Full wwPDB EM Validation Report ⓘ

Dec 19, 2022 – 10:06 am GMT

PDB ID	:	6Z5S
EMDB ID	:	EMD-11081
Title	:	RC-LH1(14)-W complex from Rhodopseudomonas palustris
Authors	:	Swainsbury, D.J.K.; Qian, P.; Hitchcock, A.; Hunter, C.N.
Deposited on	:	2020-05-27
Resolution	:	2.65 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

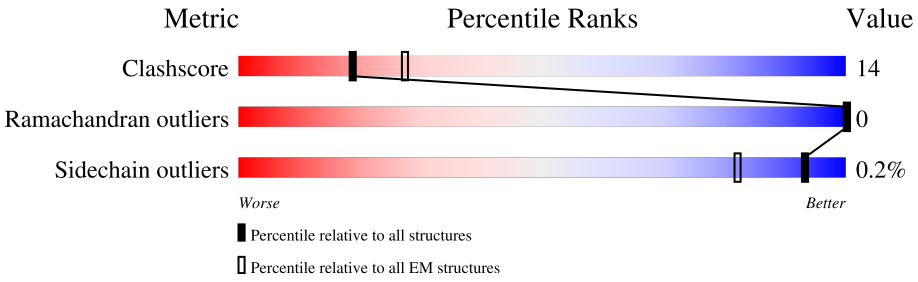
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.65 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	W	102	72% 21% 8%
2	M	307	81% 16%
3	L	277	74% 25%
4	H	255	75% 23%
5	1	63	43% 30% 27%
5	3	63	5% 54% 19% 27%
5	5	63	6% 49% 24% 27%
5	A	63	43% 21% 37%

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Mol	Chain	Length	Quality of chain
5	C	63	46% 25% 27%
5	E	63	52% 21% 27%
5	G	63	46% 27% 27%
5	J	63	57% 14% 29%
5	N	63	57% 16% 27%
5	P	63	59% 14% 27%
5	R	63	51% 22% 27%
5	T	63	56% 16% 27%
5	V	63	56% 17% 27%
5	Y	63	48% 25% 27%
6	2	65	42% 31% 28%
6	4	65	49% 22% 29%
6	6	65	40% 25% 35%
6	B	65	55% 17% 28%
6	D	65	58% 15% 26%
6	F	65	55% 18% 26%
6	I	65	55% 17% 28%
6	K	65	52% 20% 28%
6	O	65	49% 25% 26%
6	Q	65	49% 25% 26%
6	S	65	48% 26% 26%
6	U	65	54% 18% 28%
6	X	65	48% 25% 28%
6	Z	65	46% 26% 28%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	QAK	M	401	X	-	-	-
9	BPH	L	403	X	-	-	-
9	BPH	M	403	X	-	-	-

2 Entry composition (i)

There are 17 unique types of molecules in this entry. The entry contains 22794 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 Light harvesting complex 1 Protein W.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	W	94	Total	C	N	O	S	0	0
			682	455	114	110	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	M	299	Total	C	N	O	S	0	0
			2381	1582	389	398	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	L	276	Total	C	N	O	S	0	0
			2185	1467	350	359	9		

- Molecule 4 is a protein called H subunit of photosynthetic reaction center complex.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	251	Total	C	N	O	S	0	0
			1894	1221	321	347	5		

- Molecule 5 is a protein called Light-harvesting complex 1 alpha chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	1	46	Total	C	N	O	S	0	0
			397	274	67	55	1		
5	5	46	Total	C	N	O	S	0	0
			397	274	67	55	1		
5	3	46	Total	C	N	O	S	0	0
			397	274	67	55	1		
5	Y	46	Total	C	N	O	S	0	0
			397	274	67	55	1		

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Mol	Chain	Residues	Atoms	AltConf	Trace
5	V	46	Total C N O S 397 274 67 55 1	0	0
5	T	46	Total C N O S 408 283 68 56 1	1	0
5	A	40	Total C N O 352 248 58 46	0	0
5	C	46	Total C N O S 397 274 67 55 1	0	0
5	R	46	Total C N O S 397 274 67 55 1	0	0
5	P	46	Total C N O S 397 274 67 55 1	0	0
5	N	46	Total C N O S 397 274 67 55 1	0	0
5	J	45	Total C N O S 392 271 66 54 1	0	0
5	G	46	Total C N O S 397 274 67 55 1	0	0
5	E	46	Total C N O S 397 274 67 55 1	0	0

- Molecule 6 is a protein called Light-harvesting complex 1 beta chain.

Mol	Chain	Residues	Atoms	AltConf	Trace
6	2	47	Total C N O S 393 271 60 61 1	1	0
6	6	42	Total C N O S 356 247 54 54 1	1	0
6	4	46	Total C N O S 374 256 58 59 1	0	0
6	Z	47	Total C N O S 393 271 60 61 1	1	0
6	X	47	Total C N O S 393 271 60 61 1	1	0
6	U	47	Total C N O S 393 271 60 61 1	1	0
6	B	47	Total C N O S 382 262 59 60 1	0	0
6	D	48	Total C N O S 399 274 61 63 1	1	0
6	S	48	Total C N O S 399 274 61 63 1	1	0

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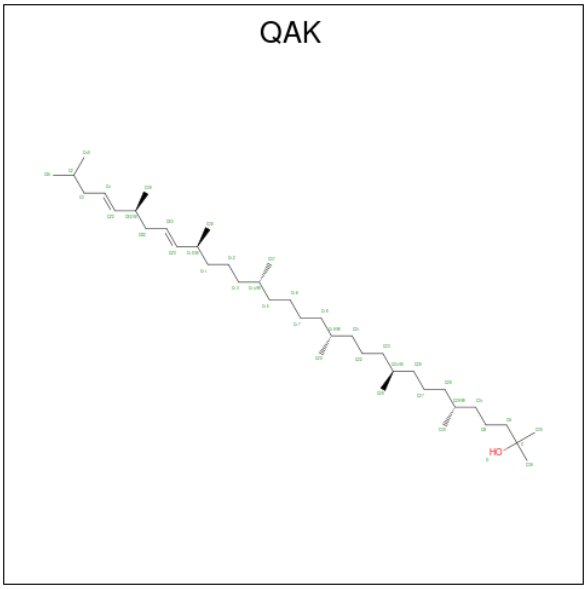
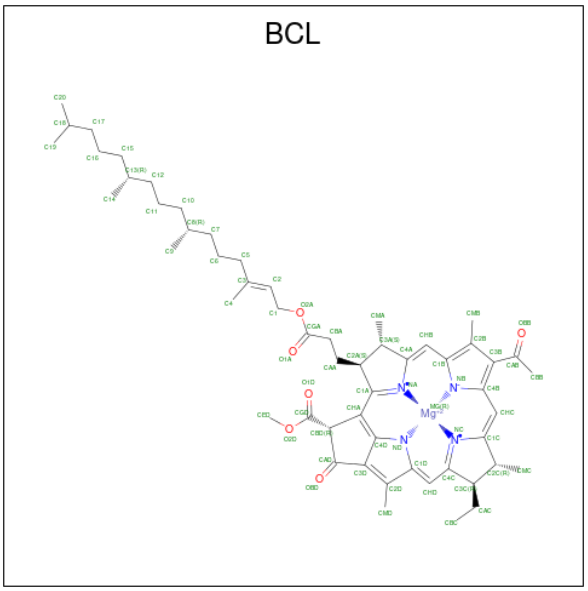
Mol	Chain	Residues	Atoms					AltConf	Trace
6	Q	48	Total	C	N	O	S	1	0
			399	274	61	63	1		
6	O	48	Total	C	N	O	S	0	0
			388	265	60	62	1		
6	K	47	Total	C	N	O	S	0	0
			382	262	59	60	1		
6	I	47	Total	C	N	O	S	0	0
			382	262	59	60	1		
6	F	48	Total	C	N	O	S	0	0
			388	265	60	62	1		

- Molecule 7 is (6 {R},10 {S},14 {R},19 {R},23 {S},24 {E},27 {S},28 {E})-2,6,10,14,19,23,27,31-octamethyldotriaconta-24,28-dien-2-ol (three-letter code: QAK) (formula: $C_{40}H_{78}O$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
7	M	1	Total	C	O	0
			41	40	1	

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



Mol	Chain	Residues	Atoms					AltConf
8	M	1	Total	C	Mg	N	O	0
			132	110	2	8	12	
8	M	1	Total	C	Mg	N	O	0
			132	110	2	8	12	
8	L	1	Total	C	Mg	N	O	0
			132	110	2	8	12	
8	L	1	Total	C	Mg	N	O	0
			132	110	2	8	12	
8	1	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	2	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	5	1	Total	C	Mg	N	O	0
			132	110	2	8	12	
8	5	1	Total	C	Mg	N	O	0
			132	110	2	8	12	
8	3	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	4	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	Y	1	Total	C	Mg	N	O	0
			132	110	2	8	12	
8	Y	1	Total	C	Mg	N	O	0
			132	110	2	8	12	
8	V	1	Total	C	Mg	N	O	0
			132	110	2	8	12	
8	V	1	Total	C	Mg	N	O	0
			132	110	2	8	12	

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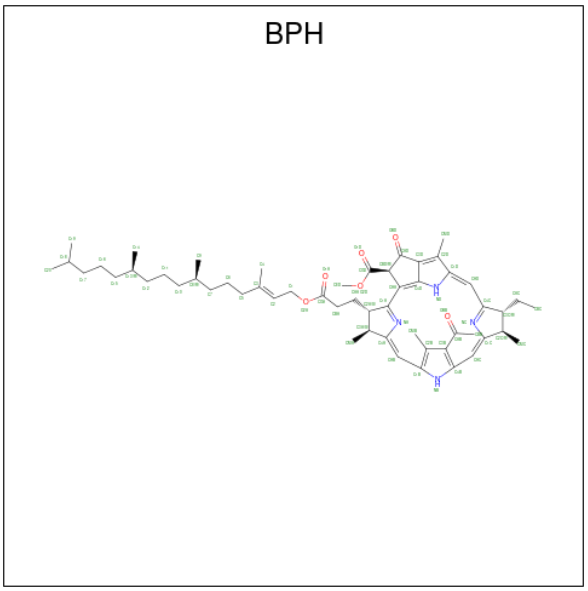
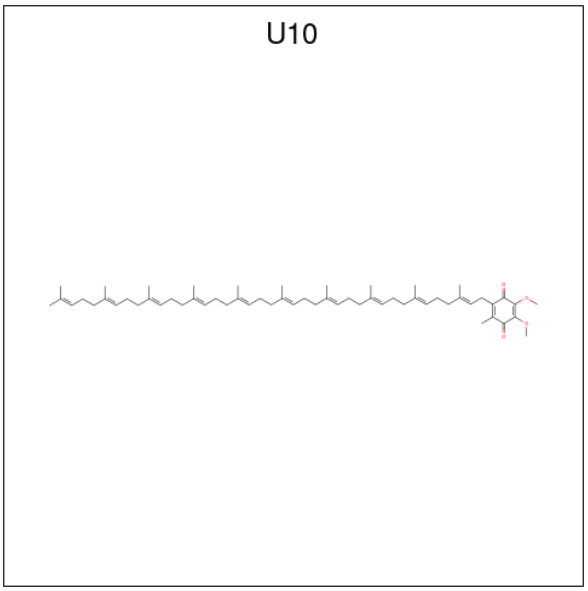
Mol	Chain	Residues	Atoms					AltConf
8	T	1	Total	C	Mg	N	O	0
			132	110	2	8	12	
8	T	1	Total	C	Mg	N	O	0
			132	110	2	8	12	
8	A	1	Total	C	Mg	N	O	0
			132	110	2	8	12	
8	A	1	Total	C	Mg	N	O	0
			132	110	2	8	12	
8	C	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	D	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	R	1	Total	C	Mg	N	O	0
			132	110	2	8	12	
8	R	1	Total	C	Mg	N	O	0
			132	110	2	8	12	
8	P	1	Total	C	Mg	N	O	0
			132	110	2	8	12	
8	P	1	Total	C	Mg	N	O	0
			132	110	2	8	12	
8	N	1	Total	C	Mg	N	O	0
			132	110	2	8	12	
8	N	1	Total	C	Mg	N	O	0
			132	110	2	8	12	
8	J	1	Total	C	Mg	N	O	0
			132	110	2	8	12	
8	J	1	Total	C	Mg	N	O	0
			132	110	2	8	12	
8	G	1	Total	C	Mg	N	O	0
			132	110	2	8	12	
8	G	1	Total	C	Mg	N	O	0
			132	110	2	8	12	
8	E	1	Total	C	Mg	N	O	0
			132	110	2	8	12	
8	E	1	Total	C	Mg	N	O	0
			132	110	2	8	12	

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



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

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



Mol	Chain	Residues	Atoms			AltConf
10	M	1	Total	C	O	0
			48	44	4	

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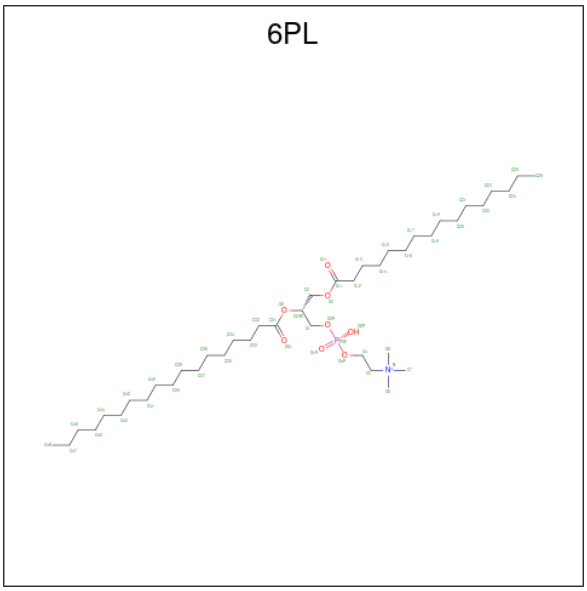
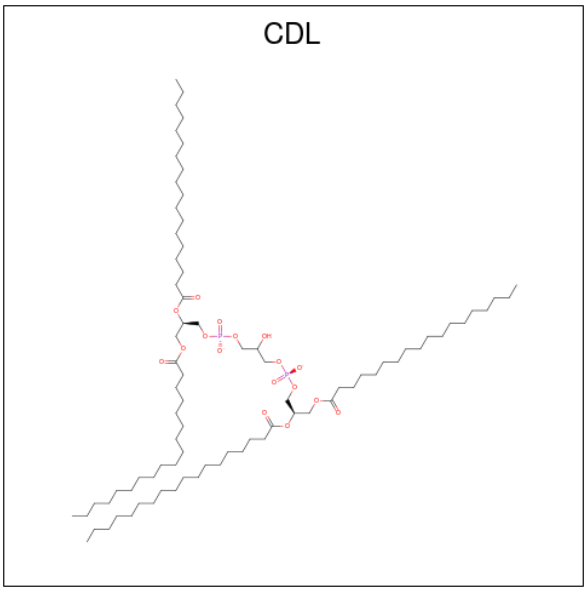
Mol	Chain	Residues	Atoms			AltConf
10	L	1	Total 19	C 15	O 4	0
10	1	1	Total 40	C 36	O 4	0

- Molecule 11 is (4S,7R)-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITOYLOXY) METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSAN-1-AMINIUM 4-OXIDE (three-letter code: 6PL) (formula: $C_{42}H_{85}NO_8P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
11	M	1	Total 52	C 42	N 1	O 8	P 1	0
11	H	1	Total 52	C 42	N 1	O 8	P 1	0
11	E	1	Total 40	C 30	N 1	O 8	P 1	0

- Molecule 12 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$) (labeled as "Ligand of Interest" by depositor).

