C3C-C4C-CHD	-3.50	115.90	123.39
8	q	102	BCL	CHD-C1D-C2D	-3.49	118.16	125.48
16	D	104	A1EF2	C12-C11-C10	3.49	123.34	111.88
16	g	103	A1EF2	C39-C22-C21	-3.49	118.04	122.92
16	g	103	A1EF2	C38-C17-C18	-3.48	118.05	122.92
16	J	106	A1EF2	C38-C17-C18	-3.48	118.05	122.92
16	D	105	A1EF2	C20-C19-C18	3.48	130.60	123.47
16	g	101	A1EF2	C24-C25-C26	3.47	132.27	127.31
8	B	101	BCL	C3C-C4C-CHD	-3.47	115.98	123.39
11	H	303	PGV	O01-C1-C2	3.46	118.96	111.50
16	n	101	A1EF2	C19-C20-C21	3.45	130.54	123.47
8	n	102	BCL	C4-C3-C5	3.45	121.07	115.27
8	I	102	BCL	C3C-C4C-CHD	-3.44	116.03	123.39
8	g	102	BCL	C3C-C4C-CHD	-3.43	116.06	123.39
16	N	103	A1EF2	C29-C28-C27	-3.43	112.50	123.22
8	Q	101	BCL	C4-C3-C5	3.43	121.04	115.27
16	J	101	A1EF2	C19-C20-C21	3.42	130.48	123.47
8	L	301	BCL	CMC-C2C-C3C	3.41	127.60	113.83
16	C	104	A1EF2	C38-C17-C18	-3.41	118.14	122.92
8	g	102	BCL	C1C-NC-C4C	-3.41	105.17	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	j	101	BCL	C3C-C4C-CHD	-3.41	116.12	123.39
8	n	102	BCL	CBC-CAC-C3C	-3.40	105.89	113.47
16	q	101	A1EF2	C39-C22-C21	-3.40	118.16	122.92
8	G	104	BCL	C1C-NC-C4C	-3.40	105.18	106.71
8	d	102	BCL	C4-C3-C5	3.39	120.98	115.27
16	J	104	A1EF2	C39-C22-C21	-3.39	118.18	122.92
16	D	104	A1EF2	C38-C17-C18	-3.38	118.19	122.92
8	P	102	BCL	C1-C2-C3	-3.38	120.20	126.04
16	a	103	A1EF2	C29-C28-C27	-3.38	112.68	123.22
10	L	304	U10	C22-C23-C24	-3.37	119.54	127.66
8	K	102	BCL	C1-C2-C3	-3.37	120.21	126.04
8	o	102	BCL	CED-O2D-CGD	3.37	123.56	115.94
16	M	411	A1EF2	C38-C17-C18	-3.37	118.20	122.92
16	N	102	A1EF2	C39-C22-C21	-3.37	118.21	122.92
16	E	105	A1EF2	C38-C17-C18	-3.37	118.21	122.92
8	g	102	BCL	CBC-CAC-C3C	-3.37	105.97	113.47
8	A	702	BCL	C1D-ND-C4D	3.36	108.72	106.33
8	e	102	BCL	C3C-C4C-CHD	-3.36	116.22	123.39
8	P	102	BCL	CBC-CAC-C3C	-3.35	106.02	113.47
16	E	105	A1EF2	C12-C11-C10	3.34	122.87	111.88
8	q	102	BCL	CMC-C2C-C3C	3.34	127.31	113.83
13	B	102	LMT	C1-O1'-C1'	-3.34	108.30	113.84
16	J	104	A1EF2	C12-C11-C10	3.34	122.86	111.88
10	M	407	U10	C32-C33-C34	-3.34	119.62	127.66
13	D	101	LMT	O1B-C4'-C3'	3.34	116.16	107.28
8	N	101	BCL	C1-C2-C3	-3.33	120.29	126.04
16	q	101	A1EF2	C38-C17-C18	-3.33	118.26	122.92
8	i	101	BCL	CBC-CAC-C3C	-3.33	106.06	113.47
16	a	103	A1EF2	C23-C22-C21	3.32	124.04	118.94
8	C	103	BCL	C4B-C3B-C2B	-3.31	103.03	108.36
10	L	303	U10	C8-C7-C6	3.31	120.96	112.05
8	j	101	BCL	CBC-CAC-C3C	-3.29	106.14	113.47
10	L	304	U10	C7-C8-C9	-3.29	121.32	126.79
16	O	103	A1EF2	C38-C17-C18	-3.28	118.33	122.92
8	d	102	BCL	C3C-C4C-CHD	-3.28	116.39	123.39
16	C	104	A1EF2	C12-C11-C10	3.28	122.65	111.88
16	N	103	A1EF2	C38-C17-C18	-3.27	118.34	122.92
16	g	103	A1EF2	C16-C17-C18	3.27	123.96	118.94
8	A	702	BCL	CMC-C2C-C3C	3.27	127.02	113.83
16	B	103	A1EF2	C39-C22-C21	-3.27	118.35	122.92
16	J	101	A1EF2	C39-C22-C21	-3.26	118.36	122.92
16	N	103	A1EF2	C39-C22-C21	-3.25	118.37	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	D	102	BCL	CMC-C2C-C3C	3.25	126.93	113.83
8	C	103	BCL	C4-C3-C5	3.25	120.73	115.27
8	q	102	BCL	CHC-C4B-C3B	-3.24	120.81	132.35
8	D	102	BCL	C3C-C4C-CHD	-3.24	116.46	123.39
8	o	102	BCL	CMC-C2C-C3C	3.24	126.89	113.83
16	J	106	A1EF2	C12-C11-C10	3.24	122.52	111.88
16	B	103	A1EF2	C38-C17-C18	-3.24	118.39	122.92
16	D	104	A1EF2	C39-C22-C21	-3.24	118.39	122.92
8	o	102	BCL	C1D-ND-C4D	3.23	108.63	106.33
8	f	102	BCL	CMC-C2C-C3C	3.23	126.84	113.83
8	Q	101	BCL	CMC-C2C-C3C	3.22	126.84	113.83
8	K	102	BCL	CMC-C2C-C3C	3.22	126.84	113.83
16	g	103	A1EF2	C23-C22-C21	3.22	123.89	118.94
16	g	101	A1EF2	C39-C22-C21	-3.22	118.41	122.92
16	J	106	A1EF2	C23-C22-C21	3.22	123.89	118.94
16	c	104	A1EF2	C39-C22-C21	-3.22	118.41	122.92
16	J	103	A1EF2	C38-C17-C18	-3.22	118.41	122.92
16	g	101	A1EF2	C28-C27-C26	-3.22	117.37	126.42
16	N	102	A1EF2	C12-C11-C10	3.22	122.46	111.88
8	B	101	BCL	C4B-C3B-C2B	-3.22	103.18	108.36
8	k	102	BCL	C3C-C4C-CHD	-3.22	116.52	123.39
16	N	102	A1EF2	C38-C17-C18	-3.21	118.42	122.92
8	B	101	BCL	CMC-C2C-C3C	3.21	126.78	113.83
16	J	104	A1EF2	C38-C17-C18	-3.21	118.43	122.92
8	I	102	BCL	CMC-C2C-C3C	3.21	126.78	113.83
16	J	106	A1EF2	C16-C17-C18	3.21	123.87	118.94
8	o	102	BCL	C4B-C3B-C2B	-3.21	103.20	108.36
8	L	308	BCL	C2C-C3C-C4C	-3.19	96.55	101.34
8	K	102	BCL	C3C-C4C-CHD	-3.19	116.57	123.39
16	J	101	A1EF2	C12-C11-C10	3.19	122.38	111.88
8	P	102	BCL	C4B-C3B-C2B	-3.19	103.23	108.36
16	p	101	A1EF2	C39-C22-C21	-3.19	118.46	122.92
8	c	102	BCL	CBC-CAC-C3C	-3.19	106.37	113.47
8	O	102	BCL	C1C-NC-C4C	-3.19	105.27	106.71
8	j	101	BCL	CMC-C2C-C3C	3.19	126.68	113.83
8	F	103	BCL	CMC-C2C-C3C	3.18	126.67	113.83
16	D	105	A1EF2	C38-C17-C18	-3.18	118.47	122.92
8	O	102	BCL	CMC-C2C-C3C	3.18	126.66	113.83
8	E	103	BCL	C4B-C3B-C2B	-3.18	103.25	108.36
8	g	102	BCL	CMC-C2C-C3C	3.18	126.65	113.83
16	C	104	A1EF2	C39-C22-C21	-3.18	118.47	122.92
16	O	103	A1EF2	C39-C22-C21	-3.18	118.47	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	Q	101	BCL	CHD-C1D-C2D	-3.17	118.83	125.48
8	K	102	BCL	C4B-C3B-C2B	-3.17	103.26	108.36
16	g	103	A1EF2	C29-C28-C27	-3.17	113.32	123.22
8	L	308	BCL	CMC-C2C-C3C	3.17	126.62	113.83
8	C	103	BCL	CMC-C2C-C3C	3.17	126.62	113.83
16	e	101	A1EF2	C39-C22-C21	-3.17	118.48	122.92
8	p	102	BCL	CMC-C2C-C3C	3.17	126.60	113.83
8	E	103	BCL	C1-C2-C3	-3.16	120.57	126.04
16	c	104	A1EF2	C28-C27-C26	-3.16	117.54	126.42
8	Q	101	BCL	C1-C2-C3	-3.16	120.58	126.04
16	J	101	A1EF2	C38-C17-C18	-3.16	118.50	122.92
8	D	102	BCL	C4B-C3B-C2B	-3.16	103.28	108.36
8	E	103	BCL	O2A-CGA-CBA	3.15	121.80	111.91
8	B	101	BCL	O2D-CGD-O1D	-3.15	117.68	123.84
8	k	102	BCL	C4-C3-C5	3.15	120.57	115.27
8	p	102	BCL	C1C-NC-C4C	-3.15	105.29	106.71
8	o	102	BCL	CBC-CAC-C3C	-3.14	106.47	113.47
8	J	102	BCL	C1C-NC-C4C	-3.14	105.29	106.71
8	n	102	BCL	C3C-C4C-CHD	-3.14	116.68	123.39
8	p	102	BCL	CHC-C4B-C3B	-3.14	121.17	132.35
8	N	101	BCL	CBC-CAC-C3C	-3.13	106.50	113.47
8	a	102	BCL	CMC-C2C-C3C	3.13	126.45	113.83
8	J	102	BCL	C1-C2-C3	-3.13	120.63	126.04
8	E	103	BCL	CMC-C2C-C3C	3.12	126.43	113.83
8	k	102	BCL	CBC-CAC-C3C	-3.12	106.52	113.47
16	E	105	A1EF2	C29-C28-C27	-3.12	113.48	123.22
8	d	102	BCL	CBC-CAC-C3C	-3.12	106.52	113.47
8	Q	101	BCL	CHC-C4B-C3B	-3.12	121.25	132.35
8	G	104	BCL	CMC-C2C-C3C	3.12	126.40	113.83
16	d	101	A1EF2	C39-C22-C21	-3.11	118.56	122.92
8	p	102	BCL	CBC-CAC-C3C	-3.11	106.54	113.47
11	L	306	PGV	C02-O01-C1	-3.11	110.13	117.79
8	e	102	BCL	CMC-C2C-C3C	3.11	126.38	113.83
8	C	103	BCL	C1D-ND-C4D	3.11	108.55	106.33
8	c	102	BCL	CMC-C2C-C3C	3.11	126.37	113.83
10	M	407	U10	C25-C24-C26	3.11	120.50	115.27
16	k	101	A1EF2	C39-C22-C21	-3.11	118.57	122.92
8	M	401	BCL	CMC-C2C-C3C	3.10	126.35	113.83
16	e	101	A1EF2	C38-C17-C18	-3.10	118.58	122.92
13	H	302	LMT	O1B-C4'-C3'	3.10	115.53	107.28
13	X	103	LMT	O1B-C4'-C3'	3.10	115.53	107.28
8	G	104	BCL	CHD-C4C-NC	3.10	128.52	125.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	i	101	BCL	C4B-C3B-C2B	-3.10	103.37	108.36
16	O	103	A1EF2	C29-C28-C27	-3.10	113.55	123.22
16	J	106	A1EF2	C29-C28-C27	-3.09	113.56	123.22
8	E	103	BCL	C4-C3-C5	3.09	120.47	115.27
8	k	102	BCL	CMC-C2C-C3C	3.09	126.31	113.83
8	A	702	BCL	C4B-C3B-C2B	-3.09	103.39	108.36
8	O	102	BCL	CHD-C4C-NC	3.09	128.51	125.08
8	a	102	BCL	C1C-NC-C4C	-3.09	105.32	106.71
16	q	101	A1EF2	C16-C17-C18	3.08	123.67	118.94
16	o	101	A1EF2	C39-C22-C21	-3.08	118.61	122.92
8	L	308	BCL	C1-C2-C3	-3.08	120.71	126.04
8	A	702	BCL	C1-C2-C3	-3.08	120.72	126.04
16	p	101	A1EF2	C38-C17-C18	-3.08	118.61	122.92
8	C	103	BCL	C3C-C4C-CHD	-3.08	116.81	123.39
8	i	101	BCL	CMC-C2C-C3C	3.08	126.23	113.83
8	J	102	BCL	C4-C3-C5	3.08	120.44	115.27
8	n	102	BCL	CMC-C2C-C3C	3.07	126.23	113.83
8	L	301	BCL	C1D-ND-C4D	3.07	108.52	106.33
8	L	301	BCL	C4B-C3B-C2B	-3.07	103.42	108.36
8	b	103	BCL	CMC-C2C-C3C	3.07	126.22	113.83
8	D	102	BCL	C4-C3-C5	3.07	120.44	115.27
8	A	702	BCL	CBC-CAC-C3C	-3.07	106.64	113.47
16	J	106	A1EF2	C19-C20-C21	3.07	129.76	123.47
16	d	101	A1EF2	C28-C27-C26	-3.07	117.80	126.42
8	J	102	BCL	CMC-C2C-C3C	3.06	126.19	113.83
8	G	104	BCL	C4-C3-C5	3.06	120.42	115.27
8	M	404	BCL	CMC-C2C-C3C	3.06	126.18	113.83
8	k	102	BCL	C1-C2-C3	-3.06	120.75	126.04
8	J	102	BCL	CHD-C1D-ND	-3.06	121.64	124.45
16	J	104	A1EF2	C29-C28-C27	-3.06	113.68	123.22
8	D	102	BCL	O2D-CGD-O1D	-3.06	117.86	123.84
8	k	102	BCL	C4B-C3B-C2B	-3.06	103.44	108.36
8	e	102	BCL	CBC-CAC-C3C	-3.06	106.67	113.47
8	P	102	BCL	CMC-C2C-C3C	3.05	126.15	113.83
16	J	104	A1EF2	C23-C22-C21	3.05	123.63	118.94
8	J	102	BCL	C4B-C3B-C2B	-3.05	103.45	108.36
8	O	102	BCL	C4-C3-C5	3.05	120.40	115.27
16	b	102	A1EF2	C39-C22-C21	-3.05	118.66	122.92
16	f	101	A1EF2	C38-C17-C18	-3.04	118.66	122.92
16	f	101	A1EF2	C39-C22-C21	-3.04	118.66	122.92
8	N	101	BCL	CHD-C1D-ND	-3.04	121.66	124.45
8	M	401	BCL	CBC-CAC-C3C	-3.04	106.70	113.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	a	102	BCL	C1D-ND-C4D	3.04	108.49	106.33
8	J	102	BCL	O2D-CGD-O1D	-3.03	117.91	123.84
8	q	102	BCL	C3C-C4C-CHD	-3.03	116.92	123.39
8	K	102	BCL	CBC-CAC-C3C	-3.03	106.72	113.47
16	o	101	A1EF2	C38-C17-C18	-3.03	118.68	122.92
8	K	102	BCL	O2D-CGD-O1D	-3.03	117.92	123.84
16	D	105	A1EF2	C39-C22-C21	-3.02	118.69	122.92
8	J	102	BCL	CHD-C4C-NC	3.02	128.43	125.08
8	c	102	BCL	C1D-ND-C4D	3.02	108.48	106.33
16	D	104	A1EF2	C16-C17-C18	3.02	123.58	118.94
16	J	103	A1EF2	C39-C22-C21	-3.02	118.69	122.92
8	d	102	BCL	C1C-NC-C4C	-3.02	105.35	106.71
8	O	102	BCL	CBC-CAC-C3C	-3.02	106.74	113.47
8	b	103	BCL	C1D-ND-C4D	3.02	108.48	106.33
8	a	102	BCL	CBC-CAC-C3C	-3.02	106.75	113.47
16	g	103	A1EF2	C24-C25-C26	-3.01	123.01	127.31
8	E	103	BCL	CHD-C1D-ND	-3.01	121.69	124.45
8	N	101	BCL	CMC-C2C-C3C	3.01	125.98	113.83
8	L	301	BCL	C3C-C4C-CHD	-3.01	116.96	123.39
16	C	104	A1EF2	C16-C17-C18	3.01	123.56	118.94
10	L	304	U10	C20-C19-C21	3.01	120.33	115.27
8	P	102	BCL	C4A-NA-C1A	-3.01	105.35	106.71
16	I	105	A1EF2	C38-C17-C18	-3.01	118.71	122.92
8	o	102	BCL	C1-C2-C3	-3.00	120.85	126.04
8	F	103	BCL	CHD-C1D-ND	-3.00	121.70	124.45
8	f	102	BCL	CBC-CAC-C3C	-3.00	106.79	113.47
8	M	404	BCL	C4B-C3B-C2B	-2.99	103.55	108.36
16	E	105	A1EF2	C39-C22-C21	-2.99	118.73	122.92
8	G	104	BCL	C1-C2-C3	-2.99	120.87	126.04
16	D	105	A1EF2	C19-C20-C21	2.99	129.60	123.47
16	E	105	A1EF2	C16-C17-C18	2.99	123.53	118.94
8	I	102	BCL	C1-C2-C3	-2.99	120.88	126.04
16	q	101	A1EF2	C23-C22-C21	2.98	123.52	118.94
10	L	303	U10	C17-C18-C19	-2.98	120.48	127.66
16	c	104	A1EF2	C38-C17-C18	-2.98	118.75	122.92
16	N	102	A1EF2	C19-C20-C21	2.98	129.58	123.47
16	B	103	A1EF2	C19-C20-C21	2.97	129.57	123.47
16	p	101	A1EF2	C20-C19-C18	2.97	129.56	123.47
8	c	102	BCL	C1C-NC-C4C	-2.97	105.37	106.71
8	I	102	BCL	C4B-C3B-C2B	-2.96	103.59	108.36
8	d	102	BCL	CMC-C2C-C3C	2.96	125.78	113.83
8	Q	101	BCL	CBC-CAC-C3C	-2.96	106.87	113.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	M	401	BCL	C3C-C4C-CHD	-2.96	117.07	123.39
8	b	103	BCL	C3C-C4C-CHD	-2.96	117.07	123.39
16	a	103	A1EF2	C38-C17-C18	-2.96	118.78	122.92
8	F	103	BCL	C4B-C3B-C2B	-2.95	103.61	108.36
8	M	404	BCL	CHD-C4C-NC	2.94	128.35	125.08
8	G	104	BCL	O2D-CGD-O1D	-2.94	118.08	123.84
16	O	103	A1EF2	C16-C17-C18	2.94	123.46	118.94
13	a	101	LMT	C1B-O1B-C4'	-2.94	110.69	117.96
8	i	101	BCL	CHD-C1D-ND	-2.94	121.75	124.45
8	n	102	BCL	C1D-ND-C4D	2.94	108.42	106.33
16	b	102	A1EF2	C38-C17-C18	-2.93	118.81	122.92
16	b	102	A1EF2	C24-C25-C26	2.93	131.50	127.31
8	J	102	BCL	CBC-CAC-C3C	-2.93	106.94	113.47
16	q	101	A1EF2	C20-C19-C18	2.93	129.48	123.47
8	F	103	BCL	O2D-CGD-O1D	-2.93	118.11	123.84
16	M	411	A1EF2	C16-C17-C18	2.93	123.43	118.94
16	n	101	A1EF2	C38-C17-C18	-2.92	118.83	122.92
8	M	404	BCL	C4-C3-C5	2.92	120.19	115.27
13	L	311	LMT	C1B-O1B-C4'	-2.92	110.73	117.96
16	k	101	A1EF2	C38-C17-C18	-2.92	118.83	122.92
8	N	101	BCL	CHD-C4C-NC	2.92	128.32	125.08
8	K	102	BCL	C4-C3-C5	2.92	120.18	115.27
8	C	103	BCL	O2D-CGD-O1D	-2.92	118.13	123.84
8	O	102	BCL	O2A-CGA-CBA	2.92	121.06	111.91
16	g	103	A1EF2	C19-C20-C21	2.91	129.44	123.47
8	p	102	BCL	C3C-C4C-CHD	-2.91	117.18	123.39
8	b	103	BCL	CBC-CAC-C3C	-2.91	106.99	113.47
16	I	105	A1EF2	C39-C22-C21	-2.91	118.85	122.92
16	d	101	A1EF2	C38-C17-C18	-2.90	118.86	122.92
16	J	103	A1EF2	C28-C27-C26	-2.90	118.26	126.42
8	L	301	BCL	CBC-CAC-C3C	-2.90	107.00	113.47
8	c	102	BCL	C3C-C4C-CHD	-2.90	117.19	123.39
16	N	102	A1EF2	C23-C22-C21	2.90	123.39	118.94
16	g	101	A1EF2	C38-C17-C18	-2.90	118.86	122.92
8	K	102	BCL	C1D-ND-C4D	2.89	108.39	106.33
8	a	102	BCL	C3C-C4C-CHD	-2.89	117.22	123.39
8	B	101	BCL	C1D-ND-C4D	2.88	108.38	106.33
16	N	103	A1EF2	C16-C17-C18	2.88	123.36	118.94
8	M	401	BCL	C4B-C3B-C2B	-2.88	103.73	108.36
8	B	101	BCL	CBC-CAC-C3C	-2.87	107.07	113.47
13	L	312	LMT	C1B-O5B-C5B	2.87	119.33	113.69
8	j	101	BCL	C2A-C3A-C4A	-2.87	97.23	101.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	F	103	BCL	CBC-CAC-C3C	-2.87	107.07	113.47
16	N	103	A1EF2	C19-C20-C21	2.87	129.36	123.47
8	M	404	BCL	C1D-ND-C4D	2.87	108.37	106.33
8	L	308	BCL	C4-C3-C5	2.87	120.10	115.27
8	I	102	BCL	O2D-CGD-O1D	-2.87	118.23	123.84
8	F	103	BCL	CHD-C4C-NC	2.87	128.26	125.08
8	g	102	BCL	C1D-ND-C4D	2.86	108.37	106.33
8	p	102	BCL	O2A-CGA-CBA	2.86	120.90	111.91
10	L	304	U10	C25-C24-C26	2.86	120.08	115.27
8	A	702	BCL	O2A-CGA-CBA	2.86	120.89	111.91
8	L	301	BCL	CHD-C1D-C2D	-2.86	119.49	125.48
16	b	102	A1EF2	C28-C27-C26	-2.84	118.42	126.42
8	M	401	BCL	O2A-CGA-CBA	2.84	120.83	111.91
16	c	104	A1EF2	C24-C25-C26	2.84	131.37	127.31
8	L	308	BCL	C4B-C3B-C2B	-2.84	103.79	108.36
8	e	102	BCL	C1D-ND-C4D	2.84	108.35	106.33
10	M	407	U10	C20-C19-C21	2.84	120.05	115.27
8	M	404	BCL	CBC-CAC-C3C	-2.84	107.15	113.47
8	N	101	BCL	O2D-CGD-O1D	-2.84	118.29	123.84
8	O	102	BCL	C4B-C3B-C2B	-2.83	103.81	108.36
8	i	101	BCL	CHD-C4C-NC	2.83	128.22	125.08
16	N	102	A1EF2	C29-C28-C27	-2.83	114.39	123.22
8	F	103	BCL	C1-C2-C3	-2.83	121.15	126.04
8	d	102	BCL	C1D-ND-C4D	2.83	108.34	106.33
9	L	302	BPH	C2B-C1B-NB	-2.82	107.58	109.53
8	G	104	BCL	C4B-C3B-C2B	-2.82	103.82	108.36
8	o	102	BCL	O2A-CGA-CBA	2.81	120.74	111.91
16	n	101	A1EF2	C39-C22-C21	-2.81	118.98	122.92
10	L	304	U10	C27-C26-C24	-2.81	110.02	114.62
8	N	101	BCL	C1D-ND-C4D	2.81	108.33	106.33
16	a	103	A1EF2	C20-C19-C18	2.81	129.23	123.47
8	N	101	BCL	C4B-C3B-C2B	-2.80	103.85	108.36
8	L	308	BCL	O2A-CGA-CBA	2.80	120.71	111.91
10	M	407	U10	C12-C13-C14	-2.80	120.92	127.66
13	L	312	LMT	O5B-C1B-C2B	2.79	116.26	110.35
8	M	404	BCL	O2A-CGA-CBA	2.79	120.67	111.91
10	L	304	U10	C1M-C1-C6	-2.79	119.85	124.40
16	e	101	A1EF2	C16-C17-C18	2.79	123.22	118.94
16	B	103	A1EF2	C16-C17-C18	2.79	123.22	118.94
8	N	101	BCL	O2A-CGA-CBA	2.78	120.63	111.91
8	q	102	BCL	CBC-CAC-C3C	-2.78	107.28	113.47
8	c	102	BCL	CHC-C4B-C3B	-2.77	122.48	132.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	L	308	BCL	O2D-CGD-O1D	-2.77	118.42	123.84
16	J	103	A1EF2	C16-C17-C18	2.77	123.19	118.94
16	O	103	A1EF2	C19-C20-C21	2.77	129.15	123.47
10	M	407	U10	C15-C14-C16	2.77	119.92	115.27
16	N	103	A1EF2	C23-C22-C21	2.76	123.18	118.94
11	G	103	PGV	O03-C19-C20	2.76	120.58	111.91
16	N	102	A1EF2	C16-C17-C18	2.76	123.18	118.94
8	p	102	BCL	C4-C3-C5	2.76	119.92	115.27
8	E	103	BCL	O2D-CGD-O1D	-2.76	118.45	123.84
8	a	102	BCL	C4B-C3B-C2B	-2.76	103.92	108.36
16	g	103	A1EF2	C12-C11-C10	2.76	120.94	111.88
11	C	101	PGV	O03-C19-C20	2.76	120.56	111.91
8	F	103	BCL	O2A-CGA-CBA	2.76	120.56	111.91
16	D	104	A1EF2	C19-C20-C21	2.75	129.12	123.47
8	D	102	BCL	C1D-ND-C4D	2.75	108.29	106.33
16	J	104	A1EF2	C16-C17-C18	2.75	123.17	118.94
8	E	103	BCL	C1C-NC-C4C	-2.75	105.47	106.71
8	F	103	BCL	C1C-NC-C4C	-2.75	105.47	106.71
8	E	103	BCL	CHD-C4C-NC	2.75	128.13	125.08
8	D	102	BCL	O2A-CGA-CBA	2.75	120.53	111.91
8	M	404	BCL	C3C-C4C-CHD	-2.75	117.52	123.39
10	L	303	U10	C20-C19-C21	2.74	119.89	115.27
8	N	101	BCL	C4-C3-C5	2.74	119.89	115.27
9	M	405	BPH	C2B-C1B-NB	-2.74	107.63	109.53
10	M	407	U10	C30-C29-C31	2.74	119.88	115.27
13	F	101	LMT	O1B-C4'-C3'	2.74	114.57	107.28
11	C	102	PGV	O03-C19-C20	2.74	120.50	111.91
8	L	301	BCL	O2A-CGA-CBA	2.74	120.50	111.91
8	D	102	BCL	CBC-CAC-C3C	-2.74	107.38	113.47
11	K	103	PGV	O03-C19-C20	2.73	120.48	111.91
11	M	402	PGV	O03-C19-C20	2.73	120.48	111.91
8	L	308	BCL	CBC-CAC-C3C	-2.73	107.39	113.47
8	E	103	BCL	CBC-CAC-C3C	-2.73	107.39	113.47
8	f	102	BCL	C1D-ND-C4D	2.73	108.27	106.33
8	M	404	BCL	CHA-C1A-NA	-2.73	120.15	126.40
8	B	101	BCL	O2A-CGA-CBA	2.73	120.46	111.91
11	L	305	PGV	O03-C19-C20	2.72	120.45	111.91
8	P	102	BCL	C3C-C4C-CHD	-2.72	117.59	123.39
13	M	409	LMT	O1B-C4'-C3'	2.72	114.51	107.28
8	k	102	BCL	CHC-C4B-C3B	-2.71	122.69	132.35
8	F	103	BCL	C4-C3-C5	2.71	119.83	115.27
8	I	102	BCL	C4-C3-C5	2.71	119.83	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	e	102	BCL	C4-C3-C5	2.71	119.82	115.27
16	J	101	A1EF2	C23-C22-C21	2.71	123.09	118.94
8	B	101	BCL	C4-C3-C5	2.70	119.82	115.27
8	L	301	BCL	O2D-CGD-O1D	-2.70	118.55	123.84
8	g	102	BCL	C4B-C3B-C2B	-2.70	104.01	108.36
16	p	101	A1EF2	C16-C17-C18	2.70	123.08	118.94
8	o	102	BCL	C3C-C4C-CHD	-2.70	117.62	123.39
8	j	101	BCL	CHC-C4B-C3B	-2.70	122.75	132.35
8	O	102	BCL	O2D-CGD-O1D	-2.70	118.56	123.84
13	D	103	LMT	C1B-O1B-C4'	-2.70	111.29	117.96
16	M	411	A1EF2	C39-C22-C21	-2.70	119.15	122.92
8	Q	101	BCL	C1D-ND-C4D	2.70	108.25	106.33
8	f	102	BCL	C4-C3-C5	2.69	119.80	115.27
8	o	102	BCL	C1C-NC-C4C	-2.69	105.50	106.71
16	C	104	A1EF2	C19-C20-C21	2.69	128.99	123.47
8	A	702	BCL	O2D-CGD-O1D	-2.69	118.58	123.84
16	B	103	A1EF2	C23-C22-C21	2.69	123.07	118.94
8	P	102	BCL	O2A-CGA-CBA	2.69	120.34	111.91
8	i	101	BCL	C4-C3-C5	2.68	119.79	115.27
8	e	102	BCL	CHC-C4B-C3B	-2.68	122.81	132.35
16	D	104	A1EF2	C23-C22-C21	2.68	123.05	118.94
8	e	102	BCL	C4B-C3B-C2B	-2.68	104.05	108.36
16	c	104	A1EF2	C23-C22-C21	2.68	123.05	118.94
16	J	101	A1EF2	C16-C17-C18	2.67	123.04	118.94
8	G	104	BCL	CBC-CAC-C3C	-2.67	107.53	113.47
8	M	404	BCL	CED-O2D-CGD	2.67	121.97	115.94
8	M	401	BCL	C6-C5-C3	-2.67	106.46	113.45
8	Q	101	BCL	C3C-C4C-CHD	-2.67	117.70	123.39
16	p	101	A1EF2	C24-C25-C26	2.66	131.11	127.31
11	L	306	PGV	O03-C19-C20	2.66	120.27	111.91
10	M	407	U10	C4M-O4-C4	2.66	125.90	116.47
8	Q	101	BCL	C4B-C3B-C2B	-2.66	104.08	108.36
8	p	102	BCL	C1D-ND-C4D	2.66	108.23	106.33
16	E	105	A1EF2	C19-C20-C21	2.66	128.93	123.47
8	Q	101	BCL	O2D-CGD-O1D	-2.66	118.64	123.84
8	b	103	BCL	O2A-CGA-CBA	2.66	120.26	111.91
8	o	102	BCL	C4-C3-C5	2.66	119.74	115.27
8	A	702	BCL	C2A-C3A-C4A	-2.66	97.58	101.87
8	C	103	BCL	CBC-CAC-C3C	-2.65	107.56	113.47
8	D	102	BCL	C1-C2-C3	-2.65	121.45	126.04
11	E	104	PGV	O03-C19-C20	2.65	120.23	111.91
16	D	105	A1EF2	C16-C17-C18	2.65	123.01	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	M	401	BCL	C1D-ND-C4D	2.65	108.22	106.33
16	g	101	A1EF2	C23-C22-C21	2.65	123.00	118.94
16	p	101	A1EF2	C23-C22-C21	2.64	123.00	118.94
8	e	102	BCL	O2D-CGD-O1D	-2.64	118.68	123.84
16	f	101	A1EF2	C16-C17-C18	2.64	122.99	118.94
8	b	103	BCL	C4-C3-C5	2.64	119.70	115.27
8	O	102	BCL	CMD-C2D-C1D	2.64	129.36	124.71
8	g	102	BCL	O2D-CGD-O1D	-2.63	118.69	123.84
8	A	702	BCL	C3C-C4C-CHD	-2.63	117.77	123.39
11	H	304	PGV	C02-O01-C1	-2.63	111.31	117.79
8	a	102	BCL	O2D-CGD-O1D	-2.63	118.69	123.84
16	k	101	A1EF2	C23-C22-C21	2.63	122.98	118.94
8	a	102	BCL	O2A-CGA-CBA	2.63	120.15	111.91
8	o	102	BCL	CHC-C4B-C3B	-2.62	123.01	132.35
8	n	102	BCL	C4B-C3B-C2B	-2.62	104.14	108.36
11	L	313	PGV	C02-O01-C1	-2.62	111.33	117.79
8	a	102	BCL	C2A-C3A-C4A	-2.62	97.63	101.87
8	M	404	BCL	C3C-C2C-C1C	-2.62	97.64	101.87
8	I	102	BCL	CBC-CAC-C3C	-2.62	107.64	113.47
8	c	102	BCL	O2D-CGD-O1D	-2.62	118.72	123.84
16	k	101	A1EF2	C16-C17-C18	2.62	122.96	118.94
8	p	102	BCL	O2D-CGD-O1D	-2.61	118.73	123.84
10	L	303	U10	C15-C14-C16	2.61	119.67	115.27
8	n	102	BCL	O2D-CGD-O1D	-2.61	118.74	123.84
16	o	101	A1EF2	C23-C22-C21	2.61	122.94	118.94
10	L	303	U10	C25-C24-C26	2.61	119.66	115.27
8	O	102	BCL	C1D-ND-C4D	2.61	108.19	106.33
13	I	103	LMT	C1B-O1B-C4'	-2.60	111.52	117.96
10	M	407	U10	C22-C23-C24	-2.60	121.39	127.66
8	I	102	BCL	C1C-NC-C4C	-2.60	105.54	106.71
16	C	104	A1EF2	C23-C22-C21	2.60	122.93	118.94
8	b	103	BCL	O2D-CGD-O1D	-2.60	118.75	123.84
8	j	101	BCL	C4B-C3B-C2B	-2.60	104.18	108.36
16	O	103	A1EF2	C23-C22-C21	2.60	122.93	118.94
8	d	102	BCL	O2D-CGD-O1D	-2.60	118.76	123.84
8	B	101	BCL	C1-C2-C3	-2.59	121.56	126.04
16	e	101	A1EF2	C23-C22-C21	2.59	122.92	118.94
10	M	407	U10	C17-C18-C19	-2.59	121.42	127.66
8	L	301	BCL	C4-C3-C5	2.59	119.63	115.27
8	q	102	BCL	O2D-CGD-O1D	-2.59	118.78	123.84
8	p	102	BCL	CHD-C1D-C2D	-2.58	120.06	125.48
8	K	102	BCL	O2A-CGA-CBA	2.58	120.01	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	n	102	BCL	CHC-C4B-C3B	-2.58	123.17	132.35
8	j	101	BCL	C1D-ND-C4D	2.58	108.17	106.33
8	f	102	BCL	O2D-CGD-O1D	-2.57	118.81	123.84
8	a	102	BCL	C4-C3-C5	2.57	119.60	115.27
16	c	104	A1EF2	C16-C17-C18	2.57	122.89	118.94
8	j	101	BCL	C4-C3-C5	2.57	119.60	115.27
8	g	102	BCL	CHC-C4B-C3B	-2.57	123.20	132.35
8	M	404	BCL	CMD-C2D-C1D	2.57	129.24	124.71
16	o	101	A1EF2	C16-C17-C18	2.57	122.88	118.94
8	j	101	BCL	O2D-CGD-O1D	-2.57	118.82	123.84
8	f	102	BCL	O2A-CGA-CBA	2.57	119.96	111.91
8	b	103	BCL	C4B-C3B-C2B	-2.56	104.24	108.36
16	E	105	A1EF2	C23-C22-C21	2.56	122.87	118.94
8	F	103	BCL	CMD-C2D-C1D	2.56	129.22	124.71
8	j	101	BCL	O2A-CGA-CBA	2.56	119.93	111.91
8	L	301	BCL	C2A-C3A-C4A	-2.55	97.74	101.87
16	b	102	A1EF2	C23-C22-C21	2.55	122.86	118.94
8	I	102	BCL	O2A-CGA-CBA	2.55	119.92	111.91
15	M	410	CDL	OB6-CB5-C51	2.55	117.00	111.50
8	f	102	BCL	CHD-C4C-NC	2.55	127.91	125.08
8	d	102	BCL	C4B-C3B-C2B	-2.55	104.26	108.36
8	E	103	BCL	CHC-C1C-NC	2.55	128.03	124.51
8	P	102	BCL	O2D-CGD-O1D	-2.55	118.86	123.84
8	i	101	BCL	O2D-CGD-O1D	-2.54	118.86	123.84
11	M	412	PGV	O03-C19-C20	2.54	119.88	111.91
11	H	304	PGV	O03-C19-C20	2.54	119.87	111.91
10	M	407	U10	C41-C39-C40	2.54	120.21	114.60
8	O	102	BCL	CHC-C1C-NC	2.53	128.02	124.51
8	q	102	BCL	O2A-CGA-CBA	2.53	119.86	111.91
8	C	103	BCL	O2A-CGA-CBA	2.53	119.85	111.91
8	P	102	BCL	CHB-C1B-NB	-2.53	121.58	124.26
8	a	102	BCL	C1-C2-C3	-2.52	121.68	126.04
16	d	101	A1EF2	C23-C22-C21	2.52	122.81	118.94
16	o	101	A1EF2	C20-C19-C18	2.52	128.64	123.47
8	n	102	BCL	C1-C2-C3	-2.52	121.68	126.04
10	M	407	U10	C27-C28-C29	-2.52	121.59	127.66
8	I	102	BCL	CHB-C1B-NB	-2.52	121.59	124.26
8	g	102	BCL	CHD-C4C-NC	2.52	127.87	125.08
8	L	308	BCL	C3C-C4C-CHD	-2.51	118.04	123.39
8	C	103	BCL	CHA-C1A-NA	-2.51	120.66	126.40
10	L	303	U10	C22-C23-C24	-2.50	121.63	127.66
13	b	101	LMT	C1B-O1B-C4'	-2.50	111.77	117.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	f	102	BCL	C4B-C3B-C2B	-2.50	104.34	108.36
8	j	101	BCL	CHD-C4C-NC	2.50	127.85	125.08
13	B	102	LMT	O5B-C5B-C4B	2.50	114.23	109.69
8	A	702	BCL	CHC-C4B-C3B	-2.49	123.49	132.35
8	Q	101	BCL	CHA-C4D-ND	2.49	137.70	132.50
8	f	102	BCL	CHC-C4B-C3B	-2.49	123.51	132.35
8	B	101	BCL	CHC-C1C-NC	2.48	127.94	124.51
10	L	303	U10	C12-C13-C14	-2.48	121.68	127.66
8	P	102	BCL	C4-C3-C5	2.48	119.45	115.27
8	o	102	BCL	CHD-C1D-C2D	-2.48	120.28	125.48
8	b	103	BCL	CHC-C4B-C3B	-2.48	123.53	132.35
16	d	101	A1EF2	C16-C17-C18	2.48	122.75	118.94
8	P	102	BCL	CMD-C2D-C1D	2.48	129.08	124.71
16	g	103	A1EF2	C25-C24-C23	2.48	130.95	123.22
8	c	102	BCL	C4-C3-C5	2.48	119.44	115.27
8	L	301	BCL	CHA-C4D-ND	2.47	137.67	132.50
8	I	102	BCL	C1D-ND-C4D	2.47	108.09	106.33
11	L	314	PGV	O03-C19-C20	2.46	119.64	111.91
8	P	102	BCL	CHA-C4D-ND	2.46	137.65	132.50
16	b	102	A1EF2	C16-C17-C18	2.46	122.72	118.94
8	L	308	BCL	CHC-C4B-C3B	-2.45	123.62	132.35
8	K	102	BCL	C1C-NC-C4C	-2.45	105.60	106.71
16	D	105	A1EF2	C23-C22-C21	2.45	122.70	118.94
16	f	101	A1EF2	C23-C22-C21	2.45	122.70	118.94
10	M	407	U10	C10-C9-C11	2.44	119.38	115.27
8	F	103	BCL	CHC-C1C-NC	2.44	127.89	124.51
16	J	103	A1EF2	C23-C22-C21	2.44	122.69	118.94
8	Q	101	BCL	CMD-C2D-C1D	2.44	129.01	124.71
8	D	102	BCL	CHC-C1C-NC	2.44	127.88	124.51
8	c	102	BCL	O2A-CGA-CBA	2.43	119.55	111.91
8	C	103	BCL	C1-C2-C3	-2.43	121.83	126.04
8	b	103	BCL	C2A-C3A-C4A	-2.43	97.94	101.87
8	L	308	BCL	CHB-C1B-NB	-2.43	121.68	124.26
8	D	102	BCL	CMD-C2D-C1D	2.43	128.99	124.71
8	O	102	BCL	CHD-C1D-ND	-2.43	122.22	124.45
8	N	101	BCL	CMD-C2D-C1D	2.42	128.98	124.71
8	i	101	BCL	CHC-C4B-C3B	-2.42	123.75	132.35
11	L	305	PGV	C02-O01-C1	-2.42	111.84	117.79
8	q	102	BCL	CHA-C4D-ND	2.41	137.55	132.50
8	K	102	BCL	CMD-C2D-C1D	2.41	128.96	124.71
8	g	102	BCL	CHB-C1B-NB	-2.41	121.70	124.26
8	K	102	BCL	CHC-C1C-NC	2.41	127.84	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	F	102	CDL	OB4-PB2-OB3	2.41	120.12	110.68
8	A	702	BCL	CHC-C1C-NC	2.41	127.84	124.51
8	D	102	BCL	CHB-C1B-C2B	-2.41	120.43	127.24
8	B	101	BCL	CHD-C4C-NC	2.41	127.75	125.08
8	J	102	BCL	CMD-C2D-C1D	2.41	128.95	124.71
9	L	302	BPH	CMA-C3A-C4A	-2.40	109.11	114.38
8	Q	101	BCL	C1C-NC-C4C	-2.40	105.63	106.71
8	g	102	BCL	O2A-CGA-CBA	2.40	119.43	111.91
8	M	401	BCL	O2D-CGD-O1D	-2.39	119.16	123.84
8	F	103	BCL	C1D-ND-C4D	2.39	108.03	106.33
8	i	101	BCL	O2A-CGA-CBA	2.39	119.41	111.91
8	p	102	BCL	C4B-C3B-C2B	-2.39	104.52	108.36
8	M	404	BCL	C1-C2-C3	-2.39	121.91	126.04
8	a	102	BCL	CHC-C4B-C3B	-2.39	123.86	132.35
8	d	102	BCL	CHC-C4B-C3B	-2.39	123.86	132.35
16	n	101	A1EF2	C20-C19-C18	2.39	128.36	123.47
16	d	101	A1EF2	C24-C25-C26	2.39	130.71	127.31
8	k	102	BCL	O2D-CGD-O1D	-2.38	119.18	123.84
8	J	102	BCL	CHC-C4B-C3B	-2.38	123.88	132.35
10	M	407	U10	C35-C34-C36	2.38	119.28	115.27
8	n	102	BCL	C2A-C3A-C4A	-2.38	98.02	101.87
8	G	104	BCL	CHC-C1C-NC	2.38	127.80	124.51
16	J	106	A1EF2	C25-C24-C23	2.38	130.65	123.22
11	C	101	PGV	O14-P-O13	2.38	119.99	110.68
8	q	102	BCL	C2A-C3A-C4A	-2.38	98.03	101.87
15	F	102	CDL	OA4-PA1-OA3	2.38	119.99	110.68
8	E	103	BCL	CMD-C2D-C1D	2.38	128.90	124.71
8	B	101	BCL	CHA-C1A-NA	-2.37	120.96	126.40
8	n	102	BCL	O2A-CGA-CBA	2.37	119.36	111.91
8	c	102	BCL	C4B-C3B-C2B	-2.37	104.55	108.36
8	L	301	BCL	CHC-C4B-C3B	-2.36	123.94	132.35
13	M	409	LMT	C1'-C2'-C3'	2.36	114.92	110.00
8	L	308	BCL	CHA-C1A-NA	-2.36	120.99	126.40
8	M	401	BCL	CHC-C4B-C3B	-2.36	123.97	132.35
8	g	102	BCL	C4-C3-C5	2.35	119.23	115.27
8	O	102	BCL	CHC-C4B-C3B	-2.35	123.97	132.35
8	L	301	BCL	CHA-C1A-NA	-2.35	121.01	126.40
8	i	101	BCL	C1D-ND-C4D	2.35	108.00	106.33
8	n	102	BCL	CHB-C1B-NB	-2.35	121.77	124.26
8	e	102	BCL	CHD-C4C-NC	2.35	127.68	125.08
13	E	102	LMT	O1'-C1'-C2'	2.34	111.96	108.30
16	J	106	A1EF2	C24-C25-C26	-2.34	123.97	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	C	103	BCL	CHC-C1C-NC	2.34	127.75	124.51
10	L	304	U10	C3M-O3-C3	2.34	124.76	116.47
8	O	102	BCL	CHB-C1B-NB	-2.34	121.78	124.26
16	n	101	A1EF2	C16-C17-C18	2.34	122.53	118.94
16	I	105	A1EF2	C16-C17-C18	2.34	122.53	118.94
8	d	102	BCL	O2A-CGA-CBA	2.34	119.24	111.91
13	B	102	LMT	O5'-C5'-C6'	-2.33	100.63	106.44
8	C	103	BCL	CHB-C1B-C2B	-2.33	120.65	127.24
16	g	103	A1EF2	C37-C13-C12	2.33	119.19	115.27
8	o	102	BCL	CHA-C1A-NA	-2.33	121.07	126.40
8	I	102	BCL	CHA-C1A-NA	-2.33	121.07	126.40
8	G	104	BCL	CMD-C2D-C1D	2.32	128.80	124.71
8	E	103	BCL	CHA-C1A-NA	-2.32	121.09	126.40
8	c	102	BCL	C2A-C3A-C4A	-2.32	98.13	101.87
8	C	103	BCL	CMD-C2D-C1D	2.31	128.79	124.71
8	k	102	BCL	C1D-ND-C4D	2.31	107.98	106.33
8	I	102	BCL	CHC-C1C-NC	2.31	127.70	124.51
13	B	102	LMT	C1B-O1B-C4'	2.31	123.67	117.96
8	F	103	BCL	CHA-C1A-NA	-2.31	121.12	126.40
8	L	301	BCL	CHD-C4C-NC	2.30	127.64	125.08
8	L	308	BCL	CHD-C4C-NC	2.30	127.63	125.08
8	D	102	BCL	CHC-C4B-C3B	-2.30	124.16	132.35
8	E	103	BCL	C1D-ND-C4D	2.30	107.97	106.33
8	D	102	BCL	CHA-C1A-NA	-2.30	121.13	126.40
8	c	102	BCL	CHA-C4D-ND	2.30	137.31	132.50
8	i	101	BCL	C1-C2-C3	-2.29	122.08	126.04
16	g	101	A1EF2	C16-C17-C18	2.29	122.46	118.94
8	q	102	BCL	CHB-C1B-NB	-2.29	121.83	124.26
10	L	304	U10	C17-C18-C19	-2.29	122.16	127.66
8	G	104	BCL	CHD-C1D-ND	-2.28	122.36	124.45
8	L	301	BCL	CMD-C2D-C1D	2.28	128.74	124.71
8	p	102	BCL	CHA-C4D-ND	2.28	137.27	132.50
13	O	101	LMT	O1B-C4'-C3'	2.28	113.34	107.28
8	M	401	BCL	CHB-C1B-C2B	-2.28	120.81	127.24
8	F	103	BCL	CHC-C4B-C3B	-2.28	124.25	132.35
13	U	101	LMT	C1B-O1B-C4'	-2.27	112.34	117.96
8	o	102	BCL	CHA-C4D-ND	2.27	137.25	132.50
8	p	102	BCL	C1-C2-C3	-2.27	122.12	126.04
8	A	702	BCL	CHA-C4D-ND	2.27	137.24	132.50
8	O	102	BCL	CHA-C1A-NA	-2.27	121.21	126.40
8	J	102	BCL	CHC-C1C-NC	2.27	127.65	124.51
8	Q	101	BCL	O2A-CGA-CBA	2.27	119.02	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	M	401	BCL	CHA-C1A-NA	-2.26	121.21	126.40
8	L	301	BCL	CHC-C1C-NC	2.26	127.64	124.51
8	P	102	BCL	CHC-C4B-C3B	-2.26	124.30	132.35
8	Q	101	BCL	CHA-C1A-NA	-2.26	121.22	126.40
8	n	102	BCL	CHB-C1B-C2B	-2.26	120.85	127.24
8	A	702	BCL	C6-C5-C3	-2.26	107.53	113.45
8	K	102	BCL	CHB-C1B-C2B	-2.26	120.86	127.24
16	M	411	A1EF2	C14-C15-C16	2.26	130.27	123.22
8	I	102	BCL	CHB-C1B-C2B	-2.26	120.86	127.24
16	I	105	A1EF2	C23-C22-C21	2.26	122.40	118.94
16	a	103	A1EF2	C16-C17-C18	2.25	122.40	118.94
16	J	104	A1EF2	C37-C13-C12	2.25	119.06	115.27
8	n	102	BCL	CHC-C1C-NC	2.25	127.63	124.51
8	d	102	BCL	CHB-C1B-NB	-2.25	121.87	124.26
16	E	105	A1EF2	C37-C13-C12	2.25	119.06	115.27
8	J	102	BCL	CHC-C4B-NB	-2.25	121.88	124.26
16	N	102	A1EF2	C37-C13-C12	2.25	119.06	115.27
8	Q	101	BCL	C2A-C3A-C4A	-2.25	98.24	101.87
8	A	702	BCL	CHB-C1B-NB	-2.25	121.88	124.26
8	G	104	BCL	O2A-CGA-CBA	2.25	118.96	111.91
16	M	411	A1EF2	C20-C21-C22	2.25	130.52	127.31
8	i	101	BCL	CHC-C1C-NC	2.25	127.62	124.51
16	J	101	A1EF2	C37-C13-C12	2.24	119.04	115.27
8	B	101	BCL	CMD-C2D-C1D	2.24	128.66	124.71
8	d	102	BCL	CHD-C4C-NC	2.24	127.57	125.08
8	i	101	BCL	C2A-C3A-C4A	-2.24	98.25	101.87
16	M	411	A1EF2	C20-C19-C18	2.24	128.06	123.47
8	f	102	BCL	CHA-C4D-ND	2.24	137.18	132.50
8	G	104	BCL	CHA-C1A-NA	-2.24	121.28	126.40
8	o	102	BCL	C2A-C3A-C4A	-2.23	98.26	101.87
8	K	102	BCL	CHA-C1A-NA	-2.23	121.29	126.40
8	L	308	BCL	CHB-C1B-C2B	-2.23	120.94	127.24
8	N	101	BCL	CHC-C4B-C3B	-2.23	124.42	132.35
8	n	102	BCL	CHA-C4D-ND	2.23	137.16	132.50
8	I	102	BCL	CHD-C4C-NC	2.22	127.54	125.08
16	D	104	A1EF2	C37-C13-C12	2.22	119.01	115.27
11	H	303	PGV	O03-C19-C20	2.22	118.88	111.91
8	C	103	BCL	O1D-CGD-CBD	-2.22	119.94	124.48
16	e	101	A1EF2	C37-C13-C12	2.22	119.00	115.27
8	N	101	BCL	CHA-C4D-ND	2.22	137.13	132.50
8	B	101	BCL	CHC-C4B-C3B	-2.21	124.47	132.35
8	g	102	BCL	CHC-C4B-NB	-2.21	121.92	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	L	304	U10	C15-C14-C16	2.21	118.99	115.27
8	I	102	BCL	CHC-C4B-C3B	-2.21	124.49	132.35
13	c	101	LMT	C1-O1'-C1'	-2.21	110.18	113.84
16	k	101	A1EF2	C19-C18-C17	2.21	130.46	127.31
8	n	102	BCL	CHD-C4C-NC	2.20	127.53	125.08
8	O	102	BCL	CHA-C4D-ND	2.20	137.11	132.50
8	d	102	BCL	C2A-C1A-CHA	-2.20	120.00	123.86
8	J	102	BCL	O2A-CGA-CBA	2.20	118.83	111.91
8	k	102	BCL	O2A-CGA-CBA	2.20	118.82	111.91
8	E	103	BCL	CHB-C1B-C2B	-2.20	121.02	127.24
8	q	102	BCL	C4B-C3B-C2B	-2.20	104.82	108.36
8	e	102	BCL	O2A-CGA-CBA	2.20	118.82	111.91
8	J	102	BCL	C1D-ND-C4D	2.20	107.90	106.33
8	p	102	BCL	C2A-C3A-C4A	-2.20	98.32	101.87
8	c	102	BCL	CHA-C1A-NA	-2.20	121.36	126.40
8	J	102	BCL	CHB-C1B-C2B	-2.20	121.03	127.24
11	L	313	PGV	O03-C19-C20	2.20	118.80	111.91
8	N	101	BCL	CHA-C1A-NA	-2.19	121.37	126.40
8	P	102	BCL	CHA-C1A-NA	-2.19	121.37	126.40
8	f	102	BCL	CHA-C1A-NA	-2.19	121.38	126.40
8	b	103	BCL	CHA-C4D-ND	2.19	137.08	132.50
8	e	102	BCL	CHA-C4D-ND	2.19	137.08	132.50
8	a	102	BCL	C6-C5-C3	-2.19	107.71	113.45
8	a	102	BCL	CMD-C2D-C1D	2.19	128.57	124.71
8	D	102	BCL	CHA-C4D-ND	2.19	137.08	132.50
11	G	103	PGV	C02-O01-C1	-2.19	112.40	117.79
8	M	404	BCL	CHB-C1B-C2B	-2.19	121.06	127.24
8	G	104	BCL	CHC-C4B-C3B	-2.19	124.57	132.35
13	B	102	LMT	O1B-C1B-O5B	2.18	116.78	110.67
11	H	303	PGV	O14-P-O13	2.18	119.23	110.68
8	I	102	BCL	CMD-C2D-C1D	2.18	128.56	124.71
8	a	102	BCL	CHA-C4D-ND	2.18	137.06	132.50
8	j	101	BCL	CHC-C1C-NC	2.18	127.53	124.51
8	g	102	BCL	CHA-C4D-ND	2.18	137.05	132.50
8	E	103	BCL	O1D-CGD-CBD	-2.18	120.03	124.48
8	G	104	BCL	C1D-ND-C4D	2.17	107.88	106.33
10	L	304	U10	C6-C1-C2	2.17	120.90	119.18
8	M	404	BCL	CHC-C4B-C3B	-2.17	124.63	132.35
11	M	402	PGV	C02-O01-C1	-2.17	112.45	117.79
8	j	101	BCL	CHA-C1A-NA	-2.17	121.43	126.40
16	B	103	A1EF2	C37-C13-C12	2.16	118.91	115.27
8	J	102	BCL	CHA-C4D-ND	2.16	137.02	132.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	b	103	BCL	CHC-C1C-NC	2.16	127.50	124.51
16	J	106	A1EF2	C37-C13-C12	2.16	118.91	115.27
8	M	401	BCL	CMD-C2D-C1D	2.16	128.52	124.71
10	L	304	U10	O3-C3-C2	2.16	123.86	116.56
13	B	102	LMT	C6B-C5B-C4B	-2.16	107.95	113.00
8	K	102	BCL	CHB-C1B-NB	-2.15	121.98	124.26
8	d	102	BCL	CMD-C2D-C1D	2.15	128.50	124.71
8	C	103	BCL	CHA-C4D-ND	2.15	137.00	132.50
8	e	102	BCL	CHC-C1C-NC	2.15	127.48	124.51
8	g	102	BCL	CHA-C1A-NA	-2.15	121.48	126.40
8	d	102	BCL	CHA-C4D-ND	2.15	136.99	132.50
8	A	702	BCL	O2A-CGA-O1A	-2.14	118.18	123.59
13	B	102	LMT	C3B-C4B-C5B	-2.14	106.42	110.24
8	j	101	BCL	CHB-C1B-C2B	-2.14	121.19	127.24
8	j	101	BCL	CHC-C4B-NB	-2.14	121.99	124.26
8	O	102	BCL	C1-C2-C3	-2.14	122.34	126.04
8	n	102	BCL	CHA-C1A-NA	-2.14	121.51	126.40
16	N	103	A1EF2	C37-C13-C12	2.13	118.86	115.27
8	p	102	BCL	CHA-C1A-NA	-2.13	121.52	126.40
8	c	102	BCL	CHB-C1B-C2B	-2.13	121.22	127.24
8	G	104	BCL	CHB-C1B-C2B	-2.13	121.22	127.24
8	c	102	BCL	CHD-C1D-C2D	-2.13	121.01	125.48
8	F	103	BCL	C3D-C2D-C1D	-2.13	102.92	105.83
8	d	102	BCL	CHC-C4B-NB	-2.13	122.00	124.26
13	B	102	LMT	O5B-C5B-C6B	2.13	111.73	106.44
8	C	103	BCL	CHC-C4B-C3B	-2.13	124.78	132.35
16	f	101	A1EF2	C37-C13-C12	2.13	118.85	115.27
8	k	102	BCL	C2A-C3A-C4A	-2.13	98.44	101.87
8	K	102	BCL	CHC-C4B-C3B	-2.12	124.79	132.35
8	j	101	BCL	C1-C2-C3	-2.12	122.37	126.04
13	a	101	LMT	C1-O1'-C1'	-2.12	110.33	113.84
8	L	301	BCL	CHB-C1B-C2B	-2.12	121.25	127.24
16	a	103	A1EF2	C37-C13-C12	2.12	118.83	115.27
8	o	102	BCL	CHB-C1B-NB	-2.12	122.02	124.26
8	O	102	BCL	O2A-CGA-O1A	-2.12	118.25	123.59
8	K	102	BCL	CHA-C4D-ND	2.12	136.93	132.50
8	O	102	BCL	C3D-C2D-C1D	-2.11	102.95	105.83
10	M	407	U10	C37-C38-C39	-2.11	120.53	127.75
11	C	102	PGV	C02-O01-C1	-2.11	112.59	117.79
10	L	303	U10	C10-C9-C11	2.11	118.82	115.27
8	J	102	BCL	CHA-C1A-NA	-2.11	121.57	126.40
8	L	308	BCL	CMD-C2D-C1D	2.11	128.43	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	k	102	BCL	CHD-C4C-NC	2.11	127.42	125.08
16	k	101	A1EF2	C37-C13-C12	2.10	118.81	115.27
11	H	304	PGV	O01-C1-O02	-2.10	118.62	123.70
16	C	104	A1EF2	C37-C13-C12	2.10	118.81	115.27
16	J	103	A1EF2	C37-C13-C12	2.10	118.81	115.27
8	Q	101	BCL	CHC-C1C-NC	2.10	127.42	124.51
8	c	102	BCL	CHC-C1C-NC	2.10	127.42	124.51
16	d	101	A1EF2	C19-C18-C17	2.10	130.31	127.31
8	n	102	BCL	CMD-C2D-C1D	2.10	128.42	124.71
8	i	101	BCL	CMD-C2D-C1D	2.10	128.41	124.71
8	k	102	BCL	CHA-C4D-ND	2.10	136.89	132.50
8	i	101	BCL	CHA-C4D-ND	2.10	136.89	132.50
8	L	301	BCL	C1-O2A-CGA	2.10	121.95	116.44
8	k	102	BCL	CHB-C1B-C2B	-2.10	121.31	127.24
16	D	105	A1EF2	C37-C13-C12	2.10	118.80	115.27
16	o	101	A1EF2	C37-C13-C12	2.10	118.80	115.27
8	q	102	BCL	CHA-C1A-NA	-2.09	121.61	126.40
8	b	103	BCL	CHB-C1B-C2B	-2.09	121.33	127.24
8	N	101	BCL	CHC-C1C-NC	2.09	127.40	124.51
8	k	102	BCL	CHA-C1A-NA	-2.09	121.61	126.40
11	L	306	PGV	O01-C1-O02	-2.09	118.65	123.70
16	I	105	A1EF2	C37-C13-C12	2.09	118.79	115.27
8	f	102	BCL	C1-C2-C3	-2.09	122.43	126.04
8	A	702	BCL	CMD-C2D-C1D	2.09	128.39	124.71
8	b	103	BCL	CMD-C2D-C1D	2.09	128.39	124.71
8	E	103	BCL	CHC-C4B-C3B	-2.08	124.93	132.35
8	o	102	BCL	CHC-C1C-NC	2.08	127.39	124.51
8	F	103	BCL	CHA-C4D-ND	2.08	136.85	132.50
8	j	101	BCL	CHA-C4D-ND	2.08	136.85	132.50
13	B	102	LMT	O5'-C1'-O1'	-2.08	105.05	109.97
8	f	102	BCL	CHB-C1B-C2B	-2.08	121.37	127.24
8	e	102	BCL	CHA-C1A-NA	-2.08	121.64	126.40
8	O	102	BCL	O1D-CGD-CBD	-2.08	120.24	124.48
8	g	102	BCL	CHC-C1C-NC	2.07	127.38	124.51
8	g	102	BCL	CHB-C1B-C2B	-2.07	121.38	127.24
8	i	101	BCL	C2A-C1A-CHA	-2.07	120.23	123.86
8	E	103	BCL	CHA-C4D-ND	2.07	136.83	132.50
8	o	102	BCL	CMD-C2D-C1D	2.07	128.36	124.71
8	e	102	BCL	C2A-C3A-C4A	-2.07	98.53	101.87
8	j	101	BCL	CMD-C2D-C1D	2.07	128.35	124.71
16	b	102	A1EF2	C19-C18-C17	2.06	130.26	127.31
16	p	101	A1EF2	C37-C13-C12	2.06	118.74	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	K	102	BCL	CHD-C4C-NC	2.06	127.37	125.08
8	I	102	BCL	C2A-C3A-C4A	-2.06	98.54	101.87
8	J	102	BCL	C2A-C3A-C4A	-2.06	98.54	101.87
8	G	104	BCL	CHA-C4D-ND	2.06	136.80	132.50
8	M	401	BCL	C11-C12-C13	-2.06	109.27	115.92
8	A	702	BCL	CHA-C1A-NA	-2.05	121.69	126.40
8	B	101	BCL	C1C-NC-C4C	-2.05	105.78	106.71
16	n	101	A1EF2	C23-C22-C21	2.05	122.09	118.94
8	G	104	BCL	C3D-C2D-C1D	-2.05	103.03	105.83
13	D	101	LMT	O3'-C3'-C2'	-2.05	105.61	110.35
16	n	101	A1EF2	C37-C13-C12	2.05	118.72	115.27
16	g	101	A1EF2	C37-C13-C12	2.05	118.71	115.27
8	D	102	BCL	CHD-C4C-NC	2.05	127.35	125.08
8	E	103	BCL	C3D-C2D-C1D	-2.05	103.04	105.83
8	b	103	BCL	CHD-C4C-NC	2.04	127.35	125.08
10	L	304	U10	C10-C9-C11	2.04	118.70	115.27
8	B	101	BCL	CHA-C4D-ND	2.04	136.77	132.50
9	M	405	BPH	CBA-CAA-C2A	-2.04	107.85	113.81
8	b	103	BCL	CHB-C1B-NB	-2.04	122.10	124.26
16	e	101	A1EF2	C20-C19-C18	2.04	127.65	123.47
13	M	409	LMT	C1B-O1B-C4'	-2.04	112.92	117.96
13	M	409	LMT	O5'-C5'-C4'	-2.04	105.46	109.75
8	A	702	BCL	C3B-C2B-C1B	-2.04	99.83	106.39
8	a	102	BCL	C1-O2A-CGA	2.03	121.78	116.44
8	k	102	BCL	CHD-C1D-C2D	-2.03	121.21	125.48
8	Q	101	BCL	CHB-C1B-C2B	-2.03	121.49	127.24
11	L	314	PGV	C02-O01-C1	-2.03	112.79	117.79
8	A	702	BCL	CHD-C4C-NC	2.03	127.33	125.08
8	E	103	BCL	O2A-CGA-O1A	-2.03	118.47	123.59
8	L	308	BCL	C3C-C2C-C1C	-2.03	98.60	101.87
8	a	102	BCL	CHA-C1A-NA	-2.03	121.76	126.40
8	L	301	BCL	O2A-CGA-O1A	-2.02	118.48	123.59
8	o	102	BCL	O2A-CGA-O1A	-2.02	118.49	123.59
8	b	103	BCL	CHA-C1A-NA	-2.02	121.77	126.40
8	Q	101	BCL	O1D-CGD-CBD	-2.02	120.35	124.48
13	M	409	LMT	O5'-C1'-C2'	2.02	114.62	110.35
8	M	401	BCL	O2A-CGA-O1A	-2.02	118.50	123.59
8	I	102	BCL	CHA-C4D-ND	2.01	136.71	132.50
8	D	102	BCL	O2A-CGA-O1A	-2.01	118.51	123.59
8	B	101	BCL	O1D-CGD-CBD	-2.01	120.36	124.48
16	d	101	A1EF2	C37-C13-C12	2.01	118.66	115.27
13	M	409	LMT	C1B-O5B-C5B	2.01	117.64	113.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	g	102	BCL	C1-O2A-CGA	2.01	121.72	116.44
8	M	401	BCL	CHA-C4D-ND	2.01	136.70	132.50
13	L	315	LMT	C1B-O1B-C4'	-2.01	112.99	117.96
13	E	102	LMT	C1-O1'-C1'	-2.01	110.51	113.84
8	I	102	BCL	O1D-CGD-CBD	-2.00	120.39	124.48
8	L	308	BCL	C2A-C3A-C4A	-2.00	98.64	101.87