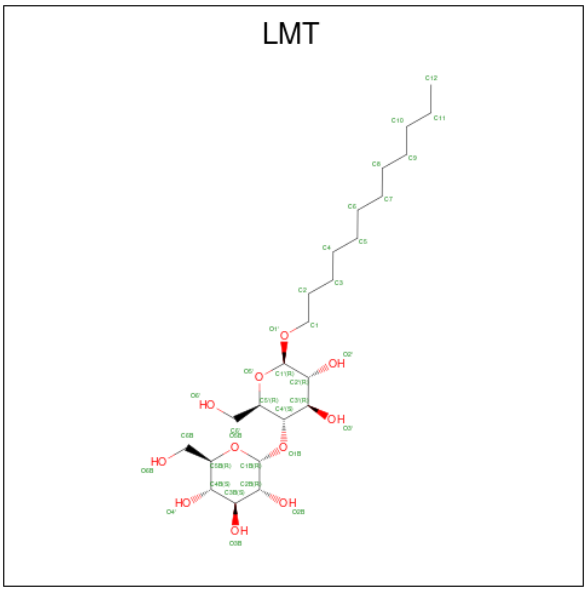


Mol	Chain	Residues	Atoms				AltConf
12	M	1	Total	C	O	P	0
			95	76	17	2	
12	L	1	Total	C	O	P	0
			89	70	17	2	
12	H	1	Total	C	O	P	0
			87	68	17	2	
12	3	1	Total	C	O	P	0
			85	66	17	2	
12	G	1	Total	C	O	P	0
			178	140	34	4	
12	G	1	Total	C	O	P	0
			178	140	34	4	

- Molecule 13 is FE (III) ION (three-letter code: FE) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 14 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
14	M	1	Total	C	O	0
			35	24	11	
14	L	1	Total	C	O	0
			35	24	11	
14	2	1	Total	C	O	0
			70	48	22	
14	2	1	Total	C	O	0
			70	48	22	
14	6	1	Total	C	O	0
			35	24	11	
14	4	1	Total	C	O	0
			35	24	11	
14	Z	1	Total	C	O	0
			35	24	11	
14	X	1	Total	C	O	0
			70	48	22	
14	X	1	Total	C	O	0
			70	48	22	
14	U	1	Total	C	O	0
			70	48	22	
14	U	1	Total	C	O	0
			70	48	22	
14	B	1	Total	C	O	0
			70	48	22	
14	B	1	Total	C	O	0
			70	48	22	
14	D	1	Total	C	O	0
			101	68	33	

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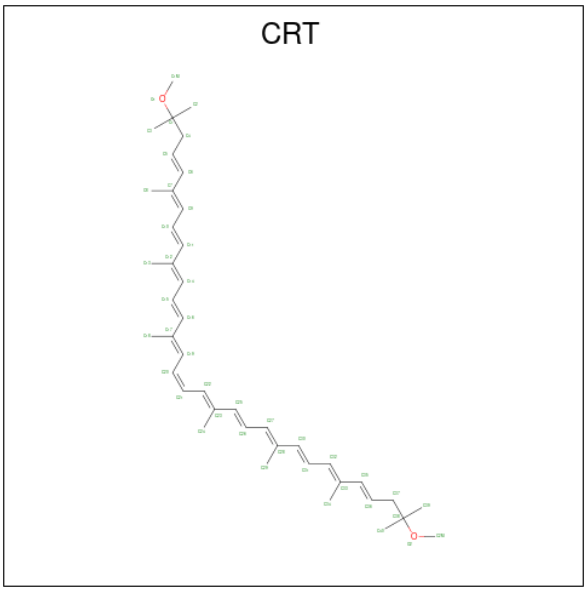
Mol	Chain	Residues	Atoms			AltConf
14	D	1	Total	C	O	0
			101	68	33	
14	D	1	Total	C	O	0
			101	68	33	
14	R	1	Total	C	O	0
			35	24	11	
14	S	1	Total	C	O	0
			70	48	22	
14	S	1	Total	C	O	0
			70	48	22	
14	Q	1	Total	C	O	0
			70	48	22	
14	Q	1	Total	C	O	0
			70	48	22	
14	O	1	Total	C	O	0
			35	24	11	
14	J	1	Total	C	O	0
			35	24	11	
14	K	1	Total	C	O	0
			70	48	22	
14	K	1	Total	C	O	0
			70	48	22	
14	I	1	Total	C	O	0
			70	48	22	
14	I	1	Total	C	O	0
			70	48	22	
14	F	1	Total	C	O	0
			70	48	22	
14	F	1	Total	C	O	0
			70	48	22	

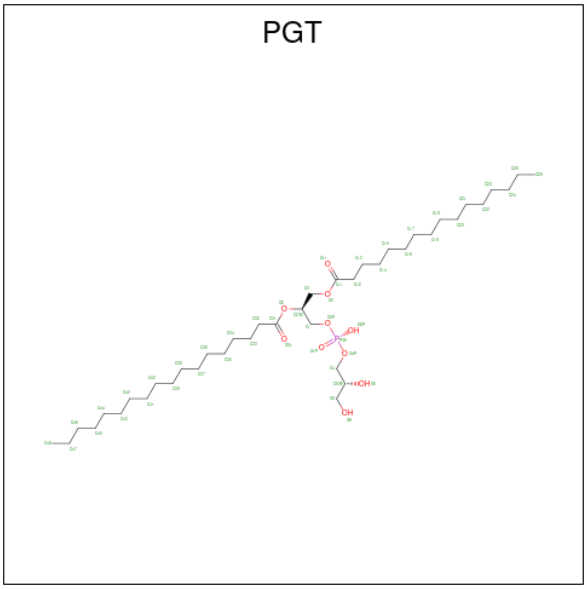
- Molecule 15 is SPIRILLOXANTHIN (three-letter code: CRT) (formula: $C_{42}H_{60}O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
15	2	1	Total C O 44 42 2	0
15	3	1	Total C O 44 42 2	0
15	Z	1	Total C O 44 42 2	0
15	X	1	Total C O 44 42 2	0
15	B	1	Total C O 44 42 2	0
15	D	1	Total C O 44 42 2	0
15	R	1	Total C O 44 42 2	0
15	S	1	Total C O 44 42 2	0
15	Q	1	Total C O 44 42 2	0
15	O	1	Total C O 44 42 2	0
15	K	1	Total C O 44 42 2	0
15	I	1	Total C O 44 42 2	0
15	F	1	Total C O 44 42 2	0

- Molecule 16 is (1S)-2-{[{[(2R)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPH

ORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL STEARATE (three-letter code: PGT) (formula: $C_{40}H_{79}O_{10}P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
16	P	1	Total	C	O	P	0
			50	39	10	1	

- Molecule 17 is water.

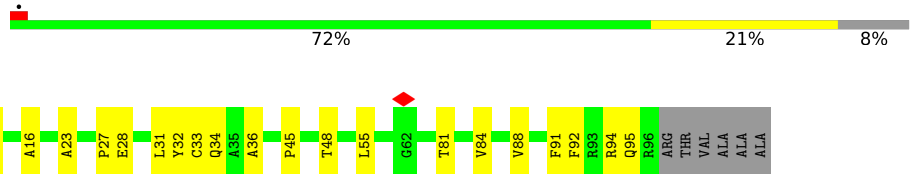
Mol	Chain	Residues	Atoms		AltConf
17	M	3	Total	O	0
			3	3	
17	L	5	Total	O	0
			5	5	
17	H	2	Total	O	0
			2	2	

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.

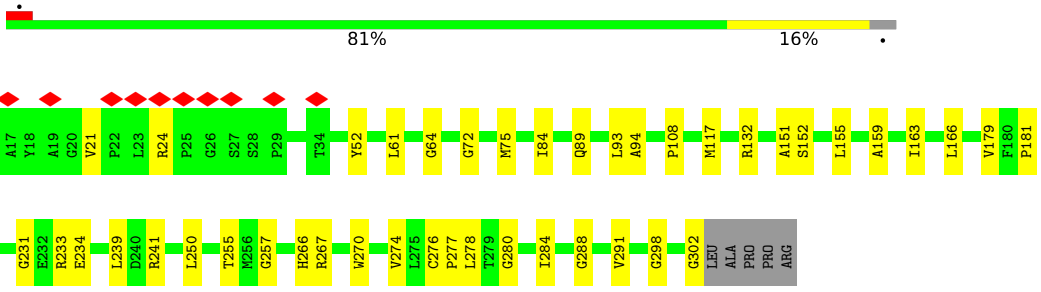
• Molecule 1: Light harvesting complex 1 Protein W

Chain W:



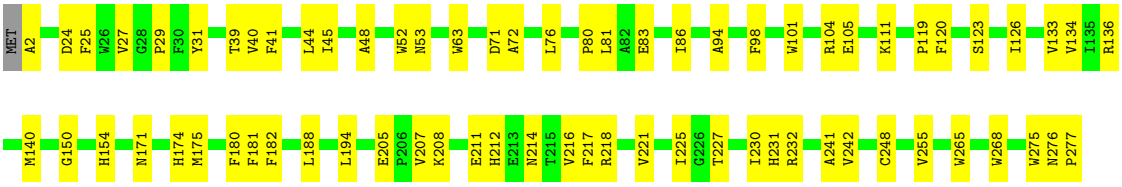
• Molecule 2: Reaction center protein M chain

Chain M:



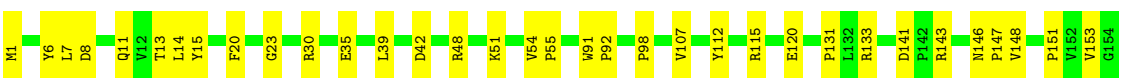
• Molecule 3: Reaction center protein L chain

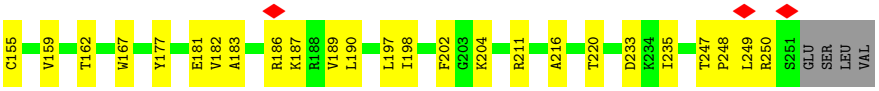
Chain L:



• Molecule 4: H subunit of photosynthetic reaction center complex

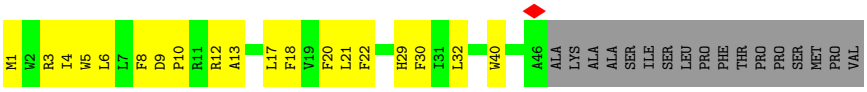
Chain H:





• Molecule 5: Light-harvesting complex 1 alpha chain

Chain 1:

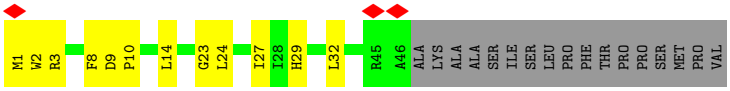


• Molecule 5: Light-harvesting complex 1 alpha chain

Chain 5:

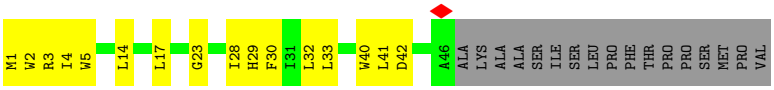
• Molecule 5: Light-harvesting complex 1 alpha chain

Chain 3:



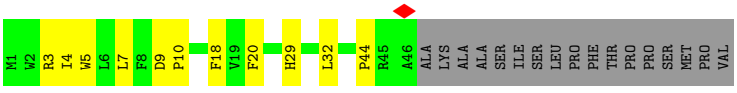
• Molecule 5: Light-harvesting complex 1 alpha chain

Chain Y:



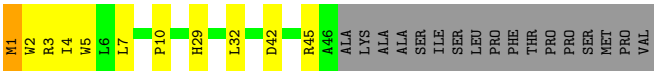
• Molecule 5: Light-harvesting complex 1 alpha chain

Chain V:



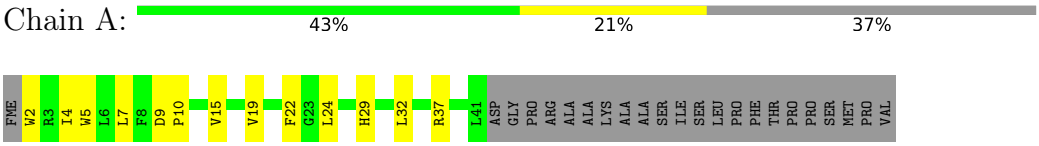
• Molecule 5: Light-harvesting complex 1 alpha chain

Chain T:



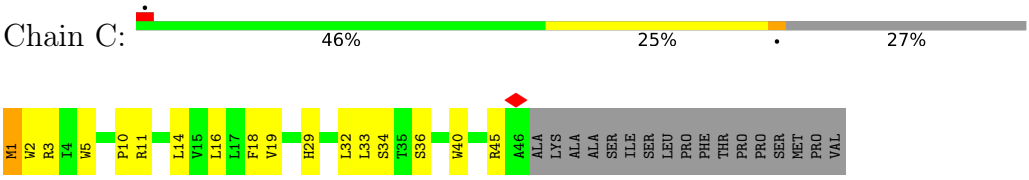
• Molecule 5: Light-harvesting complex 1 alpha chain

Chain A:



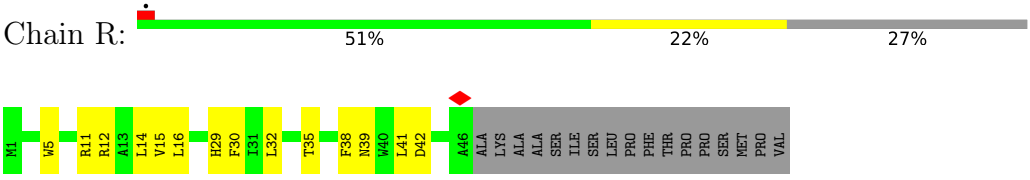
• Molecule 5: Light-harvesting complex 1 alpha chain

Chain C:



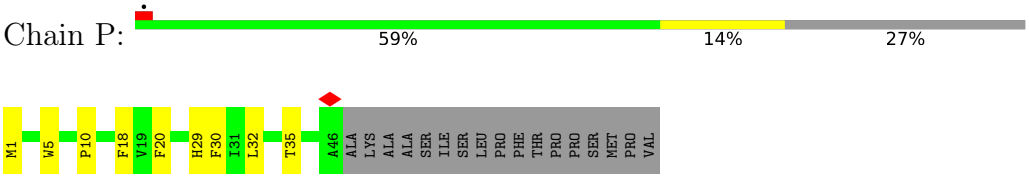
• Molecule 5: Light-harvesting complex 1 alpha chain

Chain R:



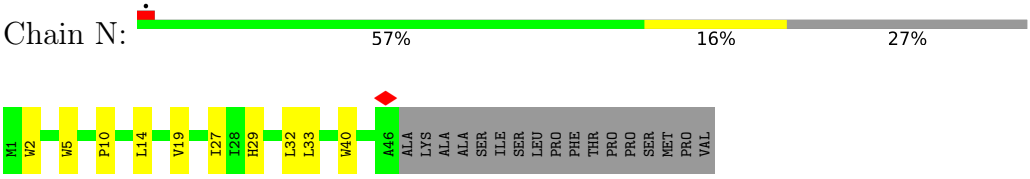
• Molecule 5: Light-harvesting complex 1 alpha chain

Chain P:



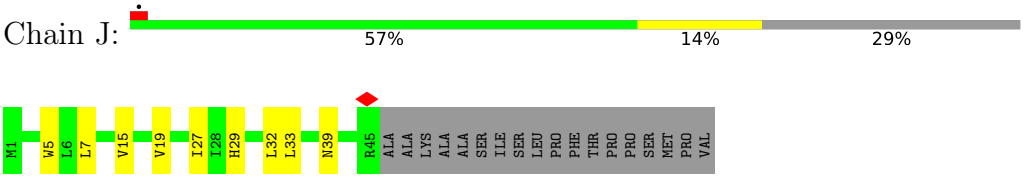
• Molecule 5: Light-harvesting complex 1 alpha chain

Chain N:



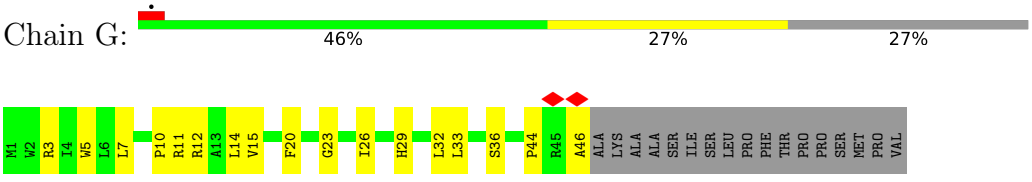
• Molecule 5: Light-harvesting complex 1 alpha chain

Chain J:



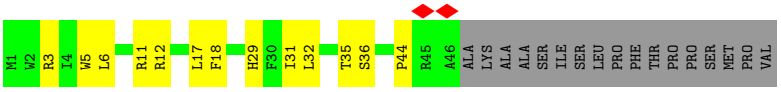
• Molecule 5: Light-harvesting complex 1 alpha chain

Chain G:



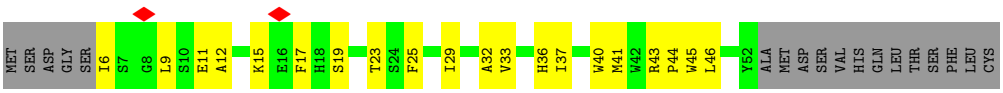
• Molecule 5: Light-harvesting complex 1 alpha chain

Chain E:



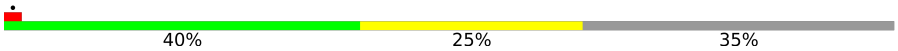
• Molecule 6: Light-harvesting complex 1 beta chain

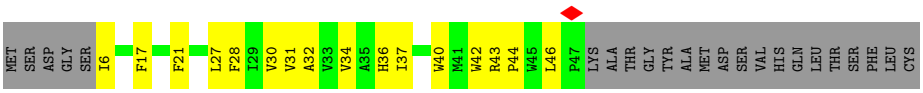
Chain 2:



• Molecule 6: Light-harvesting complex 1 beta chain

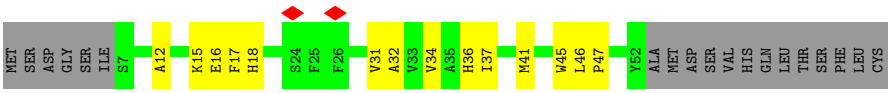
Chain 6:





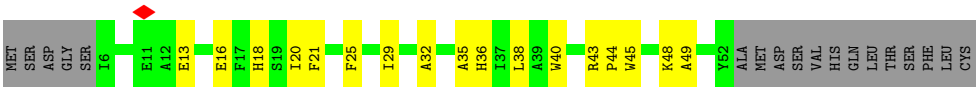
• Molecule 6: Light-harvesting complex 1 beta chain

Chain 4:



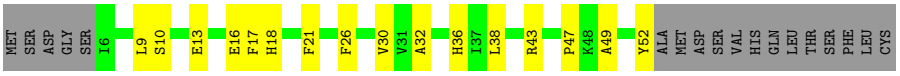
• Molecule 6: Light-harvesting complex 1 beta chain

Chain Z:



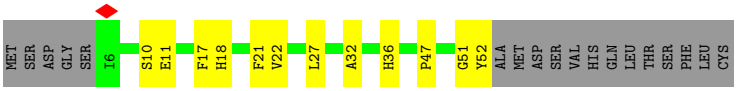
• Molecule 6: Light-harvesting complex 1 beta chain

Chain X:



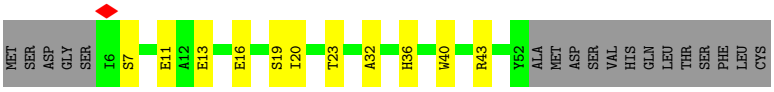
• Molecule 6: Light-harvesting complex 1 beta chain

Chain U:



• Molecule 6: Light-harvesting complex 1 beta chain

Chain B:

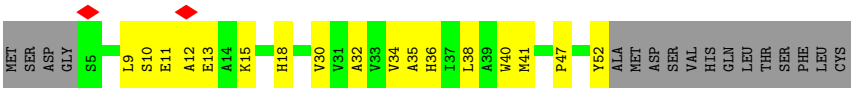


• Molecule 6: Light-harvesting complex 1 beta chain

Chain D:

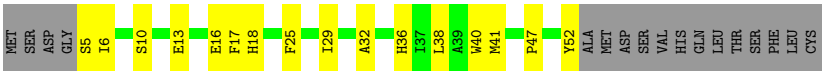
• Molecule 6: Light-harvesting complex 1 beta chain

Chain S:



• Molecule 6: Light-harvesting complex 1 beta chain

Chain Q:



• Molecule 6: Light-harvesting complex 1 beta chain

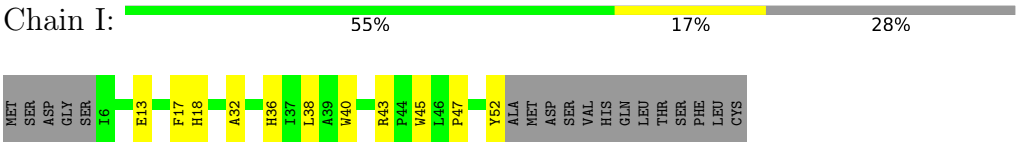
Chain O:

• Molecule 6: Light-harvesting complex 1 beta chain

Chain K:

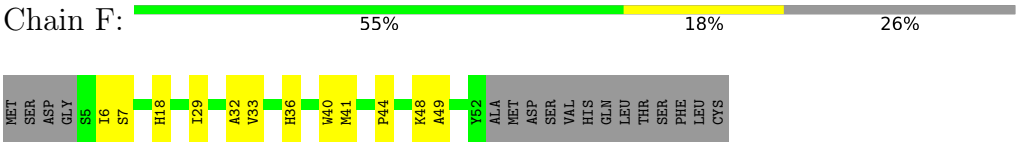
• Molecule 6: Light-harvesting complex 1 beta chain

Chain I:



• Molecule 6: Light-harvesting complex 1 beta chain

Chain F:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	377703	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	46.2	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.804	Depositor
Minimum map value	-0.205	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.015	Depositor
Recommended contour level	0.15	Depositor
Map size (Å)	419.19998, 419.19998, 419.19998	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.048, 1.048, 1.048	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: QAK, PGT, FE, LMT, FME, U10, CRT, BCL, CDL, BPH, 6PL

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	W	0.31	0/696	0.47	0/949
2	M	0.41	0/2470	0.44	0/3379
3	L	0.45	0/2271	0.44	0/3109
4	H	0.39	0/1946	0.48	0/2663
5	1	0.37	0/401	0.44	0/546
5	3	0.33	0/401	0.46	0/546
5	5	0.29	0/401	0.46	0/546
5	A	0.38	0/365	0.42	0/497
5	C	0.42	0/401	0.43	0/546
5	E	0.42	0/401	0.42	0/546
5	G	0.41	0/401	0.42	0/546
5	J	0.39	0/396	0.39	0/539
5	N	0.39	0/401	0.41	0/546
5	P	0.39	0/401	0.42	0/546
5	R	0.40	0/401	0.46	0/546
5	T	0.40	0/413	0.47	0/562
5	V	0.38	0/401	0.47	0/546
5	Y	0.36	0/401	0.43	0/546
6	2	0.37	0/409	0.42	0/558
6	4	0.32	0/389	0.45	0/531
6	6	0.36	0/371	0.41	0/507
6	B	0.41	0/397	0.43	0/542
6	D	0.41	0/415	0.41	0/566
6	F	0.41	0/403	0.47	0/550
6	I	0.41	0/397	0.42	0/542
6	K	0.41	0/397	0.39	0/542
6	O	0.38	0/403	0.46	0/550
6	Q	0.39	0/415	0.46	0/566
6	S	0.40	0/415	0.42	0/566
6	U	0.39	0/409	0.41	0/558
6	X	0.39	0/409	0.48	0/558
6	Z	0.41	0/409	0.46	0/558

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
All	All	0.40	0/18606	0.44	0/25398

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	W	682	0	727	15	0
2	M	2381	0	2323	41	0
3	L	2185	0	2130	54	0
4	H	1894	0	1909	45	0
5	1	397	0	415	23	0
5	3	397	0	415	19	0
5	5	397	0	415	17	0
5	A	352	0	372	15	0
5	C	397	0	415	17	0
5	E	397	0	415	16	0
5	G	397	0	415	17	0
5	J	392	0	410	11	0
5	N	397	0	415	11	0
5	P	397	0	415	10	0
5	R	397	0	415	14	0
5	T	408	0	423	14	0
5	V	397	0	415	14	0
5	Y	397	0	415	16	0
6	2	393	0	388	21	0
6	4	374	0	369	17	0
6	6	356	0	351	15	0
6	B	382	0	380	10	0
6	D	399	0	393	11	0
6	F	388	0	385	14	0
6	I	382	0	380	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	K	382	0	380	14	0
6	O	388	0	385	15	0
6	Q	399	0	393	18	0
6	S	399	0	393	15	0
6	U	393	0	388	13	0
6	X	393	0	388	17	0
6	Z	393	0	388	20	0
7	M	41	0	0	0	0
8	1	66	0	74	11	0
8	2	66	0	74	5	0
8	3	66	0	74	6	0
8	4	66	0	74	5	0
8	5	132	0	148	15	0
8	A	132	0	148	19	0
8	C	66	0	74	5	0
8	D	66	0	74	6	0
8	E	132	0	148	13	0
8	G	132	0	148	11	0
8	J	132	0	148	16	0
8	L	132	0	148	7	0
8	M	132	0	148	9	0
8	N	132	0	148	17	0
8	P	132	0	148	6	0
8	R	132	0	148	10	0
8	T	132	0	148	10	0
8	V	132	0	148	9	0
8	Y	132	0	148	17	0
9	L	65	0	76	6	0
9	M	65	0	76	6	0
10	1	40	0	51	2	0
10	L	19	0	17	1	0
10	M	48	0	63	6	0
11	E	40	0	54	9	0
11	H	52	0	84	9	0
11	M	52	0	84	5	0
12	3	85	0	117	10	0
12	G	178	0	259	20	0
12	H	87	0	121	12	0
12	L	89	0	124	9	0
12	M	95	0	143	12	0
13	M	1	0	0	0	0
14	2	70	0	89	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	4	35	0	45	1	0
14	6	35	0	44	3	0
14	B	70	0	88	6	0
14	D	101	0	124	9	0
14	F	70	0	90	5	0
14	I	70	0	91	4	0
14	J	35	0	45	2	0
14	K	70	0	90	4	0
14	L	35	0	44	3	0
14	M	35	0	45	2	0
14	O	35	0	45	3	0
14	Q	70	0	90	2	0
14	R	35	0	44	4	0
14	S	70	0	90	3	0
14	U	70	0	90	2	0
14	X	70	0	91	5	0
14	Z	35	0	45	3	0
15	2	44	0	60	7	0
15	3	44	0	60	5	0
15	B	44	0	60	3	0
15	D	44	0	60	1	0
15	F	44	0	60	6	0
15	I	44	0	60	5	0
15	K	44	0	60	6	0
15	O	44	0	60	3	0
15	Q	44	0	60	2	0
15	R	44	0	60	2	0
15	S	44	0	60	1	0
15	X	44	0	60	8	0
15	Z	44	0	60	13	0
16	P	50	0	73	3	0
17	H	2	0	0	0	0
17	L	5	0	0	0	0
17	M	3	0	0	1	0
All	All	22794	0	24000	674	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 14.