There are no chirality outliers.

All (1025) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	L	301	BCL	C2C-C3C-CAC-CBC
8	L	301	BCL	C4C-C3C-CAC-CBC
8	L	308	BCL	C4C-C3C-CAC-CBC
8	M	401	BCL	C4C-C3C-CAC-CBC
8	M	404	BCL	CBD-CGD-O2D-CED
8	A	702	BCL	C2C-C3C-CAC-CBC
8	A	702	BCL	C4C-C3C-CAC-CBC
8	a	102	BCL	C1A-C2A-CAA-CBA
8	a	102	BCL	C3A-C2A-CAA-CBA
8	a	102	BCL	C4C-C3C-CAC-CBC
8	B	101	BCL	C2C-C3C-CAC-CBC
8	B	101	BCL	C4C-C3C-CAC-CBC
8	b	103	BCL	C2C-C3C-CAC-CBC
8	b	103	BCL	C4C-C3C-CAC-CBC
8	C	103	BCL	C4C-C3C-CAC-CBC
8	C	103	BCL	C2-C3-C5-C6
8	C	103	BCL	C4-C3-C5-C6
8	c	102	BCL	C2C-C3C-CAC-CBC
8	c	102	BCL	C4C-C3C-CAC-CBC
8	D	102	BCL	C4C-C3C-CAC-CBC
8	d	102	BCL	C2C-C3C-CAC-CBC
8	d	102	BCL	C4C-C3C-CAC-CBC
8	E	103	BCL	C4C-C3C-CAC-CBC
8	e	102	BCL	C2C-C3C-CAC-CBC
8	e	102	BCL	C4C-C3C-CAC-CBC
8	e	102	BCL	C4-C3-C5-C6
8	F	103	BCL	C4C-C3C-CAC-CBC
8	f	102	BCL	C4C-C3C-CAC-CBC
8	G	104	BCL	C4C-C3C-CAC-CBC
8	g	102	BCL	C4C-C3C-CAC-CBC
8	I	102	BCL	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
8	i	101	BCL	C2C-C3C-CAC-CBC
8	i	101	BCL	C4C-C3C-CAC-CBC
8	i	101	BCL	C2-C3-C5-C6
8	i	101	BCL	C4-C3-C5-C6
8	J	102	BCL	C4C-C3C-CAC-CBC
8	j	101	BCL	C4C-C3C-CAC-CBC
8	K	102	BCL	C4C-C3C-CAC-CBC
8	k	102	BCL	C1A-C2A-CAA-CBA
8	k	102	BCL	C2C-C3C-CAC-CBC
8	k	102	BCL	C4C-C3C-CAC-CBC
8	k	102	BCL	C2-C3-C5-C6
8	k	102	BCL	C4-C3-C5-C6
8	N	101	BCL	C4C-C3C-CAC-CBC
8	n	102	BCL	C1A-C2A-CAA-CBA
8	n	102	BCL	C2C-C3C-CAC-CBC
8	n	102	BCL	C4C-C3C-CAC-CBC
8	O	102	BCL	C4C-C3C-CAC-CBC
8	O	102	BCL	C6-C7-C8-C10
8	o	102	BCL	C1A-C2A-CAA-CBA
8	o	102	BCL	C2C-C3C-CAC-CBC
8	o	102	BCL	C4C-C3C-CAC-CBC
8	o	102	BCL	CHA-CBD-CGD-O2D
8	o	102	BCL	CBD-CGD-O2D-CED
8	P	102	BCL	C2C-C3C-CAC-CBC
8	P	102	BCL	C4C-C3C-CAC-CBC
8	p	102	BCL	C4C-C3C-CAC-CBC
8	Q	101	BCL	C1A-C2A-CAA-CBA
8	Q	101	BCL	C2-C3-C5-C6
8	Q	101	BCL	C4-C3-C5-C6
8	q	102	BCL	C4C-C3C-CAC-CBC
10	L	303	U10	C1-C6-C7-C8
10	L	303	U10	C5-C6-C7-C8
10	L	304	U10	C9-C11-C12-C13
10	M	407	U10	C33-C34-C36-C37
10	M	407	U10	C35-C34-C36-C37
11	L	305	PGV	C04-O12-P-O13
11	L	305	PGV	C2-C1-O01-C02
11	L	313	PGV	C03-O11-P-O13
11	L	313	PGV	C04-O12-P-O13
11	L	314	PGV	C03-O11-P-O13
11	M	402	PGV	C03-O11-P-O14
11	M	412	PGV	C04-O12-P-O13

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Mol	Chain	Res	Type	Atoms
11	M	412	PGV	C04-O12-P-O14
11	M	412	PGV	C04-C05-C06-O06
11	M	412	PGV	O05-C05-C06-O06
11	H	304	PGV	C03-O11-P-O13
11	E	104	PGV	C2-C1-O01-C02
11	G	103	PGV	C03-O11-P-O12
11	G	103	PGV	C03-O11-P-O13
11	G	103	PGV	C2-C1-O01-C02
11	K	103	PGV	C03-O11-P-O13
12	X	102	LDA	C2-C1-N1-CM1
12	X	102	LDA	C2-C1-N1-CM2
12	X	102	LDA	N1-C1-C2-C3
13	B	102	LMT	O5'-C1'-O1'-C1
13	F	101	LMT	C2'-C1'-O1'-C1
13	F	101	LMT	O5'-C1'-O1'-C1
13	I	101	LMT	C2-C1-O1'-C1'
15	M	410	CDL	O1-C1-CB2-OB2
15	M	410	CDL	OB7-CB5-OB6-CB4
15	M	410	CDL	C51-CB5-OB6-CB4
15	M	413	CDL	CA4-CA3-OA5-PA1
15	M	413	CDL	CB2-OB2-PB2-OB5
15	E	101	CDL	CA3-OA5-PA1-OA2
15	E	101	CDL	CA3-OA5-PA1-OA3
15	E	101	CDL	CA4-CA3-OA5-PA1
15	E	101	CDL	OA7-CA5-OA6-CA4
15	E	101	CDL	C11-CA5-OA6-CA4
15	E	101	CDL	CB2-OB2-PB2-OB3
15	F	102	CDL	OA7-CA5-OA6-CA4
15	F	102	CDL	C11-CA5-OA6-CA4
15	F	102	CDL	OA9-CA7-OA8-CA6
15	F	102	CDL	C31-CA7-OA8-CA6
15	F	102	CDL	CB4-CB3-OB5-PB2
16	a	103	A1EF2	C25-C26-C27-C28
16	a	103	A1EF2	C40-C26-C27-C28
16	a	103	A1EF2	C26-C27-C28-C29
16	B	103	A1EF2	C27-C28-C29-C30
16	b	102	A1EF2	C11-C12-C13-C37
16	C	104	A1EF2	C29-C30-C31-C32
16	C	104	A1EF2	C41-C30-C31-C32
16	D	104	A1EF2	C27-C28-C29-C30
16	D	104	A1EF2	C28-C29-C30-C41
16	E	105	A1EF2	C27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
16	g	103	A1EF2	C28-C29-C30-C31
16	g	103	A1EF2	C28-C29-C30-C41
16	J	101	A1EF2	C25-C26-C27-C28
16	J	101	A1EF2	C40-C26-C27-C28
16	J	104	A1EF2	C27-C28-C29-C30
16	J	104	A1EF2	C28-C29-C30-C31
16	J	104	A1EF2	C28-C29-C30-C41
16	J	104	A1EF2	C41-C30-C31-C32
16	J	106	A1EF2	C28-C29-C30-C41
16	k	101	A1EF2	C27-C28-C29-C30
16	N	102	A1EF2	C25-C26-C27-C28
16	N	102	A1EF2	C40-C26-C27-C28
16	N	102	A1EF2	C27-C28-C29-C30
16	N	102	A1EF2	C30-C31-C32-C33
16	N	103	A1EF2	C27-C28-C29-C30
16	O	103	A1EF2	C27-C28-C29-C30
13	H	302	LMT	C3'-C4'-O1B-C1B
13	M	409	LMT	O5B-C1B-O1B-C4'
13	X	103	LMT	C3'-C4'-O1B-C1B
8	M	404	BCL	O1D-CGD-O2D-CED
13	D	101	LMT	O5B-C1B-O1B-C4'
13	F	101	LMT	O5B-C1B-O1B-C4'
8	j	101	BCL	O1A-CGA-O2A-C1
13	E	102	LMT	C2B-C1B-O1B-C4'
11	L	305	PGV	O02-C1-O01-C02
11	M	412	PGV	O02-C1-O01-C02
11	G	103	PGV	O02-C1-O01-C02
13	c	103	LMT	C3'-C4'-O1B-C1B
8	A	702	BCL	C3-C5-C6-C7
8	b	103	BCL	C3-C5-C6-C7
8	e	102	BCL	C3-C5-C6-C7
8	f	102	BCL	C3-C5-C6-C7
8	K	102	BCL	C3-C5-C6-C7
8	n	102	BCL	C3-C5-C6-C7
13	P	101	LMT	C3'-C4'-O1B-C1B
8	e	102	BCL	C2-C3-C5-C6
8	b	103	BCL	C2A-CAA-CBA-CGA
8	k	102	BCL	C2A-CAA-CBA-CGA
8	D	102	BCL	C3-C5-C6-C7
8	i	101	BCL	C3-C5-C6-C7
8	j	101	BCL	CBA-CGA-O2A-C1
8	o	102	BCL	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
11	E	104	PGV	O02-C1-O01-C02
16	C	104	A1EF2	C27-C28-C29-C30
16	J	101	A1EF2	C27-C28-C29-C30
16	n	101	A1EF2	C27-C28-C29-C30
11	L	306	PGV	O12-C04-C05-O05
15	F	102	CDL	OB5-CB3-CB4-OB6
8	c	102	BCL	C3-C5-C6-C7
8	d	102	BCL	CBA-CGA-O2A-C1
11	M	412	PGV	C2-C1-O01-C02
13	L	312	LMT	O5B-C5B-C6B-O6B
13	D	103	LMT	O5'-C5'-C6'-O6'
8	F	103	BCL	C5-C6-C7-C8
13	B	102	LMT	O5B-C1B-O1B-C4'
8	d	102	BCL	C3-C5-C6-C7
8	Q	101	BCL	C3-C5-C6-C7
8	d	102	BCL	O1A-CGA-O2A-C1
13	L	311	LMT	O5'-C5'-C6'-O6'
8	c	102	BCL	C4-C3-C5-C6
8	f	102	BCL	C4-C3-C5-C6
8	g	102	BCL	C4-C3-C5-C6
16	M	411	A1EF2	C4-C8-C9-C5
16	M	411	A1EF2	C41-C30-C31-C32
16	a	103	A1EF2	C11-C12-C13-C37
16	B	103	A1EF2	C11-C12-C13-C37
16	B	103	A1EF2	C41-C30-C31-C32
16	b	102	A1EF2	C4-C8-C9-C5
16	b	102	A1EF2	C41-C30-C31-C32
16	C	104	A1EF2	C11-C12-C13-C37
16	c	104	A1EF2	C4-C8-C9-C5
16	c	104	A1EF2	C11-C12-C13-C37
16	c	104	A1EF2	C41-C30-C31-C32
16	D	104	A1EF2	C11-C12-C13-C37
16	D	104	A1EF2	C41-C30-C31-C32
16	D	105	A1EF2	C11-C12-C13-C37
16	d	101	A1EF2	C4-C8-C9-C5
16	d	101	A1EF2	C11-C12-C13-C37
16	d	101	A1EF2	C41-C30-C31-C32
16	E	105	A1EF2	C11-C12-C13-C37
16	e	101	A1EF2	C4-C8-C9-C5
16	e	101	A1EF2	C11-C12-C13-C37
16	f	101	A1EF2	C4-C8-C9-C5
16	f	101	A1EF2	C11-C12-C13-C37

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Mol	Chain	Res	Type	Atoms
16	f	101	A1EF2	C41-C30-C31-C32
16	g	101	A1EF2	C4-C8-C9-C5
16	g	101	A1EF2	C11-C12-C13-C37
16	g	101	A1EF2	C41-C30-C31-C32
16	g	103	A1EF2	C11-C12-C13-C37
16	I	105	A1EF2	C4-C8-C9-C5
16	I	105	A1EF2	C11-C12-C13-C37
16	J	101	A1EF2	C11-C12-C13-C37
16	J	103	A1EF2	C4-C8-C9-C5
16	J	103	A1EF2	C11-C12-C13-C37
16	J	103	A1EF2	C41-C30-C31-C32
16	J	104	A1EF2	C11-C12-C13-C37
16	J	106	A1EF2	C11-C12-C13-C37
16	k	101	A1EF2	C4-C8-C9-C5
16	k	101	A1EF2	C11-C12-C13-C37
16	N	102	A1EF2	C11-C12-C13-C37
16	N	102	A1EF2	C41-C30-C31-C32
16	N	103	A1EF2	C11-C12-C13-C37
16	n	101	A1EF2	C4-C8-C9-C5
16	n	101	A1EF2	C11-C12-C13-C37
16	O	103	A1EF2	C11-C12-C13-C37
16	o	101	A1EF2	C4-C8-C9-C5
16	o	101	A1EF2	C11-C12-C13-C37
16	p	101	A1EF2	C4-C8-C9-C5
16	p	101	A1EF2	C11-C12-C13-C37
16	q	101	A1EF2	C4-C8-C9-C5
16	q	101	A1EF2	C11-C12-C13-C37
8	c	102	BCL	C2-C3-C5-C6
8	f	102	BCL	C2-C3-C5-C6
8	g	102	BCL	C2-C3-C5-C6
16	M	411	A1EF2	C4-C8-C9-C10
16	M	411	A1EF2	C29-C30-C31-C32
16	a	103	A1EF2	C11-C12-C13-C14
16	B	103	A1EF2	C11-C12-C13-C14
16	B	103	A1EF2	C29-C30-C31-C32
16	b	102	A1EF2	C4-C8-C9-C10
16	b	102	A1EF2	C11-C12-C13-C14
16	b	102	A1EF2	C29-C30-C31-C32
16	C	104	A1EF2	C11-C12-C13-C14
16	c	104	A1EF2	C4-C8-C9-C10
16	c	104	A1EF2	C11-C12-C13-C14
16	c	104	A1EF2	C29-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
16	D	104	A1EF2	C11-C12-C13-C14
16	D	104	A1EF2	C29-C30-C31-C32
16	D	105	A1EF2	C11-C12-C13-C14
16	d	101	A1EF2	C4-C8-C9-C10
16	d	101	A1EF2	C11-C12-C13-C14
16	d	101	A1EF2	C29-C30-C31-C32
16	E	105	A1EF2	C11-C12-C13-C14
16	e	101	A1EF2	C4-C8-C9-C10
16	e	101	A1EF2	C11-C12-C13-C14
16	f	101	A1EF2	C4-C8-C9-C10
16	f	101	A1EF2	C11-C12-C13-C14
16	f	101	A1EF2	C29-C30-C31-C32
16	g	101	A1EF2	C4-C8-C9-C10
16	g	101	A1EF2	C11-C12-C13-C14
16	g	101	A1EF2	C29-C30-C31-C32
16	g	103	A1EF2	C11-C12-C13-C14
16	I	105	A1EF2	C4-C8-C9-C10
16	I	105	A1EF2	C11-C12-C13-C14
16	J	101	A1EF2	C11-C12-C13-C14
16	J	103	A1EF2	C4-C8-C9-C10
16	J	103	A1EF2	C11-C12-C13-C14
16	J	103	A1EF2	C29-C30-C31-C32
16	J	104	A1EF2	C11-C12-C13-C14
16	J	104	A1EF2	C29-C30-C31-C32
16	J	106	A1EF2	C11-C12-C13-C14
16	k	101	A1EF2	C4-C8-C9-C10
16	k	101	A1EF2	C11-C12-C13-C14
16	N	102	A1EF2	C11-C12-C13-C14
16	N	102	A1EF2	C29-C30-C31-C32
16	N	103	A1EF2	C11-C12-C13-C14
16	n	101	A1EF2	C4-C8-C9-C10
16	n	101	A1EF2	C11-C12-C13-C14
16	O	103	A1EF2	C11-C12-C13-C14
16	o	101	A1EF2	C4-C8-C9-C10
16	o	101	A1EF2	C11-C12-C13-C14
16	p	101	A1EF2	C4-C8-C9-C10
16	p	101	A1EF2	C11-C12-C13-C14
16	q	101	A1EF2	C4-C8-C9-C10
16	q	101	A1EF2	C11-C12-C13-C14
13	O	101	LMT	O5'-C1'-O1'-C1
10	M	407	U10	C24-C26-C27-C28
8	a	102	BCL	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
8	a	102	BCL	O1A-CGA-O2A-C1
11	L	306	PGV	O12-C04-C05-C06
15	F	102	CDL	OB5-CB3-CB4-CB6
13	O	101	LMT	C3'-C4'-O1B-C1B
8	J	102	BCL	CBA-CGA-O2A-C1
8	k	102	BCL	CBA-CGA-O2A-C1
8	n	102	BCL	CBA-CGA-O2A-C1
13	L	311	LMT	C4'-C5'-C6'-O6'
16	D	105	A1EF2	C27-C28-C29-C30
16	g	103	A1EF2	C27-C28-C29-C30
16	J	106	A1EF2	C27-C28-C29-C30
13	F	101	LMT	C3'-C4'-O1B-C1B
16	g	103	A1EF2	C32-C33-C34-C35
13	D	101	LMT	C3'-C4'-O1B-C1B
13	B	102	LMT	C2B-C1B-O1B-C4'
8	c	102	BCL	C10-C11-C12-C13
8	n	102	BCL	C13-C15-C16-C17
8	k	102	BCL	O1A-CGA-O2A-C1
8	a	102	BCL	C6-C7-C8-C9
8	d	102	BCL	C11-C10-C8-C9
8	G	104	BCL	C11-C10-C8-C9
8	G	104	BCL	C14-C13-C15-C16
8	g	102	BCL	C6-C7-C8-C9
8	j	101	BCL	C6-C7-C8-C9
8	K	102	BCL	C11-C12-C13-C14
8	p	102	BCL	C6-C7-C8-C9
8	f	102	BCL	C15-C16-C17-C18
8	f	102	BCL	C2A-CAA-CBA-CGA
8	p	102	BCL	C2A-CAA-CBA-CGA
16	B	103	A1EF2	C40-C26-C27-C28
16	C	104	A1EF2	C40-C26-C27-C28
16	D	104	A1EF2	C40-C26-C27-C28
16	E	105	A1EF2	C40-C26-C27-C28
16	B	103	A1EF2	C25-C26-C27-C28
16	C	104	A1EF2	C25-C26-C27-C28
16	E	105	A1EF2	C25-C26-C27-C28
11	E	104	PGV	C19-C20-C21-C22
8	n	102	BCL	O1A-CGA-O2A-C1
8	b	103	BCL	C10-C11-C12-C13
8	d	102	BCL	C5-C6-C7-C8
8	e	102	BCL	C8-C10-C11-C12
8	j	101	BCL	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
8	b	103	BCL	C8-C10-C11-C12
8	C	103	BCL	C5-C6-C7-C8
8	k	102	BCL	C15-C16-C17-C18
13	D	103	LMT	O5B-C5B-C6B-O6B
8	J	102	BCL	O1A-CGA-O2A-C1
13	F	101	LMT	C5'-C4'-O1B-C1B
13	A	701	LMT	O5'-C5'-C6'-O6'
8	M	401	BCL	C5-C6-C7-C8
8	N	101	BCL	C10-C11-C12-C13
8	n	102	BCL	C5-C6-C7-C8
11	L	305	PGV	C19-C20-C21-C22
11	H	303	PGV	C1-C2-C3-C4
13	c	103	LMT	O5B-C5B-C6B-O6B
8	D	102	BCL	C15-C16-C17-C18
8	f	102	BCL	C8-C10-C11-C12
13	O	101	LMT	O5'-C5'-C6'-O6'
11	C	102	PGV	C20-C21-C22-C23
8	M	401	BCL	C13-C15-C16-C17
8	i	101	BCL	C10-C11-C12-C13
11	K	103	PGV	C1-C2-C3-C4
13	D	103	LMT	C2B-C1B-O1B-C4'
8	A	702	BCL	C6-C7-C8-C10
8	I	102	BCL	C6-C7-C8-C10
8	Q	101	BCL	C6-C7-C8-C10
8	i	101	BCL	C2A-CAA-CBA-CGA
8	g	102	BCL	C5-C6-C7-C8
8	k	102	BCL	C5-C6-C7-C8
13	I	101	LMT	C1-C2-C3-C4
10	M	407	U10	C34-C36-C37-C38
16	D	105	A1EF2	C26-C27-C28-C29
16	J	104	A1EF2	C26-C27-C28-C29
16	J	106	A1EF2	C26-C27-C28-C29
16	N	103	A1EF2	C26-C27-C28-C29
16	g	103	A1EF2	C32-C33-C34-C42
15	E	101	CDL	O1-C1-CA2-OA2
8	M	404	BCL	C5-C6-C7-C8
13	O	101	LMT	C5'-C4'-O1B-C1B
8	a	102	BCL	C5-C6-C7-C8
8	I	102	BCL	C10-C11-C12-C13
8	i	101	BCL	C15-C16-C17-C18
8	G	104	BCL	C5-C6-C7-C8
8	g	102	BCL	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
8	I	102	BCL	C15-C16-C17-C18
11	L	305	PGV	C03-O11-P-O12
11	L	306	PGV	C03-O11-P-O12
11	L	314	PGV	C04-O12-P-O11
11	M	402	PGV	C04-O12-P-O11
11	M	412	PGV	C04-O12-P-O11
11	M	412	PGV	C20-C19-O03-C01
13	D	101	LMT	C5'-C4'-O1B-C1B
15	M	410	CDL	CA2-C1-CB2-OB2
15	E	101	CDL	CB2-C1-CA2-OA2
8	G	104	BCL	C3-C5-C6-C7
8	L	308	BCL	C13-C15-C16-C17
11	H	304	PGV	C2-C1-O01-C02
8	c	102	BCL	C16-C17-C18-C19
12	M	403	LDA	C7-C8-C9-C10
13	B	102	LMT	O5B-C5B-C6B-O6B
11	H	304	PGV	O02-C1-O01-C02
8	K	102	BCL	C15-C16-C17-C18
13	B	102	LMT	C6-C7-C8-C9
11	L	305	PGV	O12-C04-C05-O05
13	L	312	LMT	C6-C7-C8-C9
10	L	303	U10	C15-C14-C16-C17
16	M	411	A1EF2	C11-C12-C13-C37
8	g	102	BCL	C11-C10-C8-C9
8	O	102	BCL	C6-C7-C8-C9
11	M	402	PGV	C19-C20-C21-C22
11	C	102	PGV	C23-C24-C25-C26
8	e	102	BCL	C2A-CAA-CBA-CGA
13	D	103	LMT	C4'-C5'-C6'-O6'
16	D	105	A1EF2	C40-C26-C27-C28
16	N	103	A1EF2	C40-C26-C27-C28
16	O	103	A1EF2	C40-C26-C27-C28
12	L	309	LDA	C4-C5-C6-C7
11	M	402	PGV	C04-C05-C06-O06
16	D	104	A1EF2	C25-C26-C27-C28
16	D	105	A1EF2	C25-C26-C27-C28
16	N	103	A1EF2	C25-C26-C27-C28
16	O	103	A1EF2	C25-C26-C27-C28
11	L	314	PGV	C2-C3-C4-C5
8	a	102	BCL	C16-C17-C18-C19
11	L	313	PGV	C4-C5-C6-C7
13	D	103	LMT	O1'-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
11	M	412	PGV	C6-C7-C8-C9
13	A	701	LMT	C2-C3-C4-C5
8	b	103	BCL	C3A-C2A-CAA-CBA
8	d	102	BCL	C3A-C2A-CAA-CBA
8	j	101	BCL	C3A-C2A-CAA-CBA
8	k	102	BCL	C3A-C2A-CAA-CBA
8	n	102	BCL	C3A-C2A-CAA-CBA
8	o	102	BCL	C3A-C2A-CAA-CBA
8	p	102	BCL	C3A-C2A-CAA-CBA
8	Q	101	BCL	C3A-C2A-CAA-CBA
8	q	102	BCL	C3A-C2A-CAA-CBA
13	B	102	LMT	C2-C1-O1'-C1'
13	I	103	LMT	C2-C1-O1'-C1'
8	c	102	BCL	C16-C17-C18-C20
8	N	101	BCL	C16-C17-C18-C19
8	n	102	BCL	C16-C17-C18-C19
13	A	701	LMT	C3-C4-C5-C6
10	L	304	U10	C24-C26-C27-C28
8	c	102	BCL	O2A-C1-C2-C3
8	g	102	BCL	O2A-C1-C2-C3
8	n	102	BCL	C4-C3-C5-C6
10	L	303	U10	C13-C14-C16-C17
16	M	411	A1EF2	C11-C12-C13-C14
11	L	306	PGV	C2-C1-O01-C02
11	K	103	PGV	C2-C1-O01-C02
11	C	102	PGV	C11-C10-C9-C8
11	M	412	PGV	O04-C19-O03-C01
8	N	101	BCL	C5-C6-C7-C8
12	L	310	LDA	C1-C2-C3-C4
11	L	306	PGV	O02-C1-O01-C02
11	K	103	PGV	O02-C1-O01-C02
13	a	101	LMT	O1'-C1-C2-C3
11	L	313	PGV	C5-C6-C7-C8
13	F	101	LMT	O5'-C5'-C6'-O6'
8	e	102	BCL	CBA-CGA-O2A-C1
8	f	102	BCL	CBA-CGA-O2A-C1
8	J	102	BCL	C5-C6-C7-C8
13	B	102	LMT	C1-C2-C3-C4
11	H	303	PGV	C2-C3-C4-C5
8	N	101	BCL	C15-C16-C17-C18
8	o	102	BCL	C8-C10-C11-C12
11	H	304	PGV	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
8	o	102	BCL	C4-C3-C5-C6
8	a	102	BCL	C6-C7-C8-C10
8	K	102	BCL	C11-C12-C13-C15
8	K	102	BCL	C12-C13-C15-C16
8	n	102	BCL	C2-C3-C5-C6
8	p	102	BCL	C6-C7-C8-C10
8	n	102	BCL	C8-C10-C11-C12
13	M	409	LMT	O5'-C5'-C6'-O6'
10	L	304	U10	C4-C3-O3-C3M
11	C	102	PGV	C20-C19-O03-C01
8	J	102	BCL	C13-C15-C16-C17
8	q	102	BCL	C5-C6-C7-C8
13	L	311	LMT	C1-C2-C3-C4
8	g	102	BCL	CBA-CGA-O2A-C1
13	G	102	LMT	C1-C2-C3-C4
11	L	313	PGV	C19-C20-C21-C22
8	C	103	BCL	C15-C16-C17-C18
8	e	102	BCL	O1A-CGA-O2A-C1
11	H	304	PGV	O03-C01-C02-O01
15	E	101	CDL	OB6-CB4-CB6-OB8
13	b	101	LMT	O5B-C5B-C6B-O6B
13	U	101	LMT	O5'-C5'-C6'-O6'
8	d	102	BCL	C15-C16-C17-C18
8	g	102	BCL	C15-C16-C17-C18
9	M	405	BPH	C4-C3-C5-C6
11	L	313	PGV	C1-C2-C3-C4
8	o	102	BCL	C2-C3-C5-C6
8	M	401	BCL	C11-C12-C13-C14
8	A	702	BCL	C6-C7-C8-C9
8	B	101	BCL	C6-C7-C8-C9
8	b	103	BCL	C11-C10-C8-C9
8	N	101	BCL	C14-C13-C15-C16
8	o	102	BCL	C11-C10-C8-C9
8	Q	101	BCL	C6-C7-C8-C9
12	F	104	LDA	C2-C3-C4-C5
8	d	102	BCL	C2A-CAA-CBA-CGA
11	C	101	PGV	C27-C28-C29-C30
13	M	409	LMT	O5B-C5B-C6B-O6B
13	I	101	LMT	O5'-C5'-C6'-O6'
16	J	104	A1EF2	C40-C26-C27-C28
13	D	103	LMT	O5B-C1B-O1B-C4'
16	J	104	A1EF2	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
8	f	102	BCL	O1A-CGA-O2A-C1
8	L	308	BCL	C1A-C2A-CAA-CBA
8	d	102	BCL	C1A-C2A-CAA-CBA
8	j	101	BCL	C1A-C2A-CAA-CBA
8	p	102	BCL	C1A-C2A-CAA-CBA
8	q	102	BCL	C1A-C2A-CAA-CBA
8	n	102	BCL	C16-C17-C18-C20
13	L	312	LMT	C4-C5-C6-C7
11	L	314	PGV	C03-O11-P-O12
11	M	402	PGV	C03-O11-P-O12
11	L	306	PGV	C01-C02-C03-O11
13	M	408	LMT	C4'-C5'-C6'-O6'
8	N	101	BCL	C16-C17-C18-C20
8	b	103	BCL	C15-C16-C17-C18
8	c	102	BCL	C15-C16-C17-C18
8	A	702	BCL	C4-C3-C5-C6
8	M	401	BCL	C2C-C3C-CAC-CBC
8	C	103	BCL	C2C-C3C-CAC-CBC
8	D	102	BCL	C2C-C3C-CAC-CBC
8	E	103	BCL	C2C-C3C-CAC-CBC
8	F	103	BCL	C2C-C3C-CAC-CBC
8	G	104	BCL	C2C-C3C-CAC-CBC
8	g	102	BCL	C2C-C3C-CAC-CBC
8	I	102	BCL	C2C-C3C-CAC-CBC
8	J	102	BCL	C2C-C3C-CAC-CBC
8	K	102	BCL	C2C-C3C-CAC-CBC
8	N	101	BCL	C2C-C3C-CAC-CBC
8	O	102	BCL	C2C-C3C-CAC-CBC
8	p	102	BCL	C2C-C3C-CAC-CBC
8	q	102	BCL	C2C-C3C-CAC-CBC
11	L	314	PGV	C24-C25-C26-C27
11	L	306	PGV	O03-C01-C02-C03
11	H	303	PGV	O03-C01-C02-C03
11	H	304	PGV	O03-C01-C02-C03
15	E	101	CDL	CB3-CB4-CB6-OB8
12	J	105	LDA	C5-C6-C7-C8
12	X	101	LDA	C1-C2-C3-C4
13	a	101	LMT	O5'-C5'-C6'-O6'
13	L	312	LMT	O5'-C5'-C6'-O6'
13	G	102	LMT	O5'-C5'-C6'-O6'
8	a	102	BCL	C16-C17-C18-C20
8	g	102	BCL	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
13	E	102	LMT	O5'-C5'-C6'-O6'
11	M	402	PGV	C26-C27-C28-C29
13	U	101	LMT	O1'-C1-C2-C3
11	C	102	PGV	C2-C1-O01-C02
13	H	302	LMT	O5'-C5'-C6'-O6'
13	A	701	LMT	O5B-C5B-C6B-O6B
10	M	407	U10	C30-C29-C31-C32
11	L	314	PGV	C11-C10-C9-C8
13	B	102	LMT	C11-C10-C9-C8
13	P	101	LMT	O5'-C5'-C6'-O6'
8	a	102	BCL	C13-C15-C16-C17
8	g	102	BCL	C2A-CAA-CBA-CGA
11	H	303	PGV	C20-C21-C22-C23
8	J	102	BCL	C3-C5-C6-C7
15	F	102	CDL	CB3-OB5-PB2-OB3
8	c	102	BCL	CBA-CGA-O2A-C1
11	G	103	PGV	O01-C02-C03-O11
8	q	102	BCL	C11-C12-C13-C14
13	L	312	LMT	C4B-C5B-C6B-O6B
11	C	102	PGV	O04-C19-O03-C01
8	e	102	BCL	C5-C6-C7-C8
13	L	311	LMT	C2'-C1'-O1'-C1
11	L	314	PGV	C20-C21-C22-C23
11	L	306	PGV	O03-C01-C02-O01
11	H	303	PGV	O03-C01-C02-O01
12	F	104	LDA	C4-C5-C6-C7
12	L	310	LDA	C11-C10-C9-C8
8	G	104	BCL	C4-C3-C5-C6
13	D	103	LMT	C5'-C4'-O1B-C1B
8	M	401	BCL	C11-C12-C13-C15
8	B	101	BCL	C6-C7-C8-C10
8	b	103	BCL	C11-C10-C8-C7
8	C	103	BCL	C6-C7-C8-C10
8	e	102	BCL	C6-C7-C8-C10
8	g	102	BCL	C6-C7-C8-C10
8	I	102	BCL	C11-C10-C8-C7
8	K	102	BCL	C6-C7-C8-C10
8	N	101	BCL	C12-C13-C15-C16
8	o	102	BCL	C11-C10-C8-C7
8	Q	101	BCL	C11-C10-C8-C7
9	M	405	BPH	C2-C3-C5-C6
10	M	407	U10	C28-C29-C31-C32

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Mol	Chain	Res	Type	Atoms
13	L	311	LMT	C11-C10-C9-C8
8	C	103	BCL	C6-C7-C8-C9
8	d	102	BCL	C11-C12-C13-C14
8	g	102	BCL	C14-C13-C15-C16
8	I	102	BCL	C6-C7-C8-C9
8	J	102	BCL	C11-C10-C8-C9
8	K	102	BCL	C6-C7-C8-C9
8	K	102	BCL	C14-C13-C15-C16
8	P	102	BCL	C11-C10-C8-C9
8	q	102	BCL	C11-C10-C8-C9
13	L	312	LMT	C2B-C1B-O1B-C4'
8	i	101	BCL	CBA-CGA-O2A-C1
16	g	103	A1EF2	C40-C26-C27-C28
8	I	102	BCL	C16-C17-C18-C19
8	J	102	BCL	C16-C17-C18-C19
16	g	103	A1EF2	C25-C26-C27-C28
16	J	106	A1EF2	C25-C26-C27-C28
12	I	104	LDA	N1-C1-C2-C3
15	M	410	CDL	C11-CA5-OA6-CA4
13	L	312	LMT	C5-C6-C7-C8
8	N	101	BCL	C13-C15-C16-C17
8	d	102	BCL	C13-C15-C16-C17
11	L	305	PGV	C01-C02-C03-O11
15	E	101	CDL	OB5-CB3-CB4-CB6
11	H	304	PGV	C3-C4-C5-C6
8	i	101	BCL	C8-C10-C11-C12
9	L	302	BPH	C4-C3-C5-C6
10	L	304	U10	C25-C24-C26-C27
16	O	103	A1EF2	C4-C8-C9-C5
8	G	104	BCL	C2-C3-C5-C6
13	D	103	LMT	C3'-C4'-O1B-C1B
8	k	102	BCL	C10-C11-C12-C13
11	C	102	PGV	O02-C1-O01-C02
13	E	102	LMT	O5B-C1B-O1B-C4'
13	M	408	LMT	C4-C5-C6-C7
15	M	413	CDL	CB4-CB3-OB5-PB2
15	E	101	CDL	C1-CB2-OB2-PB2
15	M	410	CDL	C57-C58-C59-C60
12	L	307	LDA	C1-C2-C3-C4
13	c	101	LMT	O1'-C1-C2-C3
13	c	103	LMT	C5'-C4'-O1B-C1B
11	L	314	PGV	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
8	p	102	BCL	C3-C5-C6-C7
11	H	304	PGV	C7-C8-C9-C10
8	A	702	BCL	C2-C3-C5-C6
11	E	104	PGV	C1-C2-C3-C4
13	L	315	LMT	C5-C6-C7-C8
8	A	702	BCL	C2A-CAA-CBA-CGA
8	J	102	BCL	C15-C16-C17-C18
11	L	305	PGV	O01-C02-C03-O11
13	I	101	LMT	C3-C4-C5-C6
8	c	102	BCL	O1A-CGA-O2A-C1
8	c	102	BCL	C13-C15-C16-C17
8	i	101	BCL	O1A-CGA-O2A-C1
11	M	402	PGV	O03-C01-C02-O01
15	M	413	CDL	OB6-CB4-CB6-OB8
13	D	101	LMT	O5'-C1'-O1'-C1
8	N	101	BCL	C3-C5-C6-C7
8	F	103	BCL	C4-C3-C5-C6
8	E	103	BCL	C2-C1-O2A-CGA
8	K	102	BCL	C2-C1-O2A-CGA
9	L	302	BPH	C2-C3-C5-C6
10	L	304	U10	C23-C24-C26-C27
8	i	101	BCL	C11-C10-C8-C9
8	k	102	BCL	C6-C7-C8-C9
8	K	102	BCL	C10-C11-C12-C13
8	M	404	BCL	C10-C11-C12-C13
8	f	102	BCL	C13-C15-C16-C17
8	J	102	BCL	C16-C17-C18-C20
8	p	102	BCL	C16-C17-C18-C19
8	q	102	BCL	C11-C12-C13-C15
8	o	102	BCL	C3-C5-C6-C7
8	O	102	BCL	C11-C10-C8-C9
13	I	103	LMT	C3-C4-C5-C6
11	H	303	PGV	C11-C12-C13-C14
8	n	102	BCL	C15-C16-C17-C18
11	C	102	PGV	C21-C22-C23-C24
8	d	102	BCL	C11-C10-C8-C7
8	E	103	BCL	C6-C7-C8-C10
8	G	104	BCL	C6-C7-C8-C10
8	J	102	BCL	C11-C10-C8-C7
8	j	101	BCL	C6-C7-C8-C10
8	N	101	BCL	C11-C10-C8-C7
8	P	102	BCL	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
8	P	102	BCL	C11-C10-C8-C7
8	q	102	BCL	C11-C10-C8-C7
16	O	103	A1EF2	C4-C8-C9-C10
8	C	103	BCL	C16-C17-C18-C19
8	C	103	BCL	C16-C17-C18-C20
8	I	102	BCL	C16-C17-C18-C20
8	p	102	BCL	C16-C17-C18-C20
13	B	102	LMT	C9-C10-C11-C12
13	L	315	LMT	C11-C10-C9-C8
8	c	102	BCL	C2A-CAA-CBA-CGA
8	c	102	BCL	C8-C10-C11-C12
15	F	102	CDL	CA3-OA5-PA1-OA4
8	o	102	BCL	C15-C16-C17-C18
8	L	301	BCL	CAD-CBD-CGD-O2D
11	K	103	PGV	C01-C02-O01-C1
16	B	103	A1EF2	C28-C29-C30-C41
16	k	101	A1EF2	C28-C29-C30-C41
11	C	101	PGV	C28-C29-C30-C31
8	a	102	BCL	C15-C16-C17-C18
11	G	103	PGV	C20-C19-O03-C01
13	L	311	LMT	O5'-C1'-O1'-C1
8	F	103	BCL	C2-C3-C5-C6
11	M	402	PGV	O03-C01-C02-C03
13	A	701	LMT	C4'-C5'-C6'-O6'
11	L	305	PGV	O12-C04-C05-C06
12	L	310	LDA	C9-C10-C11-C12
8	q	102	BCL	C10-C11-C12-C13
8	p	102	BCL	C5-C6-C7-C8
8	J	102	BCL	C4-C3-C5-C6
8	J	102	BCL	C2-C3-C5-C6
8	G	104	BCL	C6-C7-C8-C9
8	N	101	BCL	C11-C10-C8-C9
12	J	105	LDA	C11-C10-C9-C8
13	M	408	LMT	O5'-C5'-C6'-O6'
16	J	106	A1EF2	C40-C26-C27-C28
8	M	404	BCL	C16-C17-C18-C19
8	e	102	BCL	C15-C16-C17-C18
11	L	305	PGV	C04-O12-P-O11
11	H	304	PGV	C03-O11-P-O12
11	H	304	PGV	C04-O12-P-O11
11	K	103	PGV	C03-O11-P-O12
15	E	101	CDL	CB2-OB2-PB2-OB5

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Mol	Chain	Res	Type	Atoms
13	O	101	LMT	O5B-C1B-O1B-C4'
11	L	305	PGV	C03-O11-P-O13
11	L	306	PGV	C03-O11-P-O13
11	L	314	PGV	C04-O12-P-O13
11	M	402	PGV	C03-O11-P-O13
11	M	402	PGV	C04-O12-P-O13
11	G	103	PGV	C03-O11-P-O14
15	M	413	CDL	CB2-OB2-PB2-OB4
8	M	401	BCL	C16-C17-C18-C19
13	M	409	LMT	C6-C7-C8-C9
13	G	101	LMT	C4'-C5'-C6'-O6'
13	L	312	LMT	O5'-C1'-O1'-C1
8	L	308	BCL	C15-C16-C17-C18
8	M	401	BCL	C15-C16-C17-C18
11	G	103	PGV	C01-C02-C03-O11
11	K	103	PGV	C01-C02-C03-O11
12	X	102	LDA	C2-C3-C4-C5
11	C	102	PGV	C7-C8-C9-C10
12	X	102	LDA	C2-C1-N1-O1
11	E	104	PGV	C23-C24-C25-C26
8	L	308	BCL	C2C-C3C-CAC-CBC
8	a	102	BCL	C2C-C3C-CAC-CBC
8	b	103	BCL	C6-C7-C8-C10
8	f	102	BCL	C6-C7-C8-C10
8	G	104	BCL	C11-C10-C8-C7
8	g	102	BCL	C11-C10-C8-C7
11	L	306	PGV	O01-C02-C03-O11
11	C	102	PGV	O01-C02-C03-O11
11	K	103	PGV	O01-C02-C03-O11
15	M	413	CDL	OB5-CB3-CB4-OB6
16	D	104	A1EF2	C28-C29-C30-C31
16	J	106	A1EF2	C28-C29-C30-C31
16	k	101	A1EF2	C28-C29-C30-C31
11	M	402	PGV	C1-C2-C3-C4
11	G	103	PGV	O04-C19-O03-C01
11	C	102	PGV	O12-C04-C05-O05
8	i	101	BCL	C16-C17-C18-C19
15	M	410	CDL	OB6-CB4-CB6-OB8
11	H	304	PGV	C20-C21-C22-C23
13	L	315	LMT	C7-C8-C9-C10
8	e	102	BCL	O2A-C1-C2-C3
11	H	304	PGV	O03-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
13	H	301	LMT	O1'-C1-C2-C3
11	L	306	PGV	C02-C03-O11-P
13	M	409	LMT	O1'-C1-C2-C3
8	a	102	BCL	C4-C3-C5-C6
8	P	102	BCL	C4-C3-C5-C6
11	C	101	PGV	C7-C8-C9-C10
8	E	103	BCL	C6-C7-C8-C9
8	e	102	BCL	C6-C7-C8-C9
8	f	102	BCL	C11-C10-C8-C9
8	P	102	BCL	C6-C7-C8-C9
13	P	101	LMT	C5'-C4'-O1B-C1B
11	M	412	PGV	C14-C15-C16-C17
8	p	102	BCL	C4-C3-C5-C6
13	L	315	LMT	C3-C4-C5-C6
15	E	101	CDL	CB4-CB6-OB8-CB7
11	H	304	PGV	C4-C5-C6-C7
8	F	103	BCL	C13-C15-C16-C17
8	G	104	BCL	C13-C15-C16-C17
11	C	102	PGV	C01-C02-C03-O11
8	o	102	BCL	C2A-CAA-CBA-CGA
13	I	101	LMT	C5-C6-C7-C8
8	g	102	BCL	C8-C10-C11-C12
8	L	301	BCL	C2-C1-O2A-CGA
8	I	102	BCL	C2-C1-O2A-CGA
11	C	101	PGV	C03-O11-P-O13
8	b	103	BCL	C16-C17-C18-C20
11	M	412	PGV	C5-C6-C7-C8
13	M	409	LMT	C3'-C4'-O1B-C1B
11	H	304	PGV	C20-C19-O03-C01
8	G	104	BCL	C16-C17-C18-C19
8	p	102	BCL	C10-C11-C12-C13
11	G	103	PGV	O03-C01-C02-O01
9	M	405	BPH	C1-C2-C3-C5
11	L	306	PGV	C04-O12-P-O11
11	L	313	PGV	C03-O11-P-O12
11	L	313	PGV	C04-O12-P-O11
11	M	412	PGV	C03-O11-P-O12
11	C	102	PGV	C03-O11-P-O12
11	C	102	PGV	C04-O12-P-O11
11	G	103	PGV	C04-O12-P-O11
11	K	103	PGV	C04-O12-P-O11
15	M	410	CDL	CA2-OA2-PA1-OA5

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Mol	Chain	Res	Type	Atoms
15	M	410	CDL	CB3-OB5-PB2-OB2
15	M	413	CDL	CA2-OA2-PA1-OA5
15	M	413	CDL	CB3-OB5-PB2-OB2
12	I	104	LDA	C7-C8-C9-C10
12	F	104	LDA	C3-C4-C5-C6
16	N	103	A1EF2	C4-C8-C9-C5
13	E	102	LMT	C3'-C4'-O1B-C1B
8	I	102	BCL	C11-C10-C8-C9
8	n	102	BCL	C11-C10-C8-C9
11	M	412	PGV	C2-C3-C4-C5
11	L	313	PGV	C30-C31-C32-C33
11	L	306	PGV	C7-C8-C9-C10
15	M	410	CDL	C59-C60-C61-C62
13	M	408	LMT	C11-C10-C9-C8
8	O	102	BCL	C11-C10-C8-C7
12	F	104	LDA	N1-C1-C2-C3
15	M	410	CDL	OA7-CA5-OA6-CA4
13	G	102	LMT	O1'-C1-C2-C3
11	H	304	PGV	O04-C19-O03-C01
15	M	410	CDL	C11-C12-C13-C14
8	Q	101	BCL	C10-C11-C12-C13
13	E	102	LMT	C5'-C4'-O1B-C1B
13	I	101	LMT	C3'-C4'-O1B-C1B
16	J	104	A1EF2	C30-C31-C32-C33
13	M	409	LMT	C5'-C4'-O1B-C1B
11	C	101	PGV	C23-C24-C25-C26
12	L	310	LDA	C7-C8-C9-C10
8	P	102	BCL	C2-C1-O2A-CGA
13	L	312	LMT	C2'-C1'-O1'-C1
11	C	102	PGV	O03-C01-C02-O01
11	H	304	PGV	C22-C23-C24-C25
10	M	407	U10	C5-C4-O4-C4M
8	A	702	BCL	C2B-C3B-CAB-OBB
13	O	101	LMT	C2B-C1B-O1B-C4'
8	P	102	BCL	C2-C3-C5-C6
8	L	301	BCL	C11-C10-C8-C9
8	L	308	BCL	C11-C10-C8-C9
8	D	102	BCL	C14-C13-C15-C16
8	M	401	BCL	C16-C17-C18-C20
13	L	311	LMT	C5-C6-C7-C8
15	M	413	CDL	CB3-CB4-CB6-OB8
15	F	102	CDL	CA3-CA4-CA6-OA8

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Mol	Chain	Res	Type	Atoms
8	b	103	BCL	C16-C17-C18-C19
8	i	101	BCL	C16-C17-C18-C20
8	M	401	BCL	O2A-C1-C2-C3
8	b	103	BCL	O2A-C1-C2-C3
8	f	102	BCL	O2A-C1-C2-C3
9	L	302	BPH	O2A-C1-C2-C3
16	n	101	A1EF2	C39-C22-C23-C24
8	K	102	BCL	C13-C15-C16-C17
8	j	101	BCL	C4-C3-C5-C6
8	b	103	BCL	C1A-C2A-CAA-CBA
11	H	303	PGV	O02-C1-O01-C02
8	D	102	BCL	C6-C7-C8-C10
8	N	101	BCL	C6-C7-C8-C10
11	C	102	PGV	C24-C25-C26-C27
8	L	301	BCL	C2A-CAA-CBA-CGA
11	E	104	PGV	C7-C8-C9-C10
11	M	402	PGV	O01-C02-C03-O11
13	c	103	LMT	C7-C8-C9-C10
8	N	101	BCL	C4-C3-C5-C6
12	I	104	LDA	C11-C10-C9-C8
11	C	101	PGV	O02-C1-O01-C02
13	B	102	LMT	C5'-C4'-O1B-C1B
11	C	101	PGV	C4-C5-C6-C7
8	e	102	BCL	C2-C1-O2A-CGA
8	g	102	BCL	C2-C1-O2A-CGA
8	a	102	BCL	C2-C3-C5-C6
8	j	101	BCL	C2C-C3C-CAC-CBC
8	j	101	BCL	C2-C3-C5-C6
8	p	102	BCL	C2-C3-C5-C6
16	N	103	A1EF2	C4-C8-C9-C10
11	L	306	PGV	O03-C19-C20-C21
8	M	401	BCL	C11-C10-C8-C9
8	I	102	BCL	O1A-CGA-O2A-C1
8	J	102	BCL	C8-C10-C11-C12
13	L	311	LMT	C7-C8-C9-C10
10	L	303	U10	C20-C19-C21-C22
16	a	103	A1EF2	C4-C8-C9-C5
8	F	103	BCL	C16-C17-C18-C19
13	B	102	LMT	C4B-C5B-C6B-O6B
8	L	301	BCL	C11-C10-C8-C7
8	d	102	BCL	C11-C12-C13-C15
8	i	101	BCL	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
9	M	405	BPH	C1-C2-C3-C4
13	G	101	LMT	O5'-C5'-C6'-O6'
8	q	102	BCL	O2A-C1-C2-C3
11	L	305	PGV	C20-C21-C22-C23
8	b	103	BCL	CAA-CBA-CGA-O2A
10	L	303	U10	C12-C11-C9-C10
11	L	305	PGV	C3-C4-C5-C6
11	G	103	PGV	O01-C1-C2-C3
8	M	404	BCL	C14-C13-C15-C16
8	B	101	BCL	C11-C10-C8-C9
8	b	103	BCL	C6-C7-C8-C9
8	d	102	BCL	C14-C13-C15-C16
8	e	102	BCL	C14-C13-C15-C16
8	f	102	BCL	C6-C7-C8-C9
8	j	101	BCL	C11-C12-C13-C14
8	n	102	BCL	C11-C12-C13-C14
8	C	103	BCL	C3A-C2A-CAA-CBA
8	L	301	BCL	C5-C6-C7-C8
8	k	102	BCL	C8-C10-C11-C12
13	U	101	LMT	C7-C8-C9-C10
8	I	102	BCL	CBA-CGA-O2A-C1
8	N	101	BCL	C2-C3-C5-C6
16	a	103	A1EF2	C4-C8-C9-C10
11	G	103	PGV	O03-C19-C20-C21
11	K	103	PGV	C20-C21-C22-C23
13	M	408	LMT	O1'-C1-C2-C3
15	M	410	CDL	CB3-CB4-CB6-OB8
11	M	412	PGV	O01-C02-C03-O11
15	F	102	CDL	OA5-CA3-CA4-OA6
11	L	314	PGV	C21-C22-C23-C24
8	a	102	BCL	O2A-C1-C2-C3
8	i	101	BCL	O2A-C1-C2-C3
8	j	101	BCL	O2A-C1-C2-C3
8	p	102	BCL	O2A-C1-C2-C3
11	C	101	PGV	C9-C10-C11-C12
8	G	104	BCL	C16-C17-C18-C20
8	L	308	BCL	CHA-CBD-CGD-O2D
8	a	102	BCL	CHA-CBD-CGD-O2D
8	E	103	BCL	CHA-CBD-CGD-O1D
8	E	103	BCL	CHA-CBD-CGD-O2D
8	F	103	BCL	CHA-CBD-CGD-O1D
8	F	103	BCL	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
8	f	102	BCL	CHA-CBD-CGD-O1D
8	f	102	BCL	CHA-CBD-CGD-O2D
8	G	104	BCL	CHA-CBD-CGD-O1D
8	G	104	BCL	CHA-CBD-CGD-O2D
8	g	102	BCL	CHA-CBD-CGD-O2D
8	I	102	BCL	CHA-CBD-CGD-O1D
8	I	102	BCL	CHA-CBD-CGD-O2D
8	J	102	BCL	CHA-CBD-CGD-O1D
8	J	102	BCL	CHA-CBD-CGD-O2D
8	K	102	BCL	CHA-CBD-CGD-O1D
8	K	102	BCL	CHA-CBD-CGD-O2D
8	O	102	BCL	CHA-CBD-CGD-O1D
8	O	102	BCL	CHA-CBD-CGD-O2D
8	o	102	BCL	CHA-CBD-CGD-O1D
8	P	102	BCL	CHA-CBD-CGD-O1D
8	P	102	BCL	CHA-CBD-CGD-O2D
11	M	402	PGV	O01-C1-C2-C3
16	e	101	A1EF2	C32-C33-C34-C42
15	M	413	CDL	OB5-CB3-CB4-CB6
12	L	307	LDA	C11-C10-C9-C8
11	C	101	PGV	O03-C01-C02-O01
8	F	103	BCL	C15-C16-C17-C18
13	G	101	LMT	C11-C10-C9-C8
9	M	405	BPH	CHA-CBD-CGD-O1D
8	i	101	BCL	C13-C15-C16-C17
11	C	101	PGV	C2-C1-O01-C02
15	E	101	CDL	C51-CB5-OB6-CB4
16	g	103	A1EF2	C1-C3-C4-C8
8	d	102	BCL	C6-C7-C8-C10
16	c	104	A1EF2	C10-C11-C12-C13
16	O	103	A1EF2	C3-C4-C8-C9
8	G	104	BCL	C10-C11-C12-C13
13	c	103	LMT	C11-C10-C9-C8
11	L	313	PGV	C28-C29-C30-C31
11	H	303	PGV	C2-C1-O01-C02
16	a	103	A1EF2	C9-C10-C11-C12
16	b	102	A1EF2	C1-C3-C4-C8
16	C	104	A1EF2	C9-C10-C11-C12
16	D	104	A1EF2	C9-C10-C11-C12
16	D	104	A1EF2	C31-C32-C33-C34
16	D	105	A1EF2	C9-C10-C11-C12
16	d	101	A1EF2	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
16	e	101	A1EF2	C1-C3-C4-C8
16	g	103	A1EF2	C9-C10-C11-C12
16	J	101	A1EF2	C9-C10-C11-C12
16	J	104	A1EF2	C31-C32-C33-C34
16	q	101	A1EF2	C1-C3-C4-C8
16	q	101	A1EF2	C9-C10-C11-C12
11	K	103	PGV	C21-C22-C23-C24
8	C	103	BCL	C13-C15-C16-C17
11	H	304	PGV	O01-C1-C2-C3
8	o	102	BCL	C13-C15-C16-C17
8	b	103	BCL	CAA-CBA-CGA-O1A
8	B	101	BCL	C1A-C2A-CAA-CBA
8	C	103	BCL	C1A-C2A-CAA-CBA
8	F	103	BCL	C1A-C2A-CAA-CBA
11	G	103	PGV	O02-C1-C2-C3
13	O	101	LMT	C3-C4-C5-C6
16	B	103	A1EF2	C9-C10-C11-C12
16	d	101	A1EF2	C1-C3-C4-C8
16	f	101	A1EF2	C31-C32-C33-C34
16	J	106	A1EF2	C9-C10-C11-C12
8	N	101	BCL	C2-C1-O2A-CGA
13	L	312	LMT	C11-C10-C9-C8
8	Q	101	BCL	C5-C6-C7-C8
11	L	305	PGV	C22-C23-C24-C25
11	G	103	PGV	O04-C19-C20-C21
11	M	412	PGV	C03-O11-P-O13
11	C	102	PGV	C03-O11-P-O13
11	G	103	PGV	C04-O12-P-O13
11	K	103	PGV	C04-O12-P-O13
15	M	410	CDL	CB3-OB5-PB2-OB3
15	M	413	CDL	CA2-OA2-PA1-OA3
16	k	101	A1EF2	C1-C3-C4-C8
11	M	402	PGV	O02-C1-C2-C3
16	e	101	A1EF2	C30-C31-C32-C33
16	I	105	A1EF2	C10-C11-C12-C13
13	M	409	LMT	C4'-C5'-C6'-O6'
11	C	101	PGV	O03-C19-C20-C21
16	B	103	A1EF2	C31-C32-C33-C34
16	b	102	A1EF2	C31-C32-C33-C34
16	E	105	A1EF2	C31-C32-C33-C34
16	g	101	A1EF2	C31-C32-C33-C34
16	N	102	A1EF2	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
8	M	404	BCL	C11-C10-C8-C9
8	D	102	BCL	C11-C10-C8-C9
8	i	101	BCL	C6-C7-C8-C9
8	Q	101	BCL	C11-C10-C8-C9
11	C	102	PGV	C12-C13-C14-C15
11	L	306	PGV	O01-C1-C2-C3
11	C	102	PGV	C6-C7-C8-C9
8	n	102	BCL	C2A-CAA-CBA-CGA
8	M	401	BCL	CAA-CBA-CGA-O2A
8	O	102	BCL	C4-C3-C5-C6
8	M	401	BCL	C11-C10-C8-C7
8	F	103	BCL	C3A-C2A-CAA-CBA
9	M	405	BPH	C6-C7-C8-C10
10	L	303	U10	C18-C19-C21-C22
11	H	304	PGV	O02-C1-C2-C3
13	G	101	LMT	C3-C4-C5-C6
16	n	101	A1EF2	C21-C22-C23-C24
8	A	702	BCL	C2B-C3B-CAB-CBB
13	G	101	LMT	C2-C1-O1'-C1'
8	a	102	BCL	CAA-CBA-CGA-O2A
16	g	101	A1EF2	C9-C10-C11-C12
16	J	103	A1EF2	C31-C32-C33-C34
11	H	303	PGV	C7-C8-C9-C10
11	C	101	PGV	O04-C19-C20-C21
8	q	102	BCL	C2A-CAA-CBA-CGA
8	D	102	BCL	C16-C17-C18-C19
11	M	402	PGV	C11-C12-C13-C14
11	C	101	PGV	C11-C12-C13-C14

There are no ring outliers.

83 monomers are involved in 265 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	F	101	LMT	6	0
13	P	101	LMT	2	0
10	L	303	U10	4	0
15	M	413	CDL	1	0
8	p	102	BCL	5	0
8	M	401	BCL	5	0
8	I	102	BCL	2	0
12	I	104	LDA	6	0
9	M	405	BPH	15	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	n	102	BCL	4	0
8	f	102	BCL	4	0
11	E	104	PGV	4	0
13	L	312	LMT	12	0
11	C	102	PGV	3	0
13	B	102	LMT	12	0
8	N	101	BCL	5	0
13	A	701	LMT	1	0
11	C	101	PGV	5	0
8	j	101	BCL	3	0
8	a	102	BCL	6	0
8	o	102	BCL	8	0
8	L	308	BCL	3	0
8	A	702	BCL	5	0
8	F	103	BCL	2	0
8	J	102	BCL	4	0
8	c	102	BCL	4	0
13	L	311	LMT	5	0
11	K	103	PGV	4	0
8	B	101	BCL	1	0
15	E	101	CDL	2	0
13	U	101	LMT	2	0
15	M	410	CDL	7	0
16	D	105	A1EF2	1	0
13	H	302	LMT	2	0
12	M	403	LDA	2	0
8	P	102	BCL	2	0
12	J	105	LDA	2	0
13	c	103	LMT	2	0
13	O	101	LMT	1	0
8	C	103	BCL	2	0
8	k	102	BCL	3	0
11	M	402	PGV	2	0
13	D	101	LMT	2	0
13	L	315	LMT	5	0
13	a	101	LMT	4	0
11	H	304	PGV	6	0
8	K	102	BCL	2	0
8	D	102	BCL	4	0
8	b	103	BCL	2	0
8	e	102	BCL	3	0
8	g	102	BCL	5	0

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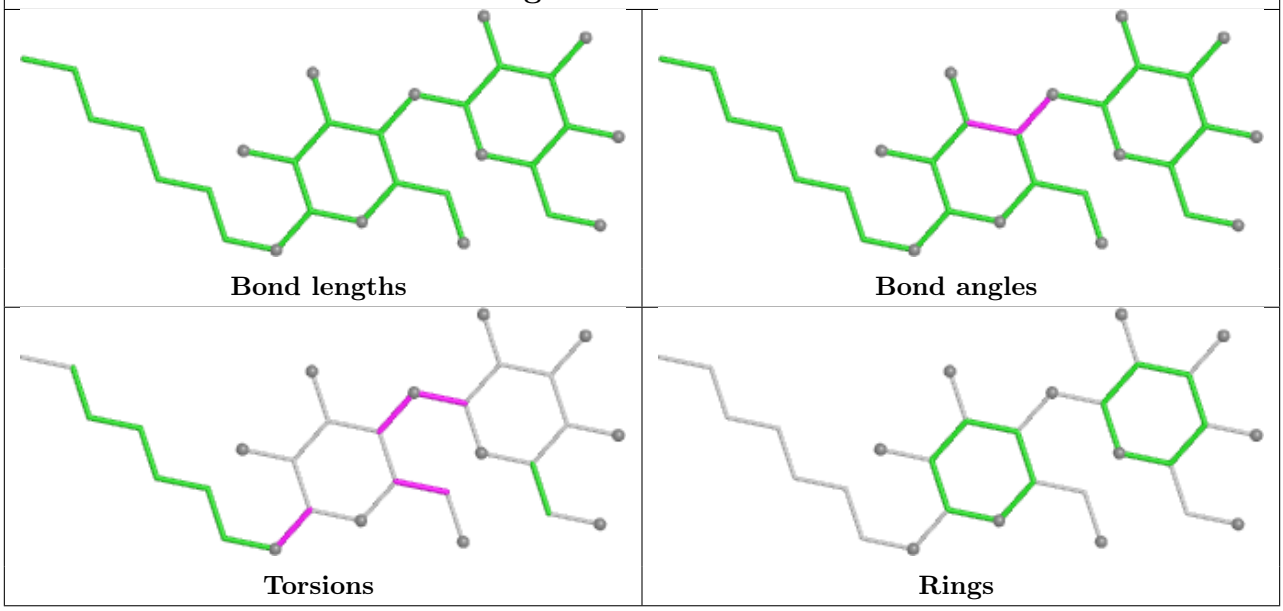
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	I	101	LMT	1	0
12	K	101	LDA	1	0
13	M	409	LMT	1	0
8	O	102	BCL	2	0
11	L	305	PGV	5	0
13	M	408	LMT	1	0
11	H	303	PGV	2	0
12	L	310	LDA	3	0
8	d	102	BCL	6	0
8	i	101	BCL	5	0
8	Q	101	BCL	1	0
13	D	103	LMT	4	0
12	L	307	LDA	1	0
8	M	404	BCL	5	0
13	H	301	LMT	1	0
13	X	103	LMT	2	0
8	L	301	BCL	1	0
8	G	104	BCL	1	0
10	L	304	U10	2	0
12	X	101	LDA	4	0
8	E	103	BCL	2	0
12	F	104	LDA	3	0
11	L	313	PGV	6	0
11	M	412	PGV	5	0
9	L	302	BPH	6	0
13	I	103	LMT	1	0
16	a	103	A1EF2	1	0
8	q	102	BCL	2	0
12	L	309	LDA	6	0
15	F	102	CDL	1	0
11	L	314	PGV	1	0
10	M	407	U10	7	0

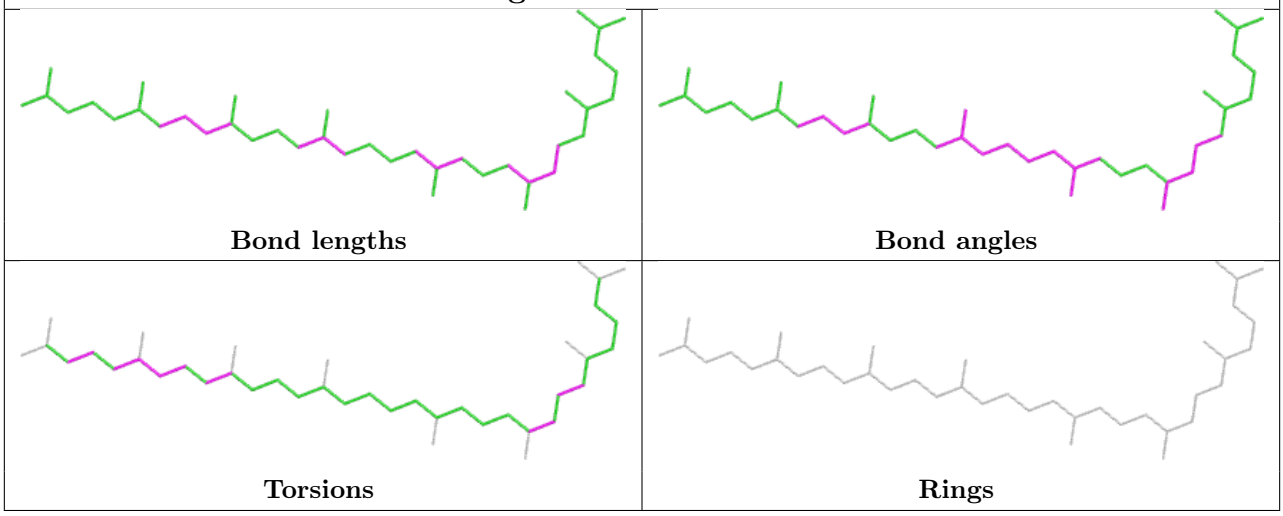
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

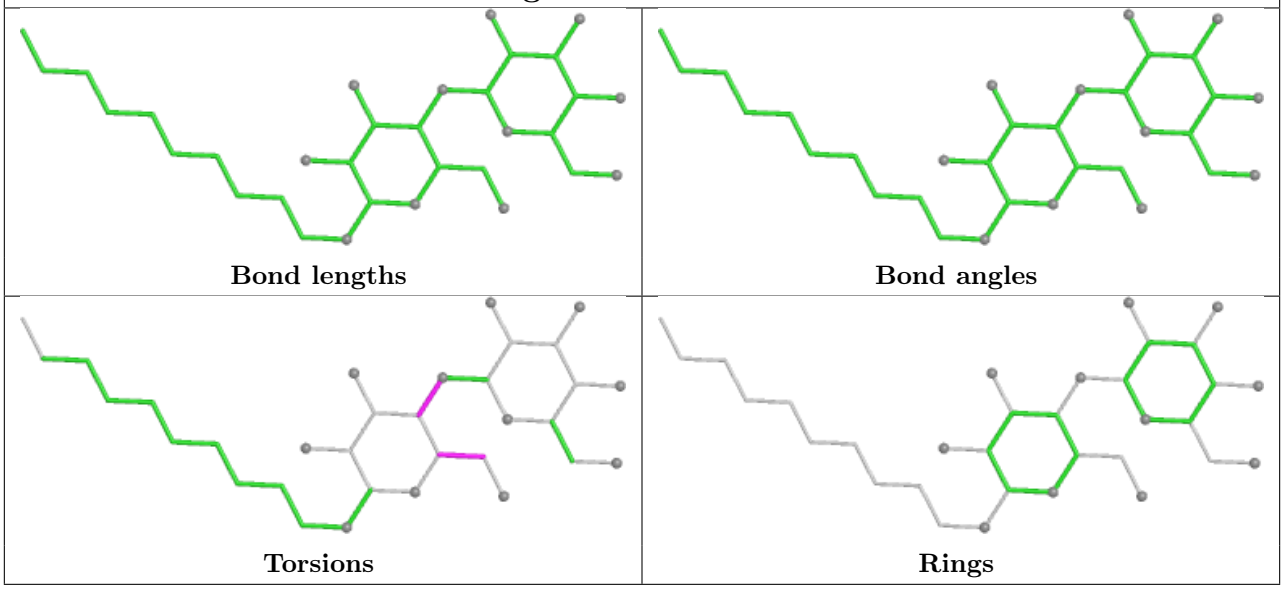
Ligand LMT F 101



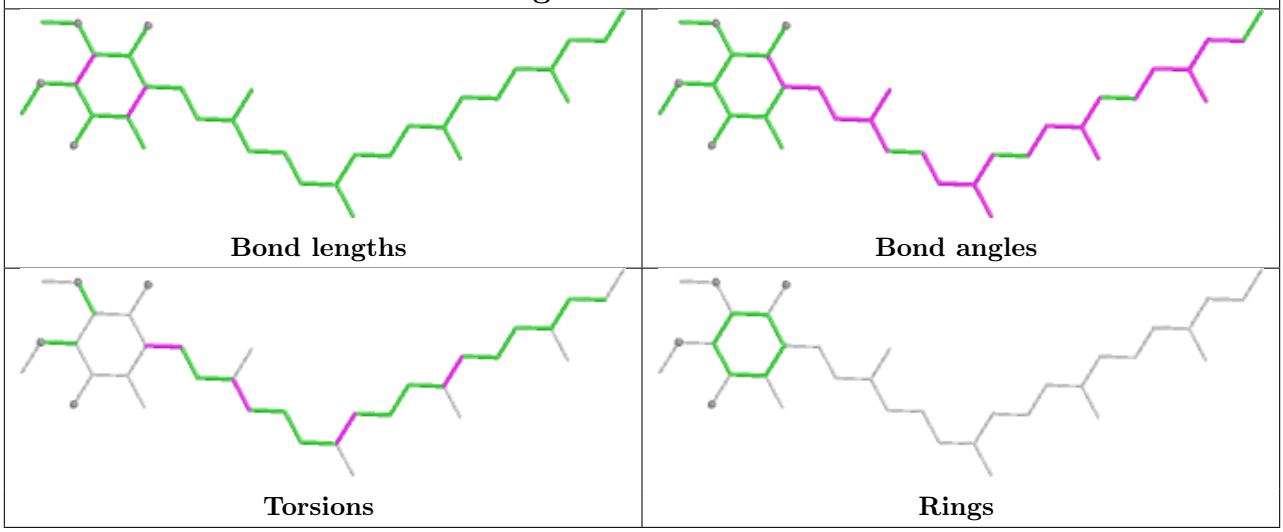
Ligand A1EF2 B 103



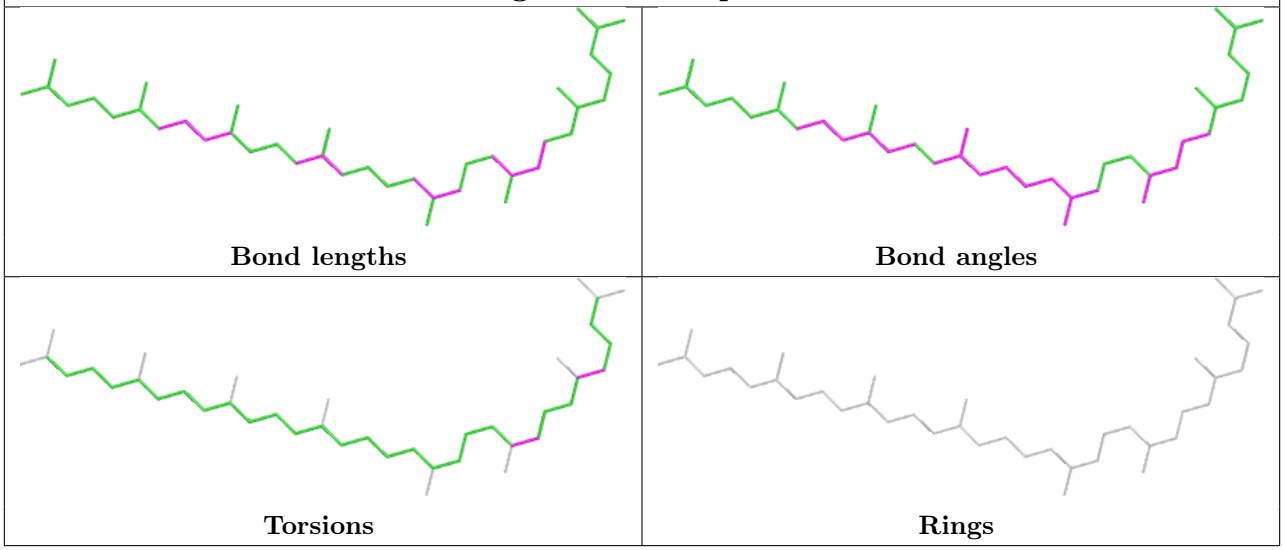
Ligand LMT P 101



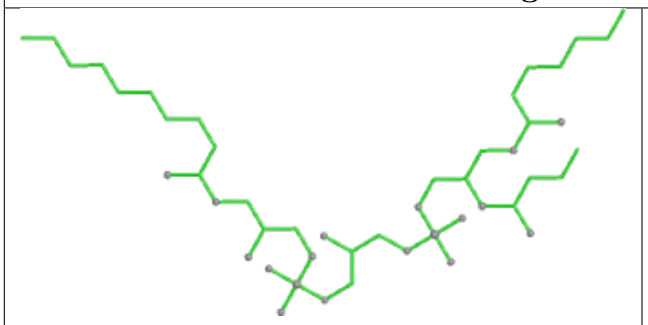
Ligand U10 L 303



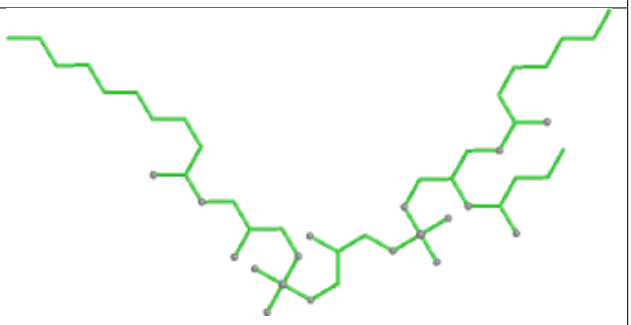
Ligand A1EF2 p 101



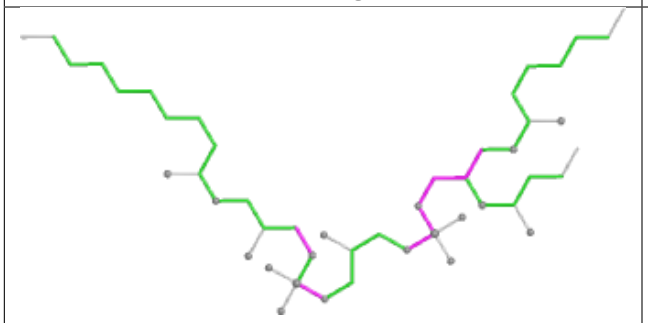
Ligand CDL M 413



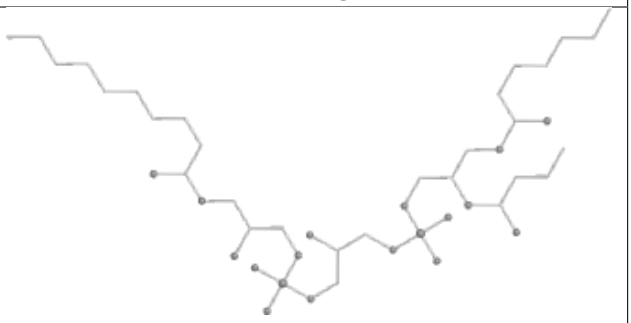
Bond lengths



Bond angles

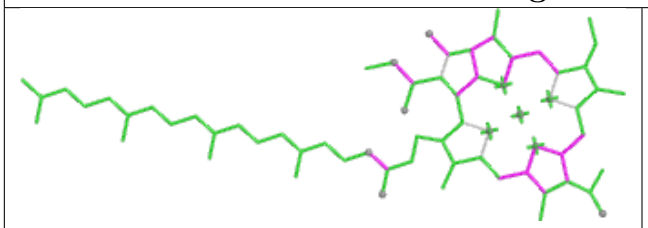


Torsions

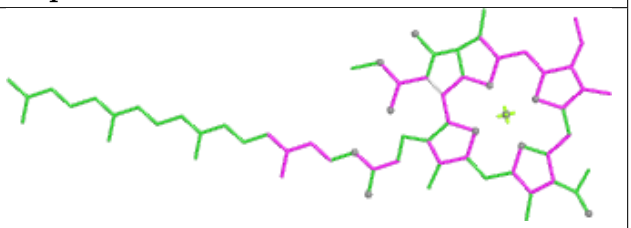


Rings

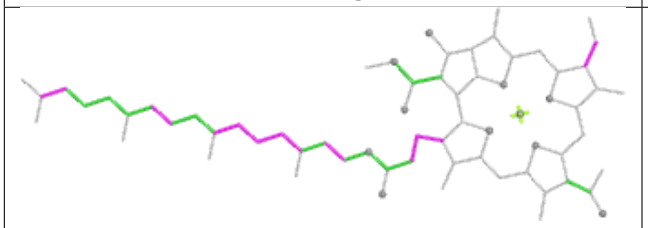
Ligand BCL p 102



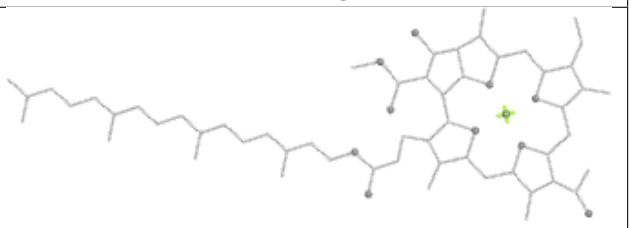
Bond lengths



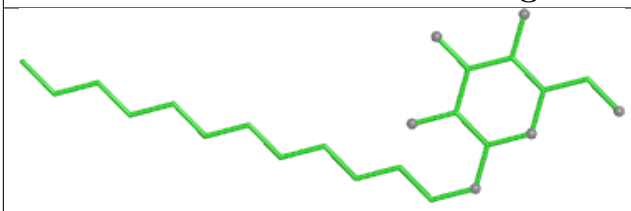
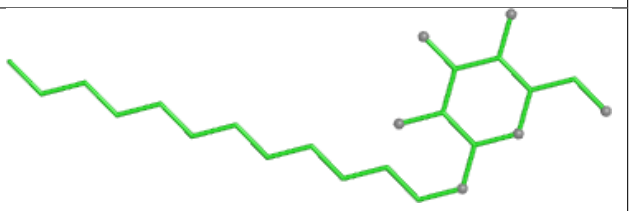
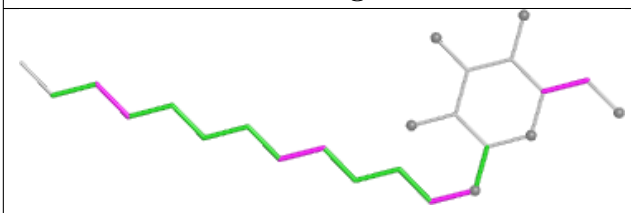
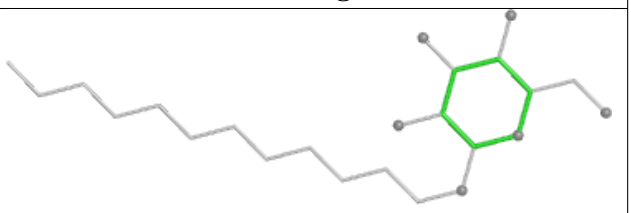
Bond angles

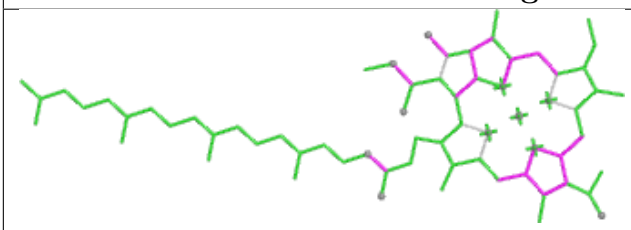
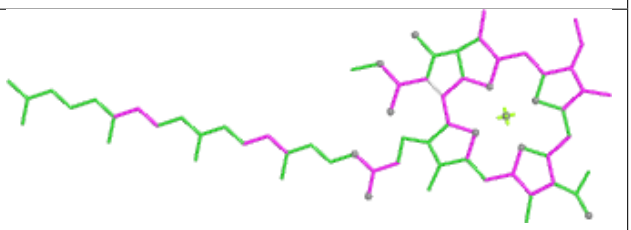
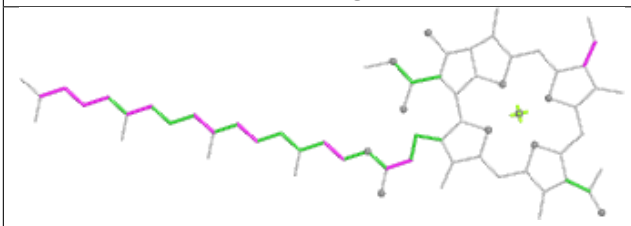
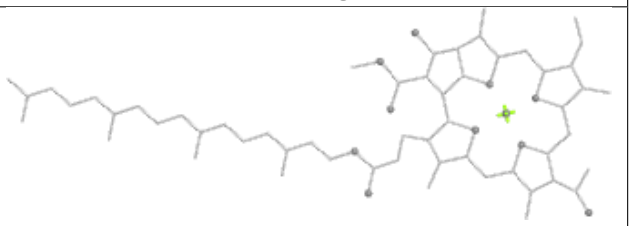


Torsions

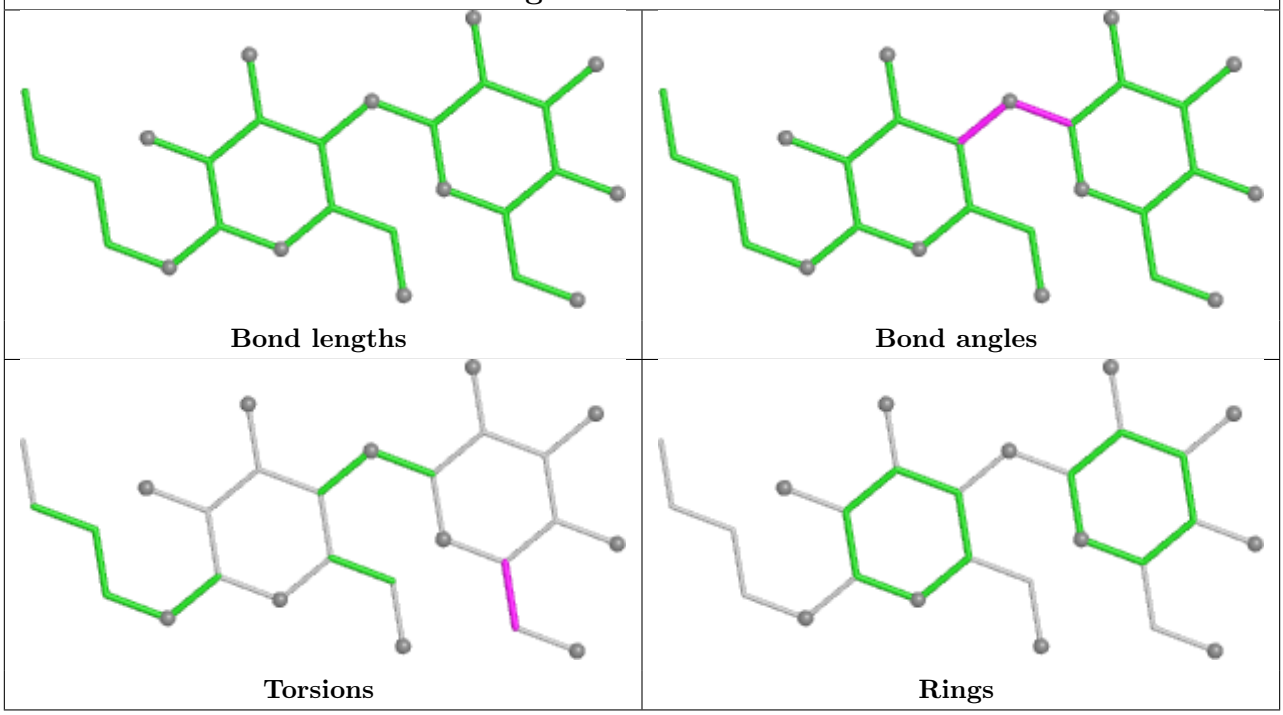


Rings

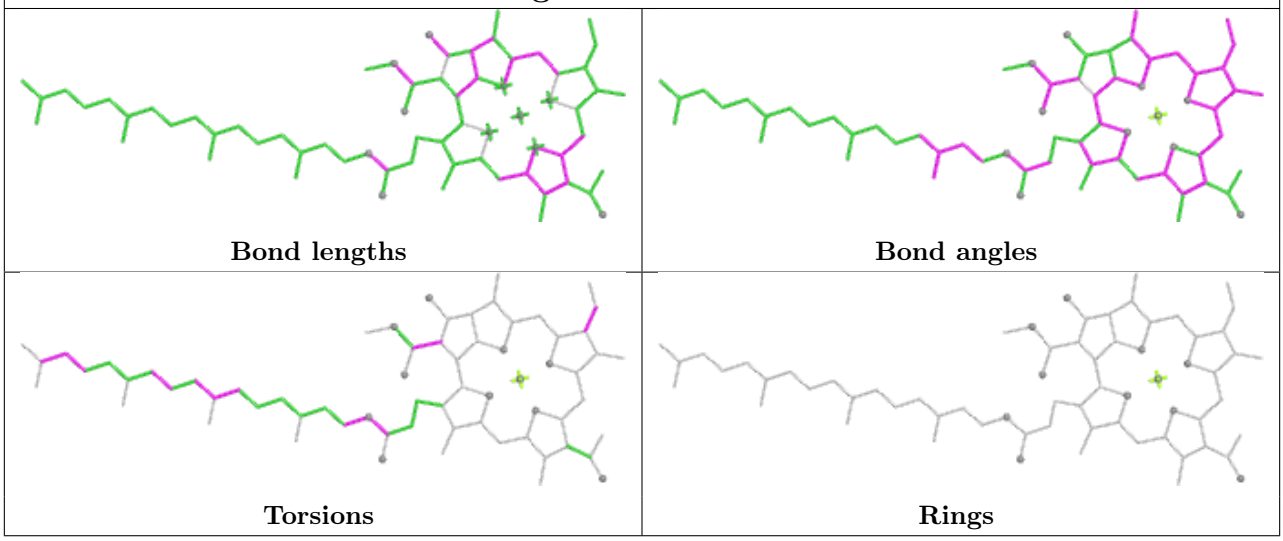
Ligand LMT G 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCL M 401	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LMT b 101



Ligand BCL I 102



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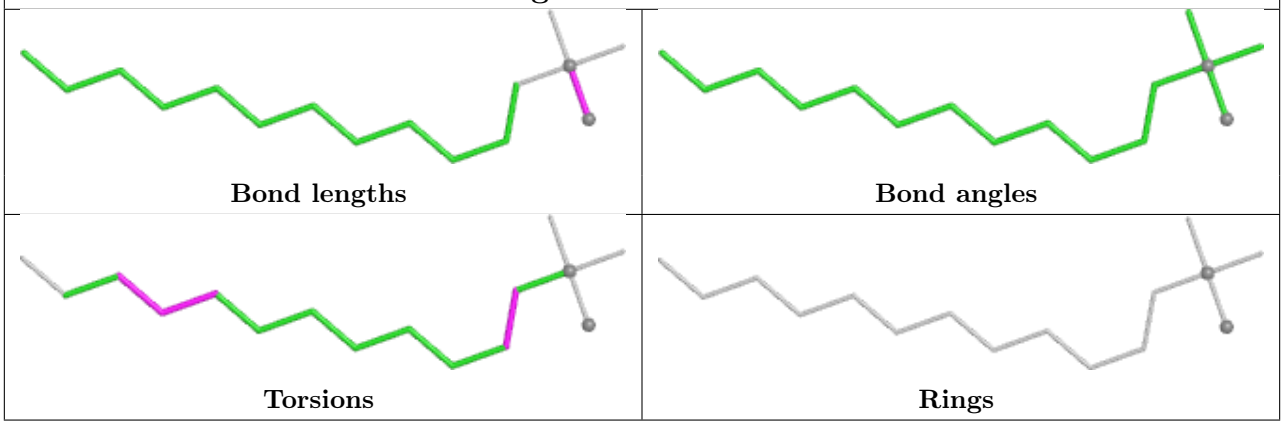
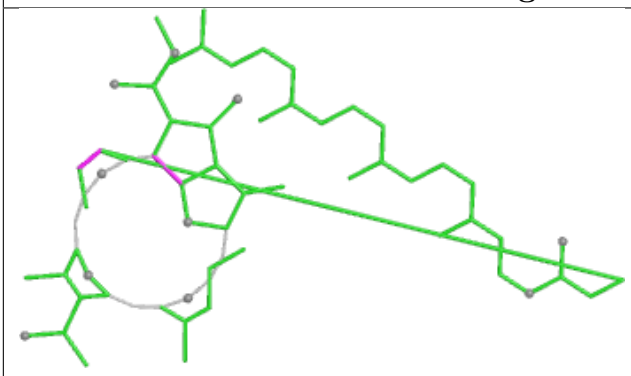
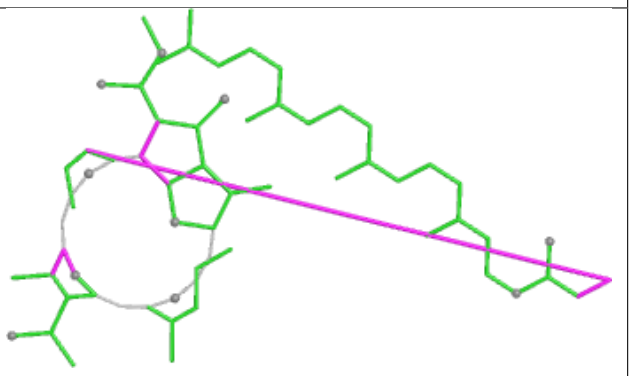
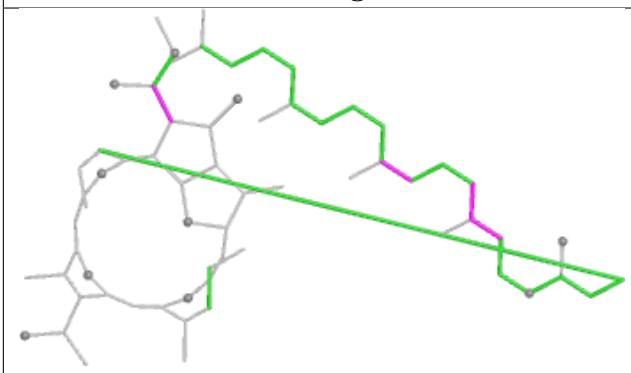
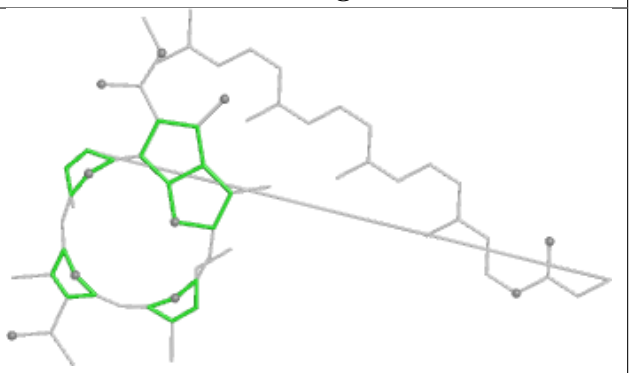
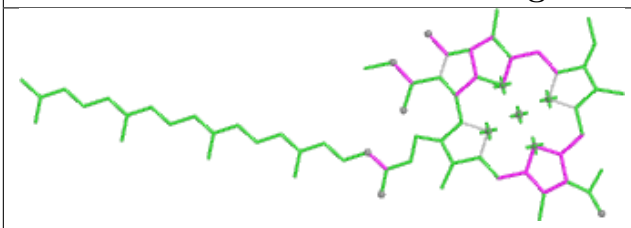
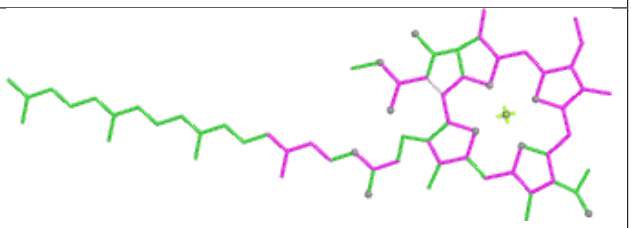
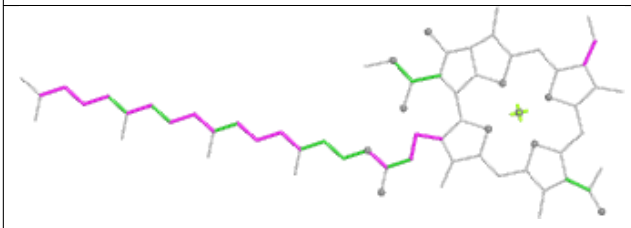
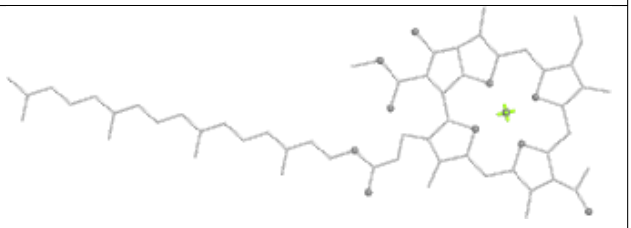


Ligand BPH M 405	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCL n 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

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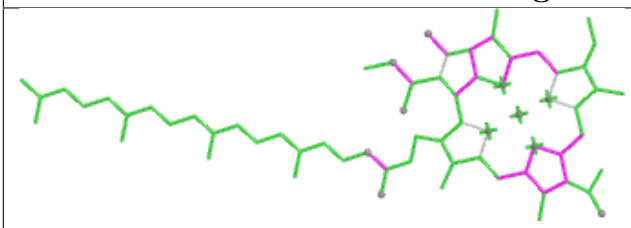
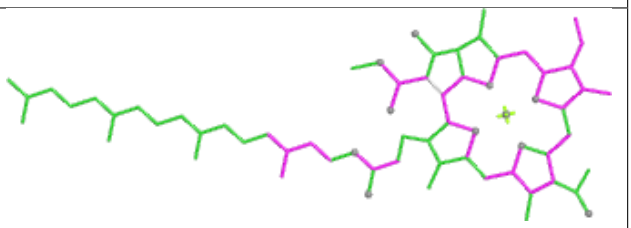
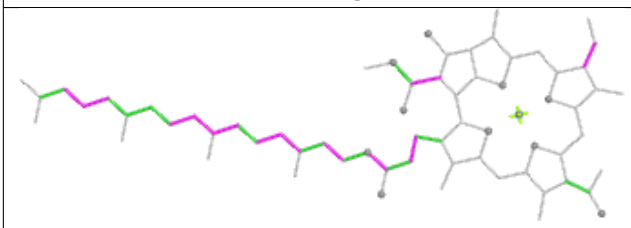
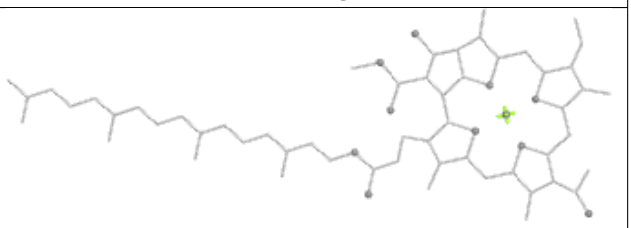
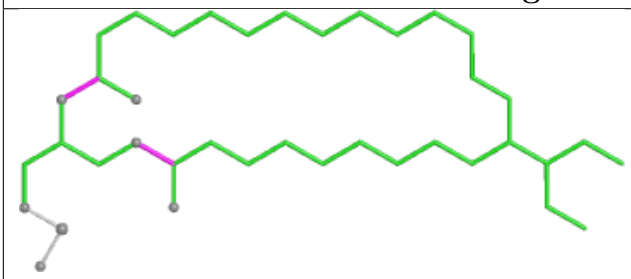
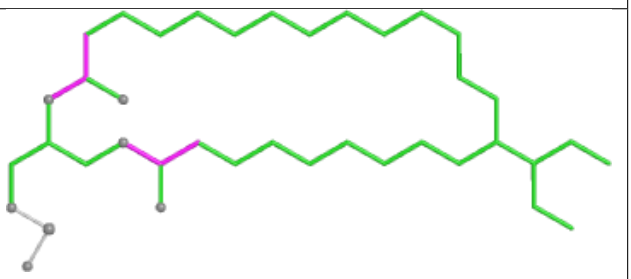
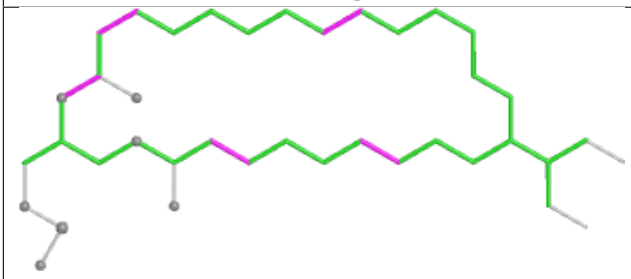
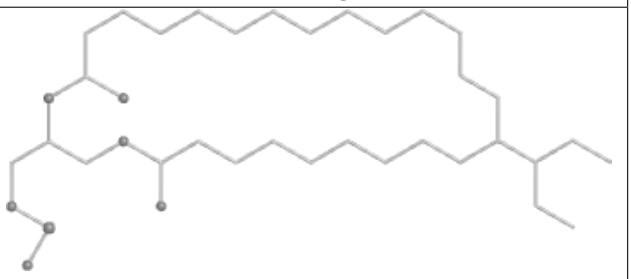
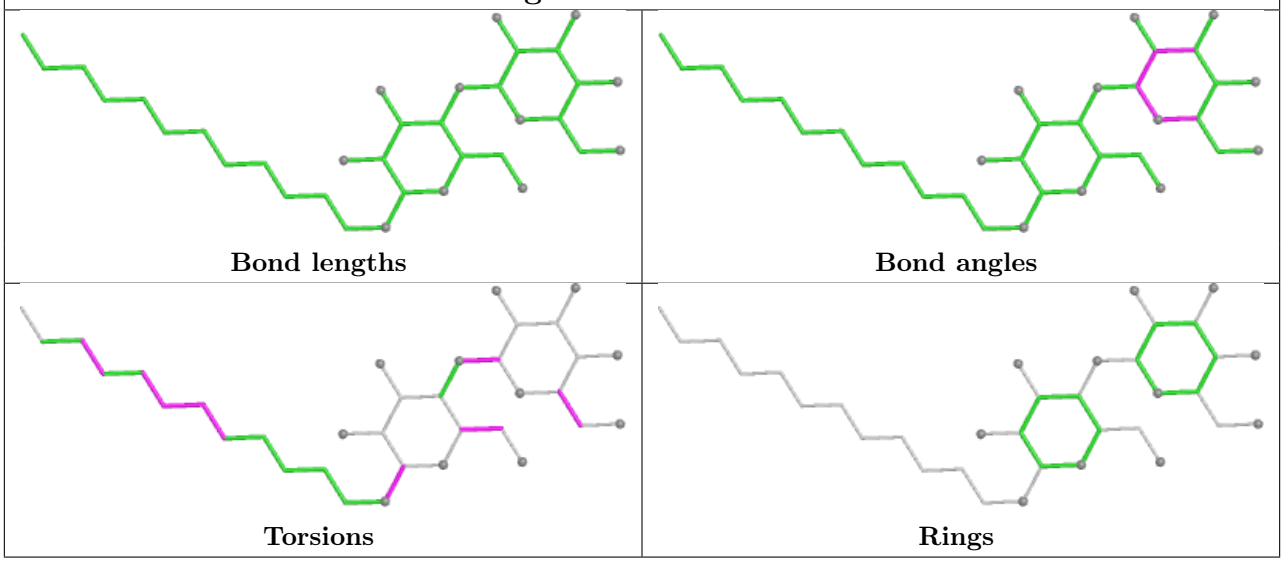
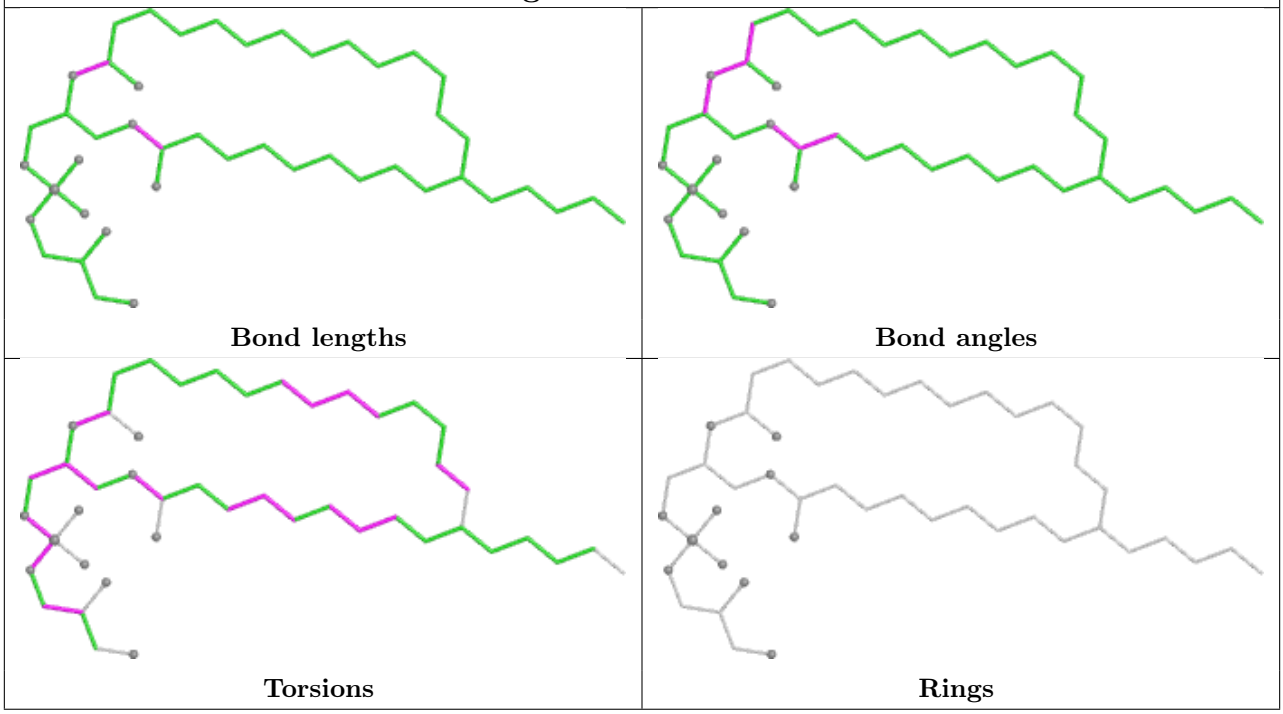
 Bond lengths	 Bond angles
 Torsions	 Rings