All (674) 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)
12:H:302:CDL:H581	11:E:101:6PL:H381	1.52	0.90
3:L:63:TRP:HE1	11:H:301:6PL:H61	1.39	0.87
3:L:221:VAL:HG23	8:L:401:BCL:H112	1.57	0.84
5:C:32:LEU:HD11	8:D:104:BCL:HHD	1.64	0.80
8:5:101:BCL:HMB2	15:3:103:CRT:H35	1.64	0.79
8:T:101:BCL:HMB2	15:S:103:CRT:H35	1.64	0.79
3:L:76:LEU:H	14:L:405:LMT:H6'2	1.47	0.78
2:M:255:THR:O	3:L:104:ARG:NH1	2.15	0.78
1:W:91:PHE:HA	1:W:94:ARG:HB2	1.64	0.78
5:J:32:LEU:HD11	8:J:103:BCL:HHD	1.65	0.77
6:O:40:TRP:HE1	14:O:101:LMT:H1B	1.51	0.76
5:3:1:FME:HCN	6:4:15:LYS:HB2	1.67	0.75
5:Y:32:LEU:HD11	8:Y:102:BCL:HHD	1.68	0.75
4:H:248:PRO:HD2	4:H:250:ARG:HE	1.52	0.74
5:V:32:LEU:HD11	8:V:102:BCL:HHD	1.69	0.74
8:G:102:BCL:HMB2	15:F:103:CRT:H35	1.67	0.74
8:A:102:BCL:H172	6:D:38:LEU:HB3	1.71	0.73
15:Z:101:CRT:H83	5:V:4:ILE:HA	1.71	0.73
5:G:32:LEU:HD11	8:G:103:BCL:HHD	1.71	0.73
3:L:31:TYR:O	3:L:104:ARG:NH2	2.21	0.73
15:B:103:CRT:H35	8:C:100:BCL:HMB2	1.70	0.73
8:P:101:BCL:HMB2	15:O:102:CRT:H35	1.69	0.72
5:1:32:LEU:HD11	8:2:101:BCL:HHD	1.69	0.72
11:M:405:6PL:H471	8:N:101:BCL:H201	1.70	0.72
5:R:32:LEU:HD11	8:R:104:BCL:HHD	1.71	0.72
6:Z:32:ALA:O	6:Z:36:HIS:ND1	2.21	0.72
5:5:37:ARG:O	6:6:43:ARG:NH1	2.22	0.71
5:T:32:LEU:HD11	8:T:102:BCL:HHD	1.71	0.71
4:H:54:VAL:HG13	4:H:55:PRO:HD3	1.73	0.71
6:6:42:TRP:HA	14:6:101:LMT:H1'	1.71	0.71
6:X:32:ALA:O	6:X:36:HIS:ND1	2.19	0.70
8:J:102:BCL:H171	12:G:104:CDL:H392	1.71	0.70
2:M:6:ASN:O	3:L:232:ARG:NE	2.19	0.70
5:Y:29:HIS:HB3	15:X:102:CRT:H2M3	1.74	0.70
6:F:32:ALA:O	6:F:36:HIS:ND1	2.22	0.70
6:O:32:ALA:O	6:O:36:HIS:ND1	2.23	0.69
3:L:24:ASP:OD1	3:L:111:LYS:NZ	2.25	0.69
6:X:10:SER:HB3	6:X:13:GLU:HB3	1.74	0.69
5:1:8:PHE:HD1	5:1:12:ARG:HH22	1.41	0.69
6:U:32:ALA:O	6:U:36:HIS:ND1	2.19	0.69
8:N:101:BCL:HMB2	15:K:103:CRT:H35	1.73	0.69
8:1:101:BCL:HMB2	15:Z:101:CRT:H35	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:I:32:ALA:O	6:I:36:HIS:ND1	2.21	0.69
5:P:5:TRP:HE1	6:Q:18:HIS:HD2	1.41	0.69
6:6:32:ALA:O	6:6:36:HIS:ND1	2.18	0.68
5:5:6:LEU:O	6:6:6:ILE:N	2.27	0.68
5:E:11:ARG:NH1	11:E:101:6PL:O1P	2.21	0.68
5:N:32:LEU:HD11	8:N:102:BCL:HHD	1.75	0.68
6:Q:13:GLU:HB2	15:Q:103:CRT:H1M1	1.74	0.68
12:L:404:CDL:HA61	5:G:33:LEU:HD23	1.76	0.67
4:H:202:PHE:HE2	4:H:204:LYS:HE2	1.59	0.67
5:3:3:ARG:HE	6:4:15:LYS:HB3	1.59	0.67
6:K:32:ALA:O	6:K:36:HIS:ND1	2.20	0.67
2:M:52:TYR:O	2:M:132:ARG:NH2	2.27	0.67
4:H:187:LYS:NZ	4:H:216:ALA:O	2.28	0.67
5:5:37:ARG:NH2	6:6:44:PRO:O	2.28	0.67
5:1:22:PHE:HB2	8:1:101:BCL:H71	1.76	0.67
5:R:39:ASN:ND2	5:R:41:LEU:O	2.26	0.67
8:J:102:BCL:HMB2	15:I:103:CRT:H35	1.75	0.67
9:M:403:BPH:HBB3	9:M:403:BPH:HHC	1.77	0.66
5:3:1:FME:SD	5:3:1:FME:N	2.66	0.66
6:4:32:ALA:O	6:4:36:HIS:ND1	2.23	0.66
2:M:233:ARG:NH1	4:H:120:GLU:OE2	2.29	0.66
5:1:17:LEU:HD21	15:2:102:CRT:H19	1.77	0.66
8:Y:101:BCL:HMB2	15:X:102:CRT:H35	1.77	0.66
12:G:104:CDL:H611	12:G:104:CDL:H192	1.77	0.66
16:P:102:PGT:H161	16:P:102:PGT:H432	1.78	0.66
6:4:34:VAL:HA	6:4:37:ILE:HD12	1.78	0.66
15:2:102:CRT:H35	8:3:101:BCL:HMB2	1.78	0.65
2:M:298:GLY:O	2:M:302:GLY:N	2.29	0.65
6:2:32:ALA:O	6:2:36:HIS:ND1	2.27	0.65
2:M:278:LEU:HD21	12:M:406:CDL:H191	1.79	0.65
5:P:5:TRP:HE1	6:Q:18:HIS:CD2	2.15	0.65
12:L:404:CDL:H772	11:H:301:6PL:H161	1.78	0.64
3:L:136:ARG:HG2	3:L:140:MET:HE2	1.79	0.64
5:1:6:LEU:HA	6:2:9:LEU:HD21	1.79	0.64
5:A:9:ASP:HB3	6:B:7:SER:HB3	1.80	0.64
5:1:6:LEU:HD12	6:2:6:ILE:HD11	1.80	0.64
14:2:103:LMT:H122	8:Y:102:BCL:H102	1.80	0.64
8:Y:102:BCL:HAA1	14:Z:102:LMT:H122	1.80	0.63
5:T:42:ASP:OD2	5:R:35:THR:OG1	2.17	0.63
5:N:29:HIS:CE1	8:N:102:BCL:HMD1	2.34	0.63
3:L:80:PRO:HG2	3:L:83:GLU:HB2	1.78	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:36:SER:OG	5:G:44:PRO:O	2.14	0.63
6:Q:32:ALA:O	6:Q:36:HIS:ND1	2.21	0.62
12:L:404:CDL:H791	12:G:101:CDL:H642	1.81	0.62
4:H:155:CYS:H	4:H:211:ARG:HA	1.65	0.62
5:J:15:VAL:HG22	12:G:101:CDL:H731	1.81	0.62
8:5:101:BCL:H2	6:6:28:PHE:HE2	1.64	0.61
10:M:404:U10:H23	12:H:302:CDL:H332	1.82	0.61
9:M:403:BPH:HBC3	9:M:403:BPH:HHD	1.81	0.61
4:H:155:CYS:HB3	4:H:248:PRO:HG3	1.82	0.61
5:T:29:HIS:CE1	8:T:102:BCL:HMD1	2.35	0.61
5:P:29:HIS:CE1	8:P:103:BCL:HMD1	2.35	0.61
5:A:32:LEU:HD11	8:A:102:BCL:HHD	1.82	0.61
2:M:216:PHE:HB2	3:L:188:LEU:HD13	1.83	0.61
8:5:101:BCL:H2	6:6:28:PHE:CE2	2.36	0.61
5:N:19:VAL:HG23	8:N:101:BCL:H161	1.83	0.60
1:W:81:THR:HA	1:W:84:VAL:HG12	1.83	0.60
5:C:29:HIS:CE1	8:D:104:BCL:HMD1	2.36	0.60
5:E:29:HIS:CE1	8:E:103:BCL:HMD1	2.36	0.60
5:Y:5:TRP:HE1	6:Z:18:HIS:CD2	2.19	0.60
5:V:29:HIS:CE1	8:V:102:BCL:HMD1	2.36	0.60
3:L:63:TRP:NE1	11:H:301:6PL:H61	2.15	0.60
4:H:54:VAL:HG21	12:G:104:CDL:H332	1.83	0.60
6:2:37:ILE:O	6:2:41:MET:HG3	2.01	0.60
5:1:3:ARG:HA	5:1:6:LEU:HD23	1.84	0.60
5:R:32:LEU:O	5:R:35:THR:HG22	2.01	0.60
6:S:40:TRP:HE1	14:S:101:LMT:H3'	1.67	0.59
6:O:5:SER:OG	6:O:6:ILE:N	2.35	0.59
5:Y:1:FME:O	6:Z:18:HIS:NE2	2.36	0.59
5:T:4:ILE:HD12	5:T:7:LEU:HD21	1.84	0.59
5:P:32:LEU:HD11	8:P:103:BCL:HHD	1.85	0.59
2:M:276:CYS:HB3	2:M:277:PRO:HD3	1.85	0.59
15:Z:101:CRT:H1M1	5:V:7:LEU:HB3	1.85	0.59
6:B:32:ALA:O	6:B:36:HIS:ND1	2.30	0.59
6:O:43:ARG:NH2	6:K:47:PRO:O	2.30	0.59
4:H:151:PRO:HA	4:H:162:THR:HA	1.85	0.59
1:W:27:PRO:HD2	1:W:31:LEU:HD13	1.85	0.58
15:3:103:CRT:H9	6:4:17:PHE:CE1	2.37	0.58
5:J:29:HIS:CE1	8:J:103:BCL:HMD1	2.38	0.58
5:3:10:PRO:HB3	6:4:17:PHE:CZ	2.38	0.58
3:L:211:GLU:N	3:L:211:GLU:OE1	2.35	0.58
5:A:22:PHE:HD2	8:A:101:BCL:H152	1.67	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:280:GLY:HA2	8:M:402:BCL:HED2	1.85	0.58
8:Y:101:BCL:H151	5:V:20:PHE:HB2	1.86	0.58
3:L:2:ALA:N	12:H:302:CDL:OB4	2.35	0.58
14:S:101:LMT:H81	14:S:102:LMT:H62	1.84	0.58
8:J:102:BCL:HMA3	8:G:103:BCL:H102	1.84	0.58
8:G:103:BCL:HMB1	8:G:103:BCL:H122	1.84	0.58
6:S:32:ALA:O	6:S:36:HIS:ND1	2.22	0.58
5:1:29:HIS:CE1	8:2:101:BCL:HMD1	2.39	0.58
8:G:102:BCL:HBB2	15:F:103:CRT:H403	1.86	0.58
6:Q:40:TRP:HE1	14:Q:101:LMT:H1B	1.69	0.58
12:G:101:CDL:H561	12:G:104:CDL:H352	1.85	0.58
1:W:91:PHE:O	1:W:95:GLN:HG2	2.04	0.57
11:M:405:6PL:H481	8:N:101:BCL:H191	1.86	0.57
5:R:29:HIS:CE1	8:R:104:BCL:HMD1	2.39	0.57
6:Z:21:PHE:HA	15:Z:101:CRT:H14	1.86	0.57
12:H:302:CDL:H832	12:H:302:CDL:H191	1.87	0.57
6:X:16:GLU:OE1	5:T:3:ARG:NH2	2.36	0.57
15:D:105:CRT:H35	8:E:102:BCL:HMB2	1.87	0.57
5:Y:5:TRP:HE1	6:Z:18:HIS:HD2	1.51	0.57
6:D:41:MET:HG2	14:D:101:LMT:H11	1.86	0.57
11:M:405:6PL:H422	11:M:405:6PL:H191	1.87	0.57
5:1:8:PHE:HB3	5:1:13:ALA:HB2	1.86	0.57
4:H:112:TYR:HB2	4:H:233:ASP:HB3	1.86	0.57
12:3:102:CDL:H611	12:3:102:CDL:H162	1.85	0.57
8:A:102:BCL:H121	14:D:103:LMT:H61	1.87	0.57
5:G:29:HIS:CE1	8:G:103:BCL:HMD1	2.39	0.57
5:E:32:LEU:HD11	8:E:103:BCL:HHD	1.86	0.57
15:I:103:CRT:H1M3	6:F:6:ILE:HD11	1.86	0.57
2:M:241:ARG:NH1	4:H:35:GLU:OE1	2.33	0.57
4:H:1:MET:HG3	4:H:7:LEU:HD23	1.86	0.56
5:3:2:TRP:HB2	6:4:18:HIS:ND1	2.20	0.56
10:M:404:U10:H311	12:H:302:CDL:H571	1.86	0.56
8:D:104:BCL:H143	8:D:104:BCL:HMB1	1.87	0.56
8:R:103:BCL:H152	5:P:20:PHE:HB2	1.87	0.56
11:M:405:6PL:H452	11:M:405:6PL:H412	1.87	0.56
6:Z:38:LEU:HB3	14:X:101:LMT:H32	1.87	0.56
14:D:102:LMT:H121	8:D:104:BCL:HAA1	1.86	0.56
12:M:406:CDL:H801	8:N:101:BCL:H162	1.87	0.56
5:5:19:VAL:HG22	8:5:101:BCL:H193	1.87	0.56
5:G:5:TRP:HE1	6:I:18:HIS:HD2	1.52	0.56
12:L:404:CDL:H411	8:E:102:BCL:H202	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Y:1:FME:O1	5:Y:2:TRP:N	2.39	0.56
8:V:101:BCL:HMB2	15:R:101:CRT:H35	1.86	0.56
6:U:10:SER:OG	6:U:11:GLU:N	2.39	0.56
5:J:27:ILE:HD12	12:G:101:CDL:H472	1.87	0.55
5:3:32:LEU:HD11	8:4:101:BCL:HHD	1.87	0.55
10:M:404:U10:H401	11:E:101:6PL:H202	1.87	0.55
12:M:406:CDL:H772	4:H:23:GLY:HA3	1.88	0.55
9:L:403:BPH:HHC	9:L:403:BPH:HBB3	1.88	0.55
10:L:406:U10:H1M1	10:L:406:U10:H103	1.88	0.55
5:R:5:TRP:HE1	6:S:18:HIS:HD2	1.53	0.55
11:E:101:6PL:H352	8:E:102:BCL:H13	1.88	0.55
6:F:41:MET:HG2	14:F:101:LMT:H12	1.87	0.55
4:H:247:THR:O	4:H:249:LEU:N	2.39	0.55
5:5:29:HIS:CE1	8:5:102:BCL:HMD1	2.42	0.55
6:4:41:MET:O	14:4:102:LMT:O2'	2.22	0.55
15:K:103:CRT:H1M3	5:G:7:LEU:HD21	1.88	0.55
1:W:4:LEU:HD23	1:W:55:LEU:HD12	1.88	0.55
5:V:10:PRO:HB3	6:X:17:PHE:CZ	2.41	0.55
5:A:2:TRP:NE1	6:B:11:GLU:OE2	2.39	0.55
5:A:29:HIS:CE1	8:A:102:BCL:HMD1	2.41	0.55
15:Z:101:CRT:H82	5:V:7:LEU:HD21	1.87	0.55
6:O:44:PRO:HG2	14:O:101:LMT:H6'2	1.88	0.55
6:X:17:PHE:HA	15:X:102:CRT:H6	1.89	0.55
5:N:10:PRO:HB3	6:O:17:PHE:CZ	2.41	0.55
2:M:151:ALA:HB1	12:M:406:CDL:H211	1.89	0.55
5:1:1:FME:SD	5:1:1:FME:N	2.79	0.55
12:L:404:CDL:H312	5:E:31:ILE:HG12	1.88	0.55
8:M:407:BCL:H152	9:L:403:BPH:H172	1.89	0.54
6:D:44:PRO:HG3	14:D:101:LMT:H1B	1.89	0.54
4:H:151:PRO:HG2	4:H:204:LYS:HD3	1.90	0.54
6:2:19:SER:O	6:2:23:THR:HG23	2.07	0.54
2:M:24:ARG:NH1	3:L:205:GLU:OE1	2.40	0.54
5:3:3:ARG:NE	6:4:15:LYS:HB3	2.23	0.54
6:S:38:LEU:HD23	6:S:41:MET:HE3	1.90	0.54
5:V:18:PHE:HB3	8:V:101:BCL:H101	1.88	0.54
12:3:102:CDL:OA4	12:3:102:CDL:O1	2.25	0.54
1:W:16:ALA:HA	1:W:88:VAL:HG11	1.90	0.54
3:L:217:PHE:O	3:L:221:VAL:HG12	2.08	0.54
6:2:43:ARG:NH1	6:Z:49:ALA:HA	2.23	0.54
15:2:102:CRT:H2M3	5:3:29:HIS:HB3	1.89	0.53
8:5:101:BCL:HMC3	14:6:101:LMT:H92	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:5:TRP:HE1	6:I:18:HIS:CD2	2.26	0.53
5:P:32:LEU:O	5:P:35:THR:HG22	2.08	0.53
1:W:23:ALA:HB1	1:W:92:PHE:HB2	1.90	0.53
5:Y:29:HIS:CE1	8:Y:102:BCL:HMD1	2.43	0.53
5:C:3:ARG:HD2	15:F:103:CRT:H41	1.90	0.53
2:M:267:ARG:NH1	17:M:501:HOH:O	2.41	0.53
5:V:9:ASP:OD1	5:V:9:ASP:N	2.41	0.53
6:I:17:PHE:HB2	15:I:103:CRT:H21A	1.90	0.53
5:Y:17:LEU:HD11	15:Z:101:CRT:H243	1.90	0.53
14:M:409:LMT:O6'	14:R:102:LMT:O2'	2.24	0.52
12:3:102:CDL:H591	12:3:102:CDL:H142	1.91	0.52
6:D:32:ALA:O	6:D:36:HIS:ND1	2.23	0.52
6:K:6:ILE:HG13	6:K:8:GLY:H	1.73	0.52
1:W:32:TYR:HB3	1:W:92:PHE:CE2	2.45	0.52
12:M:406:CDL:H122	12:M:406:CDL:HB62	1.90	0.52
6:K:17:PHE:HA	15:K:103:CRT:H6	1.90	0.52
2:M:5:GLN:HB2	6:6:6:ILE:O	2.10	0.52
5:1:10:PRO:HB3	6:2:17:PHE:CZ	2.44	0.52
6:4:31:VAL:HA	6:4:34:VAL:HG12	1.91	0.52
3:L:255:VAL:HG12	12:3:102:CDL:H312	1.92	0.52
4:H:30:ARG:NH2	12:G:101:CDL:OA4	2.42	0.52
4:H:190:LEU:HB2	4:H:235:ILE:HD13	1.90	0.52
2:M:179:VAL:O	2:M:182:HIS:ND1	2.40	0.52
5:5:32:LEU:HD22	8:5:102:BCL:HHD	1.92	0.52
5:N:5:TRP:HE1	6:O:18:HIS:HD2	1.57	0.52
5:Y:14:LEU:HD21	15:Z:101:CRT:H132	1.91	0.51
1:W:45:PRO:HA	1:W:48:THR:HG22	1.92	0.51
6:Z:13:GLU:HA	6:Z:16:GLU:HG3	1.93	0.51
5:G:23:GLY:HA3	12:G:104:CDL:H412	1.92	0.51
1:W:32:TYR:HB3	1:W:92:PHE:HE2	1.75	0.51
4:H:15:TYR:OH	11:H:301:6PL:O2P	2.29	0.51
5:C:5:TRP:HE1	6:D:18:HIS:HD2	1.58	0.51
5:3:27:ILE:HG12	12:3:102:CDL:H781	1.92	0.51
6:Z:43:ARG:HH12	6:X:49:ALA:HA	1.75	0.51
5:T:1:FME:HCN	5:T:3:ARG:HH11	1.75	0.51
12:M:406:CDL:H782	4:H:20:PHE:HA	1.92	0.51
6:Z:40:TRP:CZ2	6:Z:44:PRO:HB3	2.46	0.51
5:A:2:TRP:HA	5:A:5:TRP:CD1	2.46	0.51
8:T:102:BCL:H13	8:T:102:BCL:HMB1	1.92	0.51
12:3:102:CDL:HB32	12:3:102:CDL:H722	1.92	0.51
6:Q:10:SER:OG	6:Q:13:GLU:OE1	2.24	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:I:43:ARG:NH1	6:F:48:LYS:O	2.44	0.51
6:6:34:VAL:HA	6:6:37:ILE:HG12	1.93	0.50
5:3:29:HIS:CE1	8:4:101:BCL:HMD1	2.45	0.50
14:U:101:LMT:H2'	14:U:102:LMT:H52	1.93	0.50
6:D:38:LEU:HD13	14:D:103:LMT:H41	1.93	0.50
6:S:35:ALA:HB1	8:P:103:BCL:H151	1.92	0.50
6:F:29:ILE:O	6:F:33:VAL:HG23	2.11	0.50
5:3:1:FME:HCN	6:4:15:LYS:CB	2.37	0.50
5:V:5:TRP:HE1	6:X:18:HIS:HD2	1.58	0.50
8:G:103:BCL:HBB2	8:G:103:BCL:H13	1.93	0.50
12:H:302:CDL:H192	12:H:302:CDL:H621	1.93	0.50
8:5:102:BCL:H3A	8:5:102:BCL:H11	1.92	0.50
15:Z:101:CRT:H41	5:V:3:ARG:HB3	1.93	0.50
3:L:133:VAL:HG23	3:L:134:VAL:HG23	1.92	0.50
5:5:10:PRO:HB3	6:6:17:PHE:CE2	2.47	0.50
11:H:301:6PL:O2P	11:H:301:6PL:H51	2.12	0.50
6:2:43:ARG:HH12	6:Z:49:ALA:HA	1.75	0.50
6:S:10:SER:OG	6:S:11:GLU:OE2	2.24	0.50
4:H:181:GLU:OE2	4:H:186:ARG:HA	2.12	0.50
6:2:17:PHE:CE1	15:2:102:CRT:H9	2.46	0.50
2:M:61:LEU:HD21	8:L:401:BCL:H191	1.93	0.50
2:M:284:ILE:HG12	8:M:402:BCL:HED3	1.93	0.50
6:6:27:LEU:O	6:6:31:VAL:HG23	2.12	0.50
5:A:19:VAL:HG12	8:A:101:BCL:H111	1.94	0.50
14:D:101:LMT:H6E	14:D:102:LMT:H1B	1.94	0.50
6:2:17:PHE:HE1	15:2:102:CRT:H9	1.77	0.49
6:U:47:PRO:HB3	6:U:52:TYR:CE1	2.47	0.49
5:1:18:PHE:HB3	8:1:101:BCL:H93	1.94	0.49
6:4:12:ALA:HA	6:4:15:LYS:HG2	1.94	0.49
8:A:102:BCL:HAA1	14:B:102:LMT:H123	1.94	0.49
6:Q:5:SER:OG	6:Q:6:ILE:N	2.43	0.49
5:J:5:TRP:HE1	6:K:18:HIS:CD2	2.31	0.49
3:L:120:PHE:O	3:L:123:SER:OG	2.22	0.49
10:1:102:U10:H261	5:Y:23:GLY:HA2	1.95	0.49
5:N:5:TRP:HE1	6:O:18:HIS:CD2	2.30	0.49
5:J:5:TRP:HE1	6:K:18:HIS:HD2	1.61	0.49
3:L:53:ASN:HB2	3:L:86:ILE:HG21	1.94	0.49
3:L:71:ASP:OD1	3:L:72:ALA:N	2.45	0.49
8:L:402:BCL:H143	9:L:403:BPH:H5C2	1.94	0.49
5:5:27:ILE:HG22	12:3:102:CDL:H132	1.94	0.49
5:T:5:TRP:HE1	6:U:18:HIS:HD2	1.61	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:O:40:TRP:HZ2	14:O:101:LMT:H6D	1.77	0.49
4:H:153:VAL:HA	4:H:159:VAL:HA	1.95	0.49
4:H:167:TRP:HB2	4:H:177:TYR:HB2	1.95	0.49
6:O:35:ALA:HB1	8:J:103:BCL:H151	1.94	0.49
3:L:181:PHE:CD2	3:L:241:ALA:HB1	2.48	0.49
9:L:403:BPH:HHC	9:L:403:BPH:CBB	2.42	0.49
8:A:102:BCL:H192	14:B:102:LMT:H31	1.93	0.49
4:H:151:PRO:HG2	4:H:204:LYS:CD	2.42	0.49
6:Z:13:GLU:OE2	6:Z:13:GLU:N	2.43	0.49
8:J:103:BCL:H11	6:K:29:ILE:HD12	1.95	0.49
4:H:115:ARG:HD2	4:H:233:ASP:OD2	2.13	0.48
6:Q:25:PHE:O	6:Q:29:ILE:HG12	2.12	0.48
5:5:18:PHE:CE1	8:5:101:BCL:H51	2.48	0.48
8:Y:101:BCL:H141	8:Y:101:BCL:H162	1.64	0.48
8:A:102:BCL:H3A	8:A:102:BCL:O2A	2.12	0.48
5:C:1:FME:HE3	15:F:103:CRT:H10	1.95	0.48
6:S:11:GLU:HG2	6:S:15:LYS:HZ3	1.78	0.48
3:L:171:ASN:HB3	3:L:174:HIS:HB3	1.95	0.48
4:H:248:PRO:HD2	4:H:250:ARG:NE	2.26	0.48
8:Y:102:BCL:HAC2	6:Z:45:TRP:CZ3	2.48	0.48
6:X:38:LEU:HB3	8:T:102:BCL:H193	1.96	0.48
5:R:5:TRP:HE1	6:S:18:HIS:CD2	2.31	0.48
1:W:34:GLN:O	1:W:36:ALA:N	2.42	0.48
5:P:30:PHE:CZ	16:P:102:PGT:H371	2.49	0.48
14:B:101:LMT:H1B	14:B:101:LMT:H3'	1.63	0.48
6:F:44:PRO:HG3	14:F:101:LMT:H1B	1.96	0.48
6:Q:47:PRO:HB3	6:Q:52:TYR:CE1	2.49	0.48
6:I:40:TRP:CG	14:I:102:LMT:H62	2.49	0.48
2:M:166:LEU:HD21	5:R:30:PHE:HE2	1.77	0.48
8:1:101:BCL:C2B	15:Z:101:CRT:H371	2.43	0.48
6:Z:40:TRP:CE2	6:Z:44:PRO:HB3	2.48	0.48
8:T:102:BCL:CBB	8:T:102:BCL:H162	2.44	0.48
5:A:37:ARG:O	6:B:43:ARG:NH1	2.46	0.48
6:D:40:TRP:CG	14:D:101:LMT:H72	2.49	0.48
5:P:18:PHE:HB3	8:P:101:BCL:H92	1.96	0.48
6:O:25:PHE:O	6:O:29:ILE:HG12	2.14	0.48
8:N:101:BCL:H11	15:K:103:CRT:H291	1.95	0.48
6:K:25:PHE:O	6:K:29:ILE:HG12	2.14	0.48
3:L:242:VAL:HG21	9:L:403:BPH:HBC3	1.94	0.47
6:6:40:TRP:HH2	6:6:46:LEU:HB2	1.78	0.47
6:Q:40:TRP:CD1	14:Q:101:LMT:H4'	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:44:PRO:HG3	6:I:43:ARG:HH12	1.78	0.47
5:T:5:TRP:HE1	6:U:18:HIS:CD2	2.32	0.47
5:R:12:ARG:HA	5:R:15:VAL:HG12	1.97	0.47
5:E:6:LEU:HB3	6:F:6:ILE:HG12	1.96	0.47
6:B:13:GLU:HA	6:B:16:GLU:HG3	1.97	0.47
6:K:21:PHE:CD2	15:K:103:CRT:H14	2.50	0.47
6:X:43:ARG:NH2	6:U:47:PRO:O	2.46	0.47
5:C:5:TRP:HE1	6:D:18:HIS:CD2	2.32	0.47
4:H:211:ARG:HB3	4:H:248:PRO:HB3	1.97	0.47
5:1:21:LEU:HD23	8:1:101:BCL:H42	1.97	0.47
8:1:101:BCL:H192	8:1:101:BCL:H162	1.74	0.47
14:D:101:LMT:H101	14:D:102:LMT:H72	1.96	0.47
8:G:102:BCL:HMA3	8:E:103:BCL:H111	1.97	0.47
4:H:141:ASP:O	4:H:143:ARG:N	2.47	0.47
5:G:20:PHE:HA	12:G:104:CDL:H402	1.96	0.47
2:M:108:PRO:HG3	5:T:45:ARG:NH2	2.30	0.47
2:M:152:SER:OG	2:M:274:VAL:HG13	2.15	0.47
6:Z:43:ARG:NH1	6:X:49:ALA:HA	2.30	0.47
12:G:101:CDL:HA4	12:G:101:CDL:H111	1.62	0.47
3:L:265:TRP:O	3:L:268:TRP:HD1	1.98	0.47
8:L:401:BCL:H92	8:L:401:BCL:H61	1.68	0.47
6:2:43:ARG:NH2	6:Z:48:LYS:O	2.48	0.47
5:3:1:FME:HB3	5:3:2:TRP:CZ3	2.50	0.47
8:A:102:BCL:H111	8:A:102:BCL:H143	1.74	0.47
4:H:182:VAL:HG22	4:H:183:ALA:H	1.80	0.46
5:C:18:PHE:HB3	8:C:100:BCL:H61	1.96	0.46
14:R:102:LMT:O6'	14:R:102:LMT:O2B	2.28	0.46
6:I:38:LEU:HB3	8:E:103:BCL:H193	1.97	0.46
14:F:101:LMT:H111	14:F:102:LMT:H102	1.97	0.46
12:L:404:CDL:H771	12:G:101:CDL:H661	1.97	0.46
4:H:91:TRP:HD1	4:H:92:PRO:O	1.98	0.46
5:Y:41:LEU:O	5:Y:42:ASP:HB2	2.14	0.46
6:S:41:MET:HA	14:S:101:LMT:H6D	1.96	0.46
3:L:212:HIS:O	3:L:216:VAL:HG12	2.15	0.46
8:V:102:BCL:H93	8:V:102:BCL:H111	1.74	0.46
6:S:9:LEU:HB2	6:S:13:GLU:CG	2.45	0.46
8:G:103:BCL:H143	8:G:103:BCL:H111	1.64	0.46
2:M:257:GLY:HA2	3:L:29:PRO:HB2	1.97	0.46
4:H:189:VAL:HG12	4:H:220:THR:HG22	1.97	0.46
8:A:101:BCL:C4B	14:B:101:LMT:H102	2.45	0.46
6:2:40:TRP:CZ2	6:2:44:PRO:HB3	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:6:ILE:HG13	6:F:7:SER:H	1.80	0.46