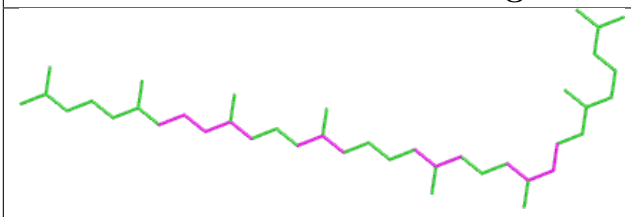
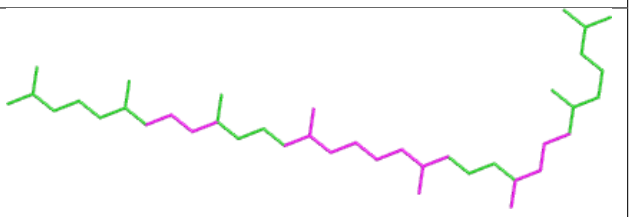
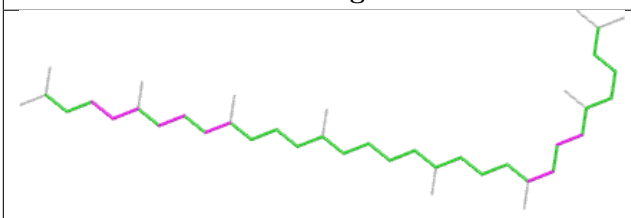
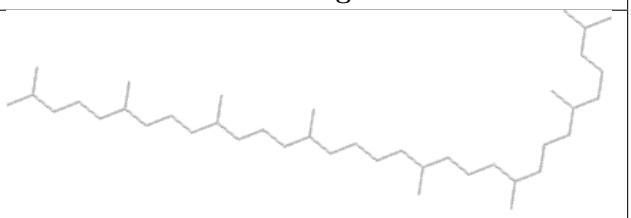
Ligand PGV E 104	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LMT L 312



Ligand PGV C 102



Ligand A1EF2 N 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

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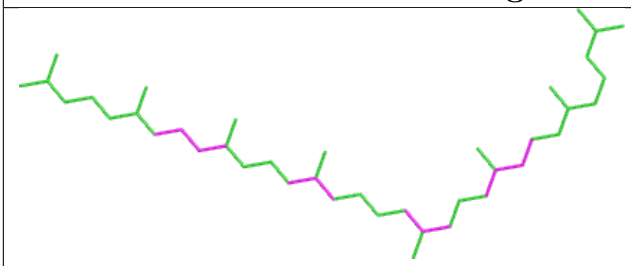
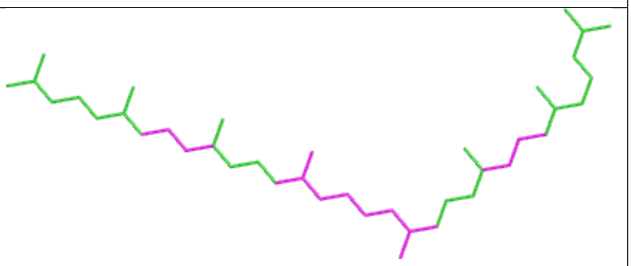
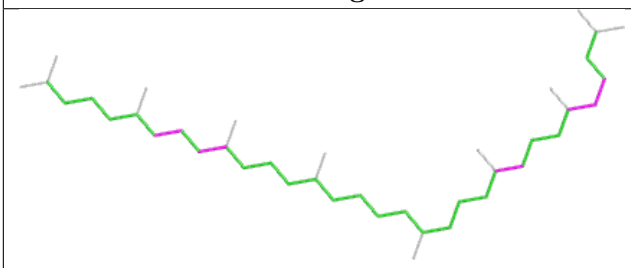
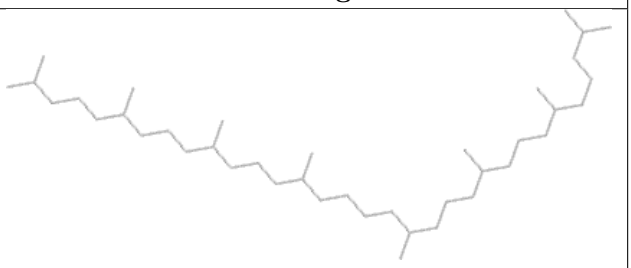
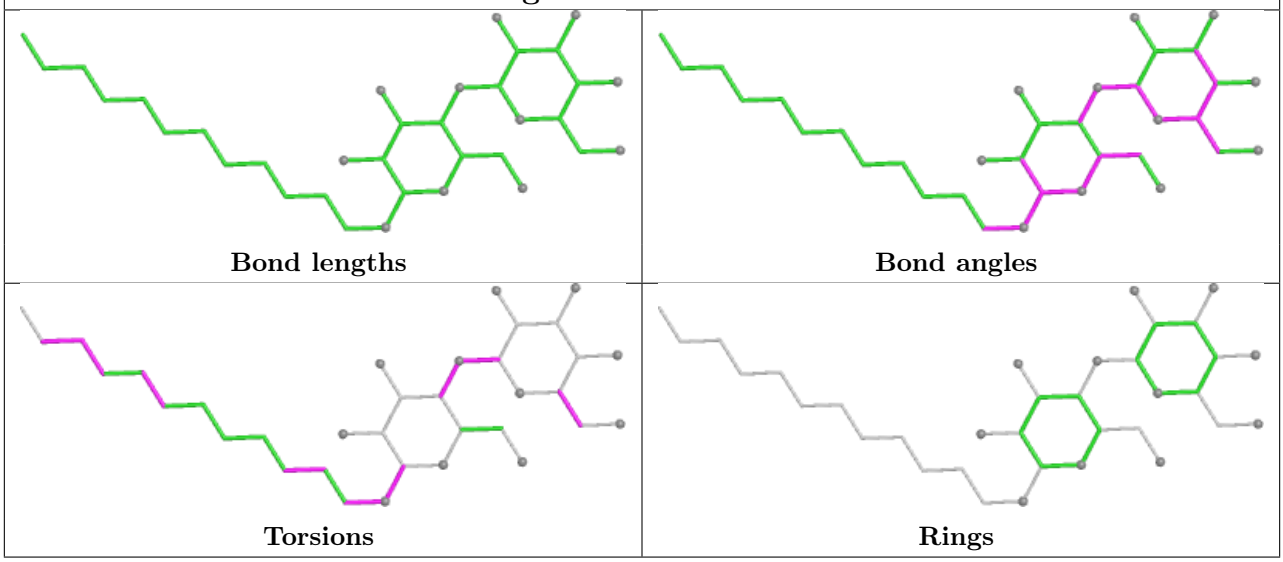
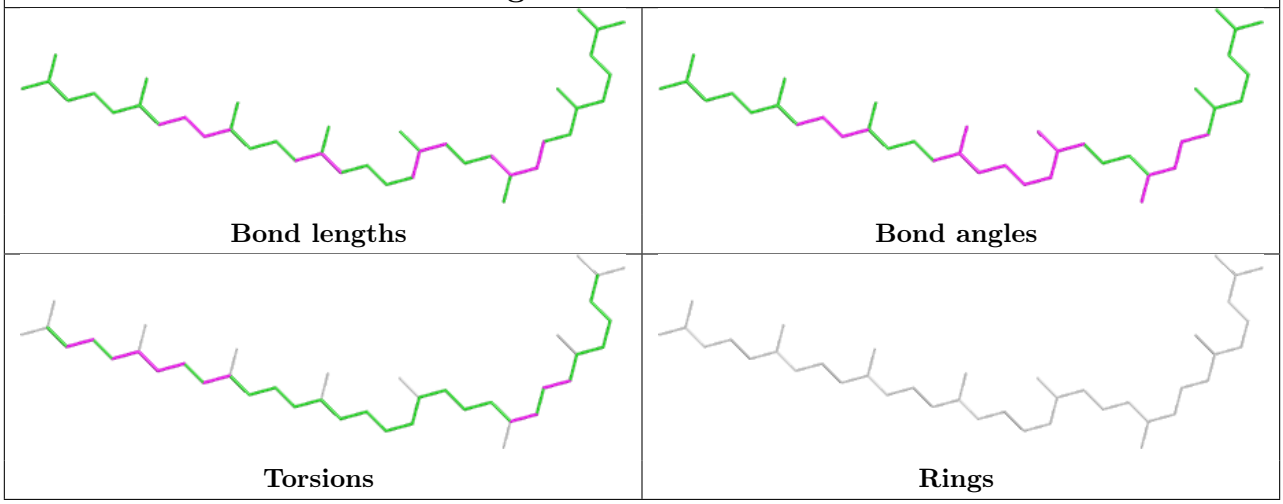
 Bond lengths	 Bond angles
 Torsions	 Rings

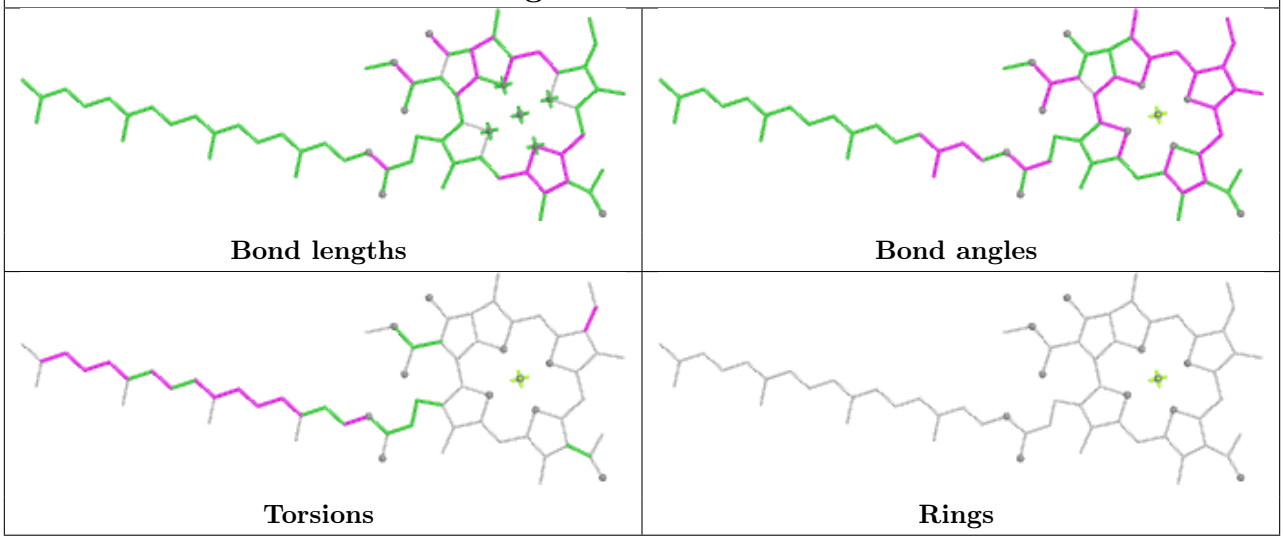
Ligand LMT B 102



Ligand A1EF2 D 104



Ligand BCL N 101



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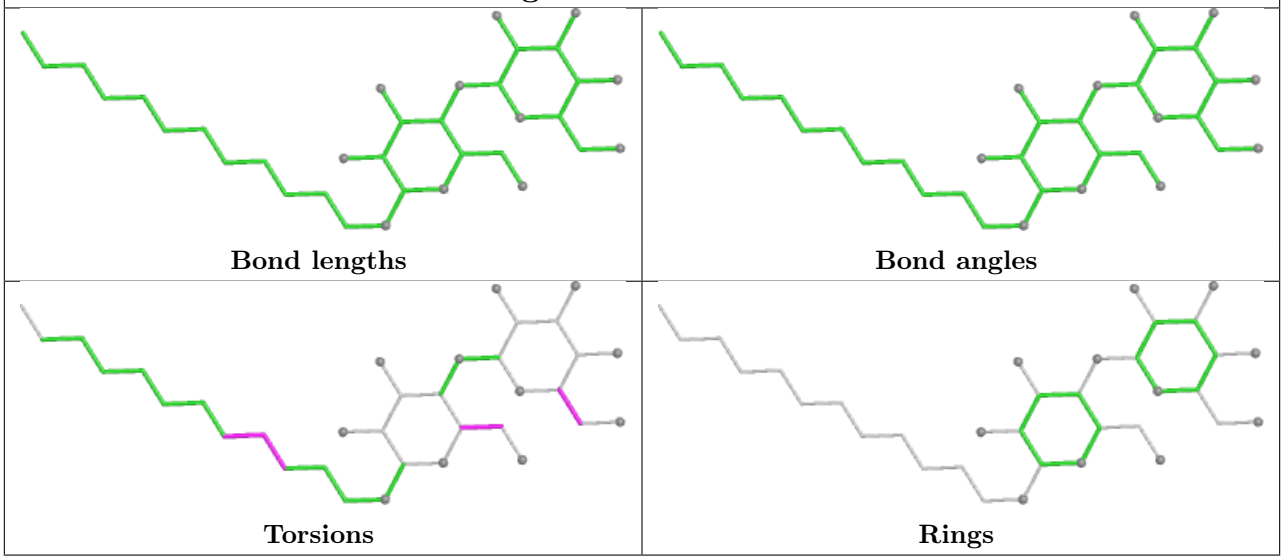
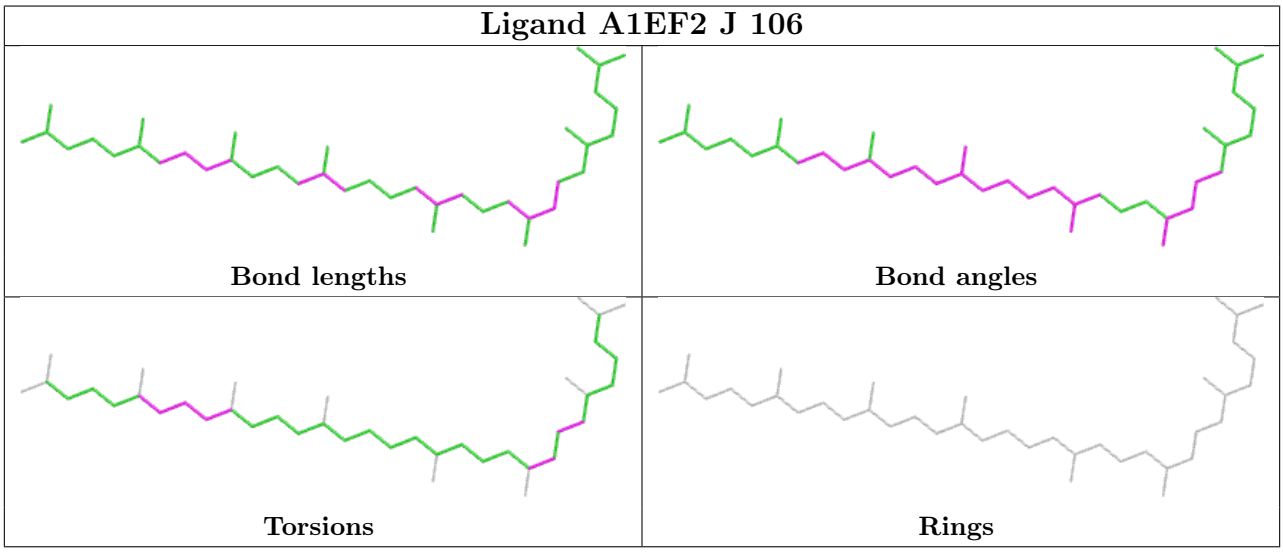
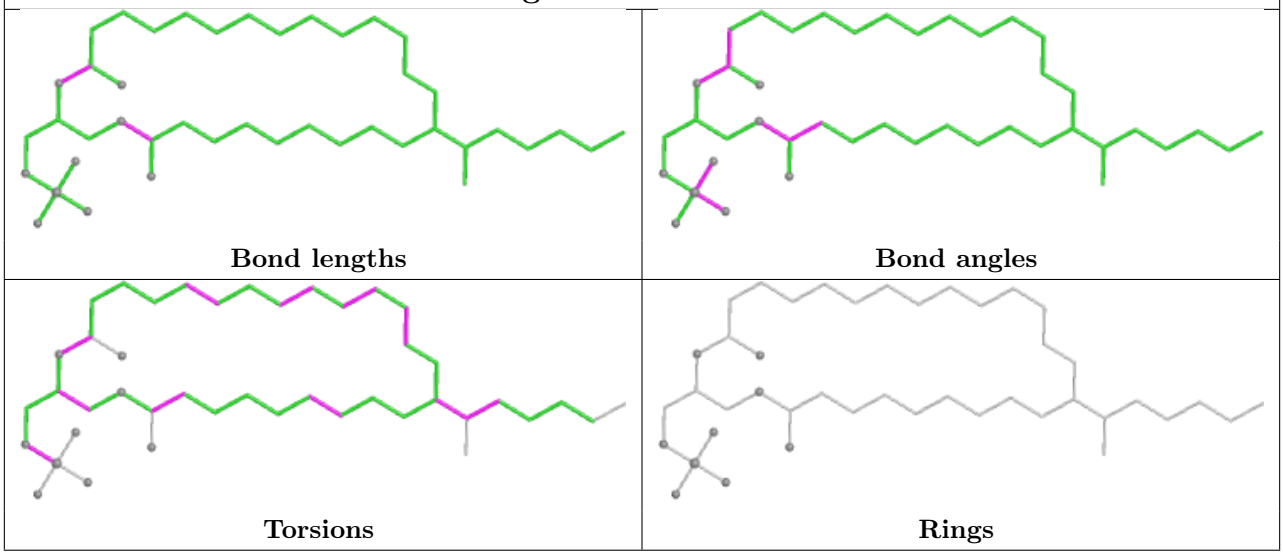
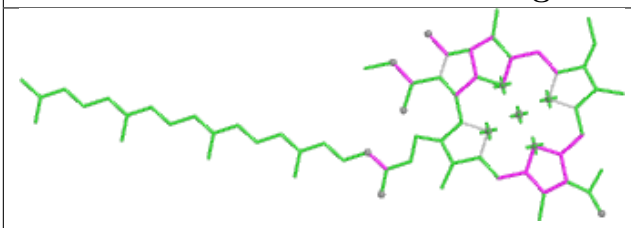
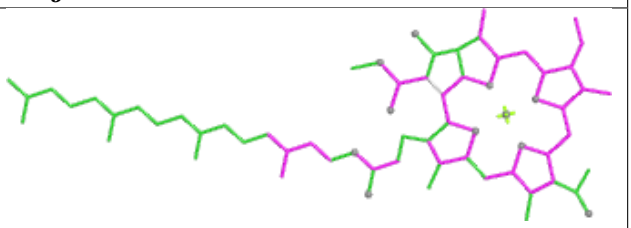
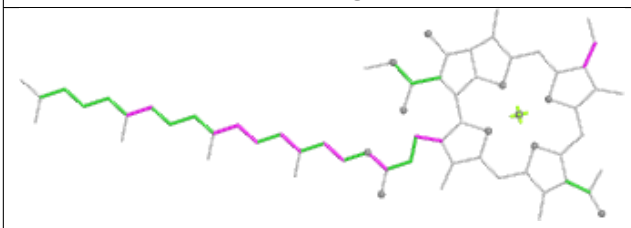
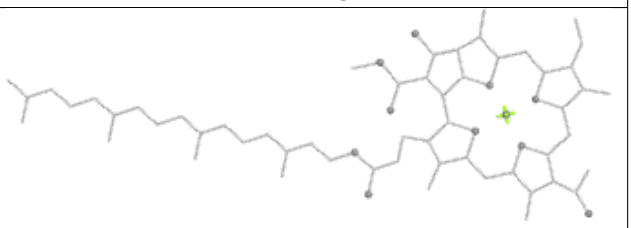


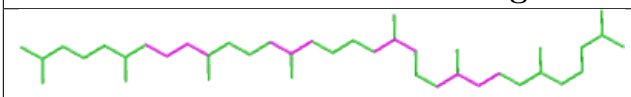
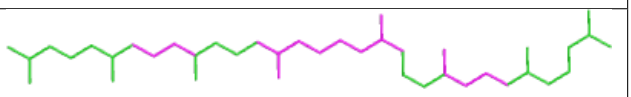
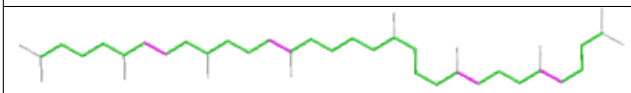
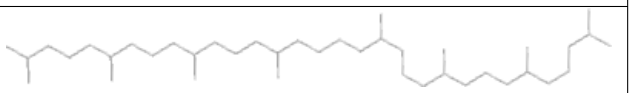
Ligand A1EF2 J 106

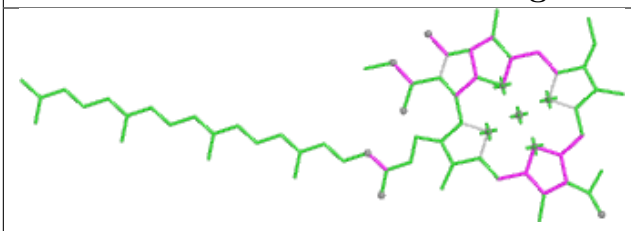
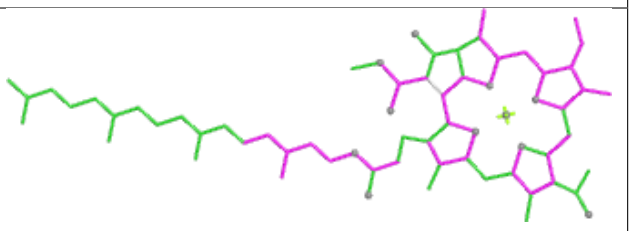
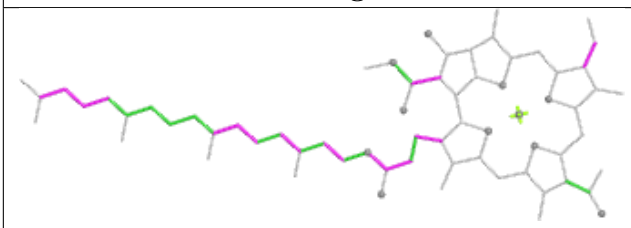
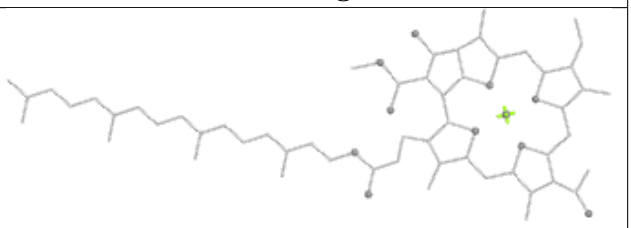


Ligand PGV C 101

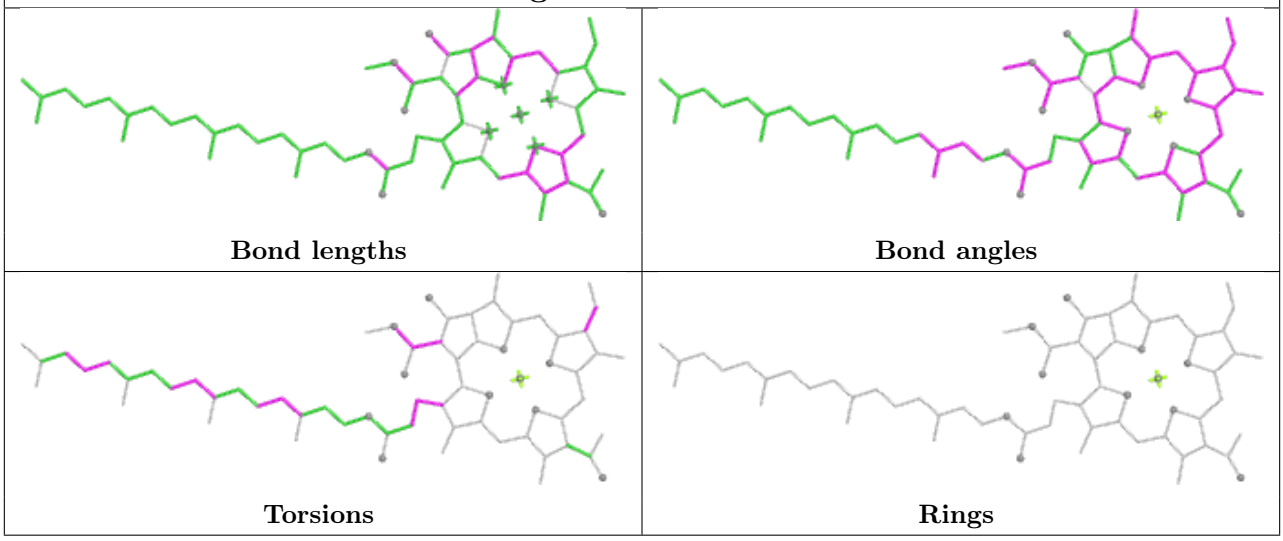


Ligand BCL j 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

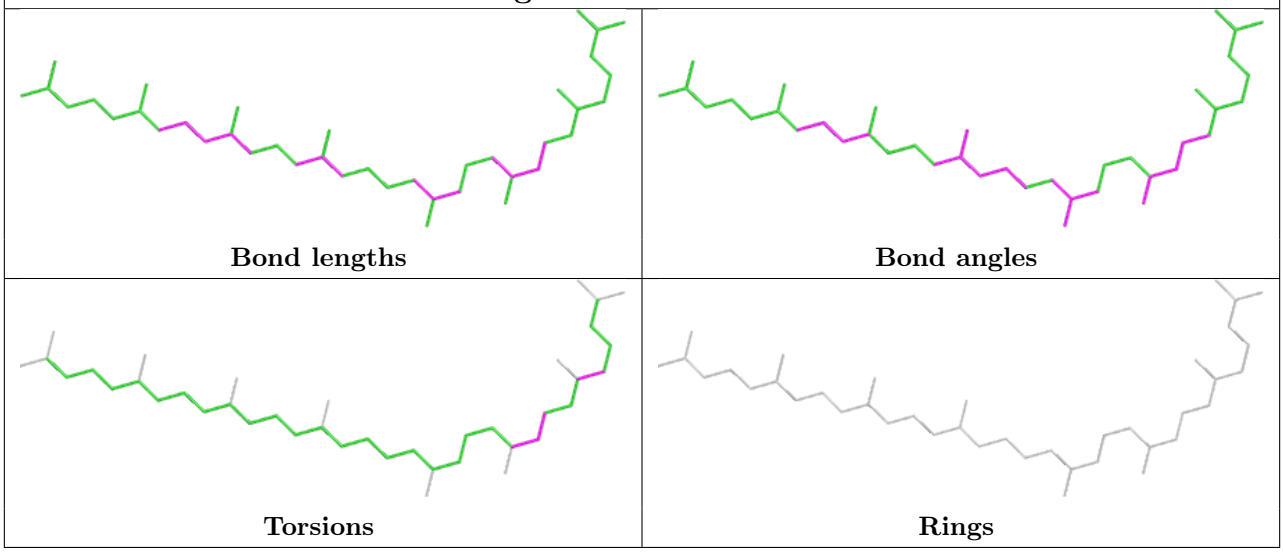
Ligand A1EF2 n 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCL a 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

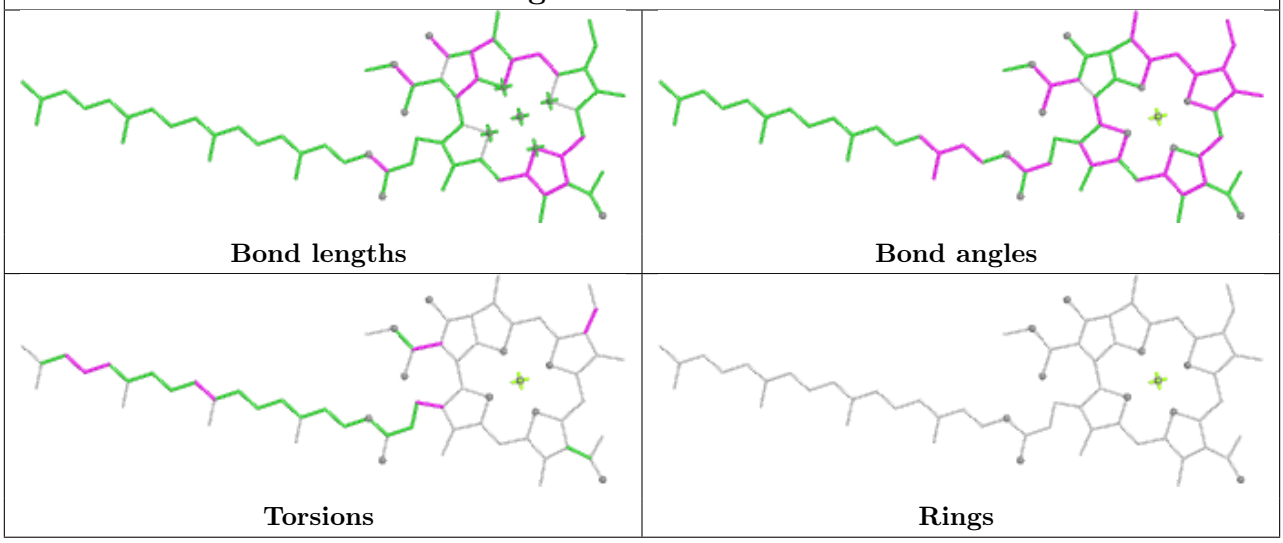
Ligand BCL o 102

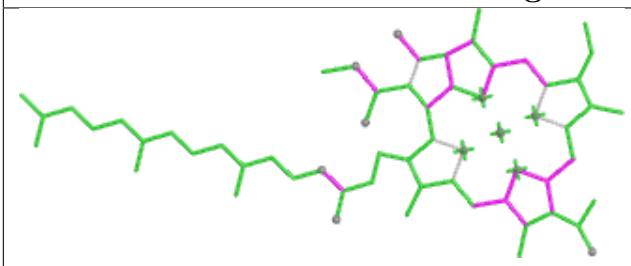
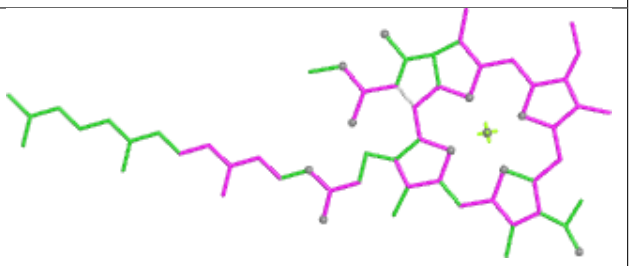
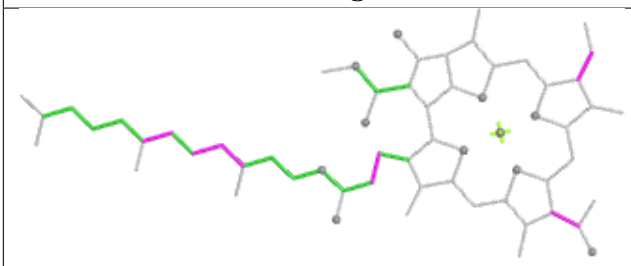
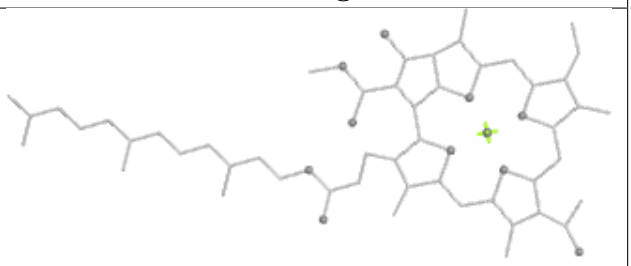


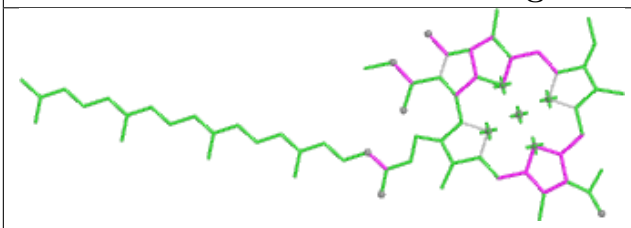
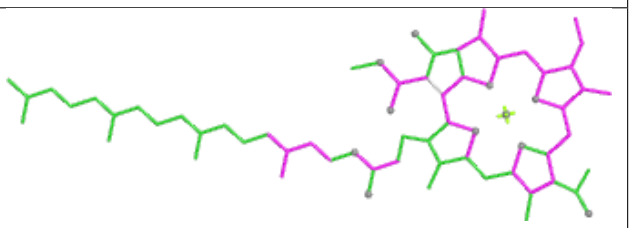
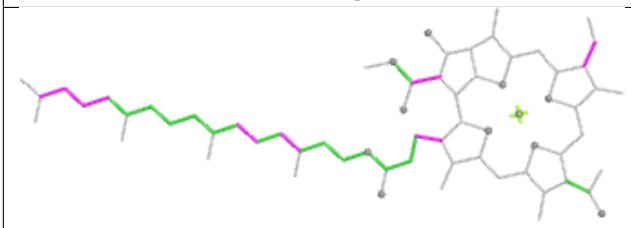
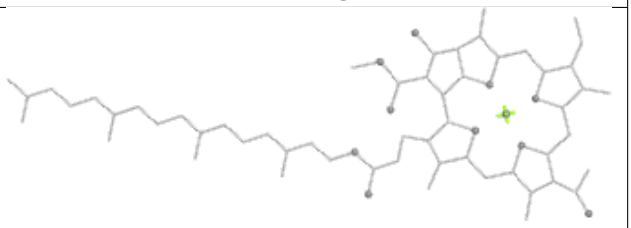
Ligand A1EF2 I 105



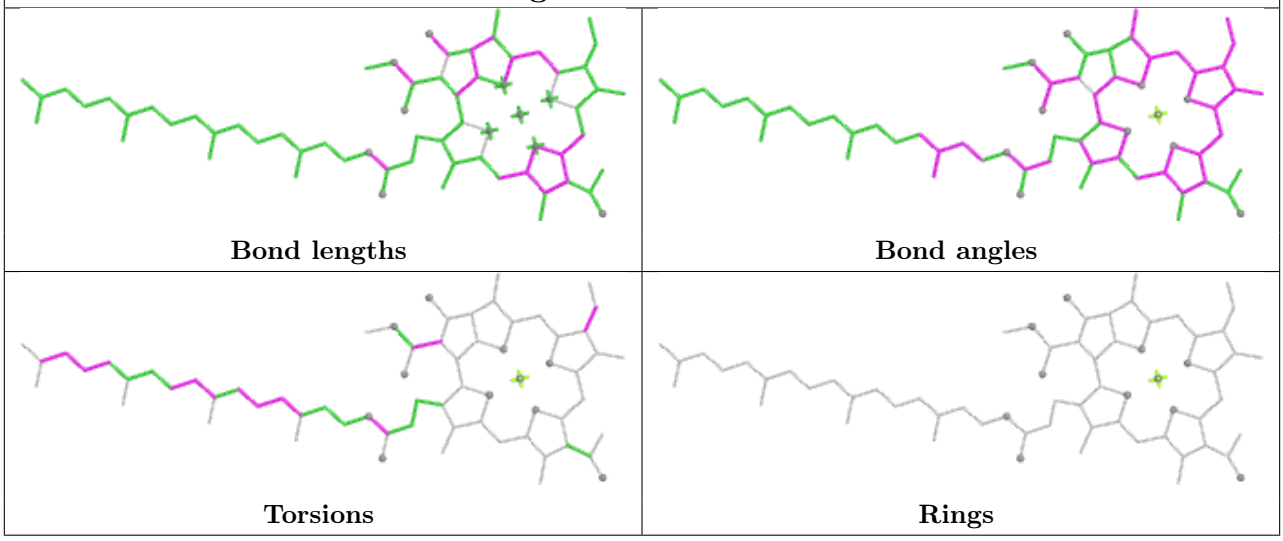
Ligand BCL L 308



Ligand BCL A 702	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCL F 103	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCL J 102



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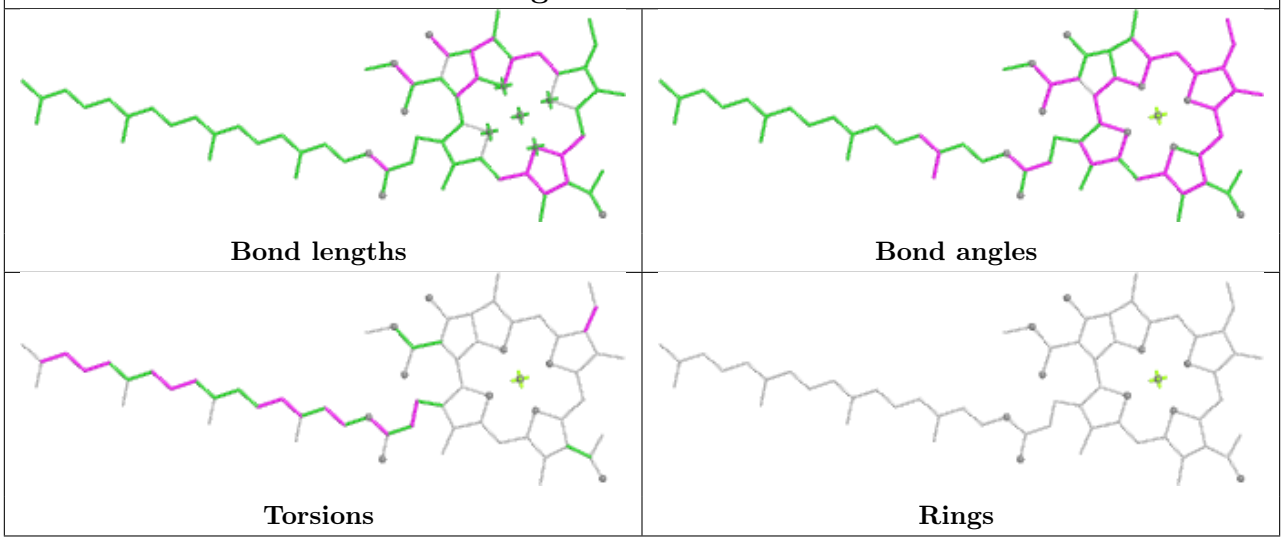

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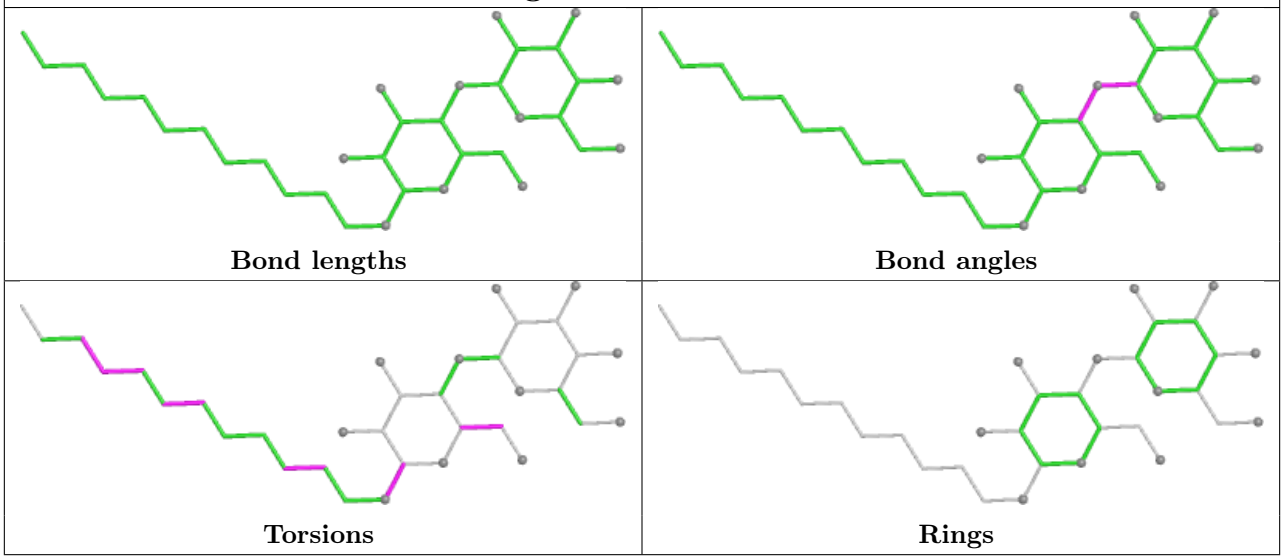

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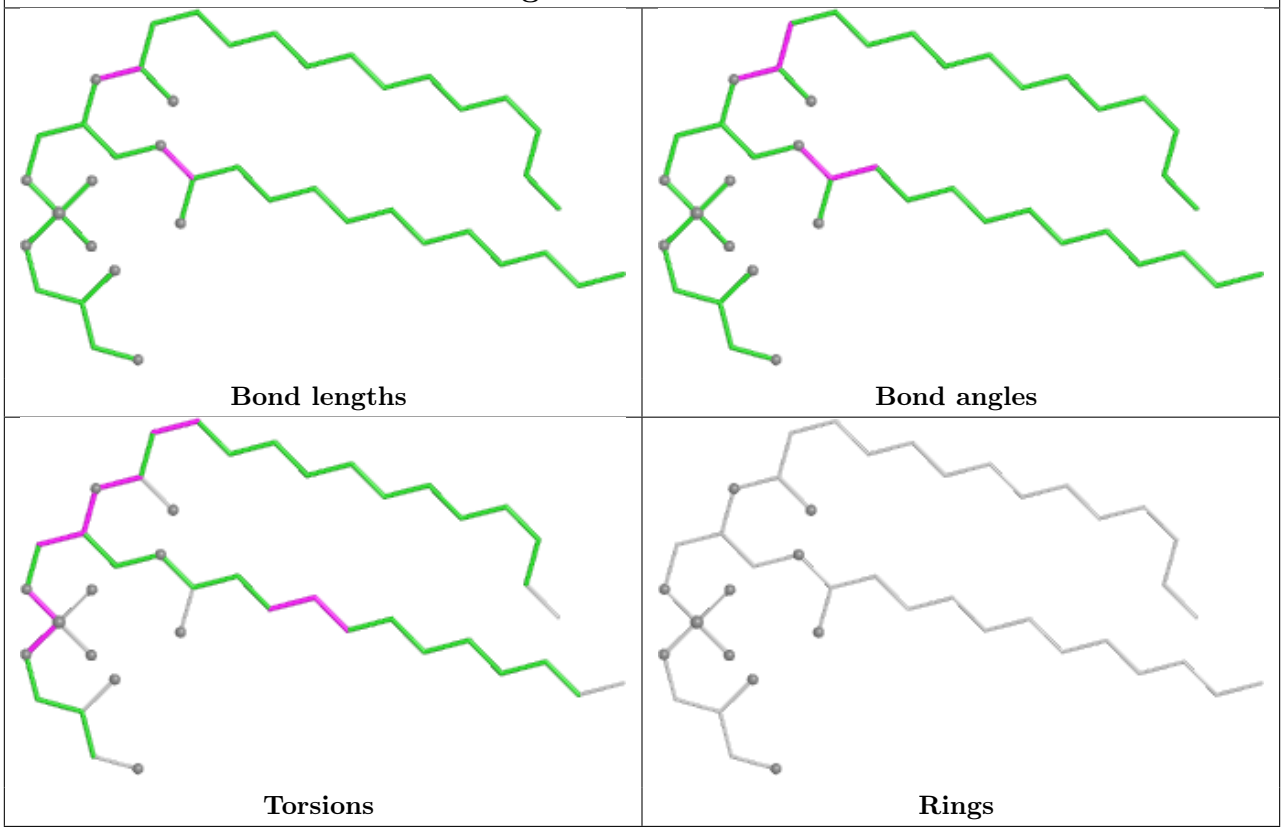

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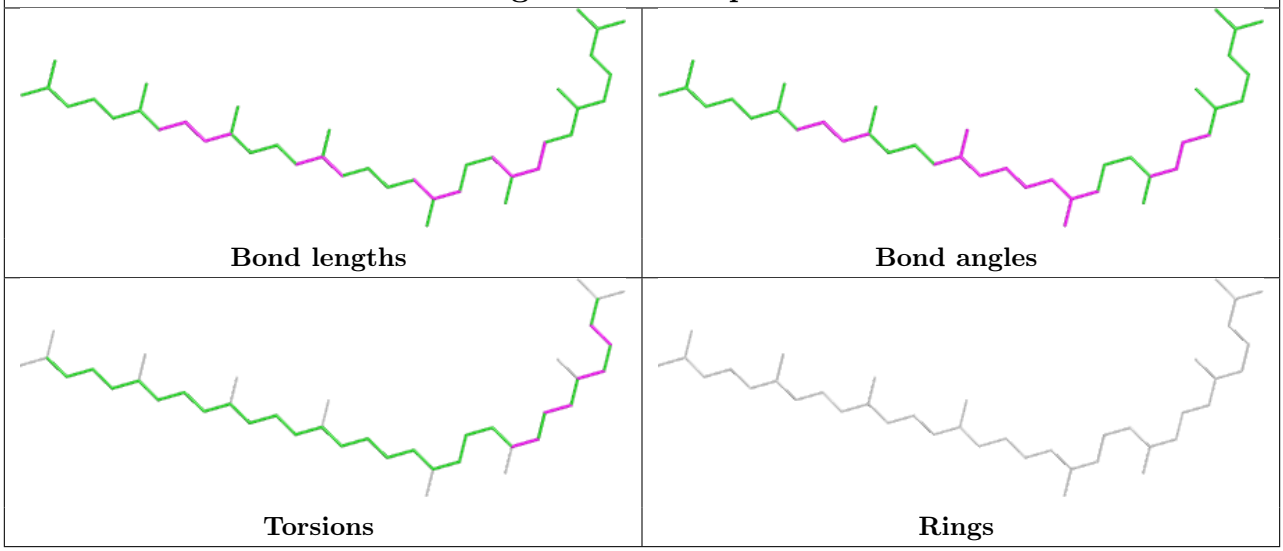

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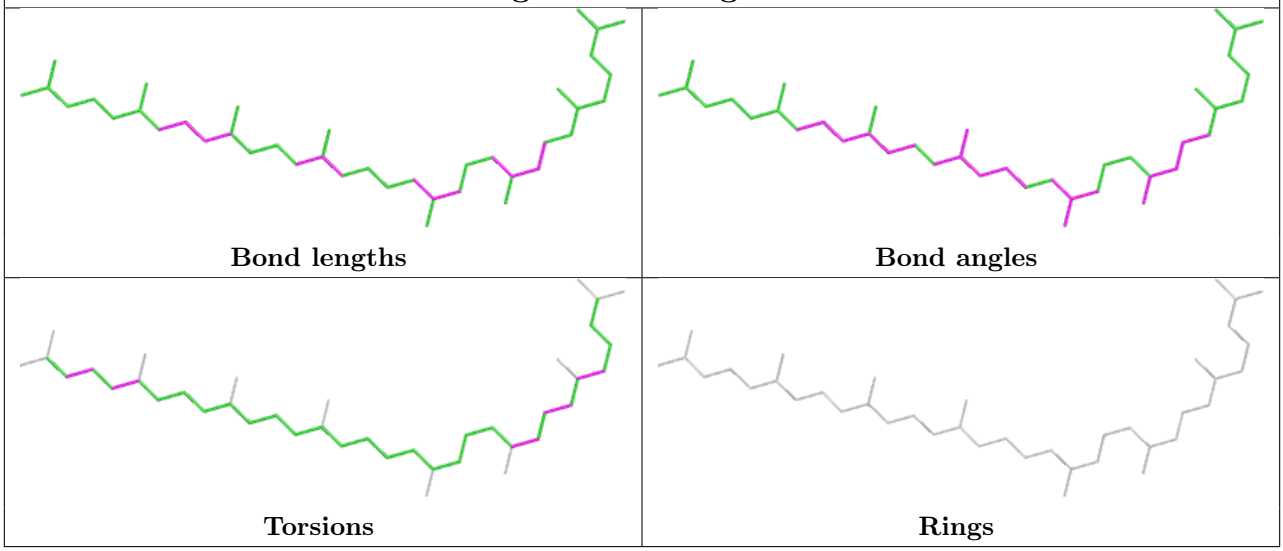

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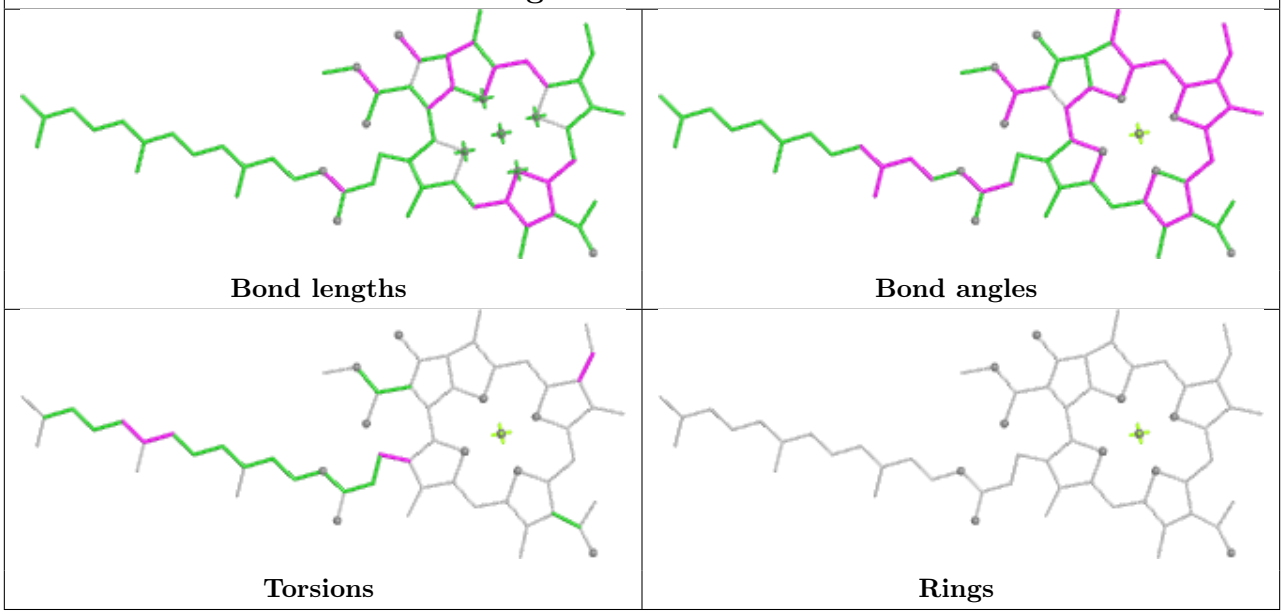

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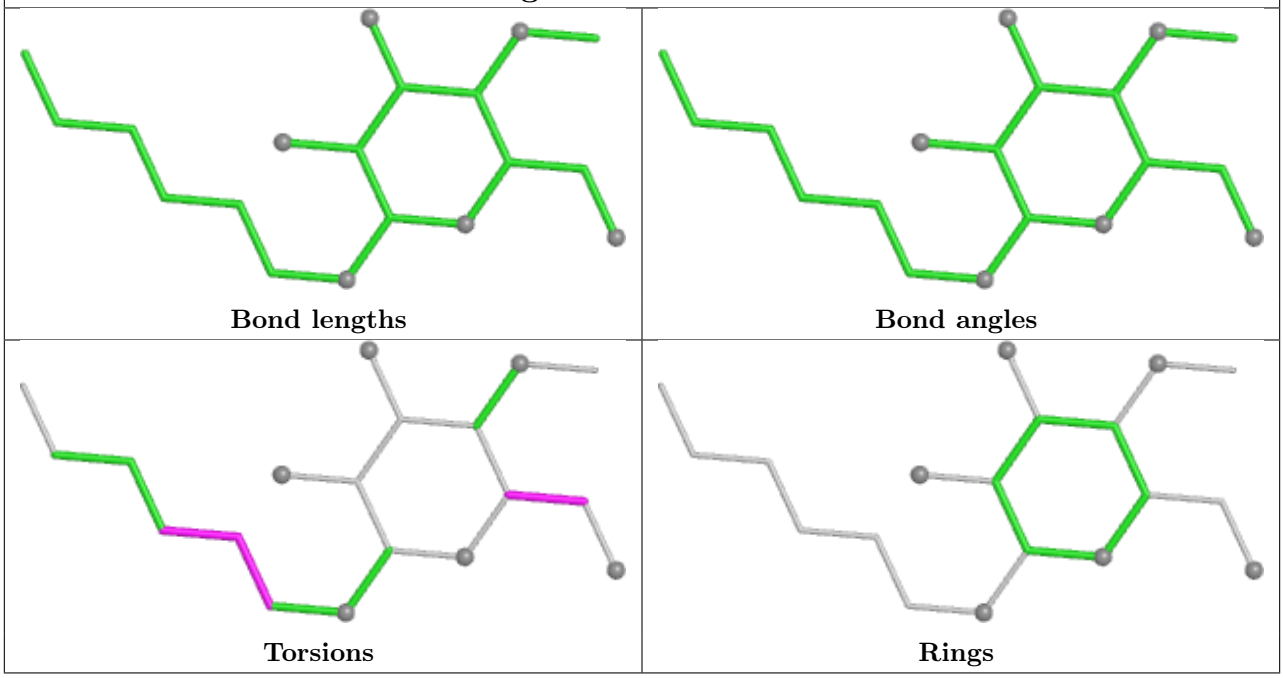

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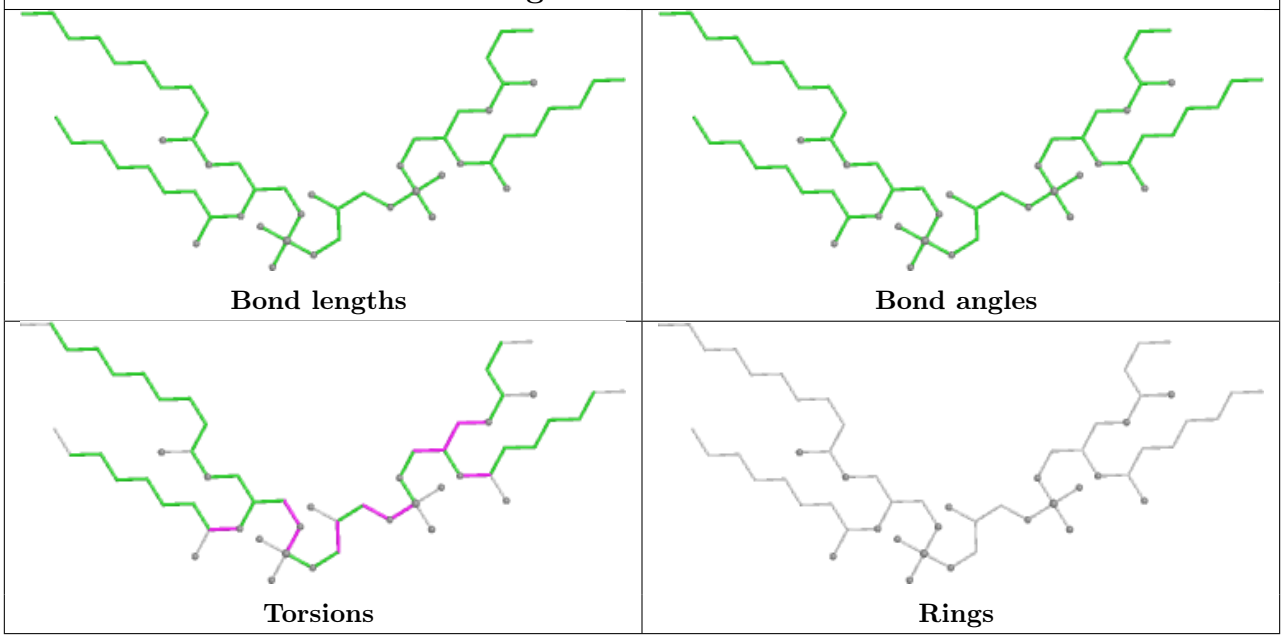

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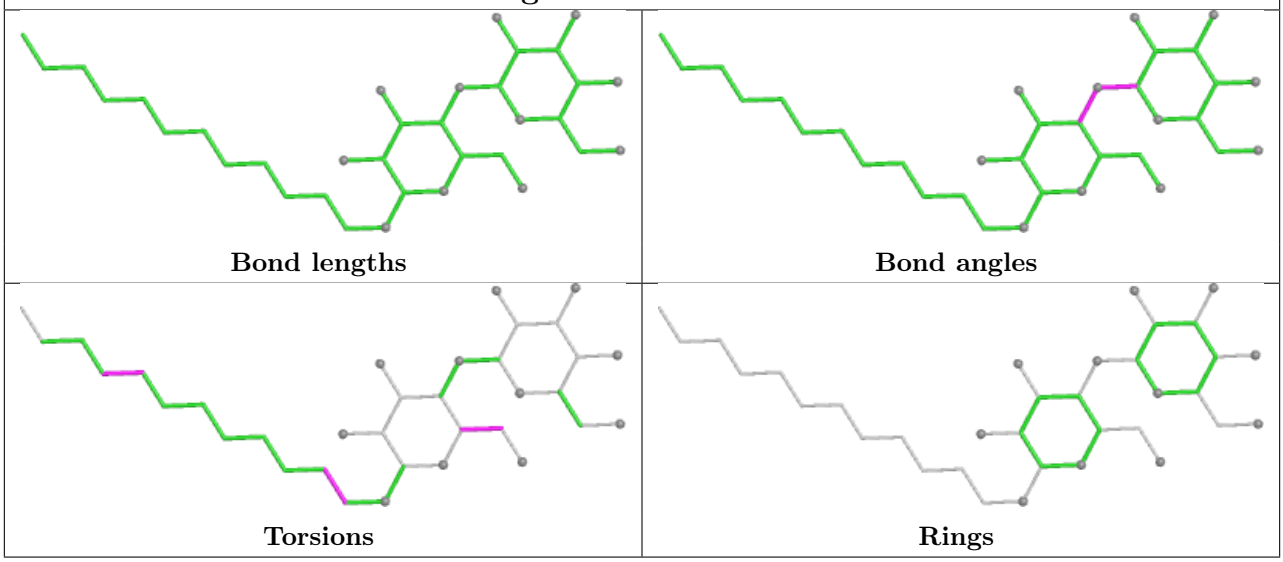
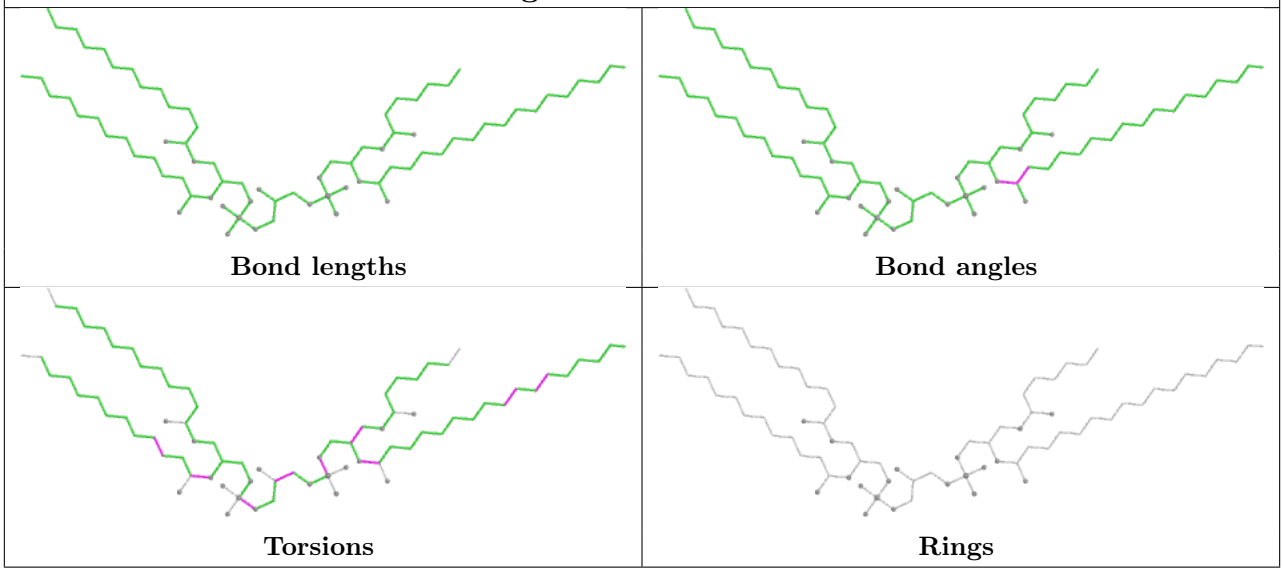


Ligand CDL M 410



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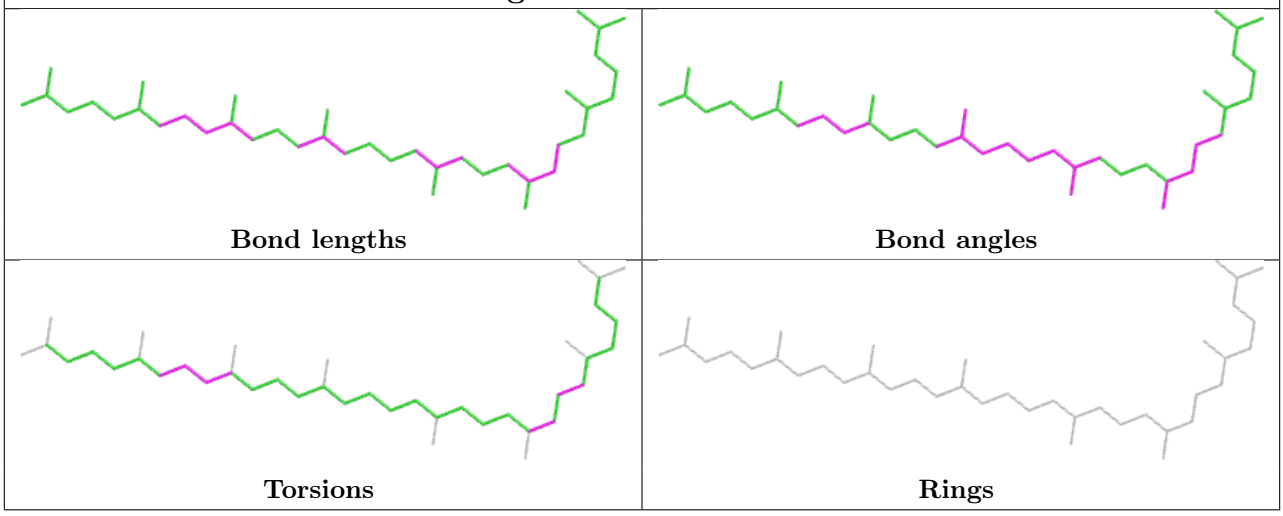

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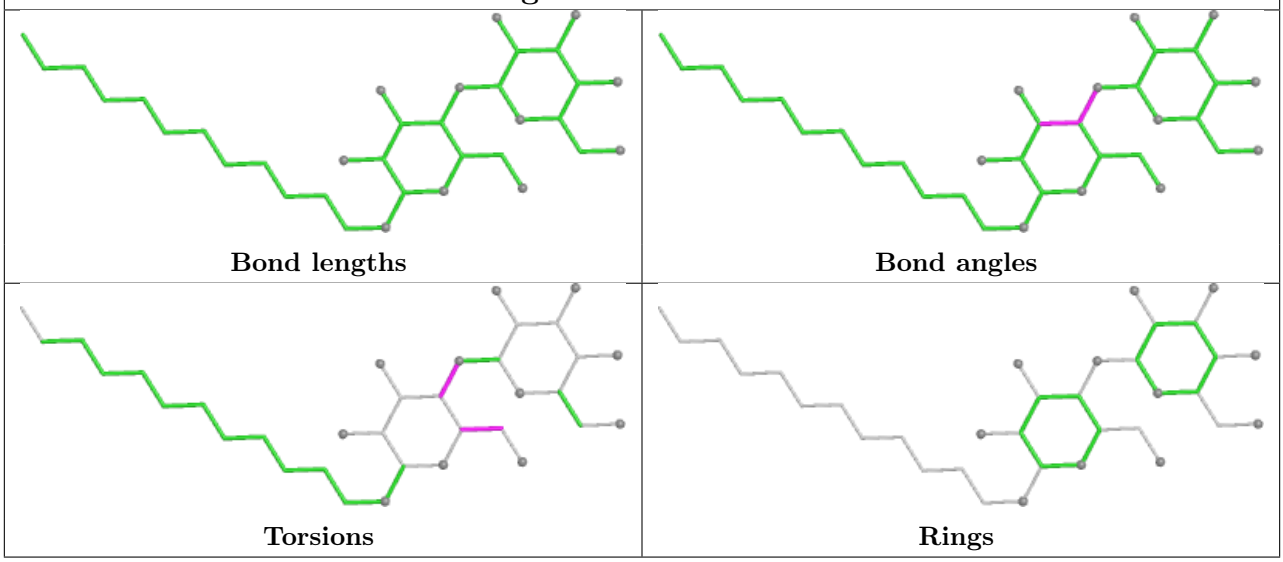

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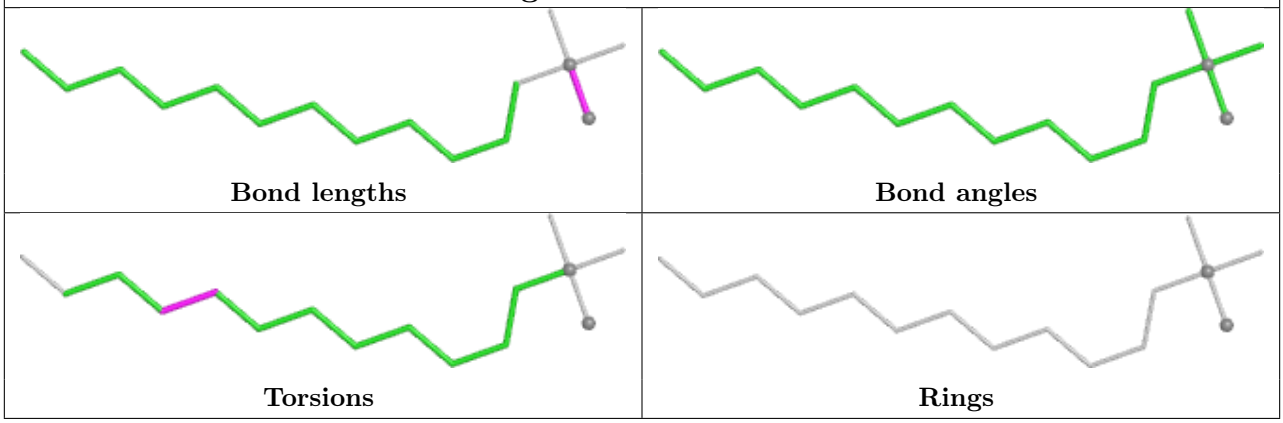
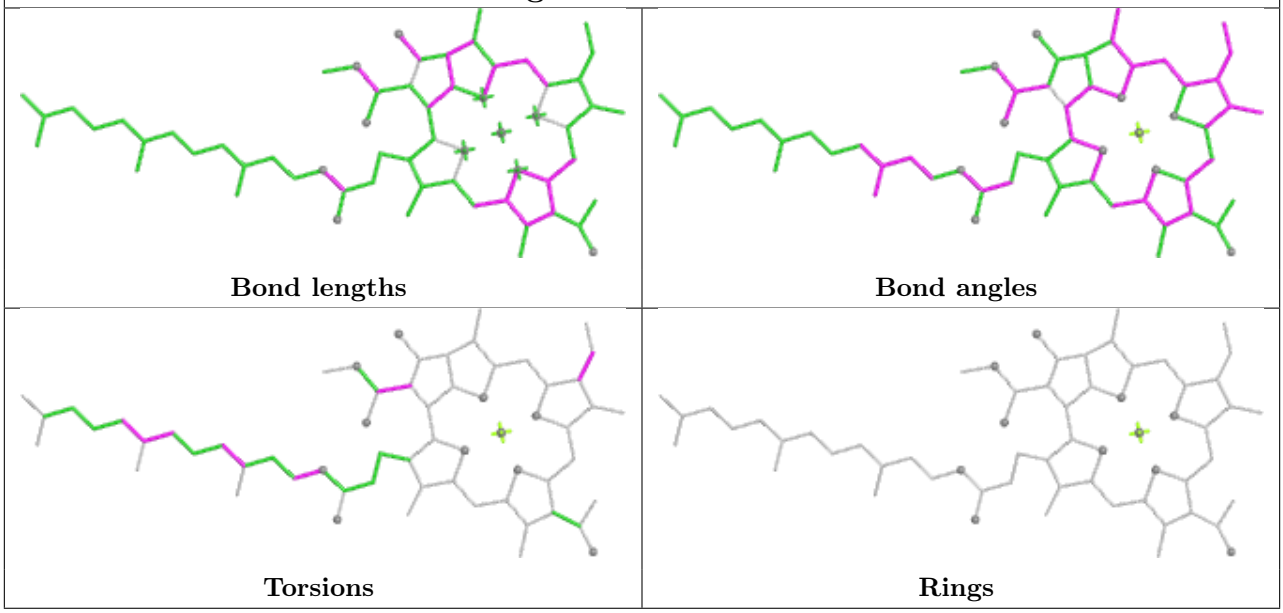


Ligand BCL P 102



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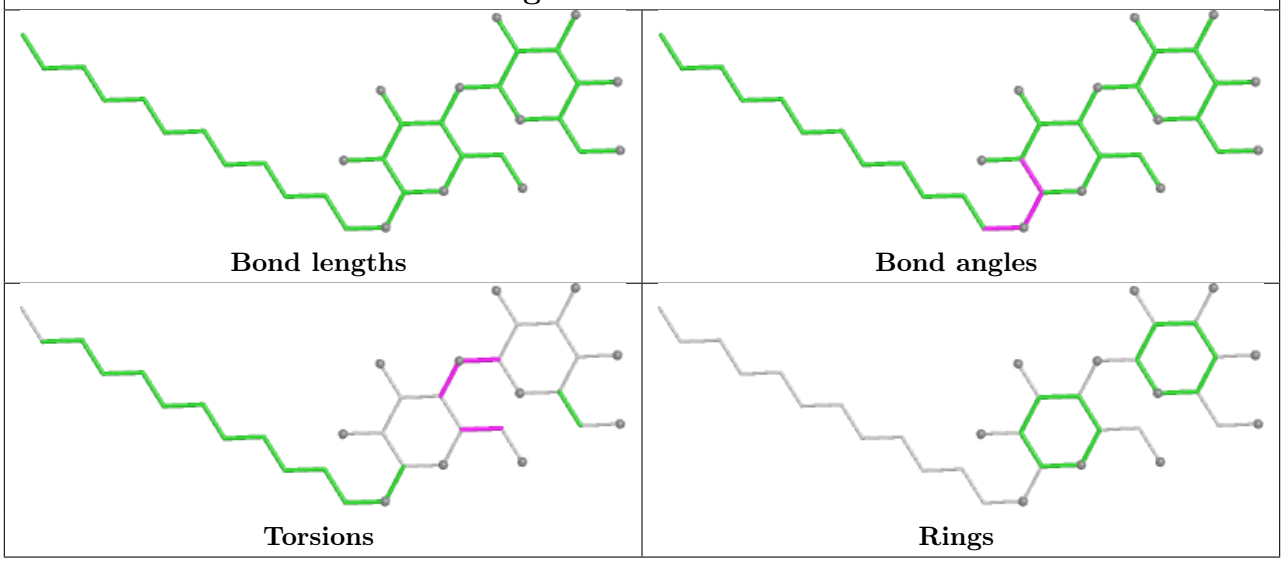

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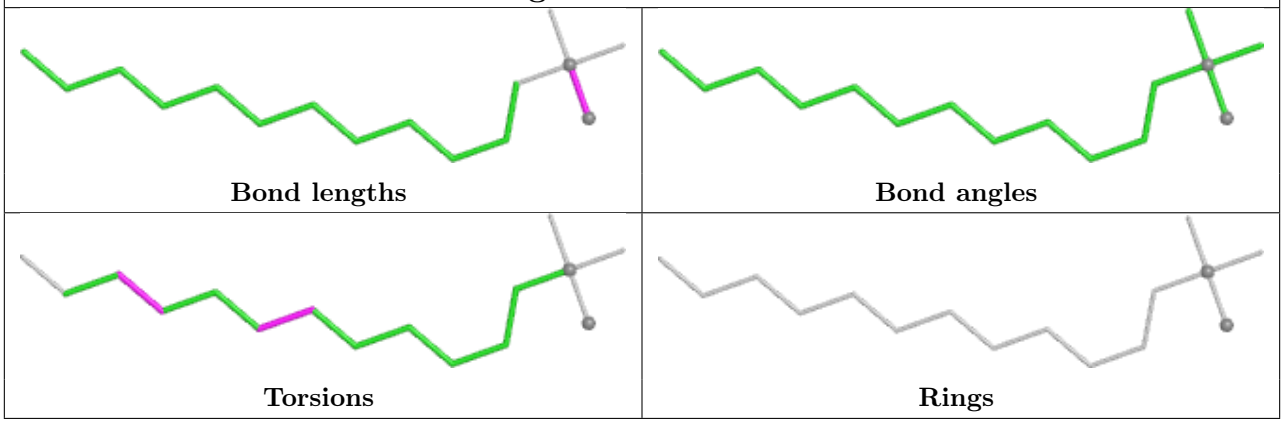

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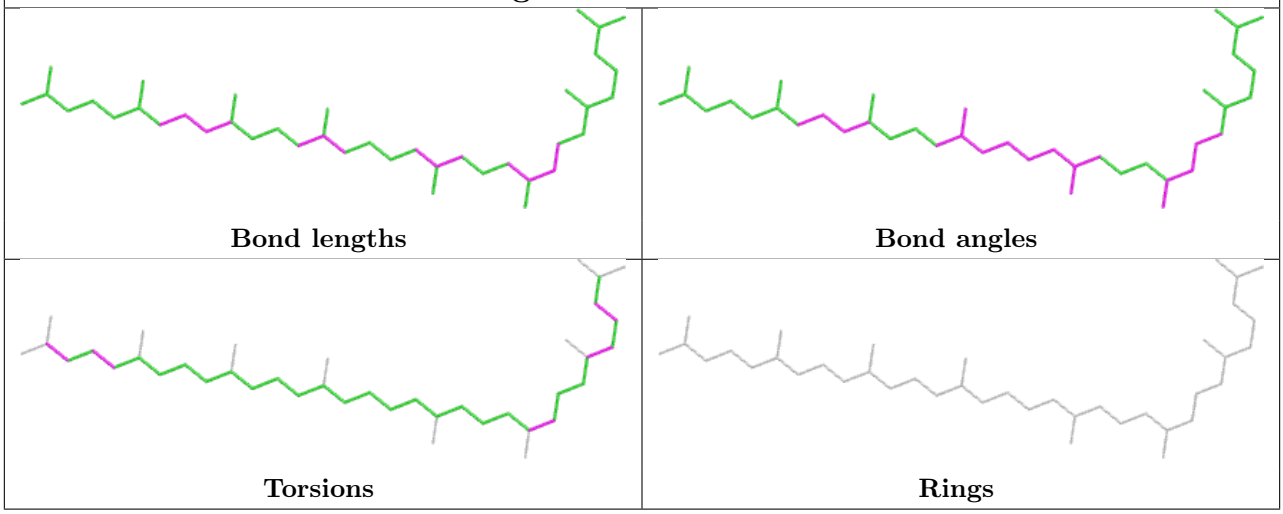

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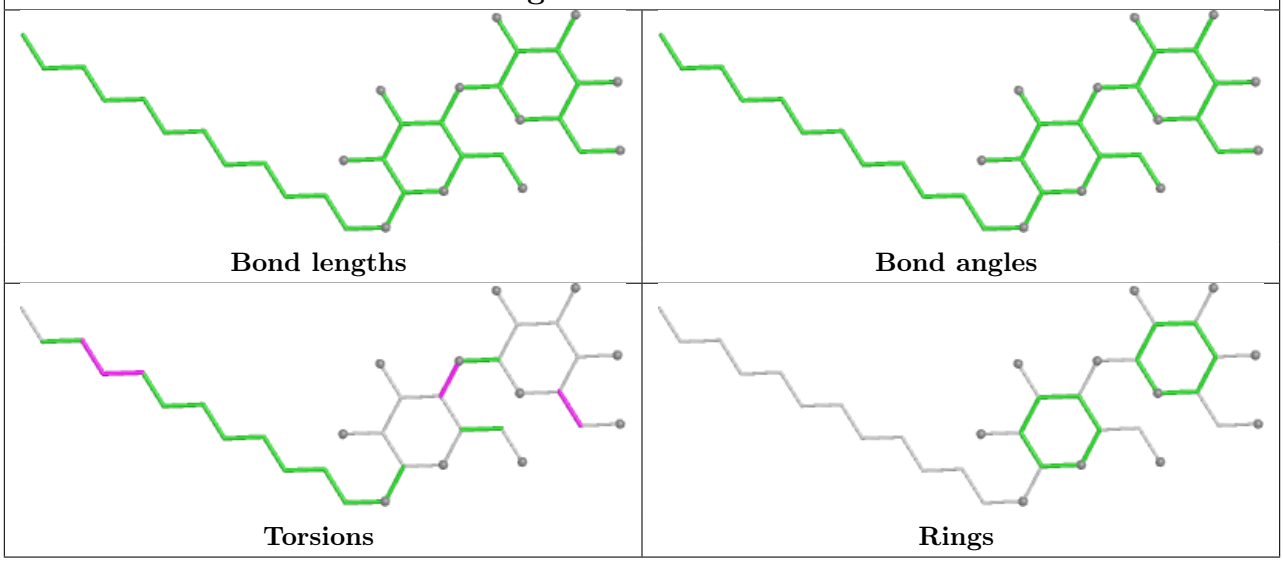

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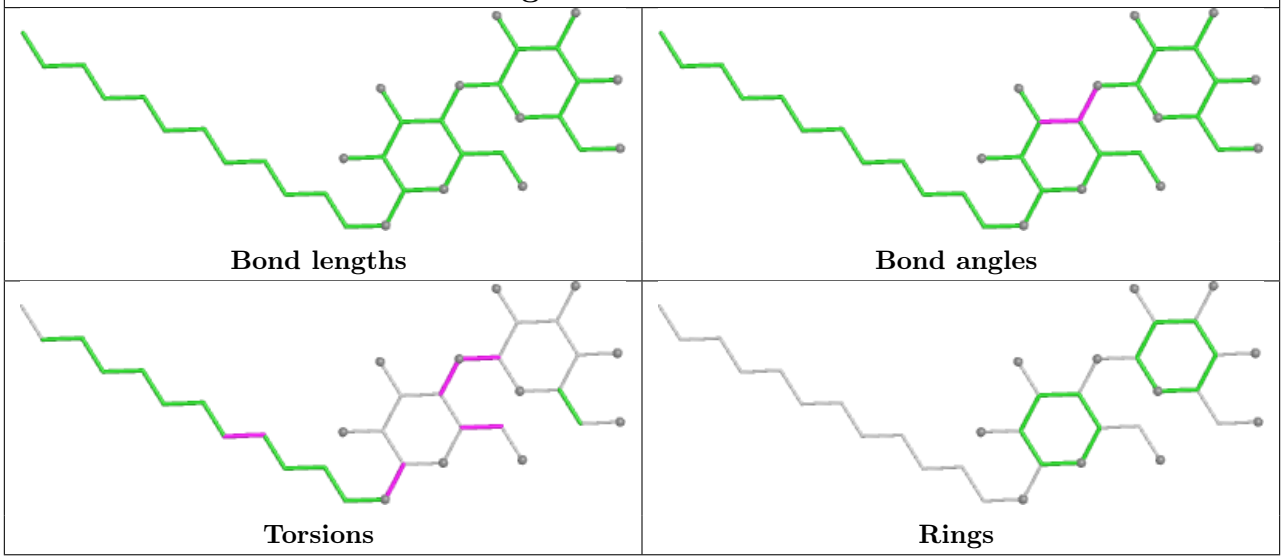

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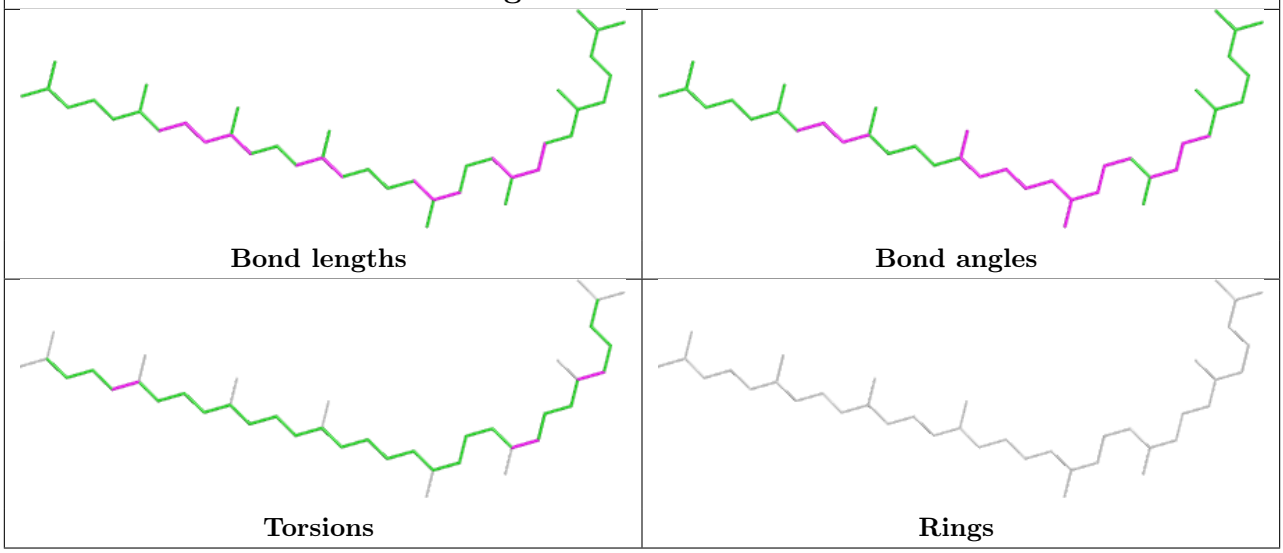
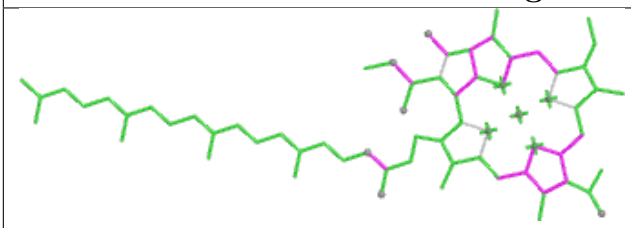
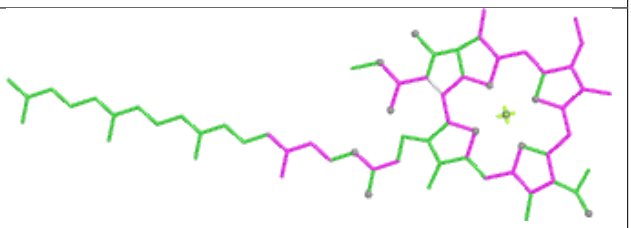
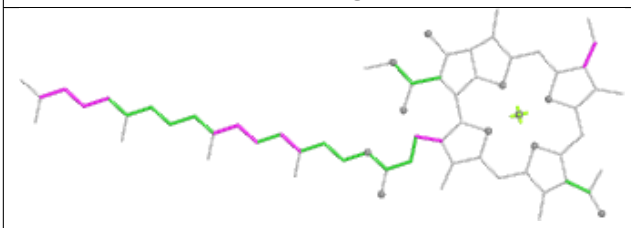
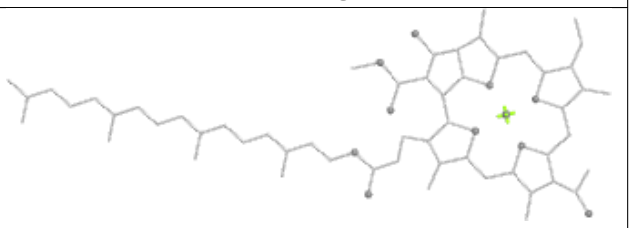


Ligand BCL C 103	
 Bond lengths	 Bond angles
 Torsions	 Rings

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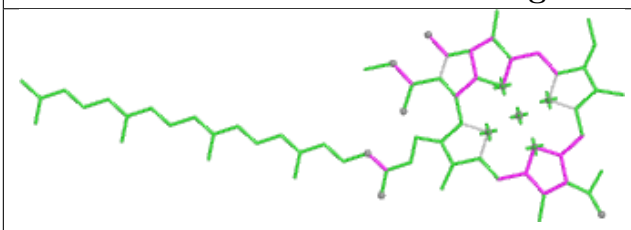
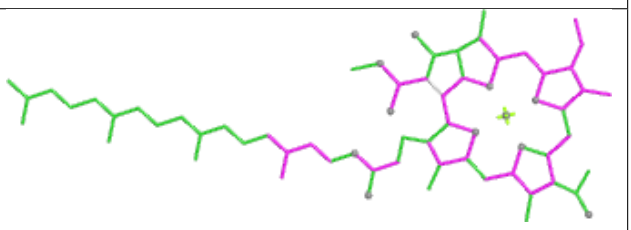
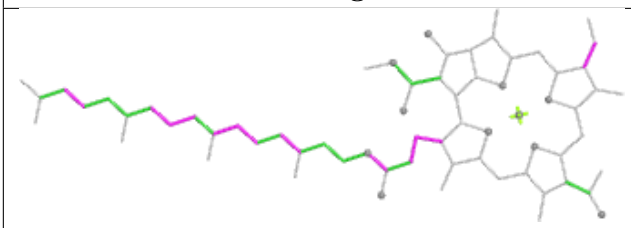
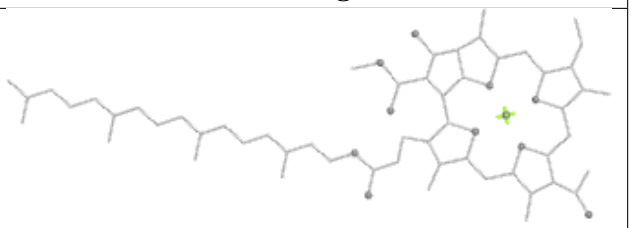
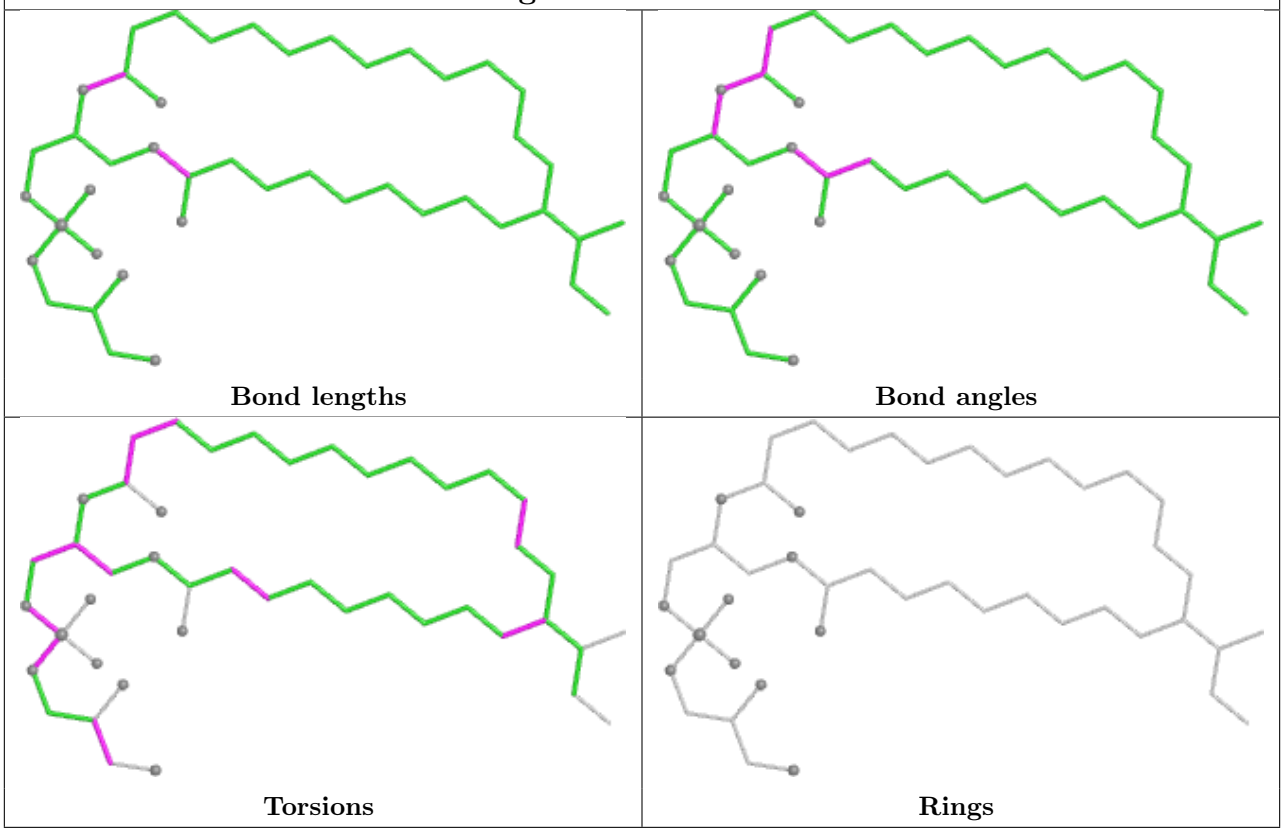
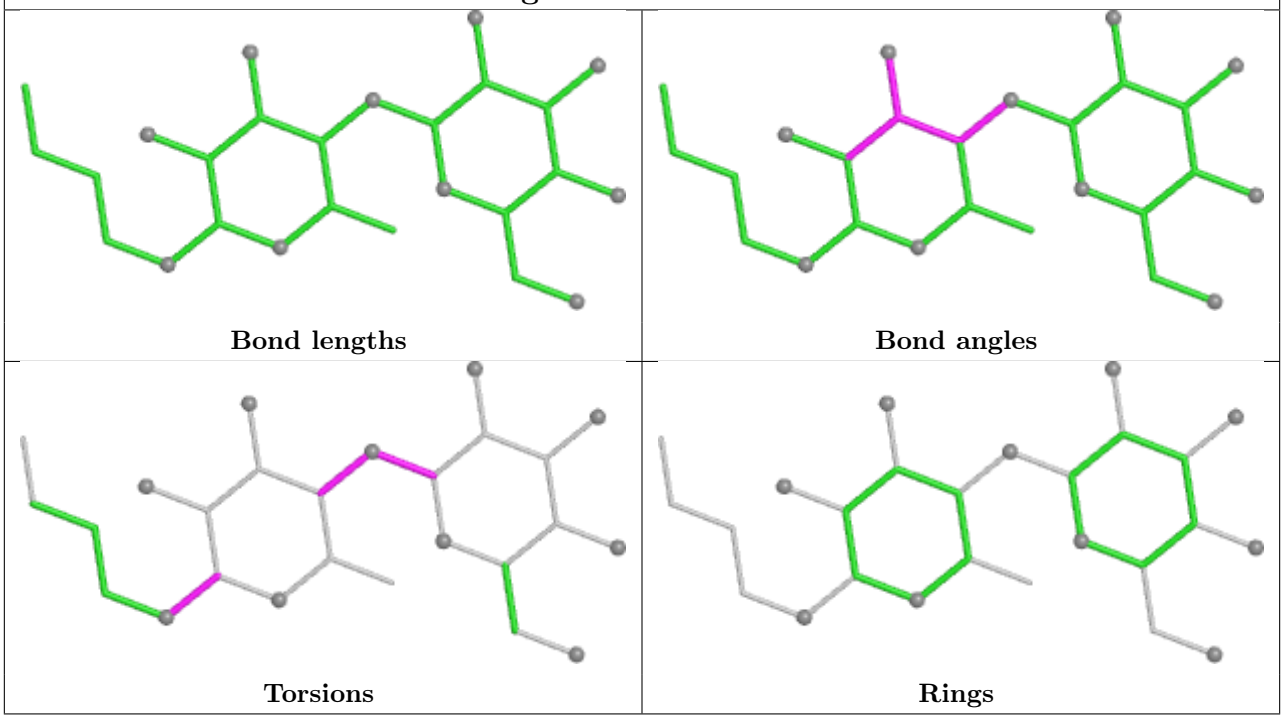
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PGV M 402



Ligand LMT D 101



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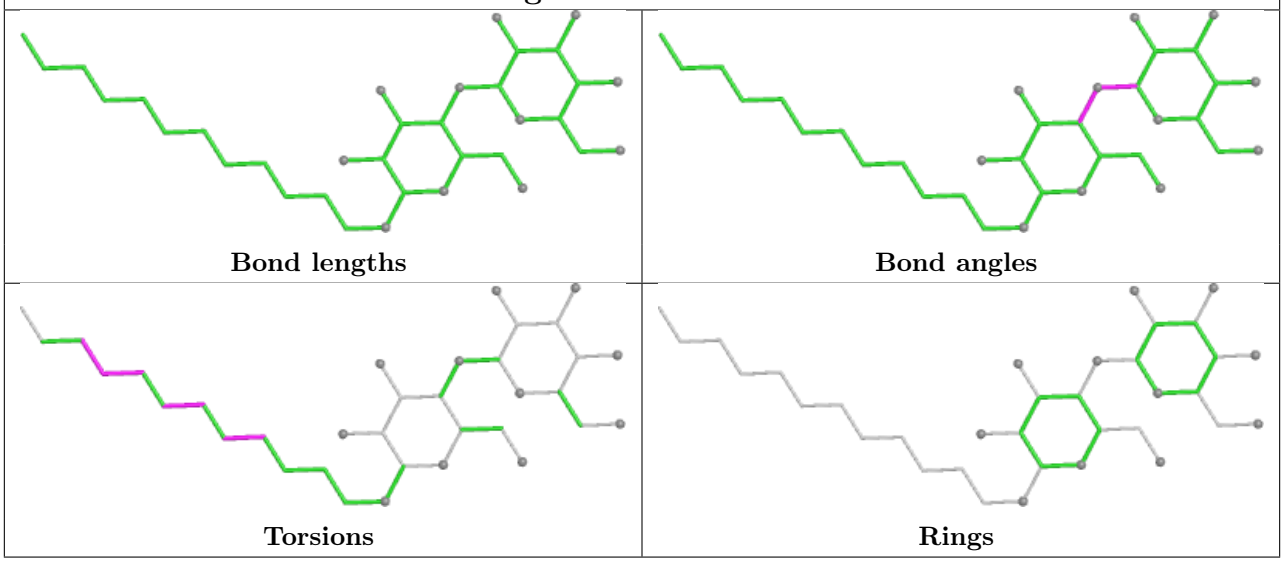
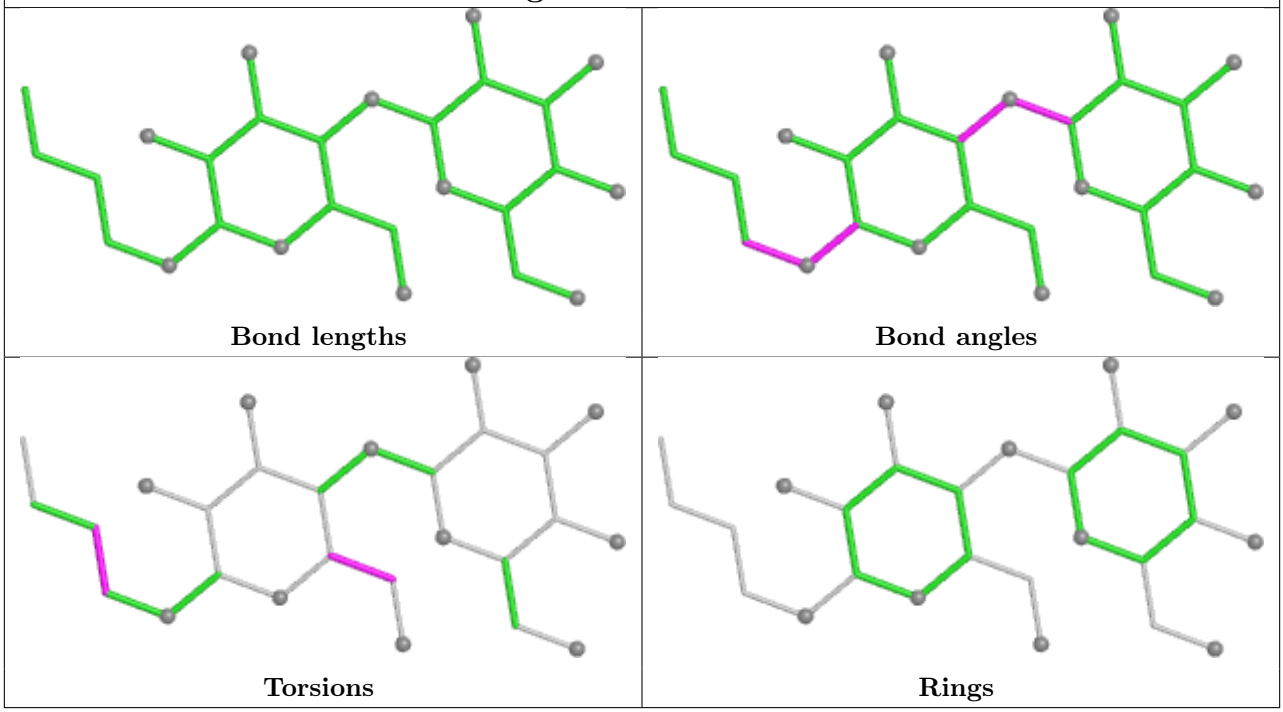


Ligand LMT a 101



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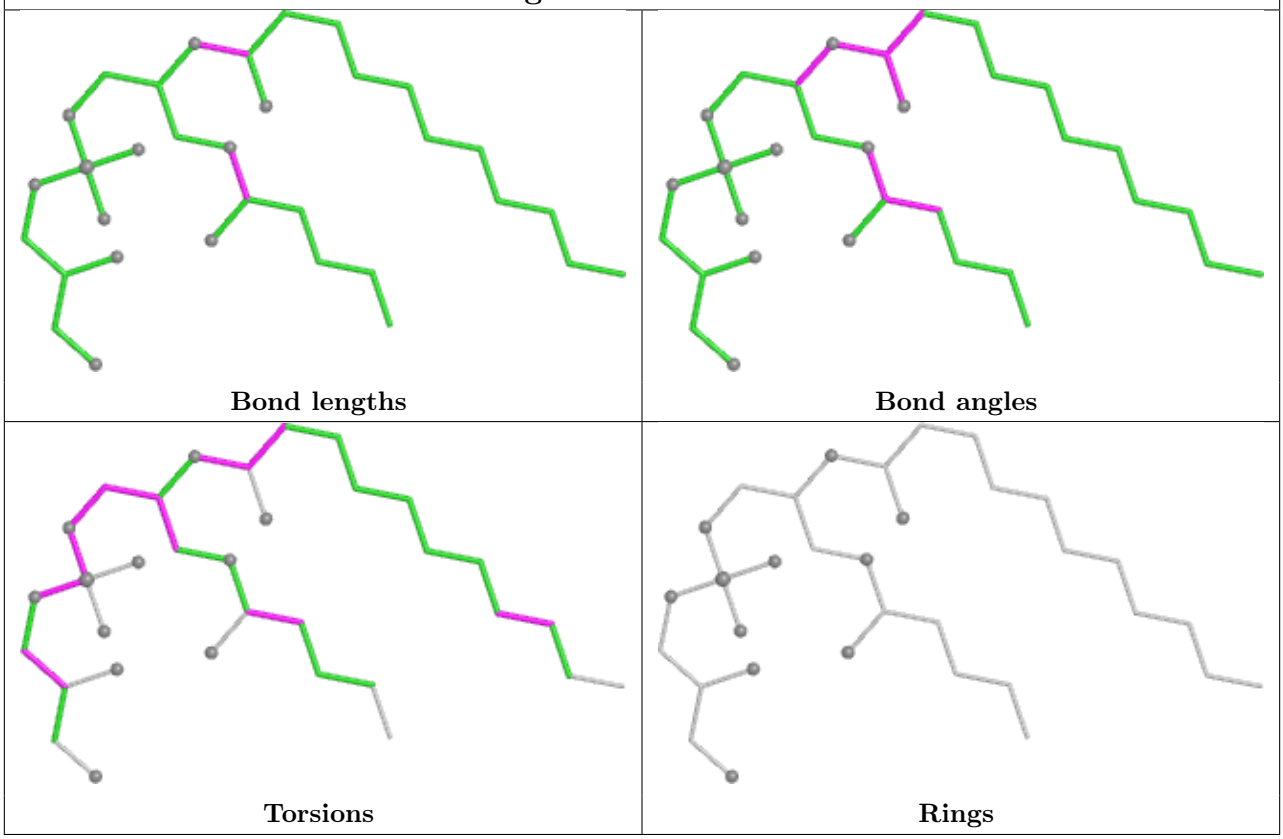

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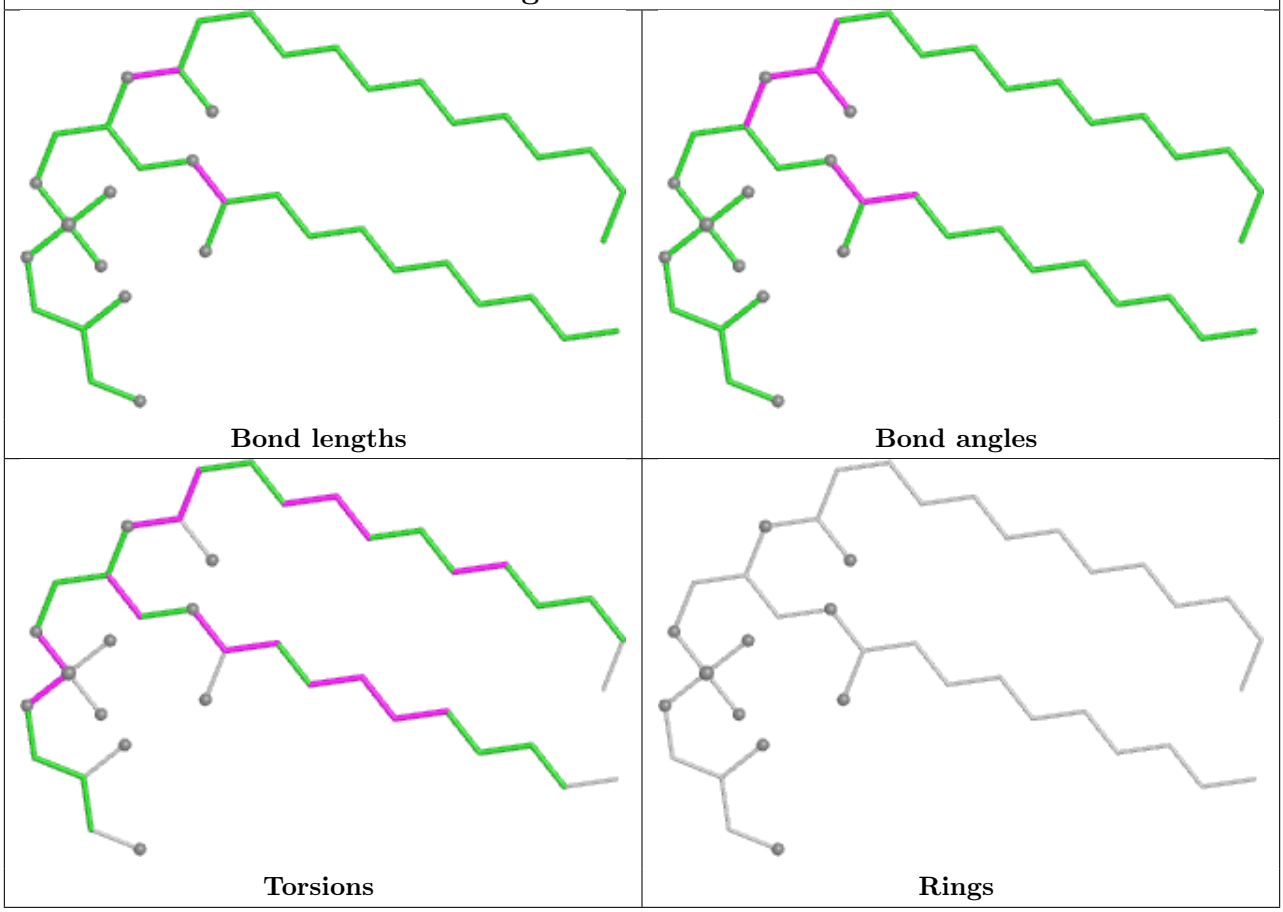
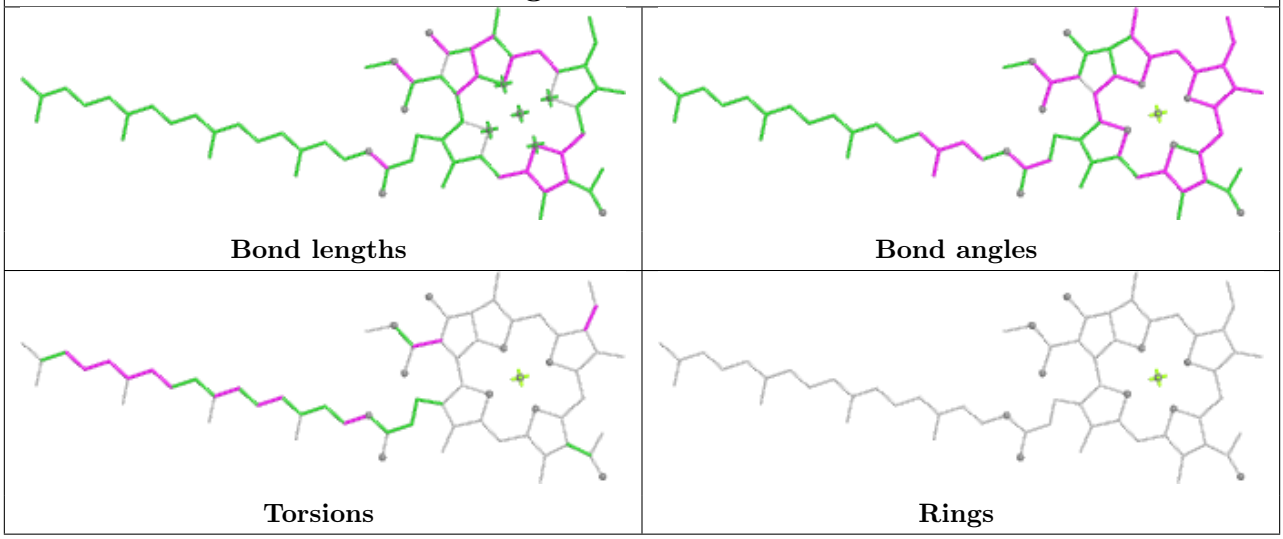
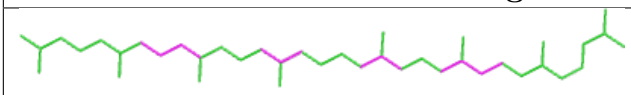
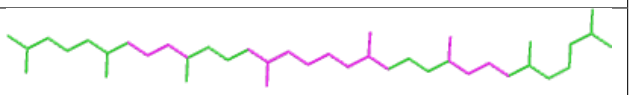
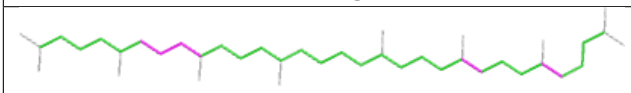
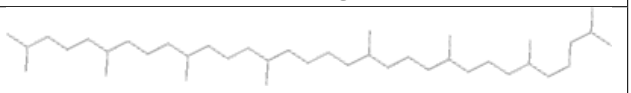