4:H:131:PRO:HB2	4:H:133:ARG:HG2	1.98	0.46
5:1:6:LEU:HD13	6:2:9:LEU:HG	1.96	0.46
8:3:101:BCL:H8	8:3:101:BCL:H121	1.52	0.46
5:V:5:TRP:HE1	6:X:18:HIS:CD2	2.32	0.46
5:E:36:SER:OG	5:E:44:PRO:O	2.33	0.46
2:M:155:LEU:HD22	12:M:406:CDL:H202	1.98	0.46
3:L:76:LEU:N	14:L:405:LMT:H6'2	2.24	0.46
14:L:405:LMT:H101	8:A:101:BCL:HMB2	1.98	0.46
6:S:11:GLU:HG2	6:S:15:LYS:NZ	2.31	0.46
6:O:13:GLU:HA	6:O:16:GLU:HG2	1.98	0.46
15:K:103:CRT:H41	5:G:3:ARG:HD3	1.97	0.46
6:F:40:TRP:HD1	14:F:101:LMT:H11	1.80	0.46
1:W:10:ILE:HD12	1:W:10:ILE:H	1.81	0.46
4:H:146:ASN:OD1	4:H:148:VAL:HG12	2.16	0.46
5:3:24:LEU:HD23	8:4:101:BCL:HED2	1.98	0.46
8:V:102:BCL:HAA1	14:X:103:LMT:H112	1.97	0.46
5:E:5:TRP:HE1	6:F:18:HIS:HD2	1.64	0.46
8:M:407:BCL:H142	12:H:302:CDL:H432	1.98	0.46
4:H:147:PRO:HG3	4:H:198:ILE:HG12	1.98	0.46
12:H:302:CDL:OB8	5:E:12:ARG:HD2	2.16	0.46
6:X:13:GLU:HG3	15:X:102:CRT:H23	1.97	0.46
15:I:103:CRT:H5	5:E:3:ARG:HB3	1.99	0.45
9:M:403:BPH:C2B	8:L:401:BCL:H2	2.47	0.45
4:H:8:ASP:OD1	4:H:11:GLN:HG2	2.16	0.45
5:3:9:ASP:N	5:3:9:ASP:OD1	2.46	0.45
8:A:101:BCL:HMB1	8:A:101:BCL:HBB3	1.97	0.45
6:S:30:VAL:O	6:S:34:VAL:HG23	2.16	0.45
12:M:406:CDL:HA61	12:M:406:CDL:H312	1.69	0.45
5:1:5:TRP:CD2	6:2:17:PHE:HE2	2.34	0.45
5:1:17:LEU:HD11	15:2:102:CRT:H243	1.98	0.45
6:2:25:PHE:O	6:2:29:ILE:HG12	2.17	0.45
8:Y:102:BCL:H161	8:Y:102:BCL:H141	1.69	0.45
8:N:102:BCL:HBB1	8:N:102:BCL:H162	1.99	0.45
8:J:103:BCL:H51	8:J:103:BCL:H8	1.78	0.45
5:1:29:HIS:CD2	15:Z:101:CRT:H372	2.51	0.45
6:2:29:ILE:O	6:2:33:VAL:HG13	2.16	0.45
6:4:45:TRP:HD1	6:4:46:LEU:HG	1.82	0.45
6:X:9:LEU:HD21	6:X:13:GLU:HG2	1.98	0.45
5:A:15:VAL:O	5:A:19:VAL:HG13	2.16	0.45
5:G:12:ARG:NH1	12:G:101:CDL:OB3	2.39	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:14:LEU:HD23	11:H:301:6PL:H32	1.99	0.45
8:Y:101:BCL:HBB2	15:X:102:CRT:H392	1.99	0.45
8:R:103:BCL:HMB2	15:Q:103:CRT:H35	1.98	0.45
8:J:103:BCL:H2C	6:K:45:TRP:CE2	2.51	0.45
8:3:101:BCL:H121	8:3:101:BCL:H172	1.98	0.45
5:C:2:TRP:CE2	6:D:15:LYS:HE3	2.52	0.45
5:G:10:PRO:O	5:G:14:LEU:HB2	2.16	0.45
2:M:94:ALA:HB2	2:M:181:PRO:HG2	1.98	0.45
3:L:276:ASN:HB3	3:L:277:PRO:HD3	1.98	0.45
8:V:102:BCL:H41	8:V:102:BCL:H61	1.58	0.45
6:Q:38:LEU:HD23	6:Q:41:MET:HE3	1.99	0.45
2:M:159:ALA:HA	2:M:163:ILE:HB	1.98	0.45
2:M:239:LEU:HD11	3:L:207:VAL:HG11	1.98	0.45
6:F:40:TRP:CD1	14:F:101:LMT:H62	2.52	0.45
1:W:27:PRO:HB2	1:W:28:GLU:OE1	2.17	0.45
3:L:105:GLU:HB3	3:L:119:PRO:HG3	1.98	0.45
6:2:11:GLU:OE2	6:2:15:LYS:HB3	2.17	0.45
5:Y:28:ILE:HG12	15:Z:101:CRT:H403	1.99	0.45
8:V:102:BCL:H142	14:X:103:LMT:H71	1.98	0.45
3:L:225:ILE:HD11	3:L:230:ILE:HD13	1.99	0.44
6:6:27:LEU:HA	6:6:30:VAL:HG12	1.99	0.44
8:Y:101:BCL:C1D	14:X:101:LMT:H82	2.47	0.44
5:R:41:LEU:O	5:R:42:ASP:HB2	2.17	0.44
6:S:9:LEU:HB2	6:S:13:GLU:HG3	1.99	0.44
3:L:150:GLY:O	3:L:154:HIS:ND1	2.50	0.44
3:L:180:PHE:HB3	3:L:241:ALA:HB2	1.98	0.44
4:H:6:TYR:CE1	14:J:101:LMT:H2B	2.52	0.44
4:H:42:ASP:OD1	4:H:42:ASP:N	2.48	0.44
8:1:101:BCL:H193	8:1:101:BCL:H141	1.98	0.44
2:M:250:LEU:HA	2:M:250:LEU:HD23	1.71	0.44
11:M:405:6PL:H211	4:H:13:THR:HG23	1.99	0.44
6:X:47:PRO:HB3	6:X:52:TYR:CE1	2.52	0.44
5:T:10:PRO:HB3	6:U:17:PHE:CE1	2.52	0.44
14:K:101:LMT:H1B	14:K:101:LMT:H6'1	1.85	0.44
8:J:102:BCL:H191	12:G:101:CDL:H191	2.00	0.44
2:M:64:GLY:HA3	9:M:403:BPH:H5C1	2.00	0.44
12:M:406:CDL:H431	12:M:406:CDL:H402	1.76	0.44
12:H:302:CDL:H1	12:H:302:CDL:OA7	2.17	0.44
5:5:11:ARG:HA	5:3:8:PHE:HE1	1.82	0.44
8:3:101:BCL:H193	8:3:101:BCL:H161	1.77	0.44
8:Y:101:BCL:H11	15:X:102:CRT:H291	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:N:10:PRO:HG2	6:O:9:LEU:HD21	1.99	0.44
2:M:270:TRP:HH2	12:M:406:CDL:H152	1.83	0.44
10:M:404:U10:H403	3:L:40:VAL:HG11	2.00	0.44
12:M:406:CDL:H673	5:N:27:ILE:HD12	1.99	0.44
6:O:9:LEU:HD13	6:O:13:GLU:HG2	1.99	0.44
2:M:234:GLU:OE2	2:M:266:HIS:CE1	2.70	0.44
6:X:9:LEU:HD23	6:X:10:SER:O	2.17	0.44
8:T:102:BCL:HHC	8:T:102:BCL:OBB	2.18	0.44
8:A:102:BCL:H143	8:C:100:BCL:CHD	2.47	0.44
6:B:19:SER:O	6:B:23:THR:HG23	2.18	0.44
8:2:101:BCL:HAA1	14:2:104:LMT:H122	2.00	0.44
8:A:101:BCL:CHD	14:B:101:LMT:H51	2.48	0.44
6:B:13:GLU:O	6:B:16:GLU:HG3	2.18	0.44
5:C:3:ARG:HB3	15:F:103:CRT:H5	2.00	0.44
6:Q:47:PRO:HB3	6:Q:52:TYR:CZ	2.53	0.44
6:K:36:HIS:CE1	14:K:101:LMT:H111	2.53	0.44
5:G:11:ARG:O	5:G:15:VAL:HG12	2.18	0.44
5:G:26:ILE:HD11	12:G:104:CDL:H451	1.99	0.44
5:5:18:PHE:CG	8:5:101:BCL:H41	2.53	0.44
6:X:21:PHE:CD1	15:X:102:CRT:H14	2.53	0.44
8:T:102:BCL:H18	8:T:102:BCL:HBB1	1.99	0.44
6:S:47:PRO:HB3	6:S:52:TYR:CZ	2.53	0.44
5:P:10:PRO:HB3	6:Q:17:PHE:CZ	2.52	0.44
5:E:17:LEU:HD21	15:F:103:CRT:C19	2.48	0.44
3:L:194:LEU:HD23	3:L:194:LEU:HA	1.81	0.43
12:3:102:CDL:H141	12:3:102:CDL:H322	2.00	0.43
8:N:101:BCL:H152	8:N:101:BCL:H111	1.81	0.43
2:M:151:ALA:HB1	12:M:406:CDL:H242	2.00	0.43
3:L:27:VAL:HG13	11:E:101:6PL:H12	1.99	0.43
5:1:40:TRP:CE3	8:1:101:BCL:HBC2	2.52	0.43
8:Y:101:BCL:H122	5:V:20:PHE:HB2	2.00	0.43
6:U:18:HIS:O	6:U:22:VAL:HG23	2.18	0.43
5:J:27:ILE:HG23	14:J:101:LMT:H72	2.00	0.43
6:I:40:TRP:CD1	14:I:102:LMT:H42	2.53	0.43
5:A:2:TRP:HA	5:A:5:TRP:HD1	1.83	0.43
5:C:36:SER:OG	5:C:45:ARG:HG2	2.17	0.43
16:P:102:PGT:HO6	16:P:102:PGT:P	2.41	0.43
6:Q:10:SER:H	6:Q:13:GLU:CD	2.21	0.43
8:E:102:BCL:HMD1	6:F:36:HIS:CE1	2.53	0.43
3:L:63:TRP:CE2	11:H:301:6PL:H321	2.54	0.43
8:2:101:BCL:H61	8:2:101:BCL:H41	1.63	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:117:MET:HB2	2:M:117:MET:HE3	1.89	0.43
9:M:403:BPH:HBB2	3:L:182:PHE:HB3	2.01	0.43
3:L:208:LYS:HD2	3:L:212:HIS:CD2	2.53	0.43
8:L:401:BCL:H91	8:L:401:BCL:H111	1.72	0.43
5:5:17:LEU:HD13	6:6:21:PHE:HZ	1.83	0.43
8:Y:102:BCL:H51	8:Y:102:BCL:H12	1.74	0.43
8:Y:102:BCL:H2C	6:Z:45:TRP:CE2	2.53	0.43
8:A:101:BCL:HMD1	6:B:36:HIS:CE1	2.53	0.43
8:R:103:BCL:H61	8:R:103:BCL:H41	1.90	0.43
8:N:101:BCL:HMA3	8:J:103:BCL:H111	2.00	0.43
8:5:101:BCL:HBB2	8:5:101:BCL:HMB1	2.01	0.43
15:Z:101:CRT:H10	15:Z:101:CRT:H81	1.87	0.43
3:L:94:ALA:HA	9:L:403:BPH:H9C2	1.99	0.43
6:4:45:TRP:CD1	6:4:46:LEU:HG	2.53	0.43
5:Y:4:ILE:HD12	5:Y:4:ILE:H	1.83	0.43
5:C:40:TRP:CD2	8:C:100:BCL:H2C	2.54	0.43
8:R:104:BCL:H12	8:R:104:BCL:H51	1.84	0.43
6:S:10:SER:C	6:S:12:ALA:H	2.21	0.43
3:L:39:THR:HG21	3:L:101:TRP:HE3	1.83	0.43
3:L:48:ALA:HB2	12:L:404:CDL:H421	2.00	0.43
12:L:404:CDL:H312	5:E:31:ILE:CG1	2.49	0.43
8:5:101:BCL:C2B	15:3:103:CRT:H371	2.49	0.43
5:N:10:PRO:O	5:N:14:LEU:HB2	2.19	0.43
6:2:36:HIS:HE1	8:2:101:BCL:HAA2	1.84	0.43
8:A:102:BCL:H61	8:A:102:BCL:H41	1.50	0.43
5:R:11:ARG:HD2	6:Q:6:ILE:HG21	2.01	0.43
8:P:103:BCL:H2	6:Q:29:ILE:HD12	2.01	0.43
5:J:19:VAL:HG21	12:G:101:CDL:H121	2.00	0.43
8:L:401:BCL:HMB1	8:L:401:BCL:HBB2	2.00	0.43
4:H:54:VAL:CG1	4:H:55:PRO:HD3	2.47	0.43
5:1:9:ASP:N	5:1:9:ASP:OD1	2.50	0.43
8:N:102:BCL:HBA1	8:N:102:BCL:H3A	1.81	0.43
14:2:103:LMT:H6D	14:Z:102:LMT:H6E	2.00	0.42
5:3:27:ILE:HG12	12:3:102:CDL:C78	2.48	0.42
5:T:10:PRO:HB3	6:U:17:PHE:CZ	2.54	0.42
12:G:101:CDL:H132	12:G:101:CDL:H372	2.01	0.42
4:H:48:ARG:HH12	6:I:13:GLU:CD	2.22	0.42
8:N:101:BCL:H142	12:G:101:CDL:H401	2.00	0.42
8:N:102:BCL:H41	8:N:102:BCL:H62	1.74	0.42
10:1:102:U10:H1M1	10:1:102:U10:H72	1.80	0.42
6:2:45:TRP:HD1	6:2:46:LEU:HG	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:5:102:BCL:H2C	8:5:102:BCL:HBC3	1.85	0.42
6:K:39:ALA:HA	8:G:103:BCL:H202	2.02	0.42
4:H:98:PRO:HB3	4:H:107:VAL:HG21	2.01	0.42
15:3:103:CRT:H1M1	6:4:16:GLU:HB2	2.00	0.42
8:V:102:BCL:H192	8:V:102:BCL:H161	1.76	0.42
5:R:14:LEU:HD12	5:R:14:LEU:HA	1.87	0.42
5:J:33:LEU:O	5:J:39:ASN:ND2	2.52	0.42
8:J:102:BCL:H111	8:J:102:BCL:H151	1.81	0.42
6:I:43:ARG:NH2	6:F:49:ALA:HA	2.34	0.42
12:L:404:CDL:H711	12:L:404:CDL:H132	2.01	0.42
4:H:39:LEU:HB2	4:H:51:LYS:HB2	2.01	0.42
5:C:10:PRO:O	5:C:14:LEU:HB2	2.19	0.42
6:D:45:TRP:CD1	6:D:46:LEU:HG	2.54	0.42
5:J:19:VAL:HG22	8:J:102:BCL:H141	2.02	0.42
12:G:101:CDL:H391	12:G:101:CDL:H152	2.01	0.42
5:E:6:LEU:HD22	6:F:6:ILE:HG21	2.00	0.42
8:M:402:BCL:H192	8:M:402:BCL:H162	1.79	0.42
3:L:227:THR:O	3:L:231:HIS:ND1	2.46	0.42
6:X:26[B]:PHE:O	6:X:30:VAL:HG13	2.20	0.42
2:M:288:GLY:N	2:M:291:VAL:O	2.51	0.42
8:5:102:BCL:H141	8:5:102:BCL:H162	1.86	0.42
8:5:102:BCL:H161	8:5:102:BCL:H192	1.74	0.42
12:3:102:CDL:H122	12:3:102:CDL:H571	2.02	0.42
6:D:45:TRP:HD1	6:D:46:LEU:HG	1.85	0.42
8:D:104:BCL:CHB	8:E:102:BCL:HMB3	2.50	0.42
8:J:103:BCL:H11	6:K:29:ILE:CD1	2.48	0.42
5:G:14:LEU:HD12	5:G:14:LEU:HA	1.85	0.42
2:M:89:GLN:O	2:M:93:LEU:HG	2.20	0.42
14:M:409:LMT:H52	14:M:409:LMT:H81	1.92	0.42
5:3:14:LEU:HD12	5:3:14:LEU:HA	1.81	0.42
5:A:7:LEU:HD22	5:C:11:ARG:HG3	2.01	0.42
8:G:103:BCL:H2C	6:I:45:TRP:CE2	2.54	0.42
3:L:98:PHE:HB3	3:L:126:ILE:HG12	2.02	0.42
5:1:4:ILE:HD11	5:1:8:PHE:HD2	1.85	0.42
5:T:7:LEU:HD23	5:T:7:LEU:H	1.85	0.42
8:T:101:BCL:H121	5:R:16:LEU:HD11	2.00	0.42
8:R:103:BCL:H91	8:R:103:BCL:H112	1.64	0.42
6:Q:13:GLU:HA	6:Q:16:GLU:HG3	2.02	0.42
3:L:171:ASN:O	3:L:175:MET:HG3	2.20	0.42
4:H:197:LEU:HD13	4:H:197:LEU:HA	1.94	0.42
8:1:101:BCL:H13	8:1:101:BCL:H101	1.61	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Y:30:PHE:CD1	15:X:102:CRT:H2M1	2.55	0.42
8:T:102:BCL:H52	8:T:102:BCL:H12	1.77	0.42
15:O:102:CRT:H10	15:O:102:CRT:H81	1.90	0.42
4:H:151:PRO:HB3	4:H:162:THR:HG22	2.03	0.41
5:5:32:LEU:HD12	5:5:32:LEU:HA	1.83	0.41
6:6:40:TRP:CZ2	6:6:44:PRO:HB3	2.55	0.41
6:Z:35:ALA:HB2	14:X:101:LMT:H112	2.01	0.41
6:Q:38:LEU:HB3	8:N:102:BCL:H193	2.01	0.41
5:N:33:LEU:HD13	5:N:40:TRP:CH2	2.55	0.41
6:I:17:PHE:HA	15:I:103:CRT:H6	2.02	0.41
8:E:102:BCL:H192	8:E:102:BCL:H162	1.87	0.41
2:M:21:VAL:HG21	3:L:212:HIS:CD2	2.55	0.41
2:M:108:PRO:HG3	5:T:45:ARG:CZ	2.50	0.41
15:2:102:CRT:H372	5:3:29:HIS:CG	2.54	0.41
5:C:16:LEU:HB3	11:E:101:6PL:C17	2.50	0.41
1:W:34:GLN:OE1	15:B:103:CRT:H82	2.20	0.41
8:1:101:BCL:C4D	14:2:103:LMT:H112	2.50	0.41
8:Y:101:BCL:H61	8:Y:101:BCL:H41	1.88	0.41
5:A:9:ASP:HA	5:A:10:PRO:HD3	1.96	0.41
6:K:44:PRO:HG2	14:K:102:LMT:H5B	2.02	0.41
2:M:84:ILE:HG12	5:1:30:PHE:CE1	2.55	0.41
2:M:197:TYR:CZ	8:M:402:BCL:HMC2	2.55	0.41
3:L:225:ILE:HD12	3:L:230:ILE:HA	2.02	0.41
6:U:21:PHE:CD2	15:R:101:CRT:H14	2.54	0.41
2:M:72:GLY:HA2	2:M:75:MET:HE2	2.02	0.41
8:M:402:BCL:HAA2	8:M:402:BCL:HBD	2.01	0.41
3:L:25:PHE:CD2	11:E:101:6PL:H82	2.56	0.41
5:C:19:VAL:HG22	8:C:100:BCL:H13	2.02	0.41
5:R:35:THR:HG23	5:R:38:PHE:H	1.86	0.41
14:R:102:LMT:H123	8:R:103:BCL:H203	2.03	0.41
5:5:29:HIS:CG	15:3:103:CRT:H372	2.56	0.41
8:R:103:BCL:H161	5:P:20:PHE:HD1	1.86	0.41
8:J:103:BCL:C3B	14:K:101:LMT:H71	2.51	0.41
5:G:36:SER:HA	5:G:46:ALA:HB3	2.02	0.41
5:5:4:ILE:HA	5:5:7:LEU:HD23	2.02	0.41
6:Z:25:PHE:CZ	6:Z:29:ILE:HD11	2.55	0.41
5:A:4:ILE:HG23	5:A:5:TRP:CD2	2.55	0.41
5:A:24:LEU:HD23	8:A:102:BCL:HED3	2.03	0.41
8:N:101:BCL:H162	8:N:101:BCL:H141	1.87	0.41
5:E:31:ILE:O	5:E:35:THR:HG23	2.20	0.41
3:L:44:LEU:HD23	3:L:44:LEU:HA	1.91	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:151:PRO:O	4:H:204:LYS:HB3	2.21	0.41
8:1:101:BCL:H61	8:1:101:BCL:H102	1.73	0.41
14:6:101:LMT:H112	14:6:101:LMT:H81	1.80	0.41
5:Y:28:ILE:HD12	8:Y:102:BCL:O1D	2.21	0.41
6:Z:20:ILE:HB	15:Z:101:CRT:H9	2.03	0.41
6:B:19:SER:OG	6:B:20:ILE:N	2.54	0.41
10:M:404:U10:H402	11:E:101:6PL:H332	2.02	0.41
10:M:404:U10:H402	11:E:101:6PL:H351	2.02	0.41
3:L:41:PHE:O	3:L:45:ILE:HG12	2.21	0.41
11:H:301:6PL:H262	12:G:104:CDL:H191	2.03	0.41
12:H:302:CDL:HB61	5:E:12:ARG:NH2	2.35	0.41
6:2:40:TRP:CZ2	14:2:104:LMT:H1'	2.55	0.41
8:4:101:BCL:H161	8:4:101:BCL:H141	1.77	0.41
5:T:1:FME:O1	5:T:2:TRP:N	2.53	0.41
6:U:27:LEU:HD23	6:U:27:LEU:HA	1.85	0.41
5:A:22:PHE:HB2	8:A:101:BCL:H72	2.02	0.41
8:D:104:BCL:H51	8:D:104:BCL:H12	1.87	0.41
5:N:2:TRP:CE2	6:O:15:LYS:HE3	2.56	0.41
6:I:40:TRP:CZ2	14:I:101:LMT:H12	2.55	0.41
8:E:103:BCL:H62	8:E:103:BCL:H41	1.53	0.41
1:W:32:TYR:CG	1:W:33:CYS:N	2.89	0.41
2:M:226:VAL:HG23	2:M:231:GLY:HA3	2.02	0.41
3:L:214:ASN:HB3	3:L:218:ARG:NH1	2.36	0.41
14:D:101:LMT:H111	14:D:101:LMT:H82	1.75	0.41
8:R:104:BCL:H172	8:R:104:BCL:HBB1	2.03	0.41
8:E:102:BCL:HHC	8:E:102:BCL:OBB	2.21	0.41
5:1:8:PHE:HB3	5:1:13:ALA:CB	2.51	0.40
5:1:20:PHE:CD2	5:1:21:LEU:HD12	2.55	0.40
6:2:12:ALA:HA	6:2:15:LYS:HZ3	1.84	0.40
5:5:2:TRP:CZ2	5:5:4:ILE:HG12	2.56	0.40
8:3:101:BCL:H102	8:3:101:BCL:H61	1.41	0.40
5:Y:33:LEU:HD13	5:Y:40:TRP:CH2	2.57	0.40
14:Z:102:LMT:H1B	14:Z:102:LMT:H3'	1.72	0.40
5:V:44:PRO:HD2	6:U:51:GLY:HA2	2.03	0.40
14:R:102:LMT:H81	14:R:102:LMT:H52	1.86	0.40
2:M:216:PHE:CB	3:L:188:LEU:HD13	2.51	0.40
8:M:402:BCL:H141	9:M:403:BPH:H4C2	2.02	0.40
8:3:101:BCL:H143	8:3:101:BCL:H112	1.76	0.40
6:B:40:TRP:NE1	14:B:102:LMT:H5'	2.35	0.40
6:I:47:PRO:HB3	6:I:52:TYR:CZ	2.56	0.40
5:5:40:TRP:HA	6:4:47:PRO:HD2	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:3:23:GLY:O	5:3:27:ILE:HG13	2.21	0.40
6:U:36:HIS:CD2	14:U:101:LMT:H101	2.56	0.40
8:N:102:BCL:HBB2	8:N:102:BCL:H13	2.03	0.40
8:J:102:BCL:H192	8:J:102:BCL:H161	1.86	0.40
8:M:407:BCL:H13	8:M:407:BCL:H172	1.67	0.40
3:L:52:TRP:HE1	5:C:34:SER:HB2	1.86	0.40
11:H:301:6PL:H172	12:H:302:CDL:H442	2.03	0.40
12:H:302:CDL:H152	12:H:302:CDL:H791	2.04	0.40
5:J:7:LEU:HD23	5:J:7:LEU:HA	1.94	0.40
5:E:18:PHE:O	8:E:102:BCL:H72	2.22	0.40
5:E:36:SER:O	5:E:44:PRO:HA	2.21	0.40
2:M:61:LEU:HD23	2:M:61:LEU:HA	1.88	0.40
3:L:81:LEU:HD12	5:C:33:LEU:HB3	2.04	0.40
6:4:45:TRP:CE2	8:4:101:BCL:H2C	2.57	0.40
15:B:103:CRT:H20	15:B:103:CRT:H181	1.97	0.40
15:O:102:CRT:H20	15:O:102:CRT:H181	1.98	0.40
14:I:101:LMT:H5'	14:I:101:LMT:H1B	1.76	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	W	92/102 (90%)	83 (90%)	9 (10%)	0	100	100
2	M	297/307 (97%)	288 (97%)	9 (3%)	0	100	100
3	L	274/277 (99%)	266 (97%)	8 (3%)	0	100	100
4	H	249/255 (98%)	226 (91%)	23 (9%)	0	100	100
5	1	44/63 (70%)	42 (96%)	2 (4%)	0	100	100
5	3	44/63 (70%)	41 (93%)	3 (7%)	0	100	100
5	5	44/63 (70%)	38 (86%)	6 (14%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	A	38/63 (60%)	35 (92%)	3 (8%)	0	100	100
5	C	44/63 (70%)	44 (100%)	0	0	100	100
5	E	44/63 (70%)	42 (96%)	2 (4%)	0	100	100
5	G	44/63 (70%)	43 (98%)	1 (2%)	0	100	100
5	J	43/63 (68%)	42 (98%)	1 (2%)	0	100	100
5	N	44/63 (70%)	42 (96%)	2 (4%)	0	100	100
5	P	44/63 (70%)	41 (93%)	3 (7%)	0	100	100
5	R	44/63 (70%)	43 (98%)	1 (2%)	0	100	100
5	T	45/63 (71%)	41 (91%)	4 (9%)	0	100	100
5	V	44/63 (70%)	43 (98%)	1 (2%)	0	100	100
5	Y	44/63 (70%)	43 (98%)	1 (2%)	0	100	100
6	2	46/65 (71%)	42 (91%)	4 (9%)	0	100	100
6	4	44/65 (68%)	41 (93%)	3 (7%)	0	100	100
6	6	41/65 (63%)	39 (95%)	2 (5%)	0	100	100
6	B	45/65 (69%)	41 (91%)	4 (9%)	0	100	100
6	D	47/65 (72%)	45 (96%)	2 (4%)	0	100	100
6	F	46/65 (71%)	41 (89%)	5 (11%)	0	100	100
6	I	45/65 (69%)	42 (93%)	3 (7%)	0	100	100
6	K	45/65 (69%)	43 (96%)	2 (4%)	0	100	100
6	O	46/65 (71%)	42 (91%)	4 (9%)	0	100	100
6	Q	47/65 (72%)	45 (96%)	2 (4%)	0	100	100
6	S	47/65 (72%)	43 (92%)	4 (8%)	0	100	100
6	U	46/65 (71%)	42 (91%)	4 (9%)	0	100	100
6	X	46/65 (71%)	44 (96%)	2 (4%)	0	100	100
6	Z	46/65 (71%)	44 (96%)	2 (4%)	0	100	100
All	All	2159/2733 (79%)	2037 (94%)	122 (6%)	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	W	65/70 (93%)	65 (100%)	0	100 100
2	M	241/247 (98%)	241 (100%)	0	100 100
3	L	222/223 (100%)	220 (99%)	2 (1%)	78 87
4	H	199/203 (98%)	199 (100%)	0	100 100
5	1	40/54 (74%)	40 (100%)	0	100 100
5	3	40/54 (74%)	40 (100%)	0	100 100
5	5	40/54 (74%)	39 (98%)	1 (2%)	47 66
5	A	37/54 (68%)	37 (100%)	0	100 100
5	C	40/54 (74%)	40 (100%)	0	100 100
5	E	40/54 (74%)	40 (100%)	0	100 100
5	G	40/54 (74%)	40 (100%)	0	100 100
5	J	40/54 (74%)	40 (100%)	0	100 100
5	N	40/54 (74%)	40 (100%)	0	100 100
5	P	40/54 (74%)	40 (100%)	0	100 100
5	R	40/54 (74%)	40 (100%)	0	100 100
5	T	41/54 (76%)	41 (100%)	0	100 100
5	V	40/54 (74%)	40 (100%)	0	100 100
5	Y	40/54 (74%)	39 (98%)	1 (2%)	47 66
6	2	40/55 (73%)	40 (100%)	0	100 100
6	4	38/55 (69%)	38 (100%)	0	100 100
6	6	37/55 (67%)	37 (100%)	0	100 100
6	B	39/55 (71%)	39 (100%)	0	100 100
6	D	41/55 (74%)	41 (100%)	0	100 100
6	F	40/55 (73%)	40 (100%)	0	100 100
6	I	39/55 (71%)	39 (100%)	0	100 100
6	K	39/55 (71%)	39 (100%)	0	100 100
6	O	40/55 (73%)	40 (100%)	0	100 100
6	Q	41/55 (74%)	41 (100%)	0	100 100
6	S	41/55 (74%)	41 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
6	U	40/55 (73%)	40 (100%)	0	100 100
6	X	40/55 (73%)	40 (100%)	0	100 100
6	Z	40/55 (73%)	40 (100%)	0	100 100
All	All	1840/2269 (81%)	1836 (100%)	4 (0%)	93 97