Ligand BCL K 102



Ligand A1EF2 N 103	
 Bond lengths	 Bond angles
 Torsions	 Rings

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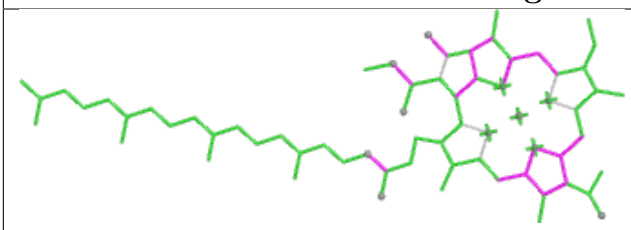
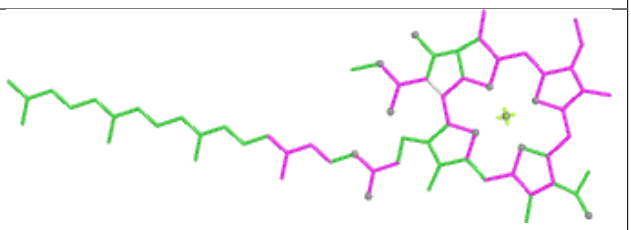
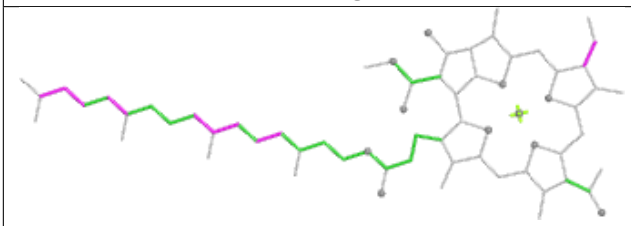
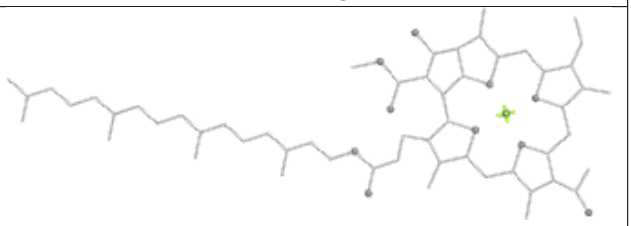
 Bond lengths	 Bond angles
 Torsions	 Rings

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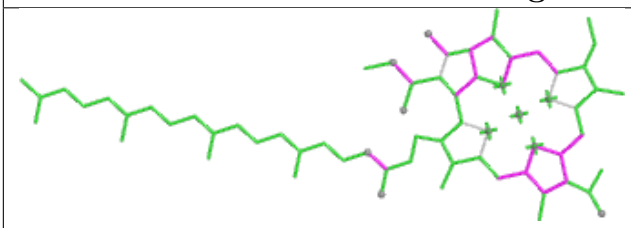
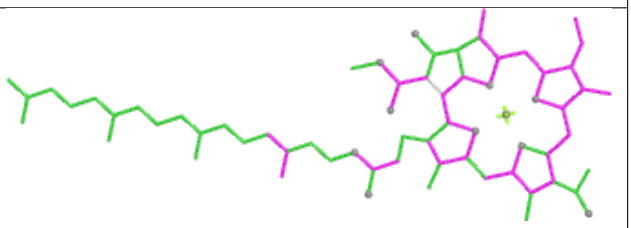
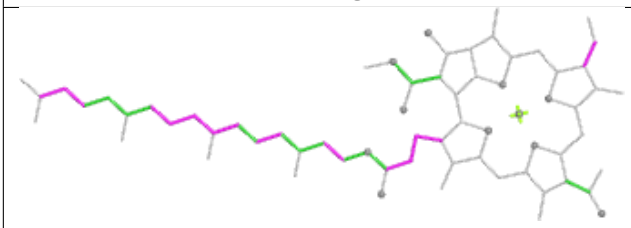
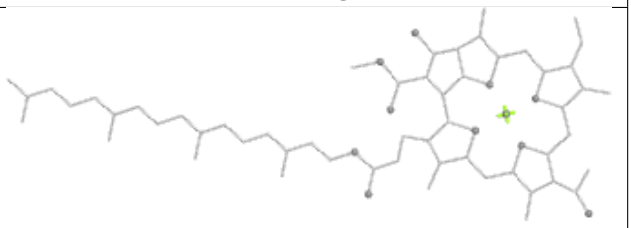
 Bond lengths	 Bond angles
 Torsions	 Rings

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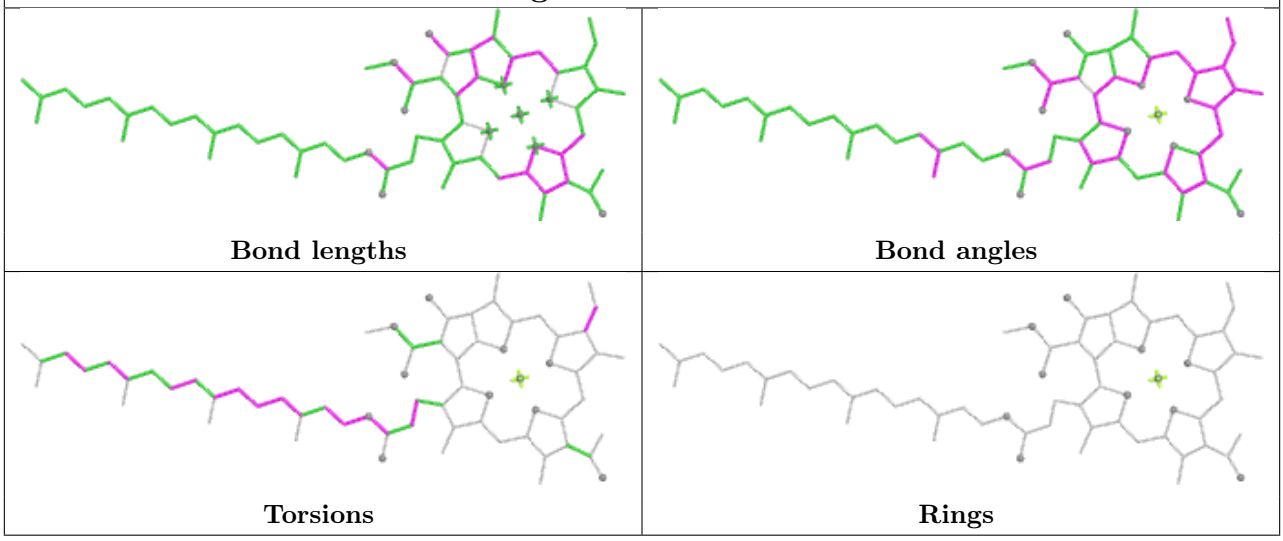
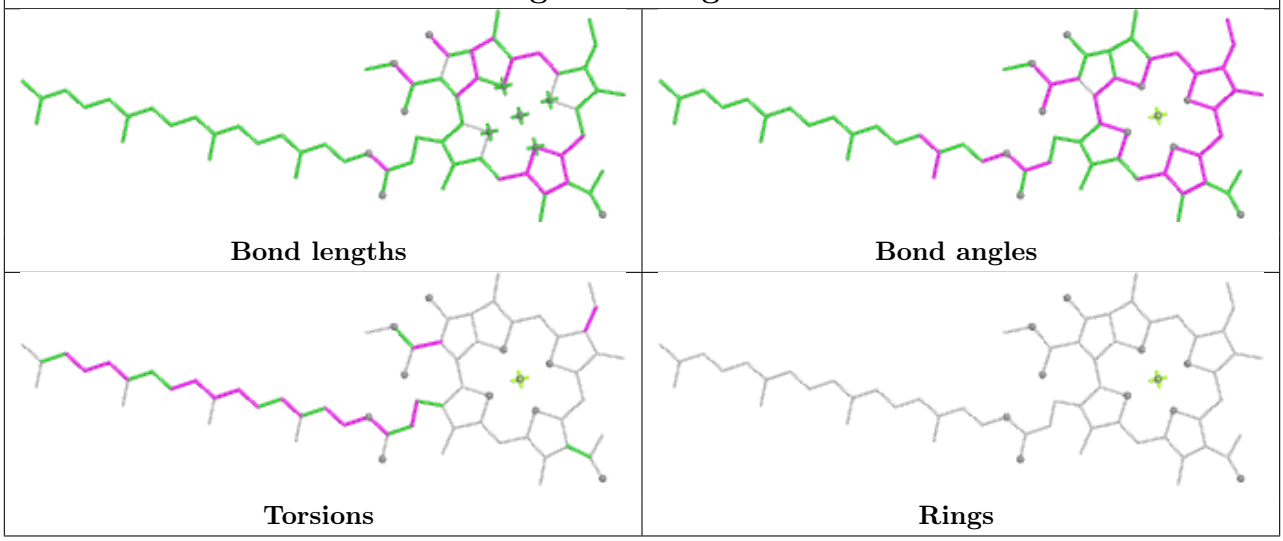
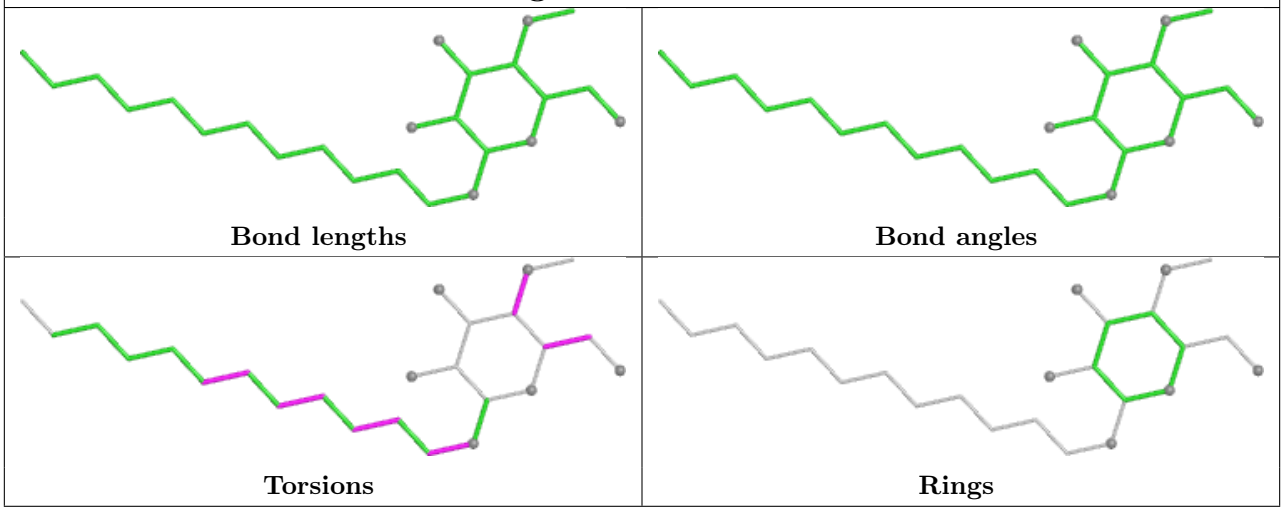


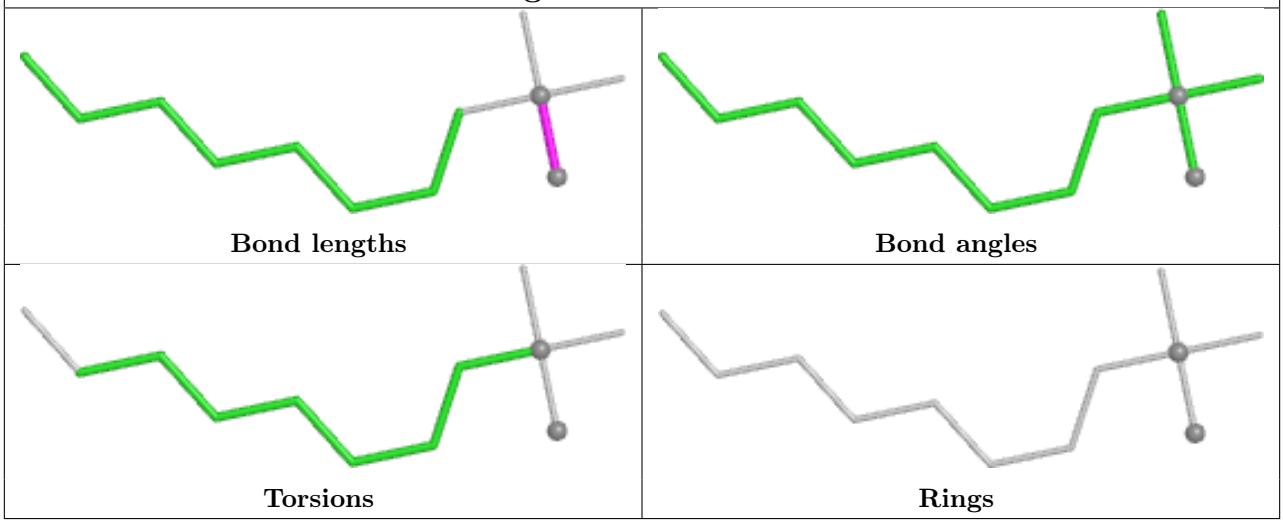
Ligand BCL g 102



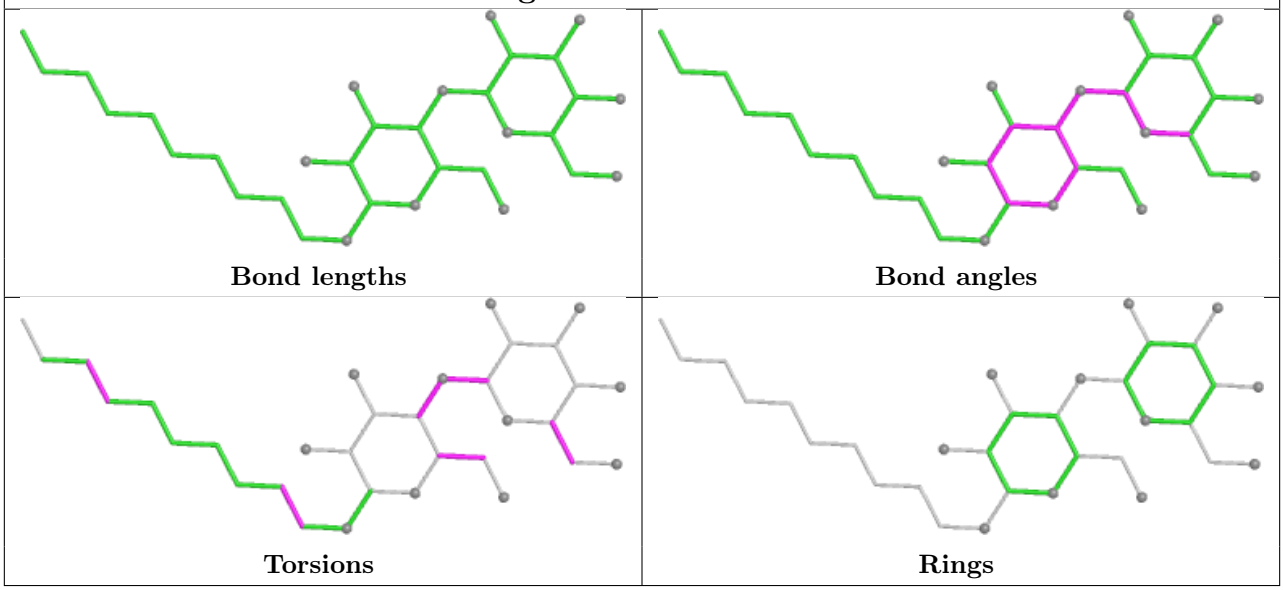
Ligand LMT I 101



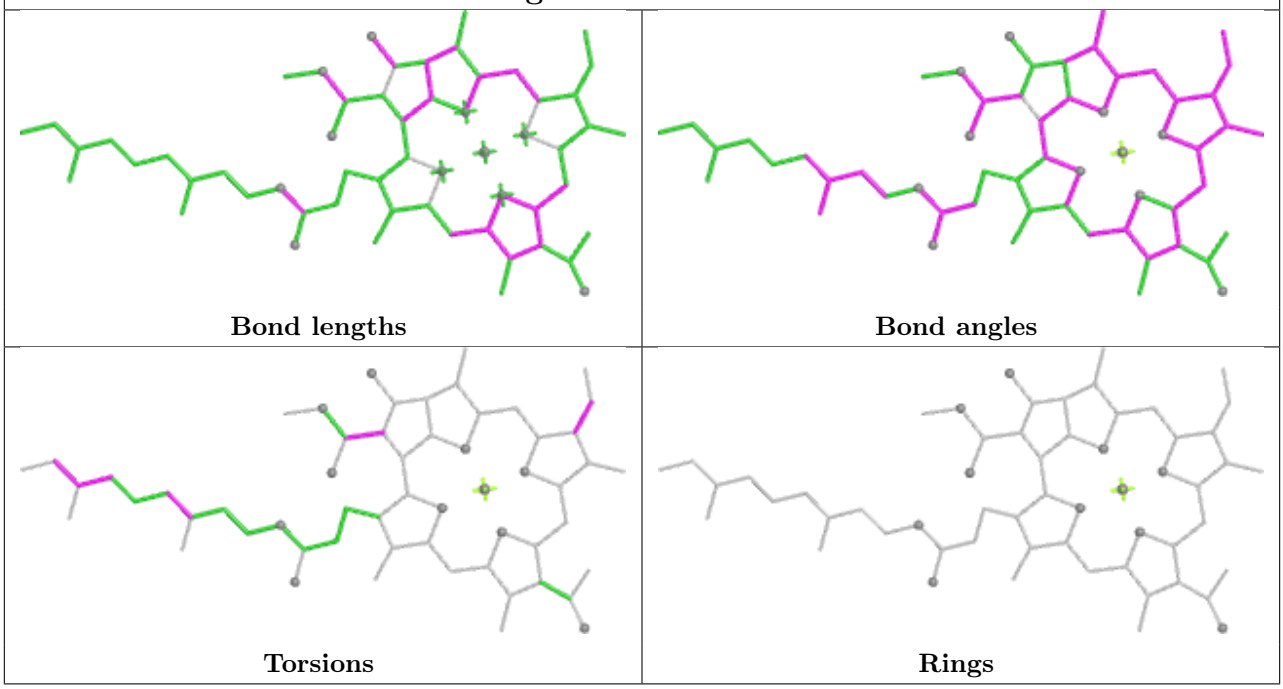
Ligand LDA K 101



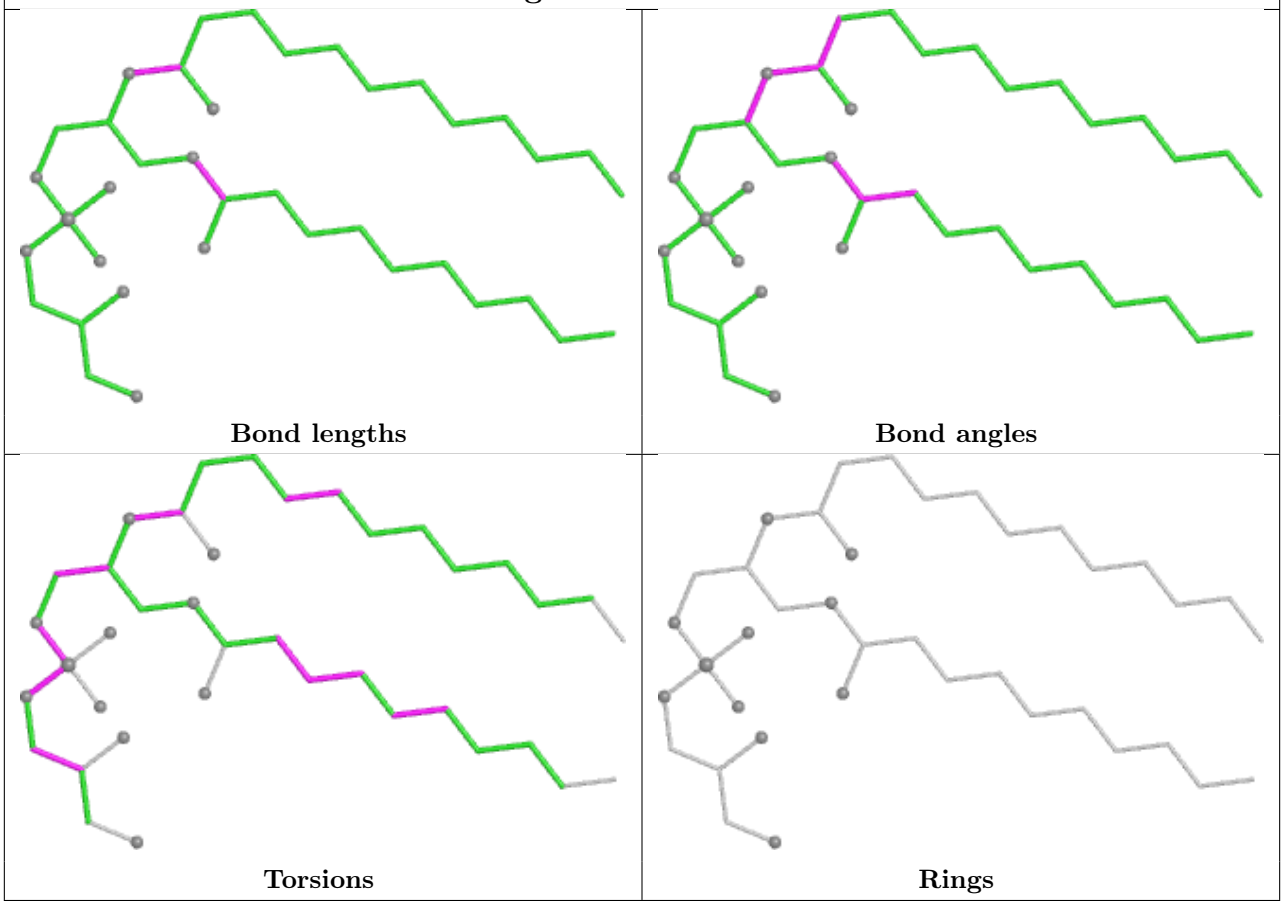
Ligand LMT M 409



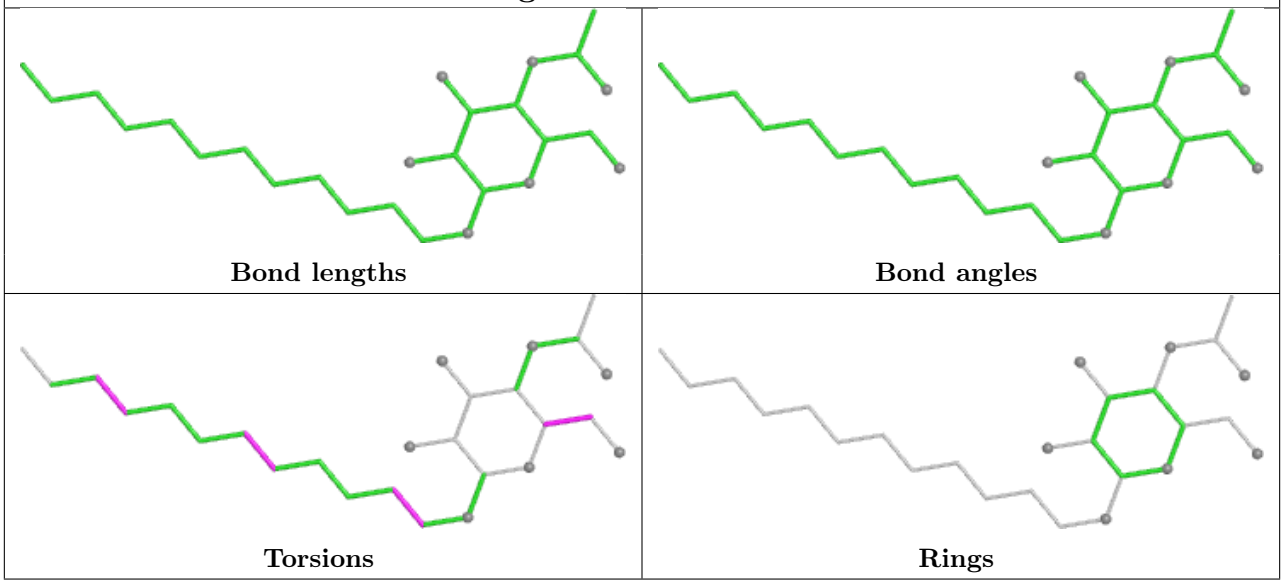
Ligand BCL O 102



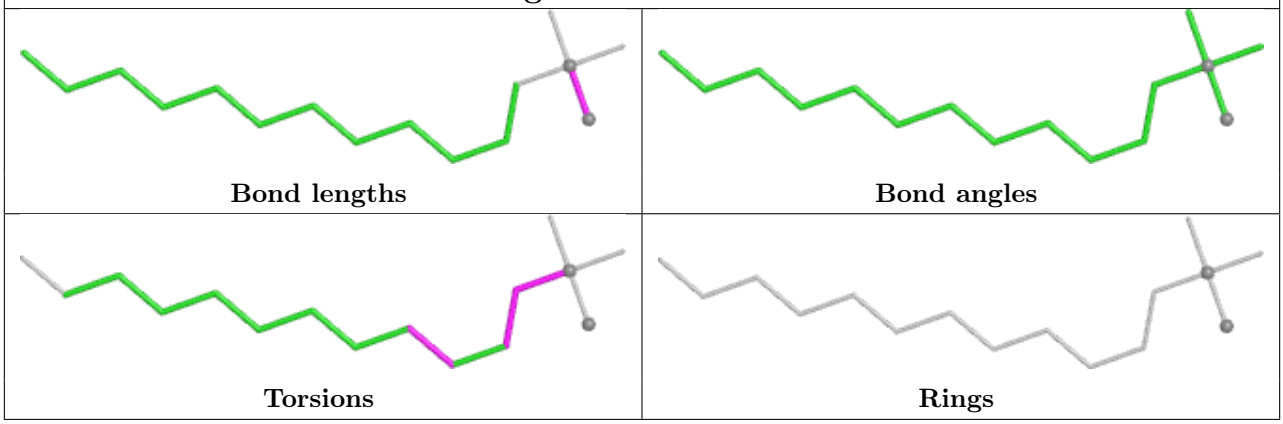
Ligand PGV L 305



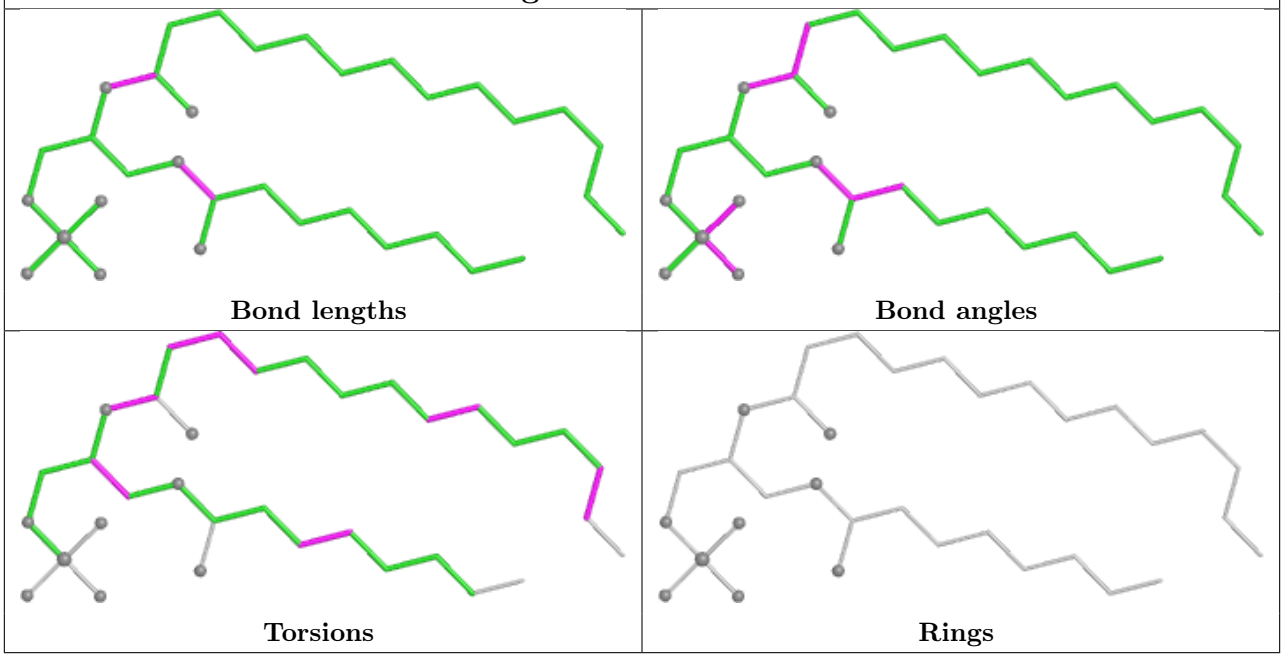
Ligand LMT M 408



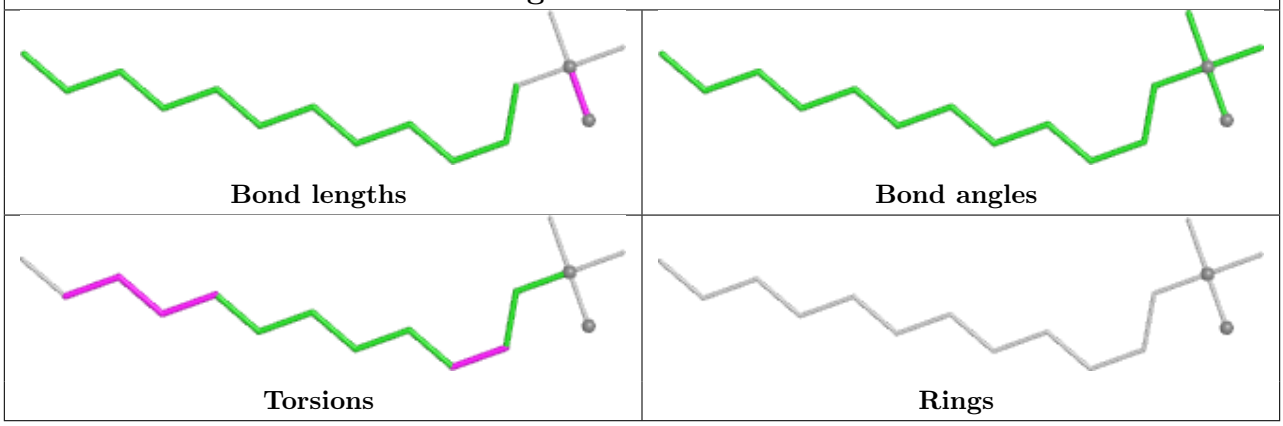
Ligand LDA X 102



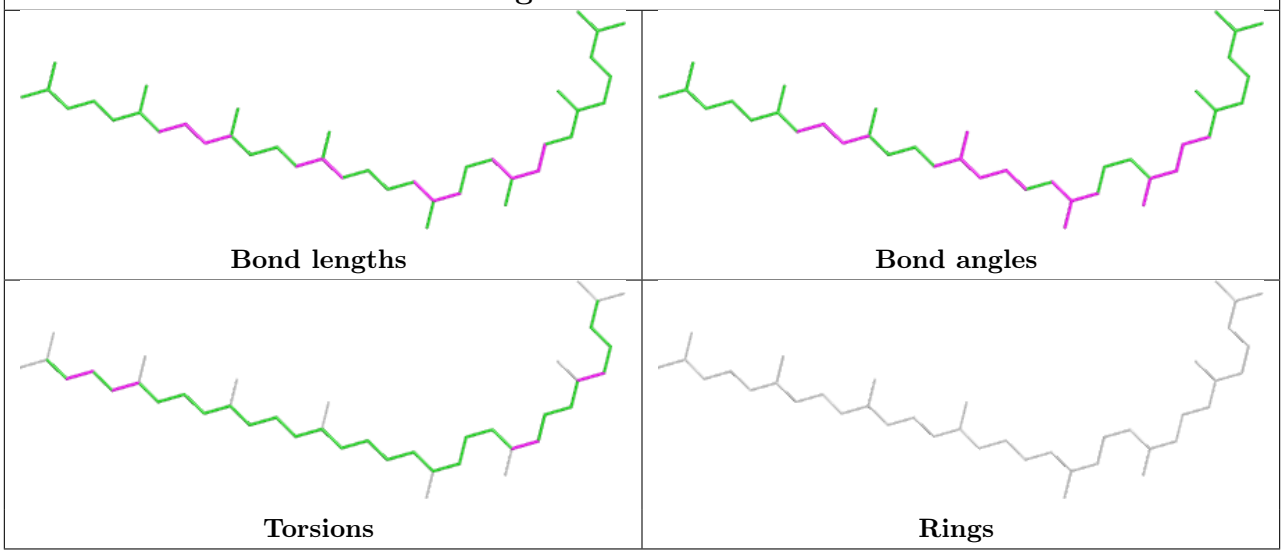
Ligand PGV H 303



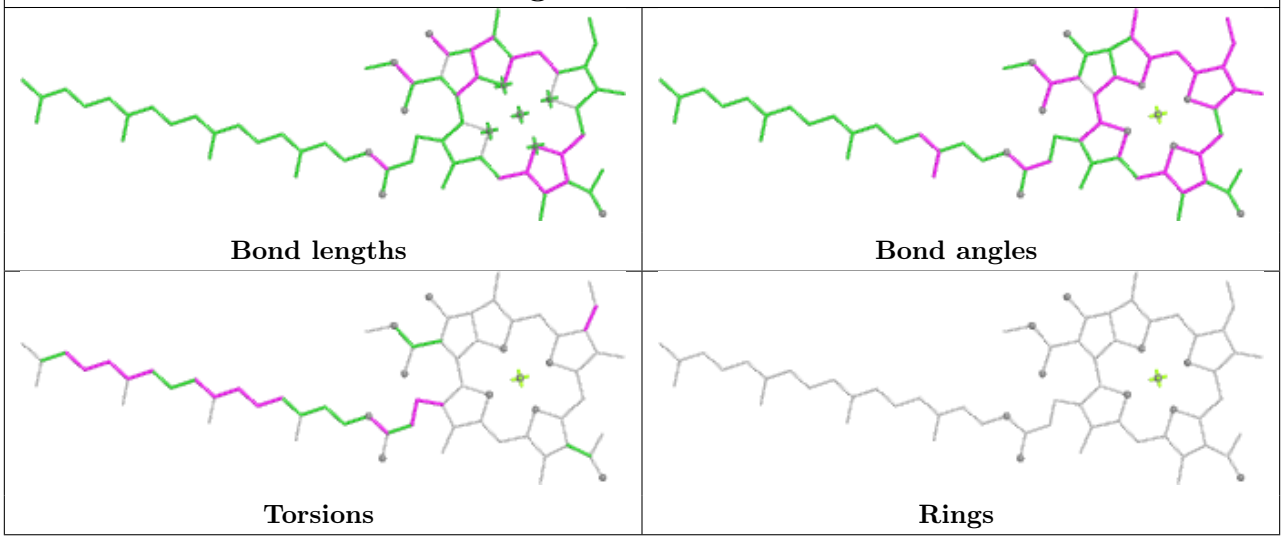
Ligand LDA L 310

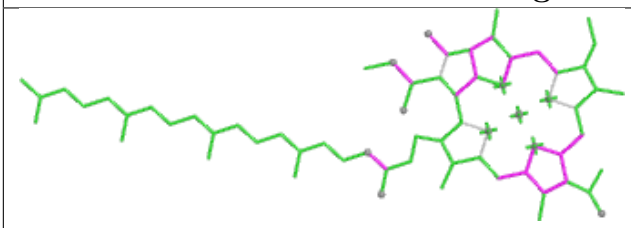
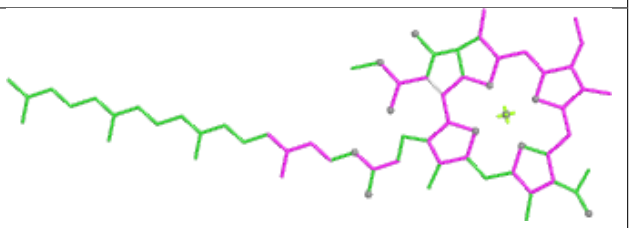
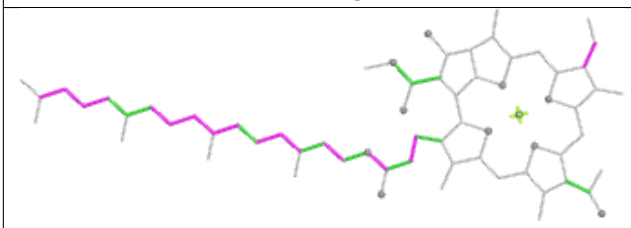
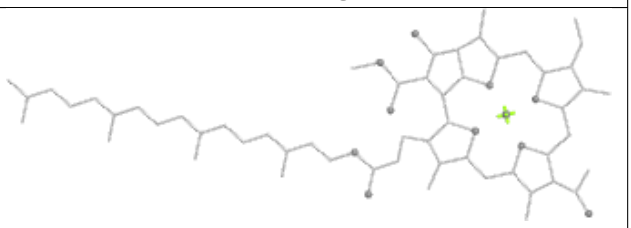


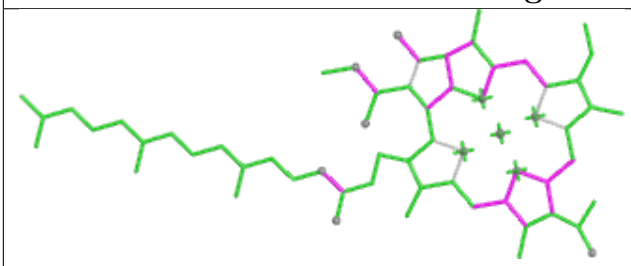
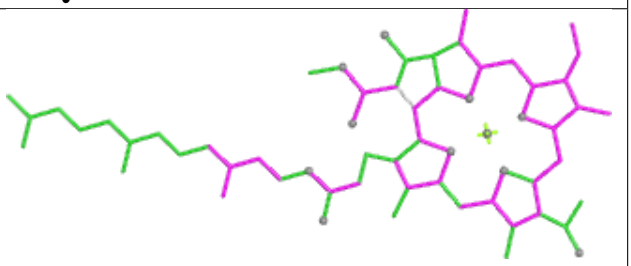
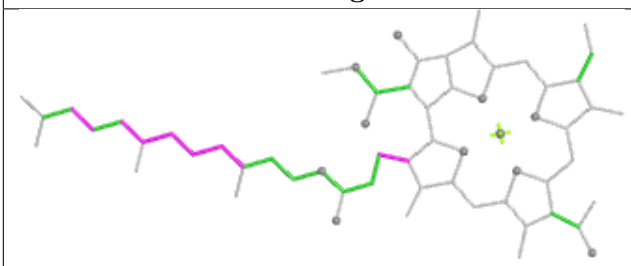
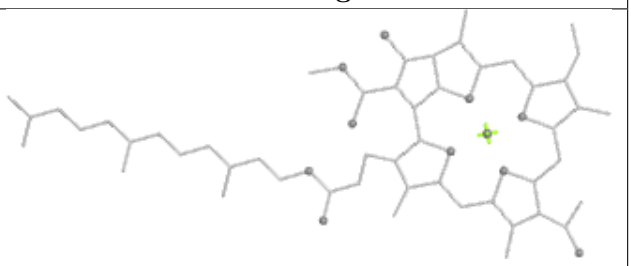
Ligand A1EF2 f 101



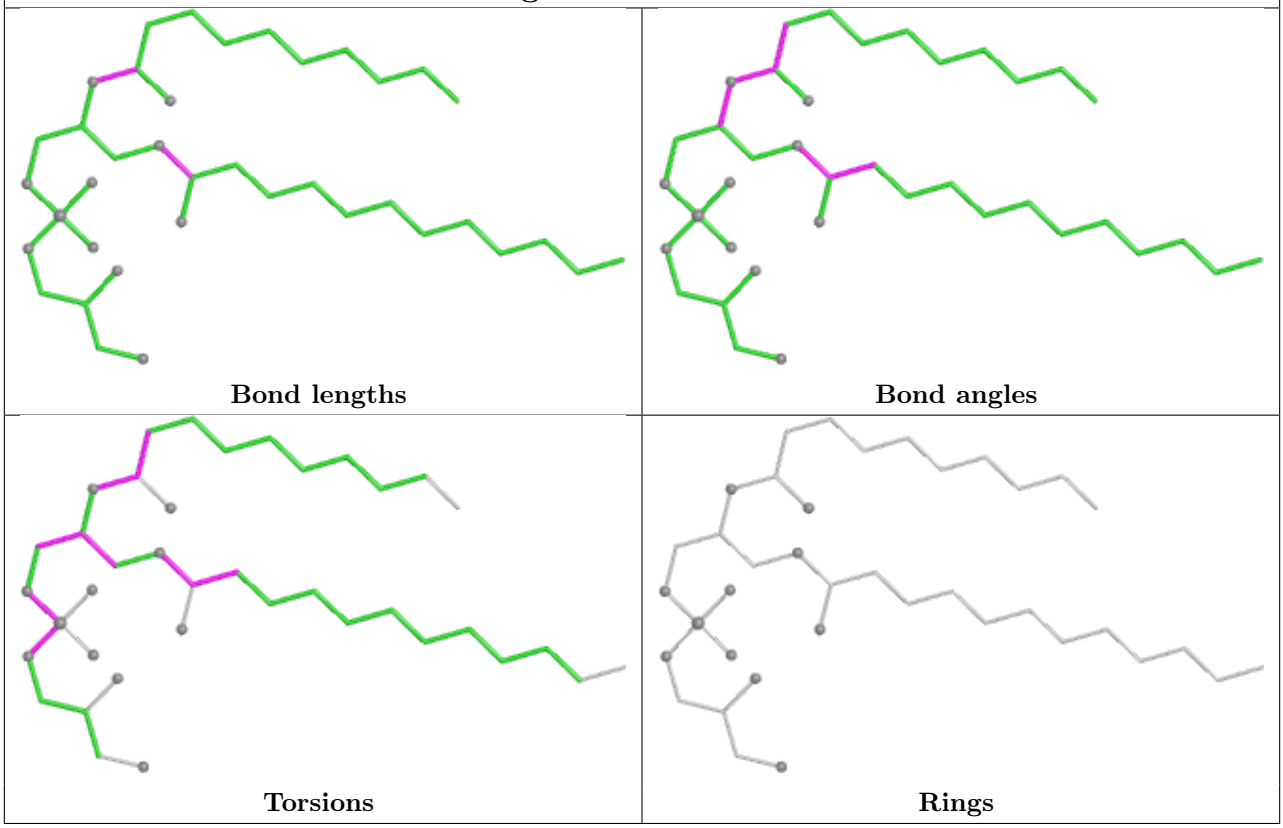
Ligand BCL d 102



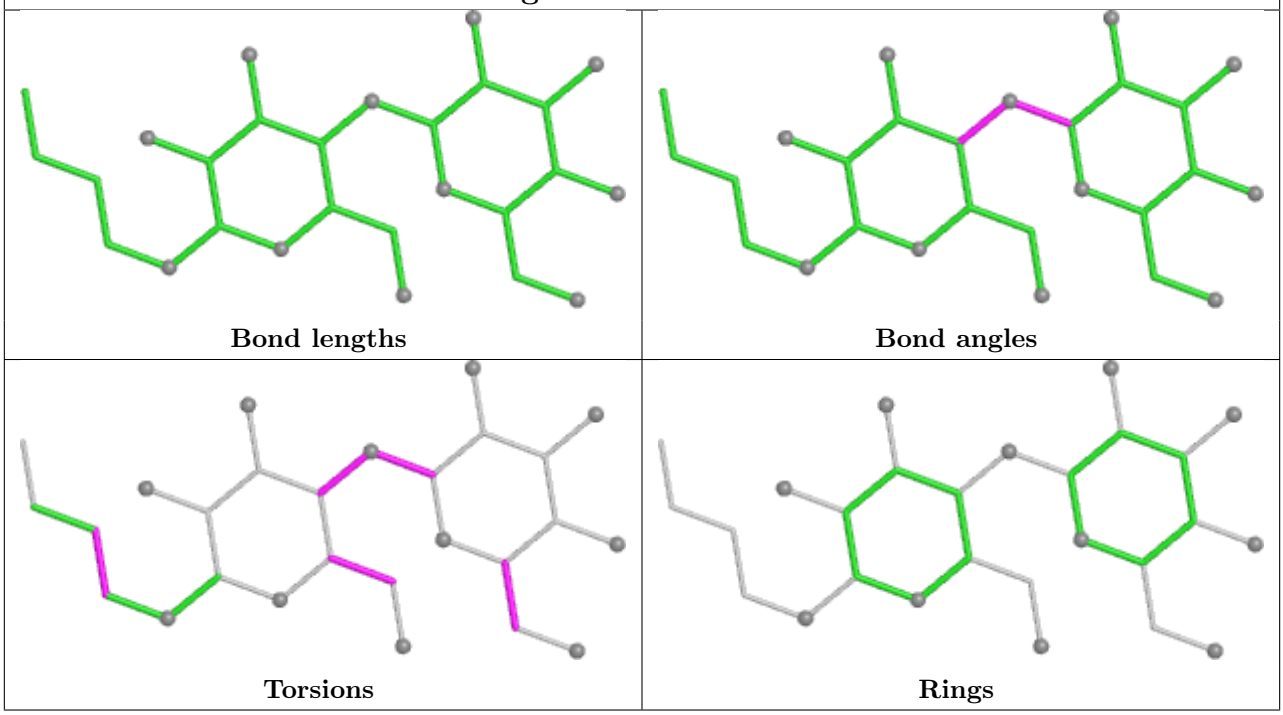
Ligand BCL i 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCL Q 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