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	L	248	CYS
3	L	275	TRP
5	5	3	ARG
5	Y	3	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
2	M	10	GLN
2	M	187	ASN
3	L	64	GLN
3	L	160	ASN
3	L	267	ASN
3	L	271	ASN
6	6	18	HIS
6	Z	18	HIS
6	X	18	HIS
6	U	18	HIS
6	B	18	HIS
6	D	18	HIS
6	S	18	HIS
6	Q	18	HIS
6	O	18	HIS
6	K	18	HIS
6	I	18	HIS
6	F	18	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

13 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	$\#\|Z\| > 2$
5	FME	R	1	5	8,9,10	0.94	0	7,9,11	0.92	0
5	FME	V	1	5	8,9,10	0.96	0	7,9,11	0.99	0
5	FME	C	1	5	8,9,10	0.98	1 (12%)	7,9,11	1.11	1 (14%)
5	FME	N	1	5	8,9,10	0.94	0	7,9,11	0.75	0
5	FME	E	1	5	8,9,10	0.93	0	7,9,11	0.76	0
5	FME	Y	1	5	8,9,10	0.93	0	7,9,11	1.14	0
5	FME	G	1	5	8,9,10	0.96	0	7,9,11	0.82	0
5	FME	5	1	5	8,9,10	0.95	0	7,9,11	0.89	0
5	FME	T	1	5	8,9,10	0.89	0	7,9,11	1.79	2 (28%)
5	FME	1	1	5	8,9,10	0.96	0	7,9,11	0.86	0
5	FME	J	1	5	8,9,10	0.96	0	7,9,11	1.06	0
5	FME	P	1	5	8,9,10	0.94	0	7,9,11	1.25	1 (14%)
5	FME	3	1	5	8,9,10	0.98	0	7,9,11	0.69	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
5	FME	R	1	5	-	1/7/9/11	-
5	FME	V	1	5	-	2/7/9/11	-
5	FME	C	1	5	-	3/7/9/11	-
5	FME	N	1	5	-	2/7/9/11	-
5	FME	E	1	5	-	3/7/9/11	-
5	FME	Y	1	5	-	3/7/9/11	-
5	FME	G	1	5	-	2/7/9/11	-
5	FME	5	1	5	-	5/7/9/11	-
5	FME	T	1	5	-	3/7/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	FME	1	1	5	-	0/7/9/11	-
5	FME	J	1	5	-	3/7/9/11	-
5	FME	P	1	5	-	5/7/9/11	-
5	FME	3	1	5	-	2/7/9/11	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	1	FME	CA-N	-2.03	1.43	1.46

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	T	1	FME	CA-N-CN	3.39	128.03	122.82
5	T	1	FME	C-CA-N	3.03	115.19	109.73
5	P	1	FME	C-CA-N	2.62	114.45	109.73
5	C	1	FME	C-CA-N	2.06	113.44	109.73

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	5	1	FME	N-CA-CB-CG
5	5	1	FME	O-C-CA-CB
5	5	1	FME	CA-CB-CG-SD
5	Y	1	FME	N-CA-CB-CG
5	Y	1	FME	C-CA-CB-CG
5	T	1	FME	N-CA-CB-CG
5	C	1	FME	N-CA-CB-CG
5	P	1	FME	N-CA-CB-CG
5	P	1	FME	O-C-CA-CB
5	J	1	FME	N-CA-CB-CG
5	J	1	FME	C-CA-CB-CG
5	G	1	FME	O-C-CA-CB
5	C	1	FME	CB-CG-SD-CE
5	5	1	FME	CB-CG-SD-CE
5	3	1	FME	CB-CG-SD-CE
5	V	1	FME	CB-CG-SD-CE
5	J	1	FME	CB-CG-SD-CE
5	G	1	FME	CB-CG-SD-CE

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Mol	Chain	Res	Type	Atoms
5	V	1	FME	N-CA-CB-CG
5	E	1	FME	N-CA-CB-CG
5	Y	1	FME	CB-CG-SD-CE
5	P	1	FME	CB-CG-SD-CE
5	R	1	FME	N-CA-CB-CG
5	T	1	FME	CB-CG-SD-CE
5	N	1	FME	CB-CG-SD-CE
5	3	1	FME	CB-CA-N-CN
5	5	1	FME	C-CA-CB-CG
5	T	1	FME	C-CA-CB-CG
5	C	1	FME	C-CA-CB-CG
5	P	1	FME	C-CA-CB-CG
5	N	1	FME	CA-CB-CG-SD
5	E	1	FME	CB-CG-SD-CE
5	P	1	FME	CB-CA-N-CN
5	E	1	FME	CB-CA-N-CN

There are no ring outliers.