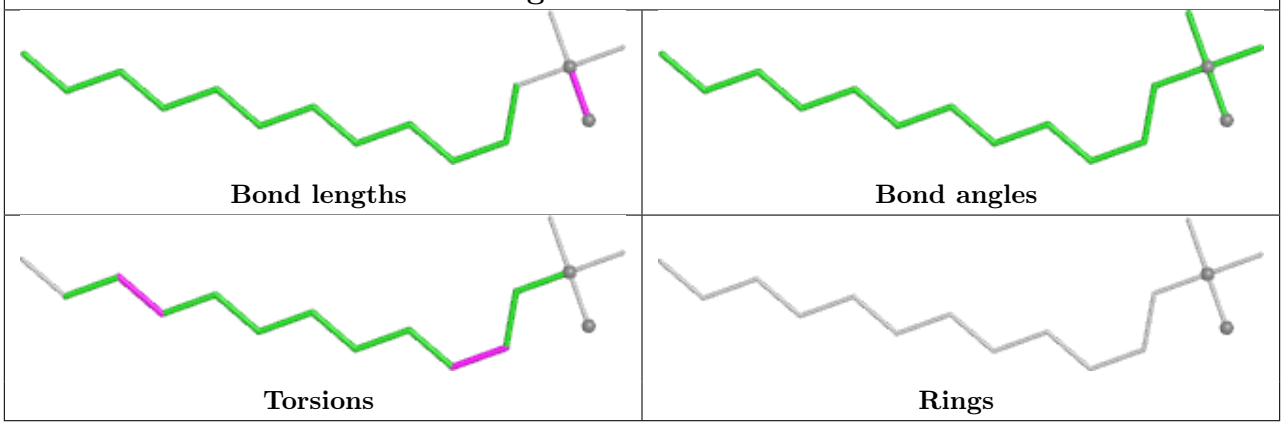
Ligand PGV G 103



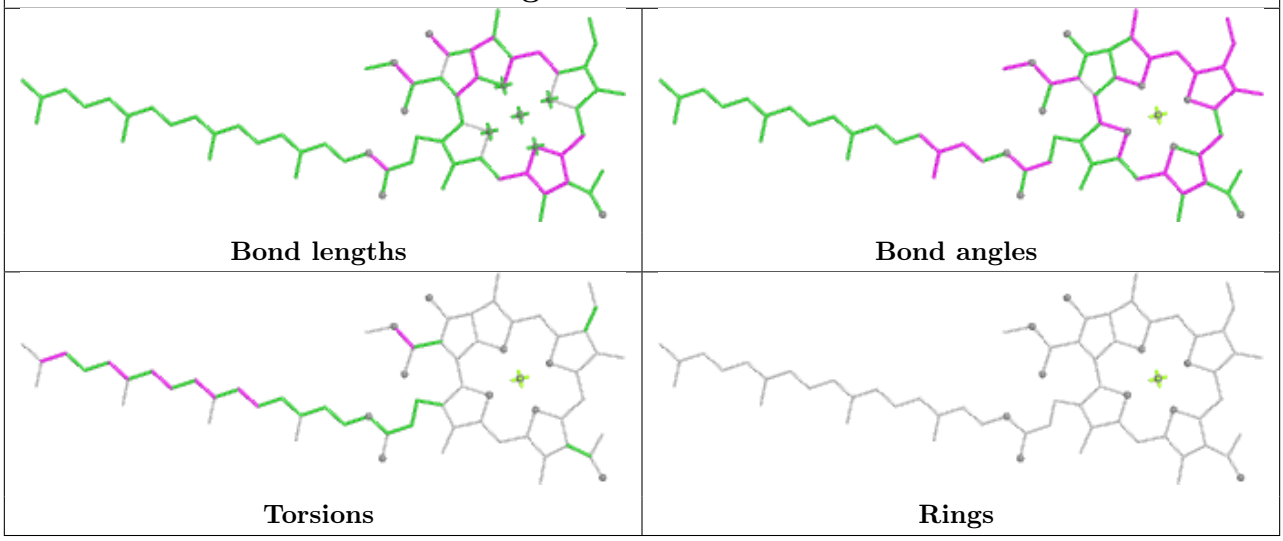
Ligand LMT D 103



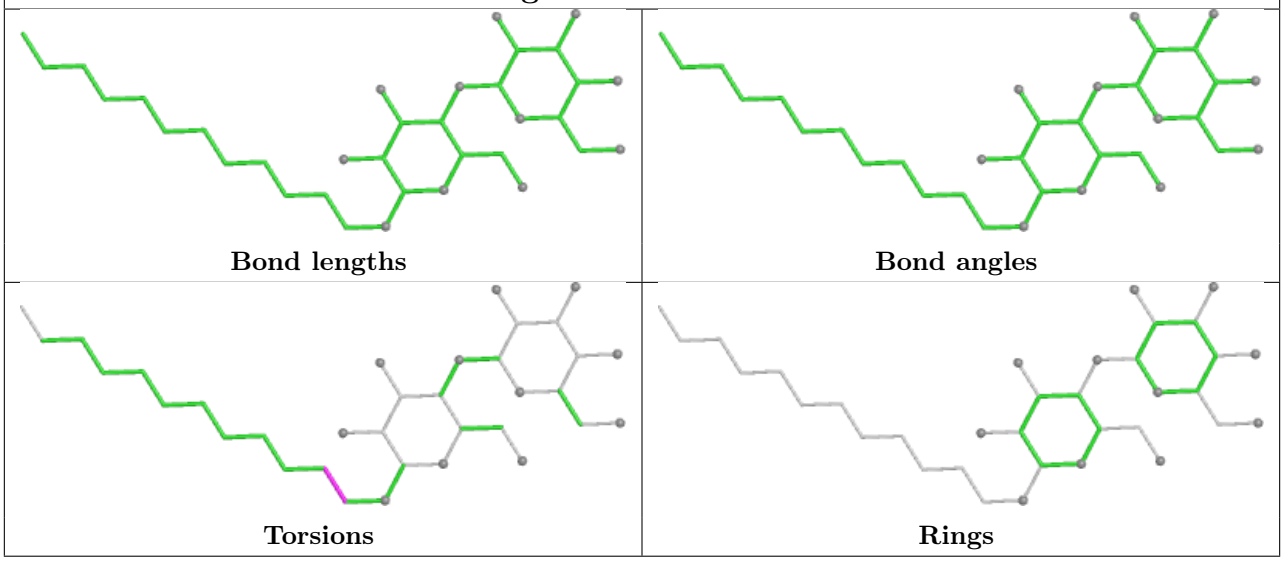
Ligand LDA L 307



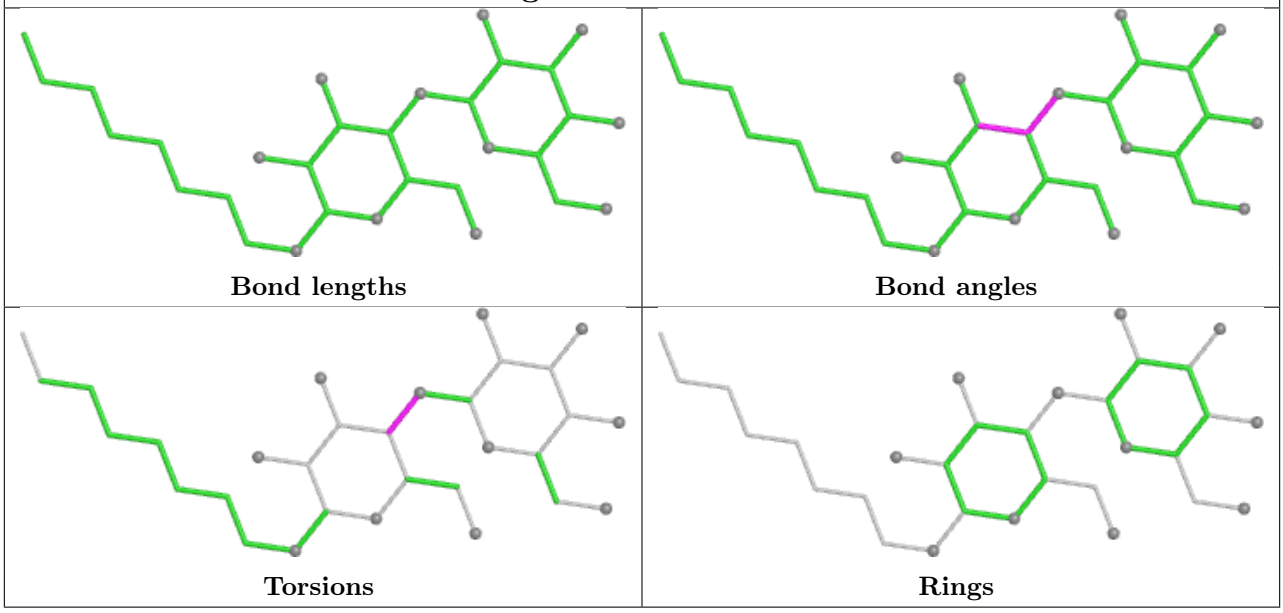
Ligand BCL M 404



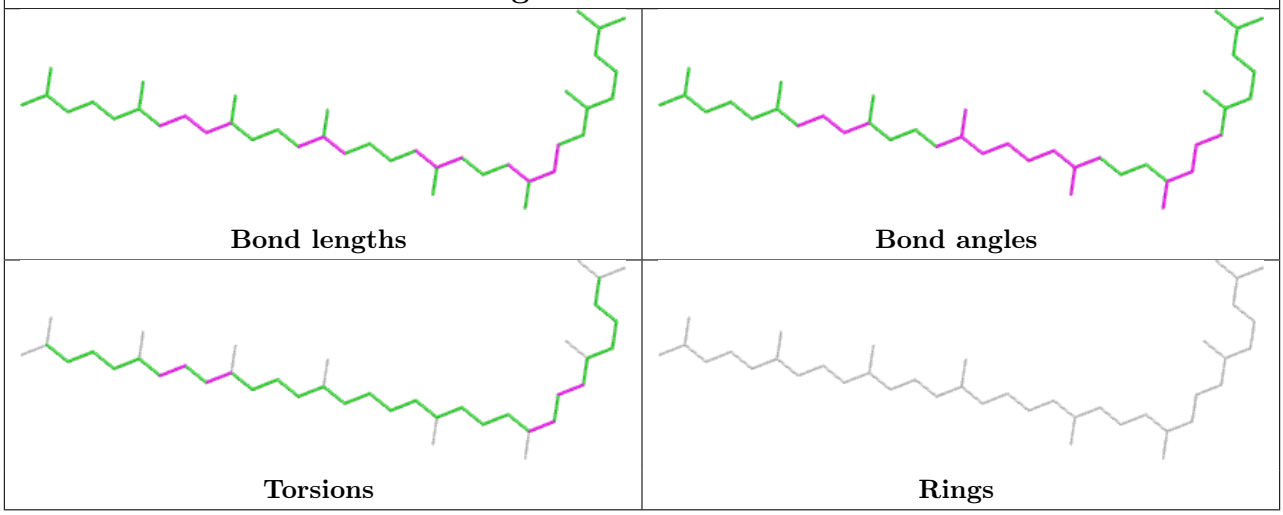
Ligand LMT H 301



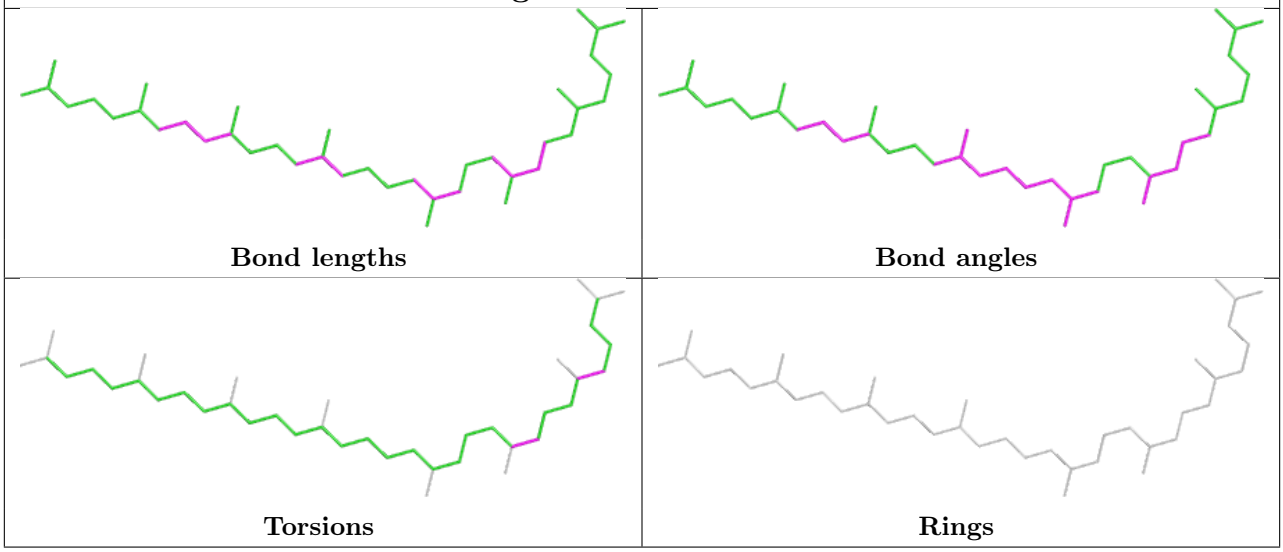
Ligand LMT X 103



Ligand A1EF2 J 101



Ligand A1EF2 o 101



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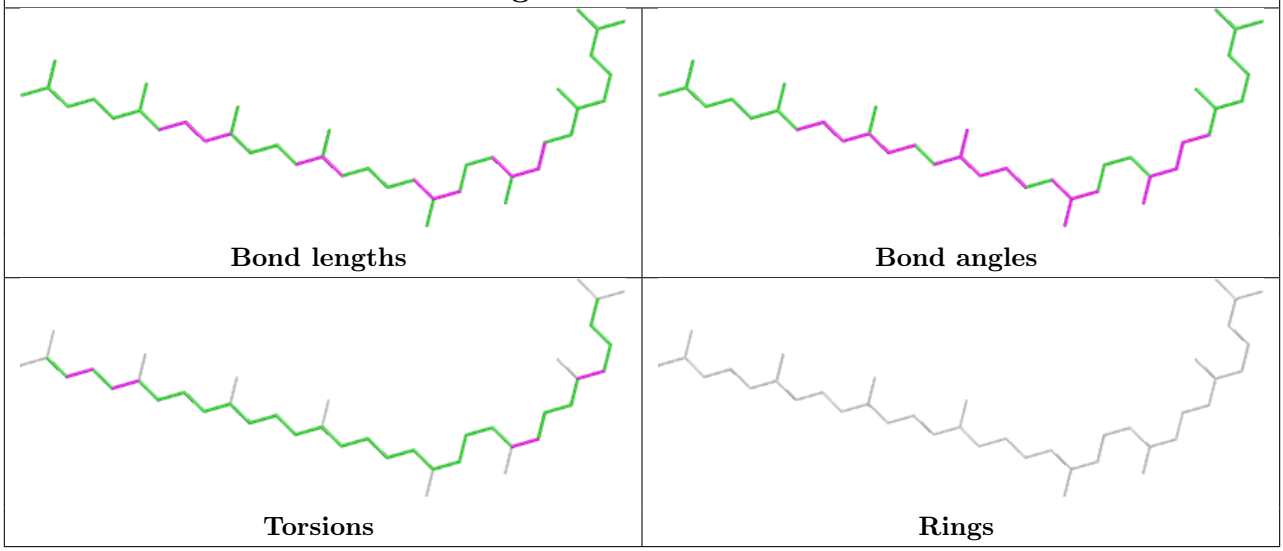
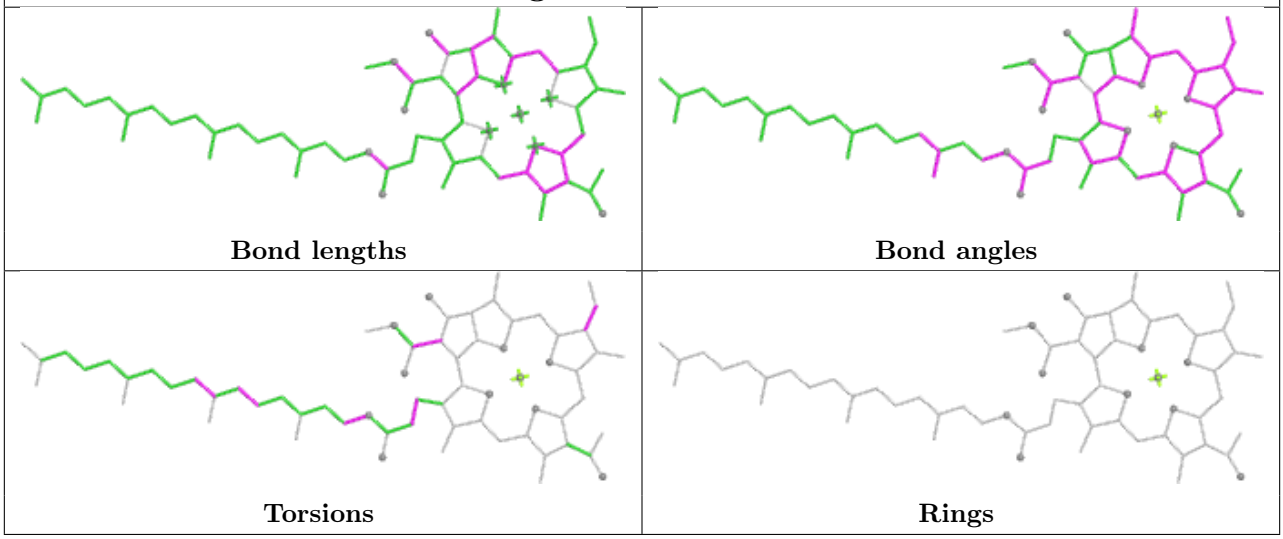
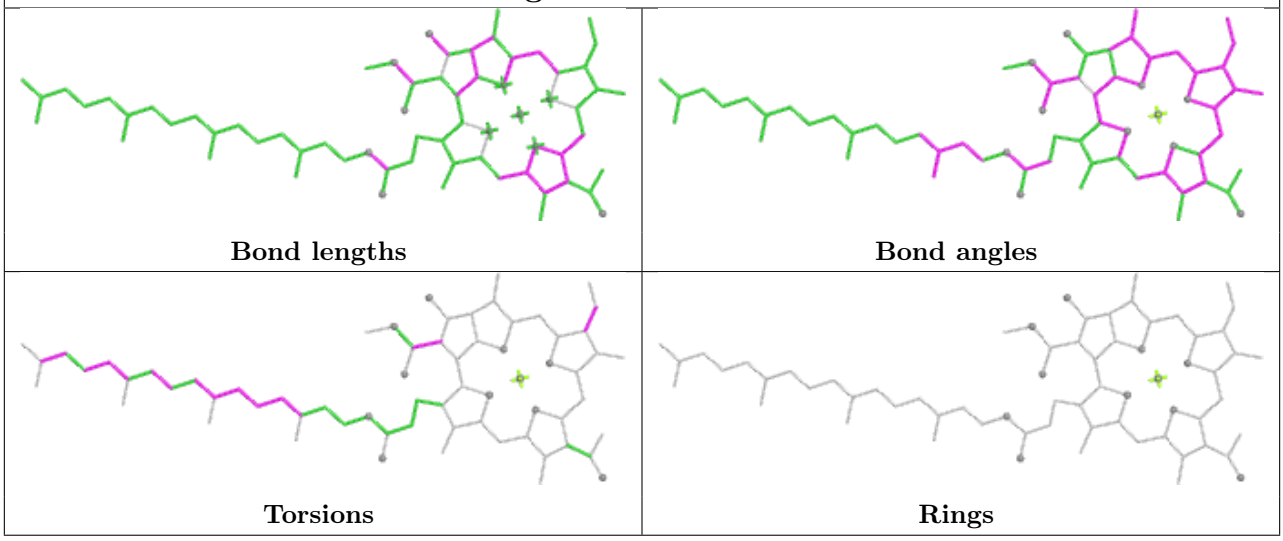


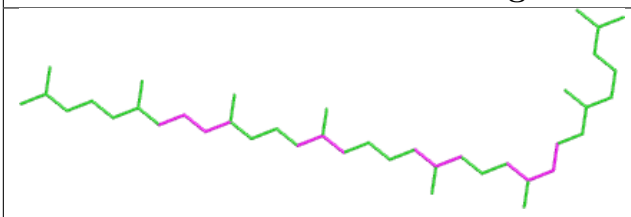
Ligand BCL L 301



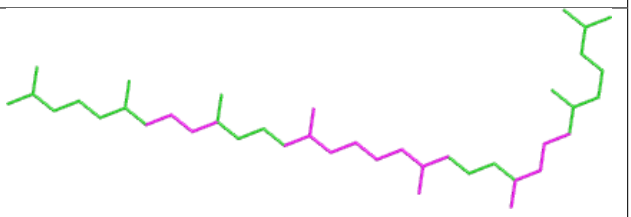
Ligand BCL G 104



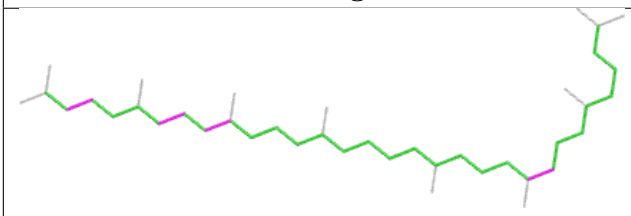
Ligand A1EF2 E 105



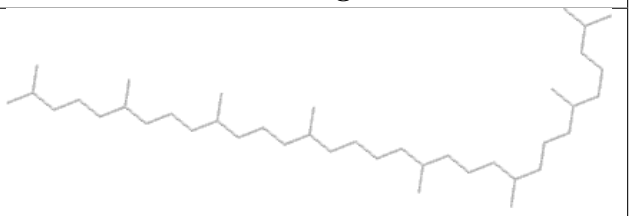
Bond lengths



Bond angles



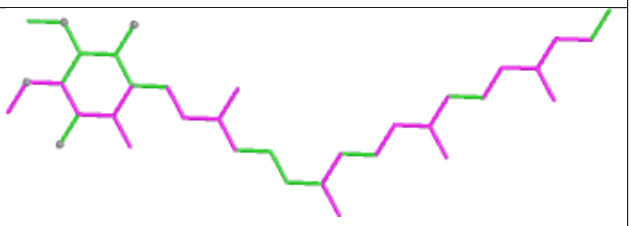
Torsions



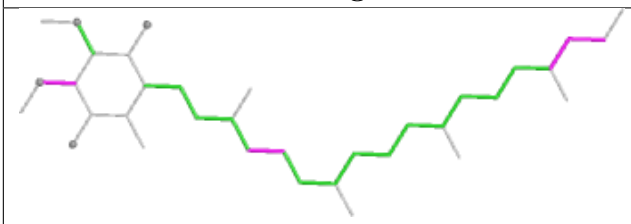
Rings

Ligand U10 L 304

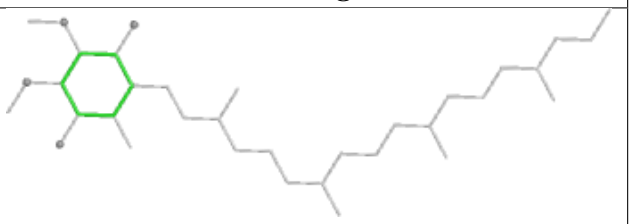
Bond lengths



Bond angles

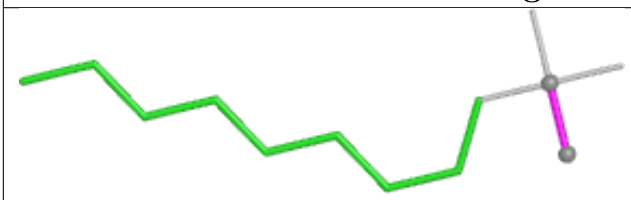


Torsions

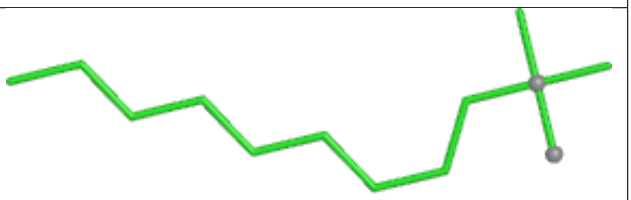


Rings

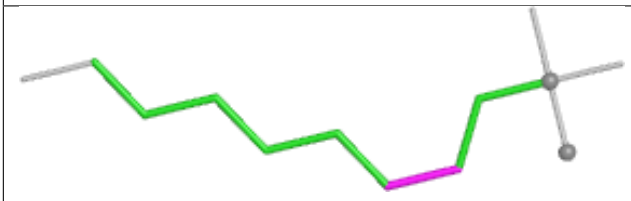
Ligand LDA X 101



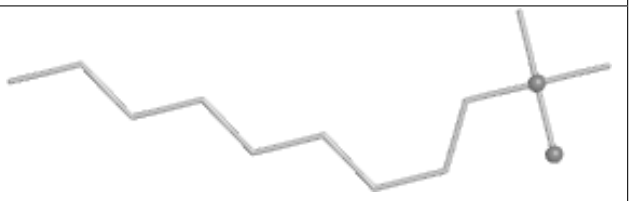
Bond lengths



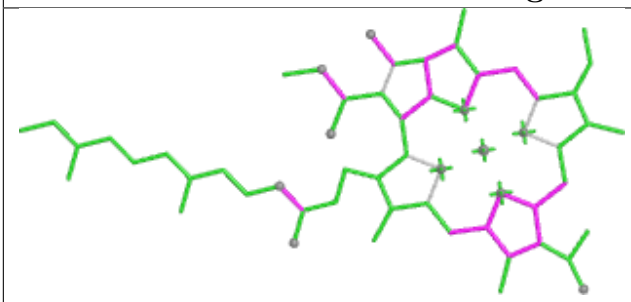
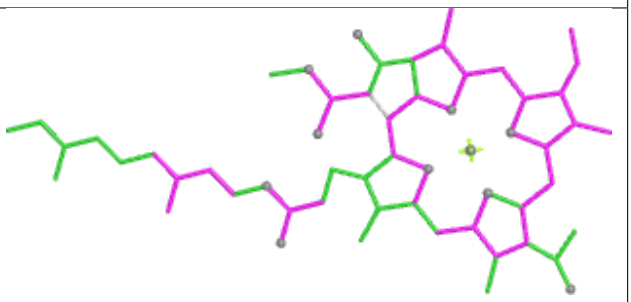
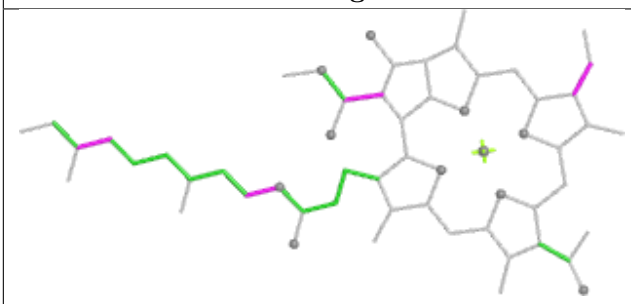
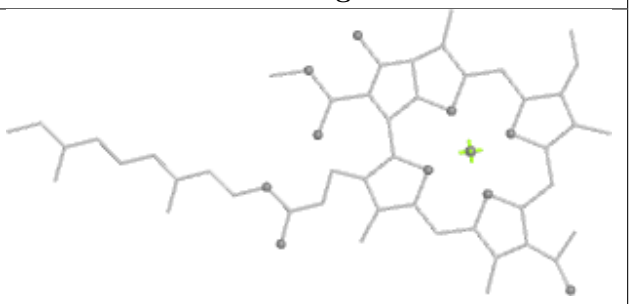
Bond angles

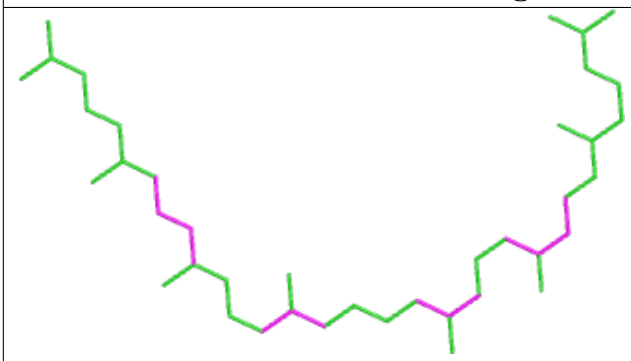
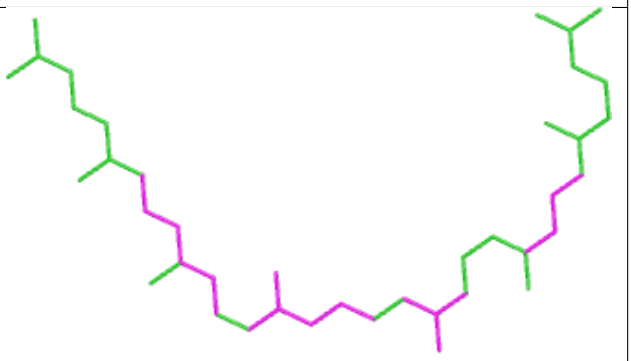
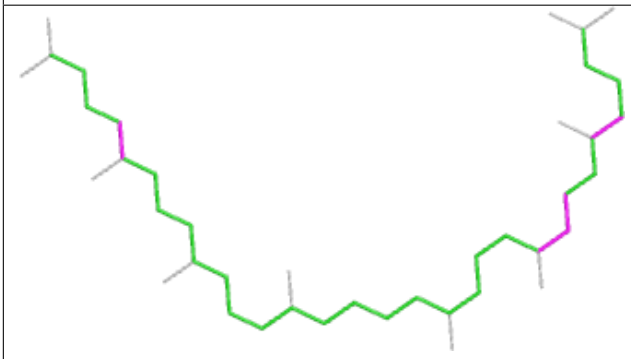
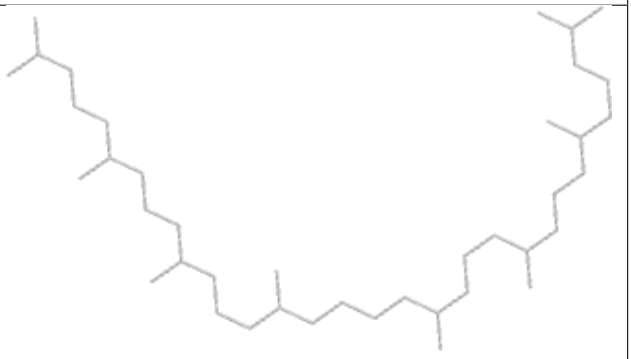


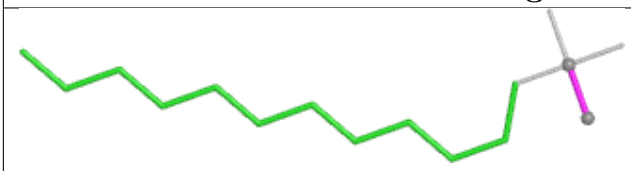
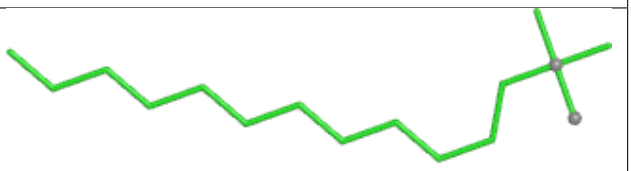
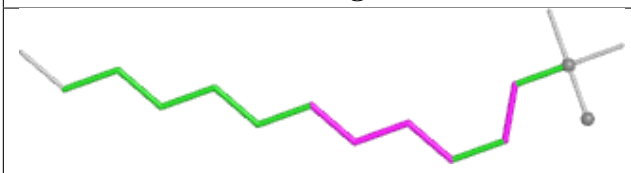
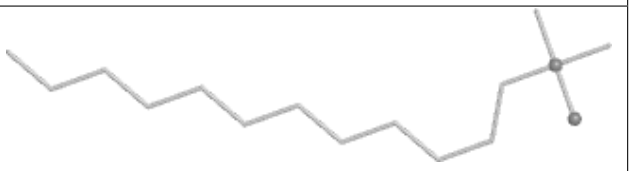
Torsions

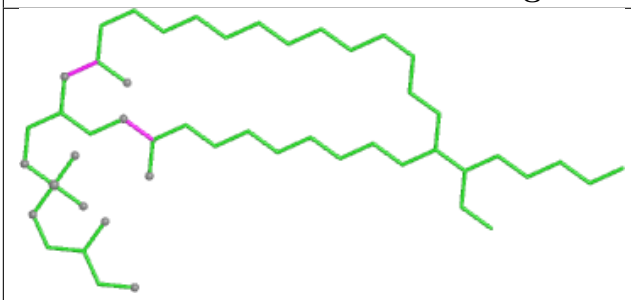
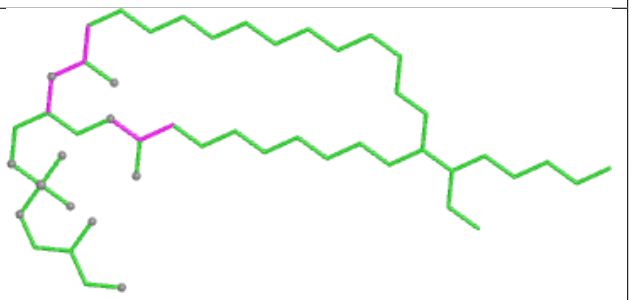
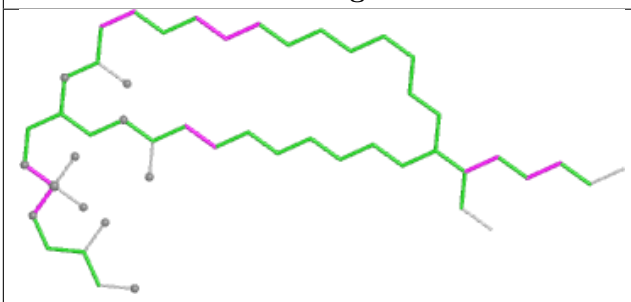
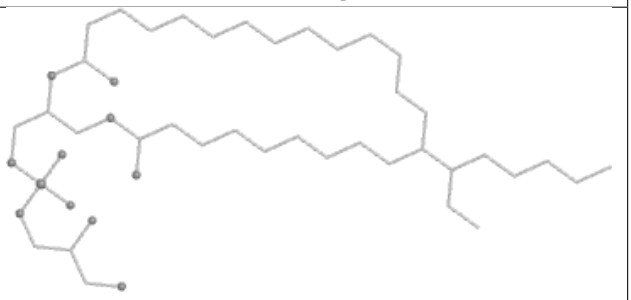


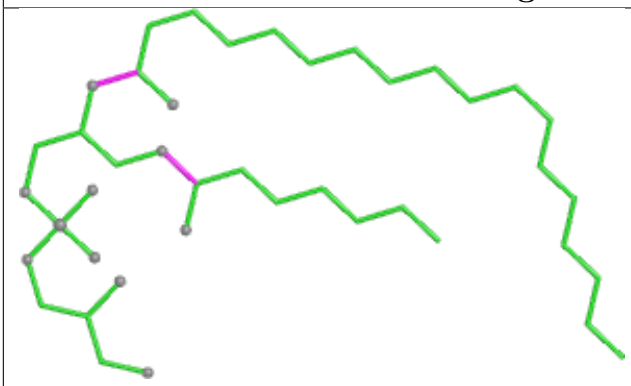
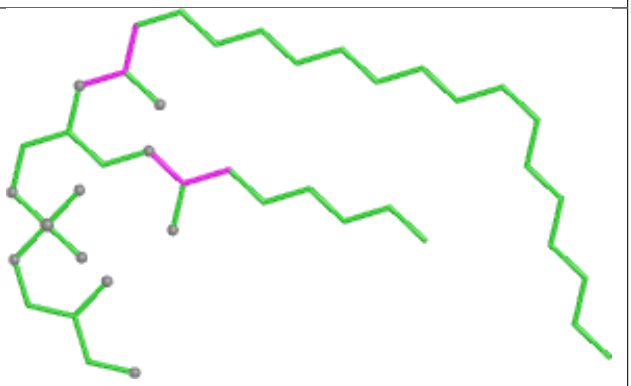
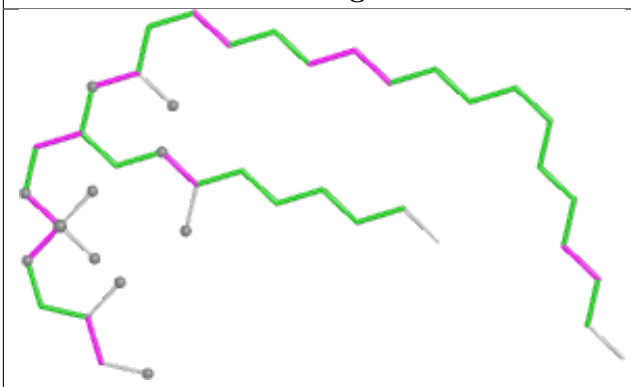
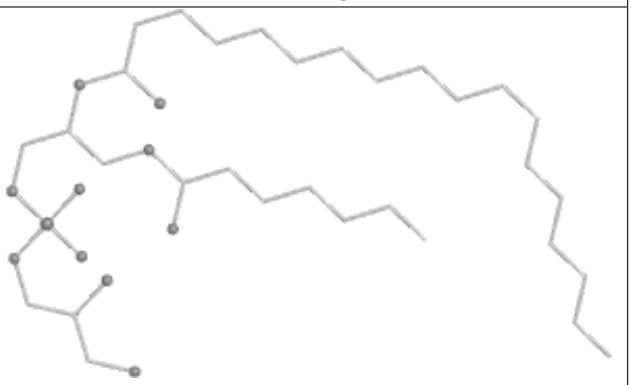
Rings

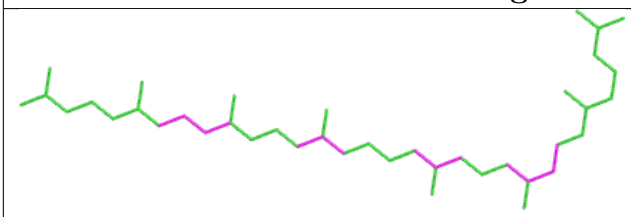
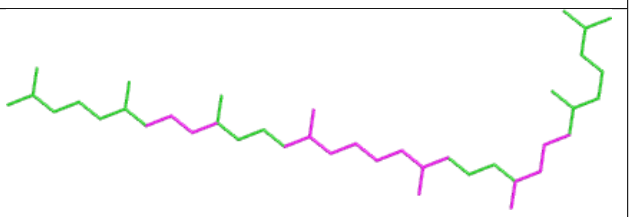
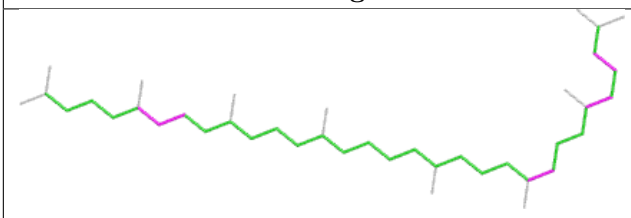
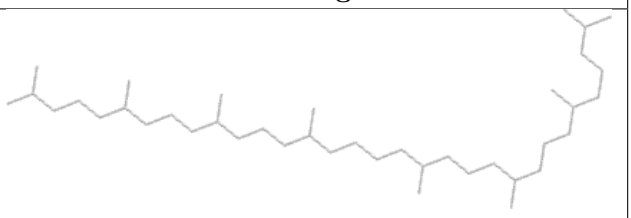
Ligand BCL E 103	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand A1EF2 c 104	
 Bond lengths	 Bond angles
 Torsions	 Rings

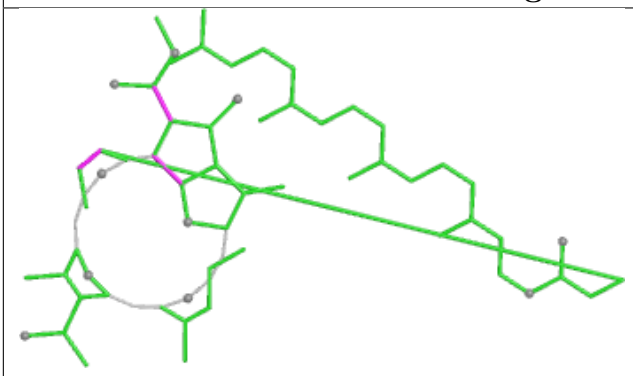
Ligand LDA F 104	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PGV L 313	
 Bond lengths	 Bond angles
 Torsions	 Rings

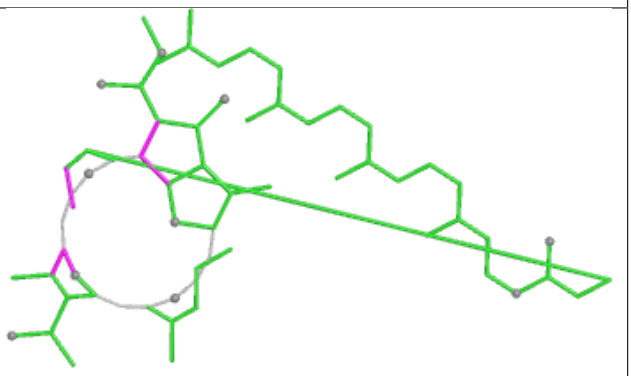
Ligand PGV M 412	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand A1EF2 k 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BPH L 302

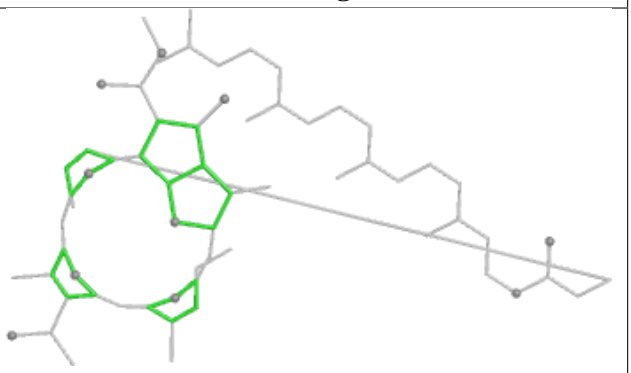


Bond lengths



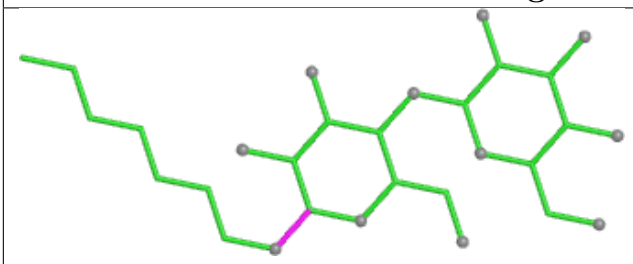
Bond angles

Torsions

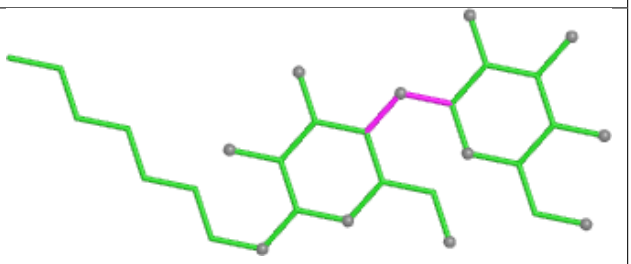


Rings

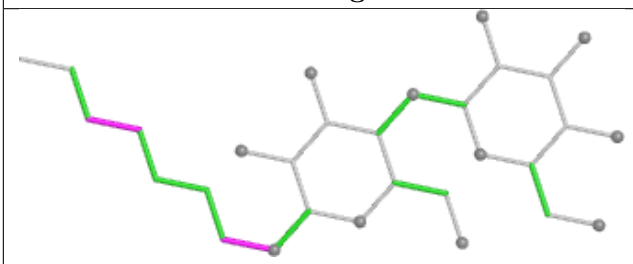
Ligand LMT I 103



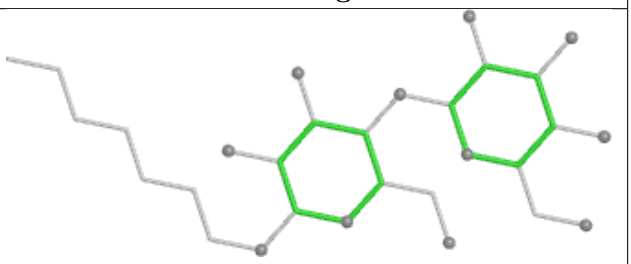
Bond lengths



Bond angles

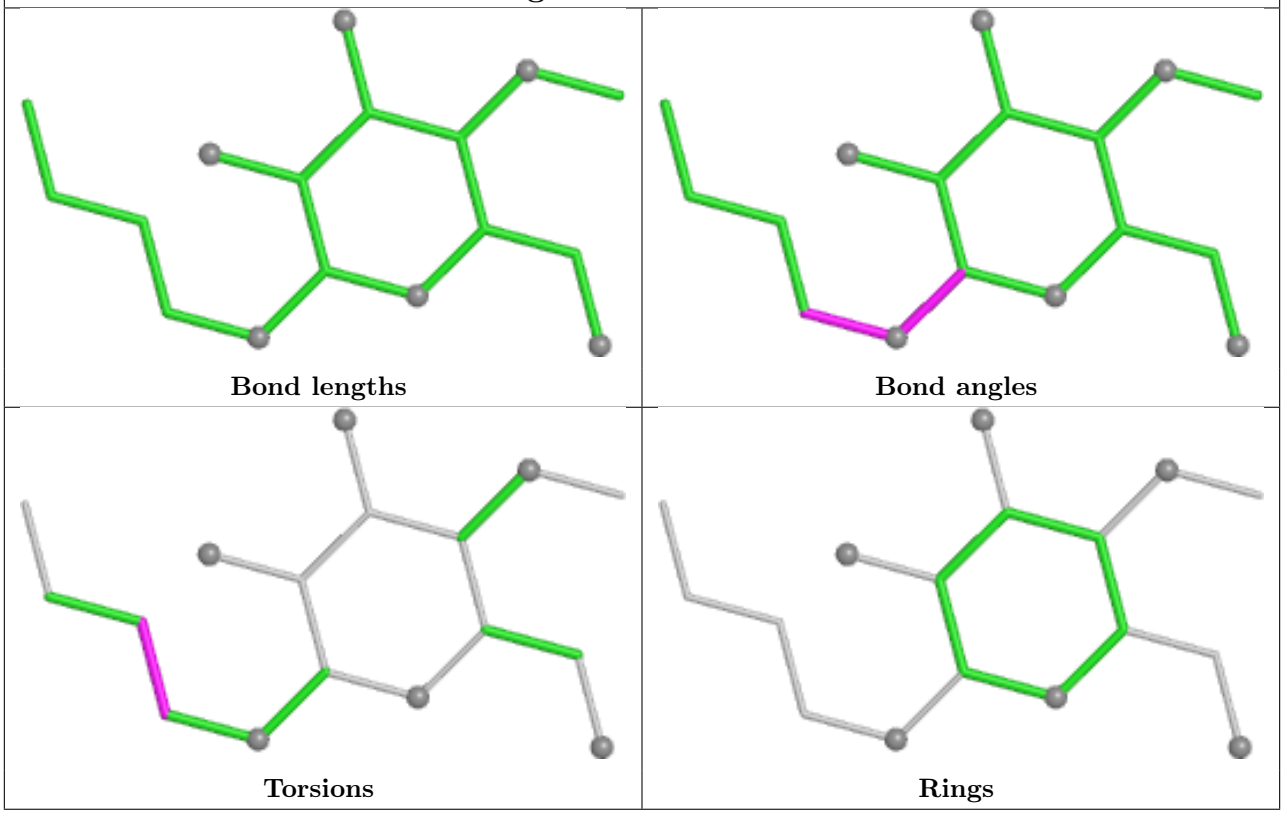


Torsions

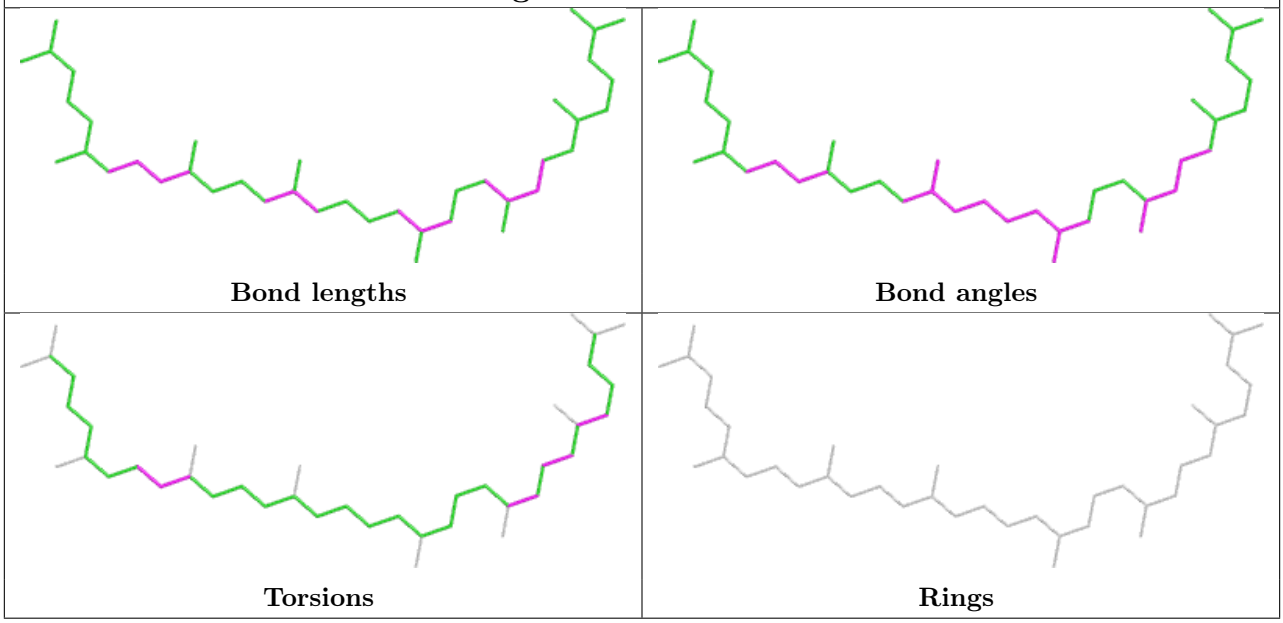


Rings

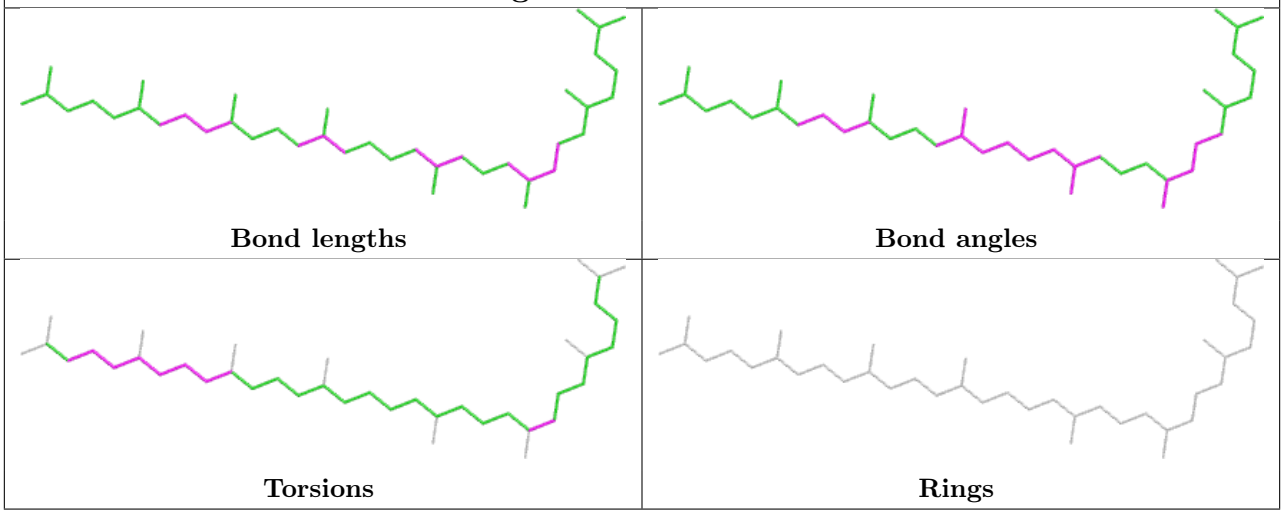
Ligand LMT c 101



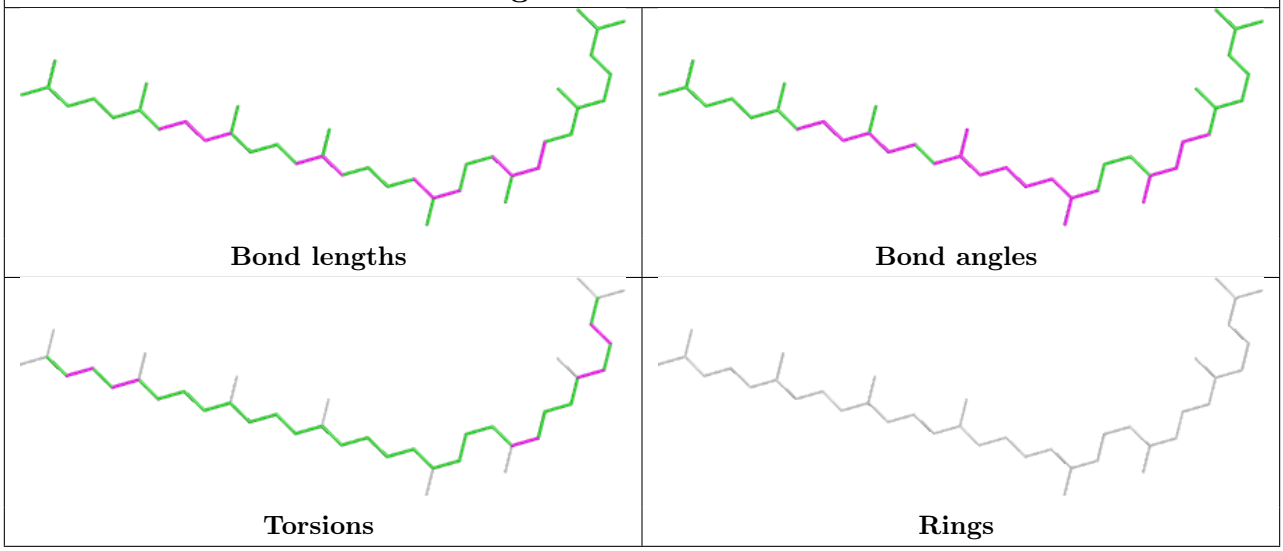
Ligand A1EF2 a 103



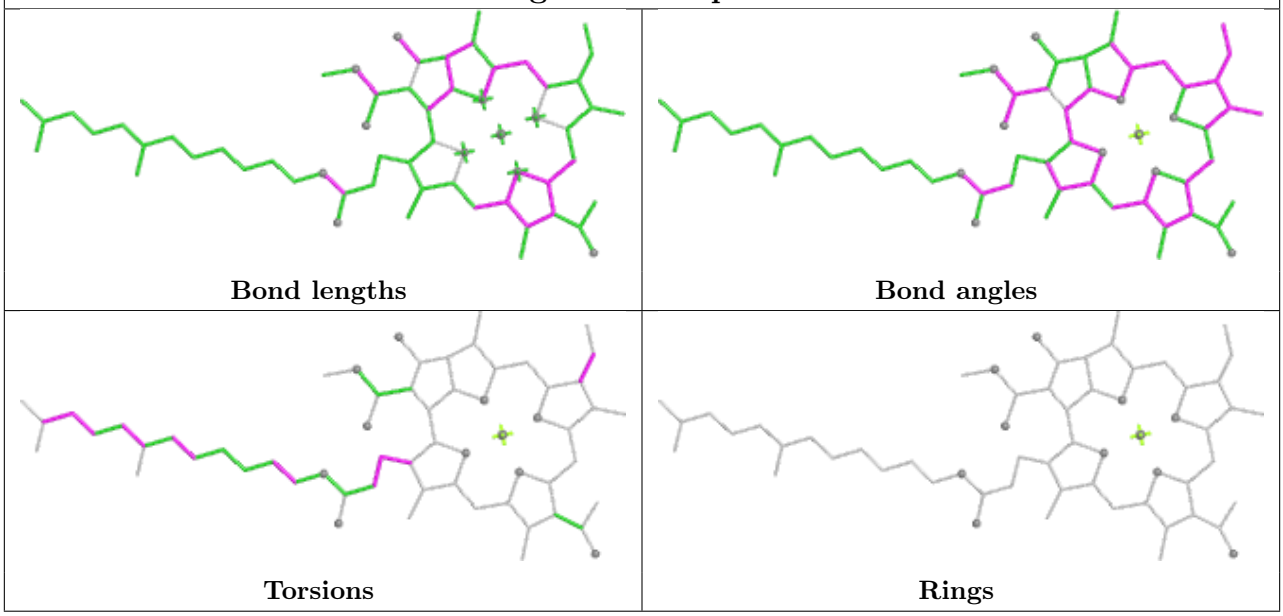
Ligand A1EF2 J 104



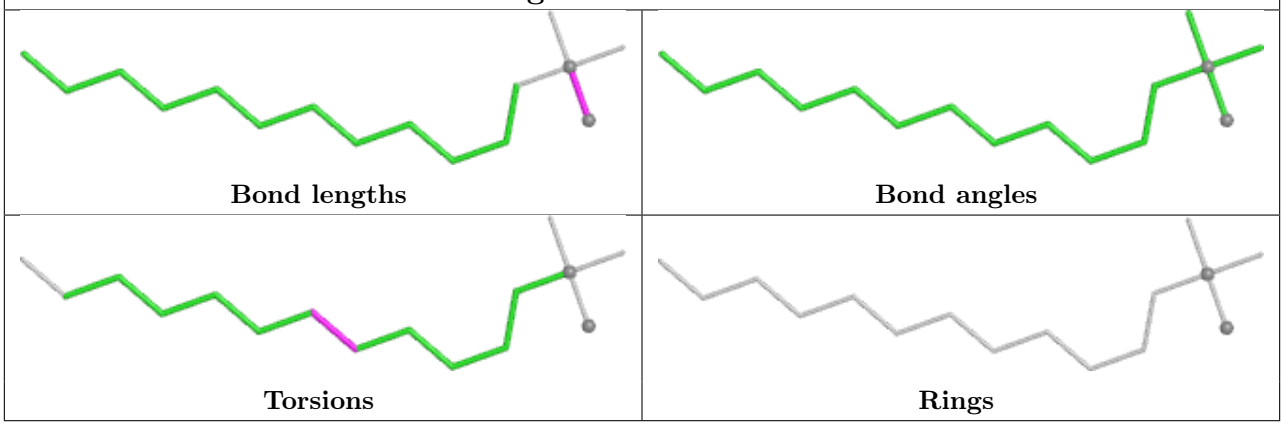
Ligand A1EF2 d 101



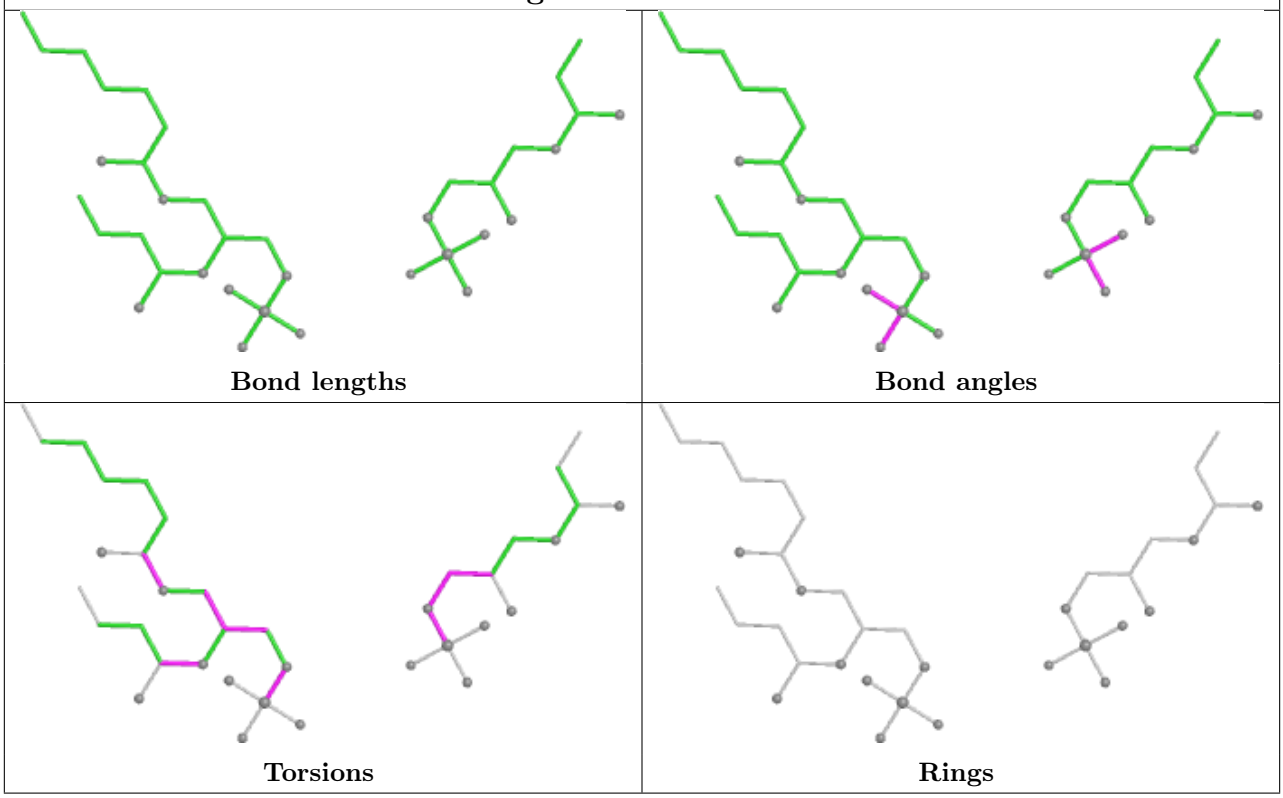
Ligand BCL q 102



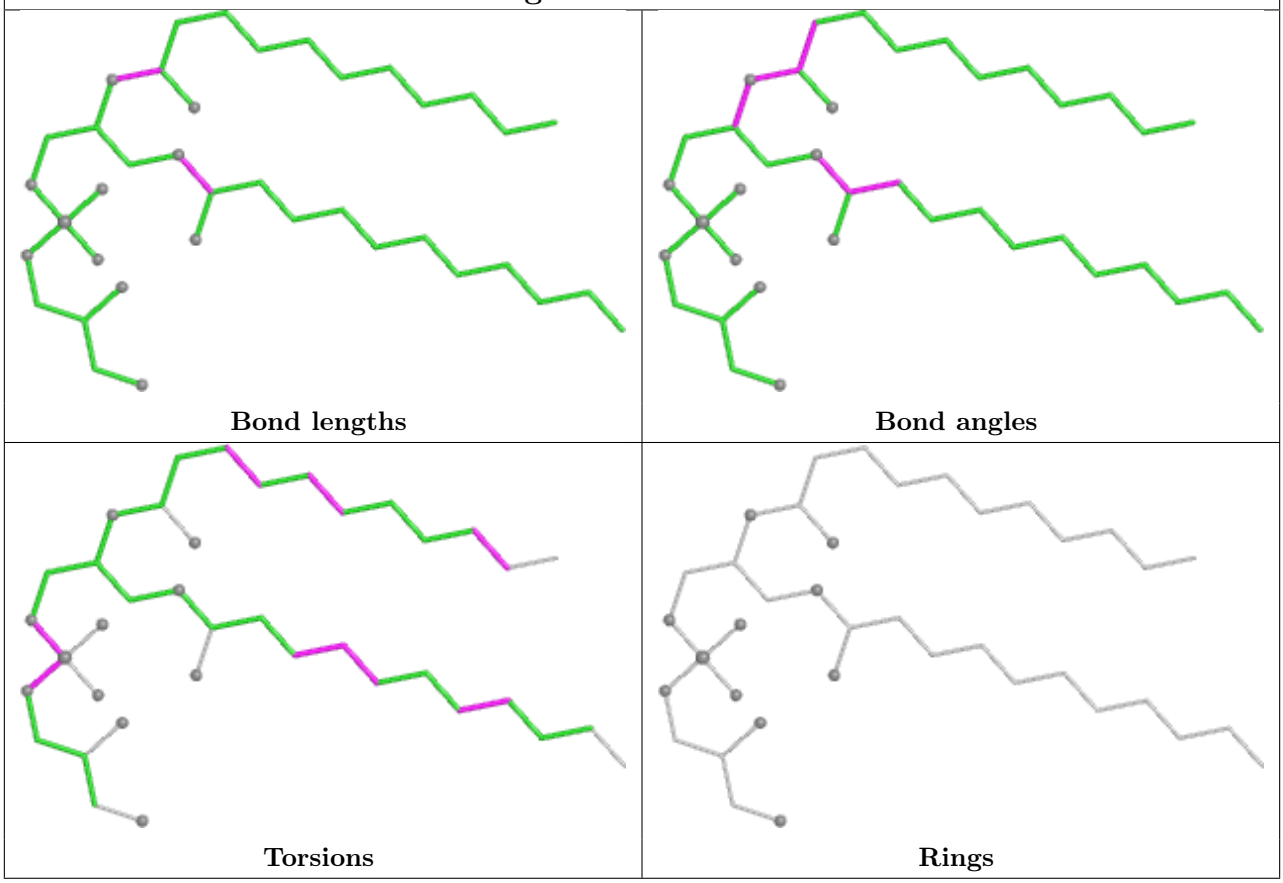
Ligand LDA L 309



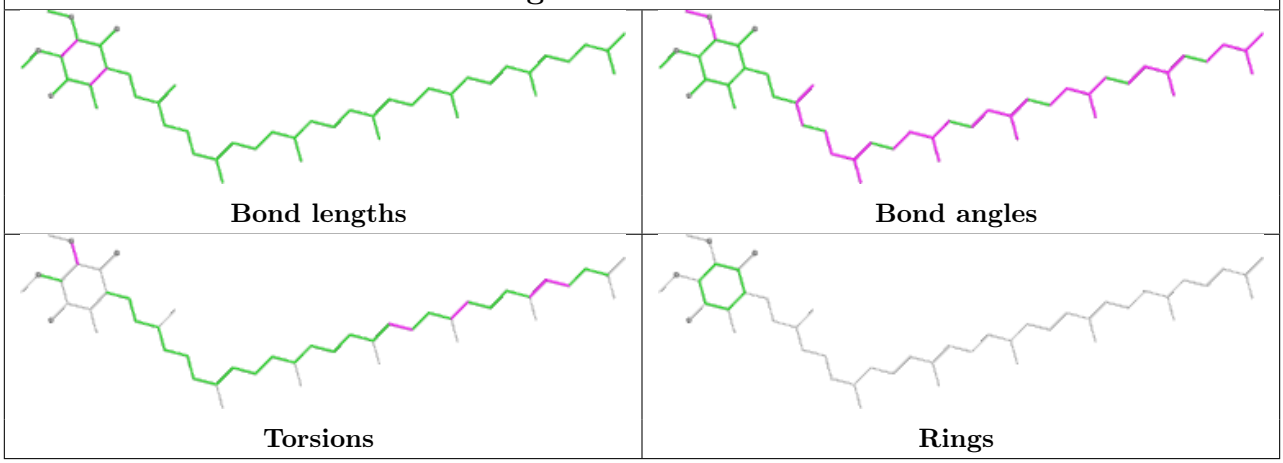
Ligand CDL F 102



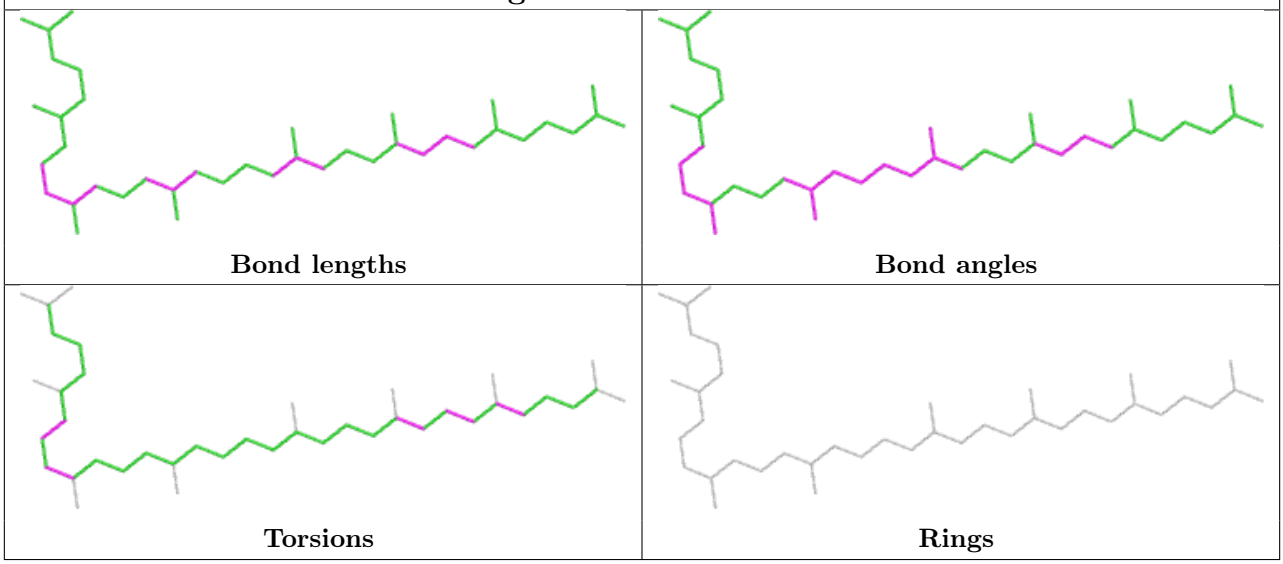
Ligand PGV L 314



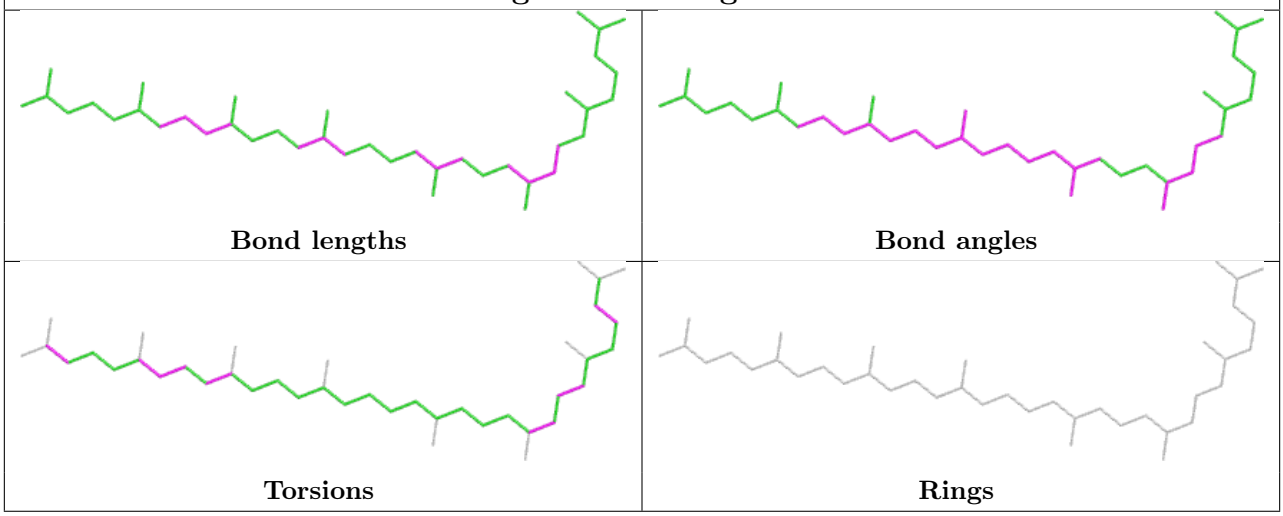
Ligand U10 M 407



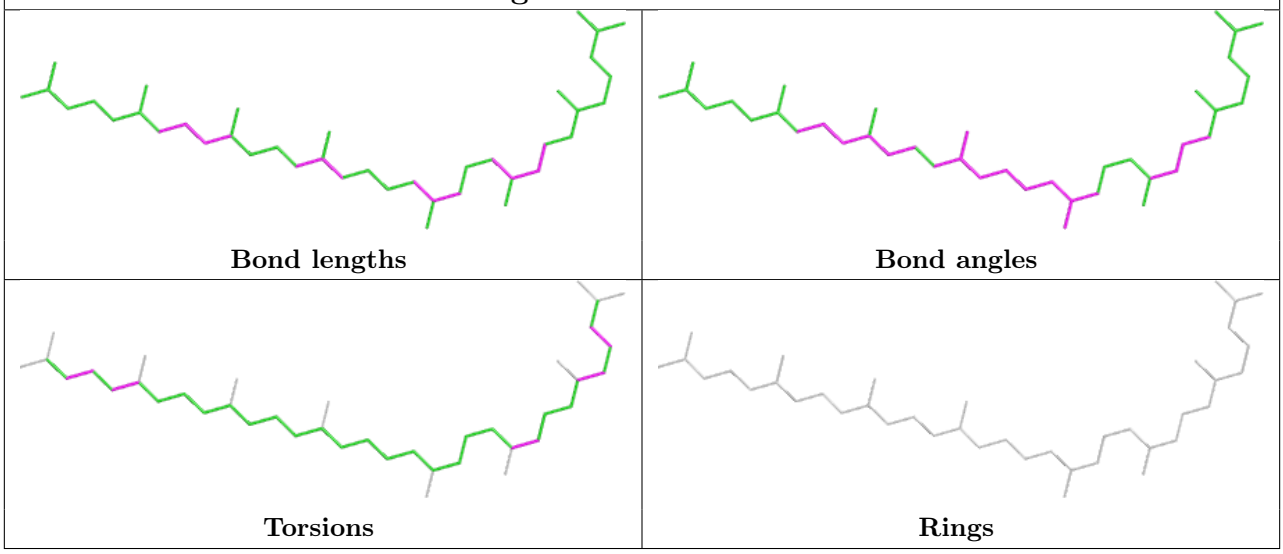
Ligand A1EF2 C 104



Ligand A1EF2 g 103



Ligand A1EF2 b 102



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

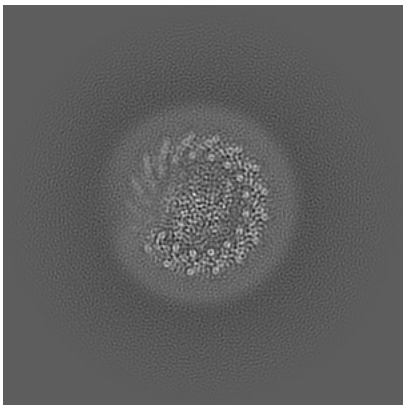
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-62409. These allow visual inspection of the internal detail of the map and identification of artifacts.

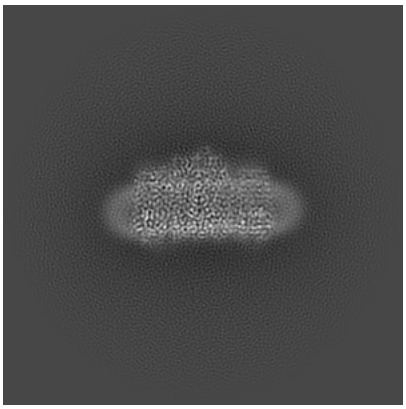
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

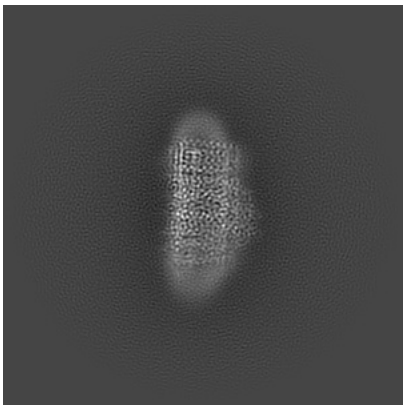
6.1.1 Primary map



X

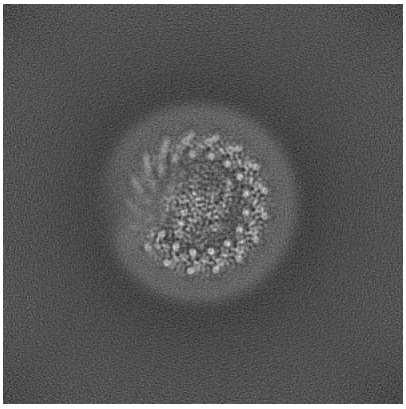


Y

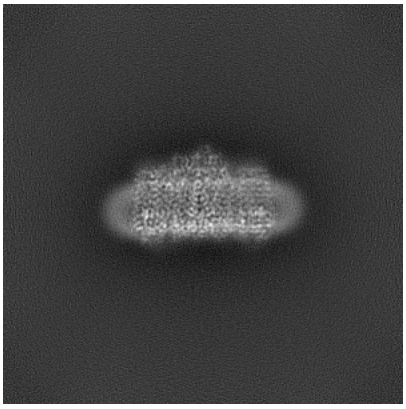


Z

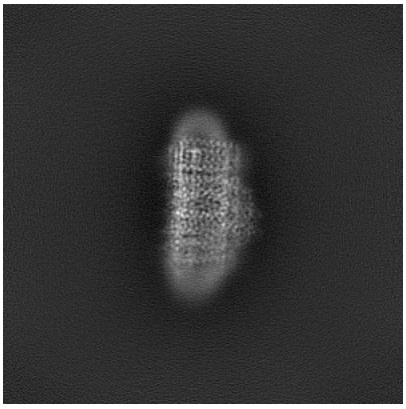
6.1.2 Raw map



X



Y

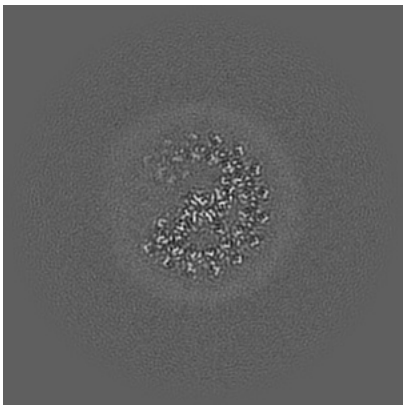


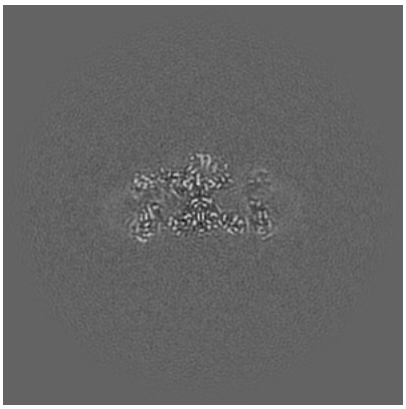
Z

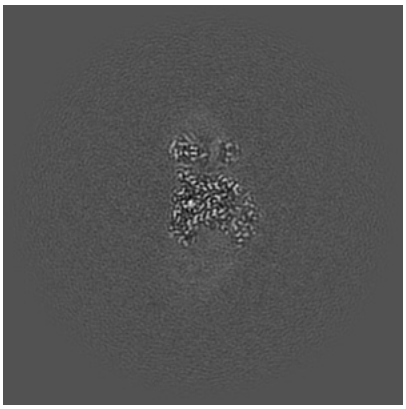
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

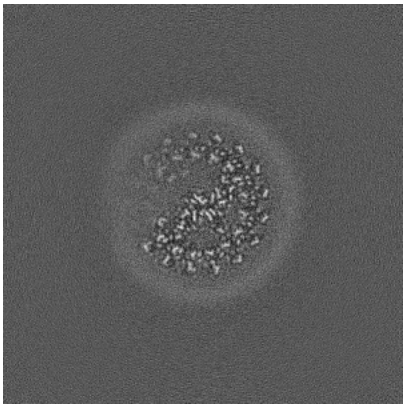
6.2.1 Primary map

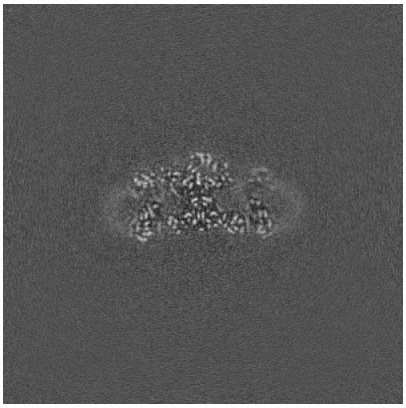

X Index: 200

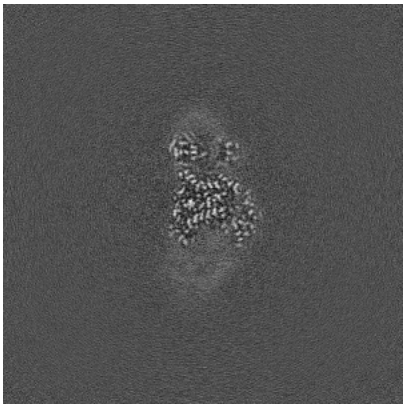

Y Index: 200


Z Index: 200

6.2.2 Raw map


X Index: 200

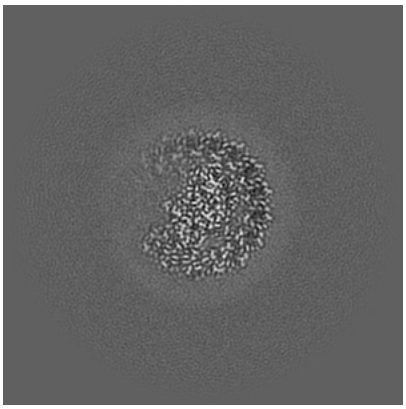

Y Index: 200

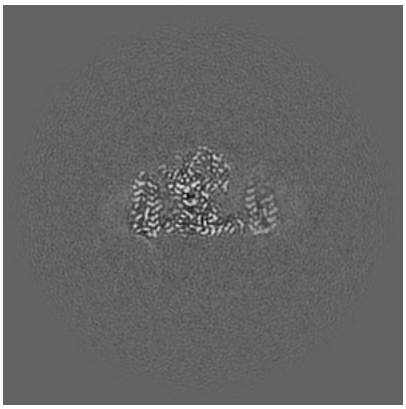

Z Index: 200

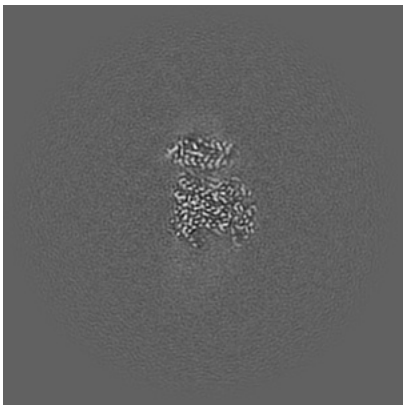
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

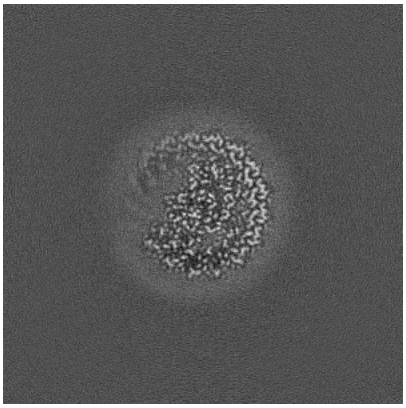
6.3.1 Primary map

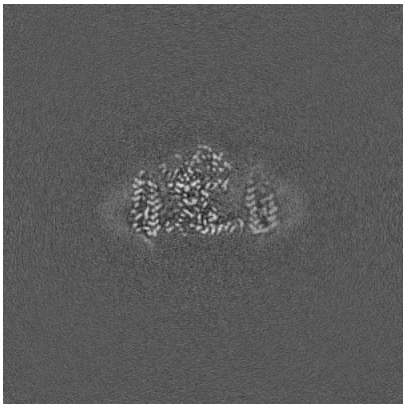

X Index: 181

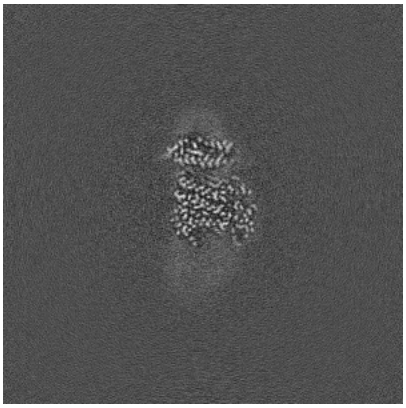

Y Index: 190


Z Index: 191

6.3.2 Raw map


X Index: 178

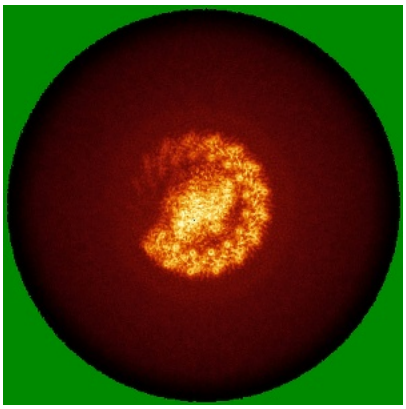

Y Index: 190

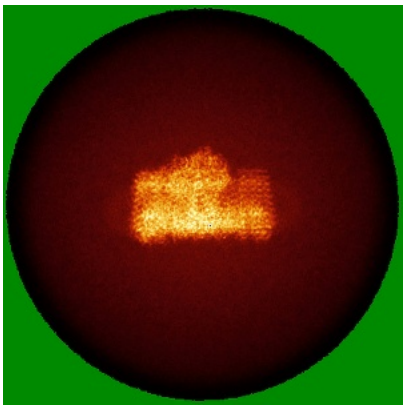

Z Index: 191

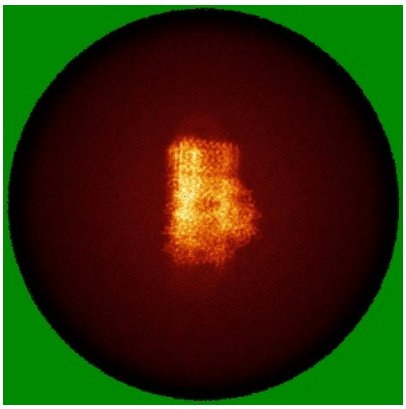
The images above show the largest variance slices of the map in three orthogonal directions.

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

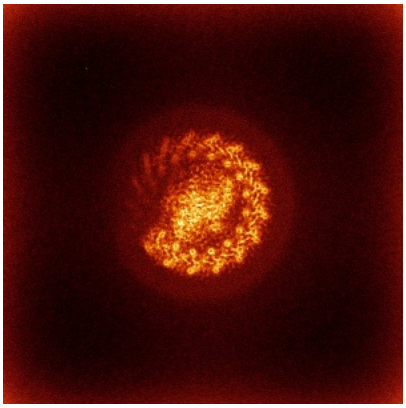
6.4.1 Primary map

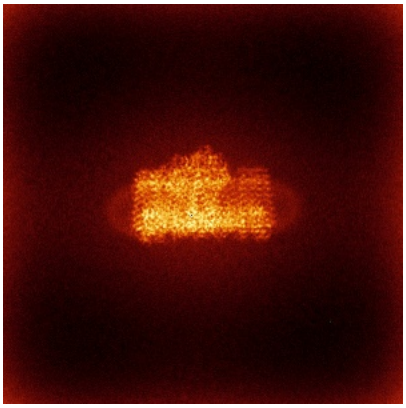

X

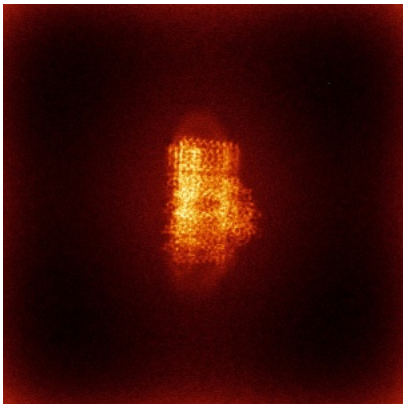

Y


Z

6.4.2 Raw map


X

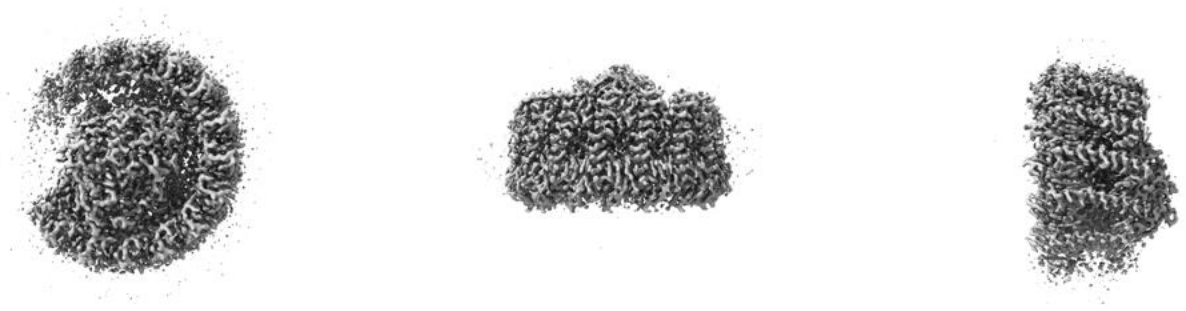

Y


Z

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

6.5 Orthogonal surface views (i)

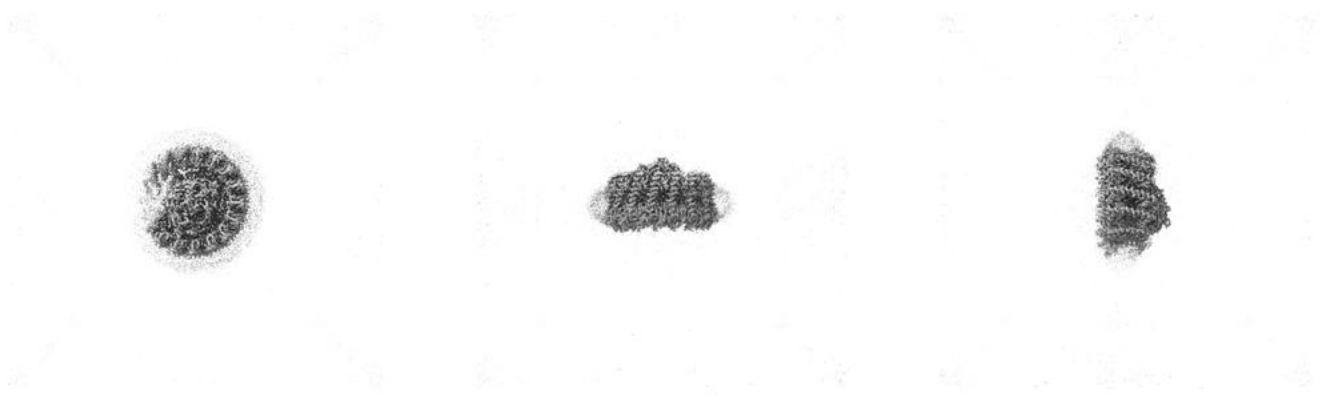
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.19. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

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

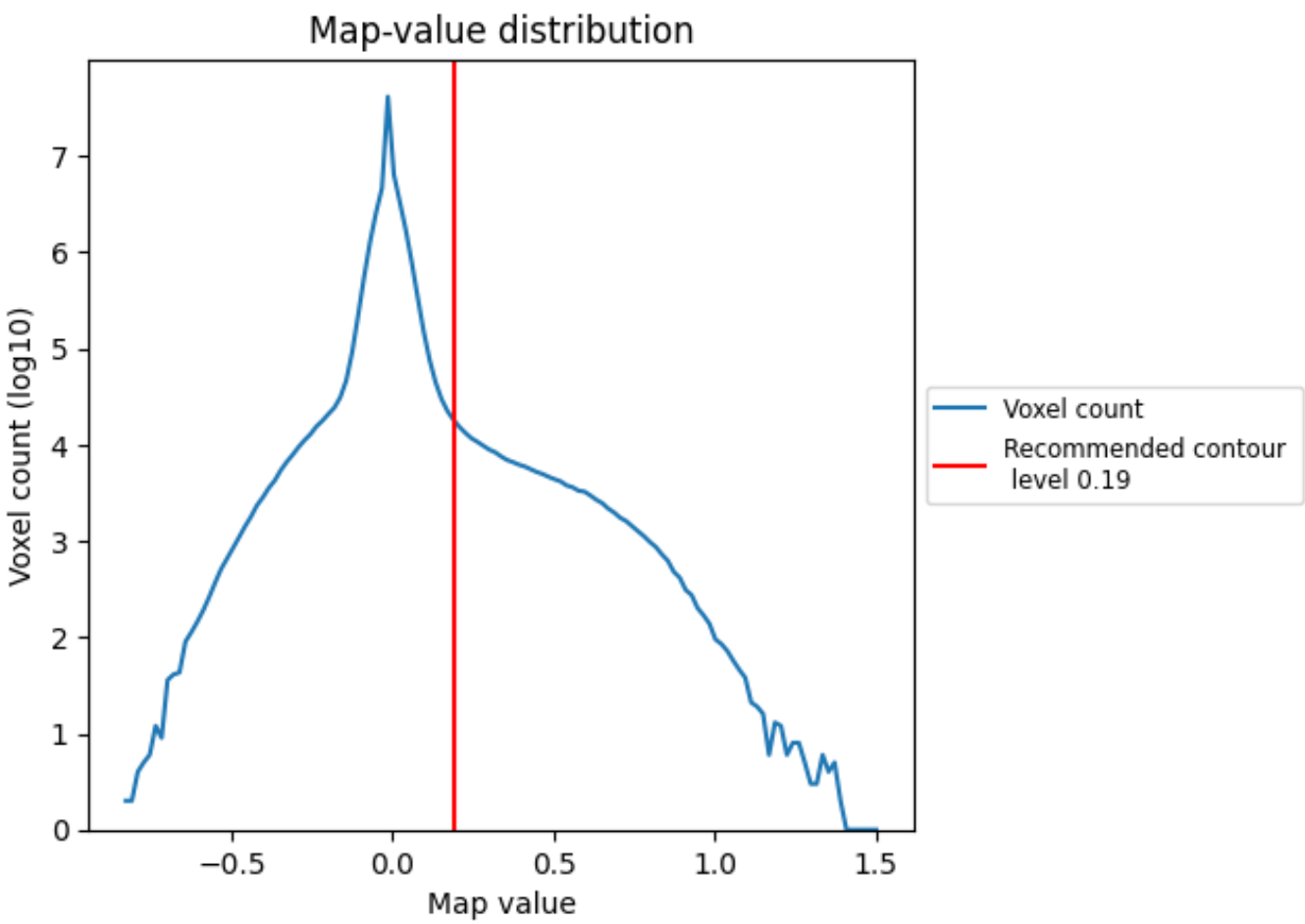
6.6 Mask visualisation (i)

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

7 Map analysis (i)

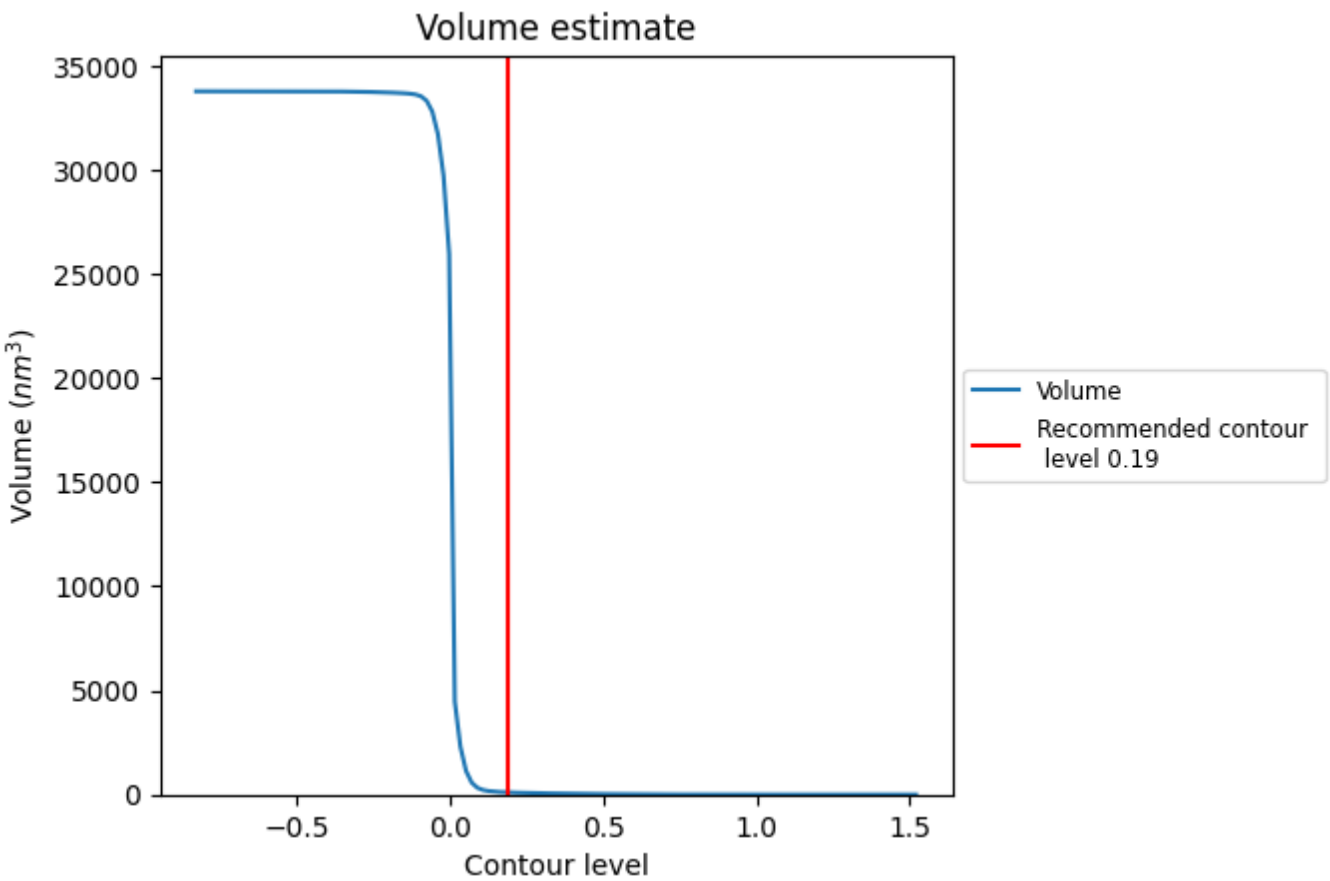
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

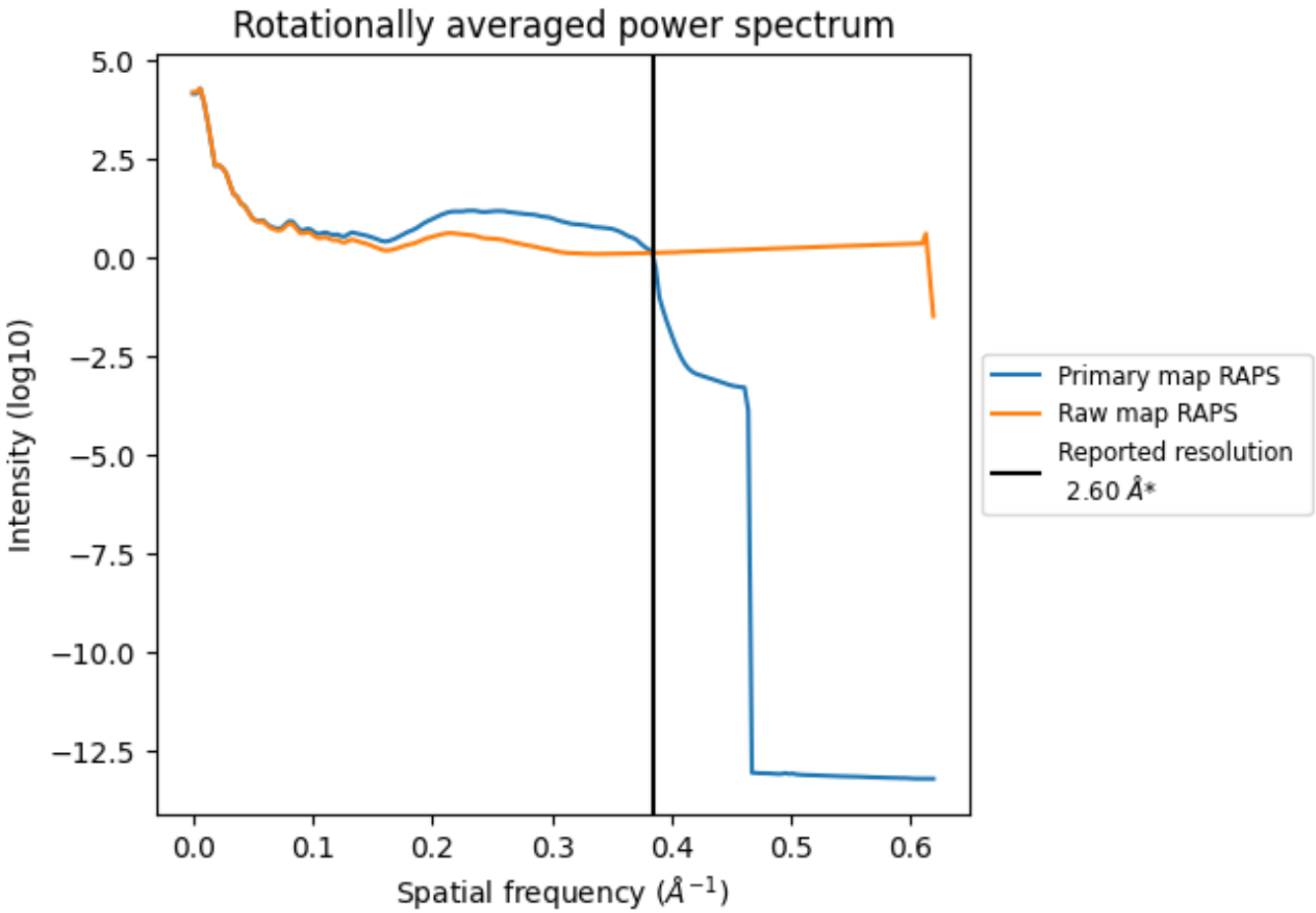
7.2 Volume estimate (i)



The volume at the recommended contour level is 104 nm^3; this corresponds to an approximate mass of 94 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

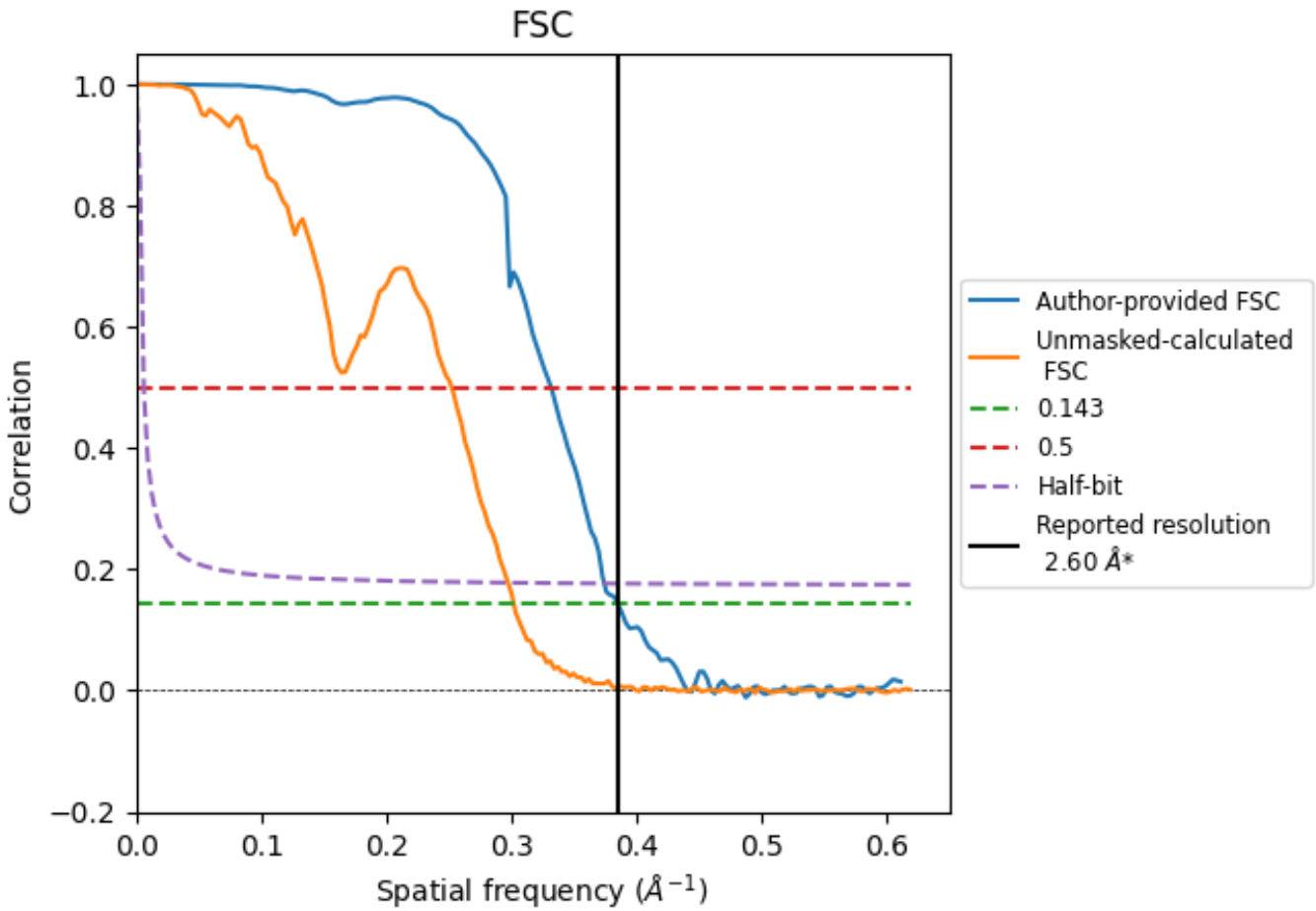


*Reported resolution corresponds to spatial frequency of 0.385 Å^{-1}

8 Fourier-Shell correlation (i)

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

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.385 Å^{-1}

8.2 Resolution estimates (i)

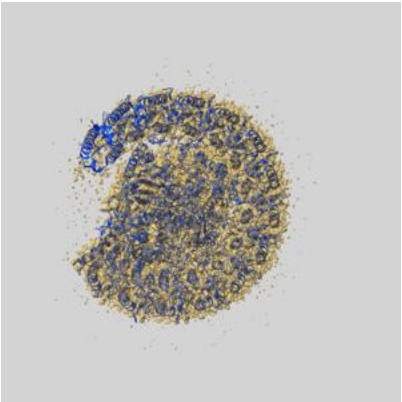
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.60	-	-
Author-provided FSC curve	2.60	3.02	2.67
Unmasked-calculated*	3.31	3.97	3.36

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.31 differs from the reported value 2.6 by more than 10 %

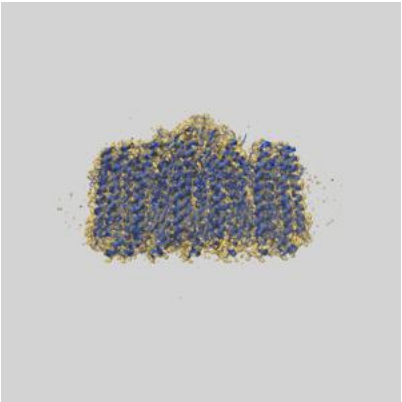
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-62409 and PDB model 9KLM. Per-residue inclusion information can be found in section 3 on page 18.

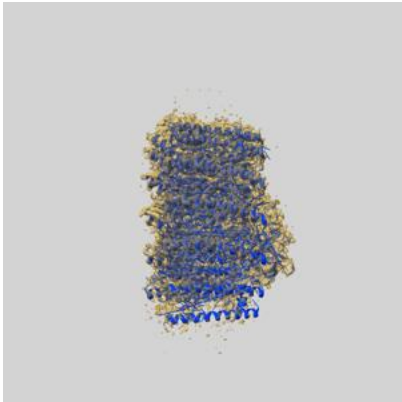
9.1 Map-model overlay (i)



X



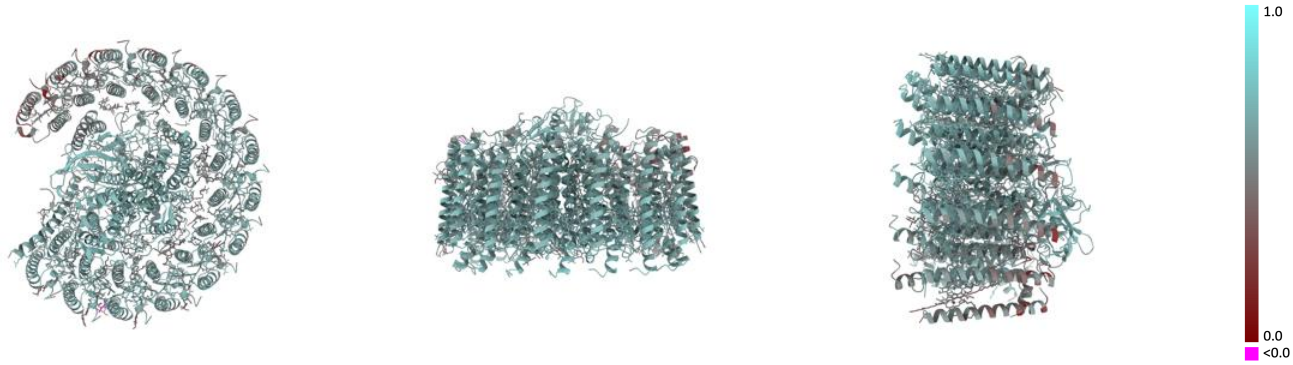
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.19 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

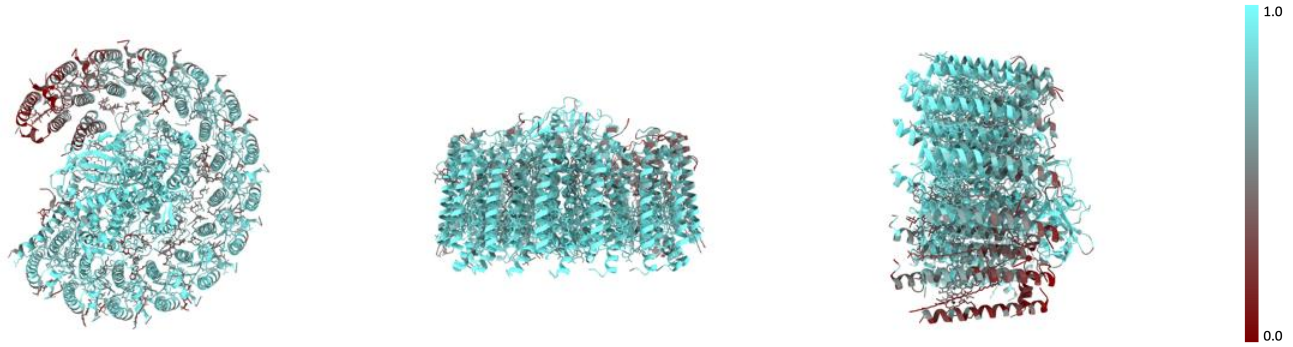
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

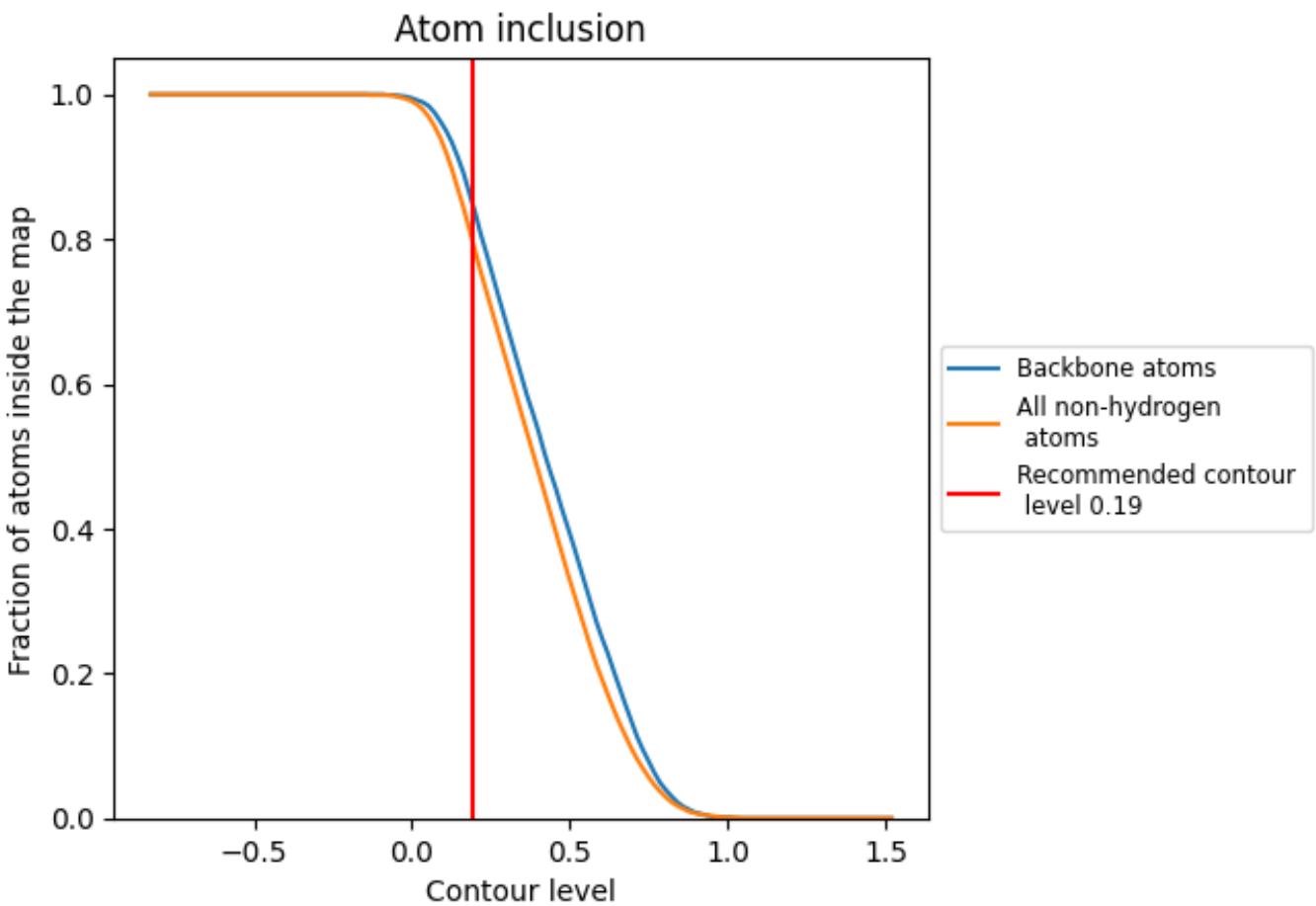
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.19).

9.4 Atom inclusion (i)



At the recommended contour level, 85% of all backbone atoms, 80% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.19) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8000	0.6150
A	0.8680	0.6330
B	0.9100	0.6480
C	0.8360	0.6270
D	0.8580	0.6340
E	0.8270	0.6150
F	0.8170	0.6150
G	0.8320	0.6230
H	0.8710	0.6370
I	0.7950	0.6040
J	0.8350	0.6270
K	0.8030	0.6190
L	0.9080	0.6520
M	0.9250	0.6570
N	0.7580	0.5950
O	0.6290	0.5620
P	0.5380	0.5310
Q	0.4130	0.5140
U	0.4390	0.5540
X	0.7650	0.6060
a	0.7980	0.6110
b	0.8270	0.6070
c	0.7800	0.6000
d	0.8490	0.6230
e	0.8520	0.6180
f	0.8140	0.6110
g	0.8220	0.6130
i	0.8140	0.6180
j	0.8180	0.6200
k	0.8000	0.5990
n	0.7320	0.5830
o	0.5560	0.5340
p	0.4170	0.5100
q	0.2360	0.4520