5 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	1	FME	1	0
5	Y	1	FME	2	0
5	T	1	FME	2	0
5	1	1	FME	1	0
5	3	1	FME	4	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 91 ligands modelled in this entry, 1 is monoatomic - leaving 90 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	$\#\|Z\| > 2$
15	CRT	O	102	-	41,43,43	1.89	12 (29%)	50,54,54	1.71	12 (24%)
8	BCL	E	103	-	58,74,74	1.63	8 (13%)	69,115,115	1.62	12 (17%)
15	CRT	K	103	-	41,43,43	1.90	12 (29%)	50,54,54	1.70	14 (28%)
15	CRT	B	103	-	41,43,43	1.88	12 (29%)	50,54,54	1.62	14 (28%)
14	LMT	U	101	-	36,36,36	1.21	6 (16%)	47,47,47	1.02	2 (4%)
15	CRT	3	103	-	41,43,43	1.94	12 (29%)	50,54,54	1.71	13 (26%)
8	BCL	L	402	-	58,74,74	1.63	9 (15%)	69,115,115	1.71	14 (20%)
12	CDL	G	101	-	87,87,99	0.30	0	93,99,111	0.41	0
8	BCL	P	103	-	58,74,74	1.64	9 (15%)	69,115,115	1.71	14 (20%)
15	CRT	2	102	-	41,43,43	1.96	12 (29%)	50,54,54	1.76	15 (30%)
8	BCL	J	103	-	58,74,74	1.65	9 (15%)	69,115,115	1.72	13 (18%)
8	BCL	V	102	-	58,74,74	1.65	9 (15%)	69,115,115	1.65	12 (17%)
11	6PL	H	301	-	51,51,51	0.30	0	57,59,59	0.40	0
14	LMT	F	101	-	36,36,36	1.20	6 (16%)	47,47,47	1.01	1 (2%)
8	BCL	M	407	-	58,74,74	1.63	9 (15%)	69,115,115	1.83	14 (20%)
14	LMT	D	102	-	36,36,36	1.16	4 (11%)	47,47,47	0.95	2 (4%)
14	LMT	S	101	-	36,36,36	1.19	5 (13%)	47,47,47	1.03	2 (4%)
9	BPH	L	403	-	51,70,70	0.60	2 (3%)	52,101,101	0.75	2 (3%)
8	BCL	Y	102	-	58,74,74	1.64	8 (13%)	69,115,115	1.64	13 (18%)
12	CDL	G	104	-	89,89,99	0.29	0	95,101,111	0.41	0
14	LMT	F	102	-	36,36,36	1.12	5 (13%)	47,47,47	0.97	2 (4%)
14	LMT	I	101	-	36,36,36	1.16	5 (13%)	47,47,47	1.02	3 (6%)
8	BCL	A	101	-	58,74,74	1.62	9 (15%)	69,115,115	1.68	16 (23%)
12	CDL	M	406	-	94,94,99	0.28	0	100,106,111	0.35	0
14	LMT	Q	102	-	36,36,36	1.25	6 (16%)	47,47,47	1.11	3 (6%)
8	BCL	Y	101	-	58,74,74	1.62	8 (13%)	69,115,115	1.74	13 (18%)
8	BCL	V	101	-	58,74,74	1.61	9 (15%)	69,115,115	1.72	13 (18%)
14	LMT	I	102	-	36,36,36	1.22	6 (16%)	47,47,47	1.02	1 (2%)
14	LMT	O	101	-	36,36,36	1.13	5 (13%)	47,47,47	1.07	2 (4%)
12	CDL	H	302	-	86,86,99	0.30	0	92,98,111	0.39	0
7	QAK	M	401	-	40,40,40	1.28	3 (7%)	45,49,49	0.81	2 (4%)
8	BCL	J	102	-	58,74,74	1.61	9 (15%)	69,115,115	1.75	13 (18%)
8	BCL	3	101	-	58,74,74	1.65	11 (18%)	69,115,115	1.69	13 (18%)
14	LMT	M	409	-	36,36,36	1.25	6 (16%)	47,47,47	1.03	3 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
8	BCL	G	102	-	58,74,74	1.61	8 (13%)	69,115,115	1.70	14 (20%)
8	BCL	D	104	-	58,74,74	1.64	10 (17%)	69,115,115	1.69	13 (18%)
14	LMT	K	102	-	36,36,36	1.18	6 (16%)	47,47,47	1.05	3 (6%)
15	CRT	X	102	-	41,43,43	1.94	12 (29%)	50,54,54	1.71	14 (28%)
8	BCL	G	103	-	58,74,74	1.64	8 (13%)	69,115,115	1.68	12 (17%)
14	LMT	2	104	-	36,36,36	1.19	5 (13%)	47,47,47	0.97	2 (4%)
14	LMT	X	101	-	36,36,36	1.28	8 (22%)	47,47,47	1.13	4 (8%)
14	LMT	K	101	-	36,36,36	1.18	5 (13%)	47,47,47	0.96	1 (2%)
14	LMT	4	102	-	36,36,36	1.21	5 (13%)	47,47,47	1.07	3 (6%)
14	LMT	U	102	-	36,36,36	1.17	5 (13%)	47,47,47	1.04	3 (6%)
15	CRT	R	101	-	41,43,43	1.86	12 (29%)	50,54,54	1.58	12 (24%)
12	CDL	3	102	-	84,84,99	0.30	0	90,96,111	0.42	0
14	LMT	Q	101	-	36,36,36	1.22	5 (13%)	47,47,47	1.06	3 (6%)
11	6PL	M	405	-	51,51,51	0.29	0	57,59,59	0.35	0
8	BCL	1	101	-	58,74,74	1.62	10 (17%)	69,115,115	1.72	14 (20%)
16	PGT	P	102	-	49,49,50	0.28	0	52,55,56	0.41	0
8	BCL	R	103	-	58,74,74	1.64	8 (13%)	69,115,115	1.69	12 (17%)
8	BCL	N	102	-	58,74,74	1.63	8 (13%)	69,115,115	1.71	14 (20%)
14	LMT	X	103	-	36,36,36	1.21	6 (16%)	47,47,47	1.03	2 (4%)
12	CDL	L	404	-	87,87,99	0.29	0	91,98,111	0.38	0
8	BCL	E	102	-	58,74,74	1.63	10 (17%)	69,115,115	1.78	15 (21%)
10	U10	L	406	-	19,19,63	2.78	8 (42%)	23,26,79	1.37	3 (13%)
8	BCL	5	102	-	58,74,74	1.70	11 (18%)	69,115,115	1.59	11 (15%)
9	BPH	M	403	-	51,70,70	0.64	2 (3%)	52,101,101	0.72	1 (1%)
14	LMT	Z	102	-	36,36,36	1.17	6 (16%)	47,47,47	1.02	3 (6%)
14	LMT	R	102	-	36,36,36	1.24	6 (16%)	47,47,47	0.97	1 (2%)
14	LMT	D	101	-	36,36,36	1.24	6 (16%)	47,47,47	1.06	3 (6%)
8	BCL	P	101	-	58,74,74	1.59	9 (15%)	69,115,115	1.72	13 (18%)
15	CRT	Z	101	-	41,43,43	1.93	12 (29%)	50,54,54	1.88	13 (26%)
8	BCL	M	402	-	58,74,74	1.65	10 (17%)	69,115,115	1.87	18 (26%)
14	LMT	6	101	-	36,36,36	1.15	5 (13%)	47,47,47	0.94	1 (2%)
10	U10	M	404	-	48,48,63	2.65	14 (29%)	58,61,79	1.71	13 (22%)
8	BCL	5	101	-	58,74,74	1.64	10 (17%)	69,115,115	1.65	16 (23%)
14	LMT	S	102	-	36,36,36	1.18	5 (13%)	47,47,47	1.18	3 (6%)
8	BCL	T	102	-	58,74,74	1.63	9 (15%)	69,115,115	1.64	13 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
14	LMT	B	101	-	36,36,36	1.21	6 (16%)	47,47,47	0.97	1 (2%)
8	BCL	R	104	-	58,74,74	1.65	10 (17%)	69,115,115	1.72	12 (17%)
14	LMT	2	103	-	36,36,36	1.22	6 (16%)	47,47,47	1.03	2 (4%)
15	CRT	I	103	-	41,43,43	1.86	13 (31%)	50,54,54	1.57	12 (24%)
14	LMT	J	101	-	36,36,36	1.20	4 (11%)	47,47,47	1.16	2 (4%)
14	LMT	D	103	-	32,32,36	1.33	7 (21%)	43,43,47	1.16	3 (6%)
15	CRT	F	103	-	41,43,43	1.90	12 (29%)	50,54,54	1.64	13 (26%)
8	BCL	N	101	-	58,74,74	1.61	8 (13%)	69,115,115	1.69	13 (18%)
8	BCL	L	401	-	58,74,74	1.63	9 (15%)	69,115,115	1.77	16 (23%)
11	6PL	E	101	-	39,39,51	0.33	0	45,47,59	0.40	0
15	CRT	D	105	-	41,43,43	1.90	12 (29%)	50,54,54	1.64	14 (28%)
15	CRT	S	103	-	41,43,43	1.86	12 (29%)	50,54,54	1.65	13 (26%)
8	BCL	C	100	-	58,74,74	1.61	8 (13%)	69,115,115	1.74	15 (21%)
10	U10	1	102	-	40,40,63	2.69	11 (27%)	48,51,79	1.75	13 (27%)
15	CRT	Q	103	-	41,43,43	1.87	12 (29%)	50,54,54	1.59	13 (26%)
8	BCL	4	101	-	58,74,74	1.71	12 (20%)	69,115,115	1.60	12 (17%)
8	BCL	T	101	-	58,74,74	1.62	8 (13%)	69,115,115	1.73	14 (20%)
14	LMT	B	102	-	36,36,36	1.17	5 (13%)	47,47,47	1.10	3 (6%)
8	BCL	A	102	-	58,74,74	1.64	8 (13%)	69,115,115	1.64	12 (17%)
14	LMT	L	405	-	36,36,36	1.19	5 (13%)	47,47,47	1.12	3 (6%)
8	BCL	2	101	-	58,74,74	1.67	10 (17%)	69,115,115	1.63	12 (17%)

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
15	CRT	O	102	-	-	1/51/51/51	-
8	BCL	E	103	-	-	13/37/137/137	-
15	CRT	K	103	-	-	0/51/51/51	-
15	CRT	B	103	-	-	0/51/51/51	-
14	LMT	U	101	-	-	8/21/61/61	0/2/2/2
15	CRT	3	103	-	-	1/51/51/51	-
8	BCL	L	402	-	-	10/37/137/137	-
12	CDL	G	101	-	-	24/98/98/110	-
8	BCL	P	103	-	-	15/37/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CRT	2	102	-	-	3/51/51/51	-
8	BCL	J	103	-	-	20/37/137/137	-
8	BCL	V	102	-	-	14/37/137/137	-
11	6PL	H	301	-	-	16/55/55/55	-
14	LMT	F	101	-	-	8/21/61/61	0/2/2/2
8	BCL	M	407	-	-	4/37/137/137	-
14	LMT	D	102	-	-	8/21/61/61	0/2/2/2
14	LMT	S	101	-	-	13/21/61/61	0/2/2/2
9	BPH	L	403	-	2/2/18/22	7/37/105/105	0/5/6/6
8	BCL	Y	102	-	-	19/37/137/137	-
12	CDL	G	104	-	-	22/100/100/110	-
14	LMT	F	102	-	-	14/21/61/61	0/2/2/2
14	LMT	I	101	-	-	9/21/61/61	0/2/2/2
8	BCL	A	101	-	-	15/37/137/137	-
12	CDL	M	406	-	-	25/105/105/110	-
14	LMT	Q	102	-	-	8/21/61/61	0/2/2/2
8	BCL	Y	101	-	-	16/37/137/137	-
8	BCL	V	101	-	-	16/37/137/137	-
14	LMT	I	102	-	-	8/21/61/61	0/2/2/2
14	LMT	O	101	-	-	6/21/61/61	0/2/2/2
12	CDL	H	302	-	-	19/97/97/110	-
7	QAK	M	401	-	1/1/8/12	25/44/44/44	-
8	BCL	J	102	-	-	16/37/137/137	-
8	BCL	3	101	-	-	15/37/137/137	-
14	LMT	M	409	-	-	9/21/61/61	0/2/2/2
8	BCL	G	102	-	-	14/37/137/137	-
8	BCL	D	104	-	-	12/37/137/137	-
14	LMT	K	102	-	-	10/21/61/61	0/2/2/2
15	CRT	X	102	-	-	2/51/51/51	-
8	BCL	G	103	-	-	20/37/137/137	-
14	LMT	2	104	-	-	9/21/61/61	0/2/2/2
14	LMT	X	101	-	-	13/21/61/61	0/2/2/2
14	LMT	K	101	-	-	11/21/61/61	0/2/2/2
14	LMT	4	102	-	-	6/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	LMT	U	102	-	-	13/21/61/61	0/2/2/2
15	CRT	R	101	-	-	0/51/51/51	-
12	CDL	3	102	-	-	14/95/95/110	-
14	LMT	Q	101	-	-	13/21/61/61	0/2/2/2
11	6PL	M	405	-	-	6/55/55/55	-
8	BCL	1	101	-	-	17/37/137/137	-
16	PGT	P	102	-	-	15/54/54/55	-
8	BCL	R	103	-	-	15/37/137/137	-
8	BCL	N	102	-	-	16/37/137/137	-
14	LMT	X	103	-	-	9/21/61/61	0/2/2/2
12	CDL	L	404	-	-	12/96/96/110	-
8	BCL	E	102	-	-	14/37/137/137	-
10	U10	L	406	-	-	1/11/35/87	0/1/1/1
8	BCL	5	102	-	-	15/37/137/137	-
9	BPH	M	403	-	2/2/18/22	2/37/105/105	0/5/6/6
14	LMT	Z	102	-	-	11/21/61/61	0/2/2/2
14	LMT	R	102	-	-	8/21/61/61	0/2/2/2
14	LMT	D	101	-	-	9/21/61/61	0/2/2/2
8	BCL	P	101	-	-	15/37/137/137	-
15	CRT	Z	101	-	-	0/51/51/51	-
8	BCL	M	402	-	-	13/37/137/137	-
14	LMT	6	101	-	-	10/21/61/61	0/2/2/2
10	U10	M	404	-	-	10/45/69/87	0/1/1/1
8	BCL	5	101	-	-	16/37/137/137	-
14	LMT	S	102	-	-	12/21/61/61	0/2/2/2
8	BCL	T	102	-	-	17/37/137/137	-
14	LMT	B	101	-	-	12/21/61/61	0/2/2/2
8	BCL	R	104	-	-	14/37/137/137	-
14	LMT	2	103	-	-	12/21/61/61	0/2/2/2
15	CRT	I	103	-	-	0/51/51/51	-
14	LMT	J	101	-	-	7/21/61/61	0/2/2/2
14	LMT	D	103	-	-	9/17/57/61	0/2/2/2
15	CRT	F	103	-	-	3/51/51/51	-
8	BCL	N	101	-	-	13/37/137/137	-
8	BCL	L	401	-	-	23/37/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	6PL	E	101	-	-	9/43/43/55	-
15	CRT	D	105	-	-	2/51/51/51	-
15	CRT	S	103	-	-	0/51/51/51	-
8	BCL	C	100	-	-	20/37/137/137	-
10	U10	1	102	-	-	16/36/60/87	0/1/1/1
15	CRT	Q	103	-	-	1/51/51/51	-
8	BCL	4	101	-	-	16/37/137/137	-
8	BCL	T	101	-	-	20/37/137/137	-
14	LMT	B	102	-	-	7/21/61/61	0/2/2/2
8	BCL	A	102	-	-	15/37/137/137	-
14	LMT	L	405	-	-	12/21/61/61	0/2/2/2
8	BCL	2	101	-	-	14/37/137/137	-

All (648) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	1	102	U10	C18-C19	6.20	1.47	1.33
10	L	406	U10	C8-C9	6.08	1.47	1.33
10	1	102	U10	C23-C24	6.01	1.47	1.33
10	1	102	U10	C28-C29	6.00	1.47	1.33
10	1	102	U10	C13-C14	5.96	1.47	1.33
10	1	102	U10	C8-C9	5.87	1.47	1.33
10	M	404	U10	C13-C14	5.83	1.47	1.33
10	M	404	U10	C33-C34	5.79	1.46	1.33
10	M	404	U10	C8-C9	5.73	1.46	1.33
10	M	404	U10	C28-C29	5.68	1.46	1.33
10	M	404	U10	O3-C3	-5.66	1.23	1.36
10	L	406	U10	O3-C3	-5.59	1.23	1.36
10	M	404	U10	C18-C19	5.59	1.46	1.33
10	M	404	U10	C23-C24	5.58	1.46	1.33
10	M	404	U10	O4-C4	-5.58	1.23	1.36
10	1	102	U10	O3-C3	-5.57	1.23	1.36
10	L	406	U10	O4-C4	-5.56	1.23	1.36
10	1	102	U10	O4-C4	-5.47	1.23	1.36
7	M	401	QAK	CZ2-C4	5.31	1.54	1.31
8	L	402	BCL	O2D-CGD	5.13	1.45	1.33
10	M	404	U10	C38-C39	5.10	1.47	1.32
8	3	101	BCL	O2D-CGD	5.06	1.45	1.33
8	M	402	BCL	O2D-CGD	5.01	1.45	1.33
8	5	101	BCL	O2D-CGD	5.01	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	M	401	QAK	CZ3-CE3	5.00	1.53	1.31
8	5	102	BCL	O2D-CGD	4.97	1.45	1.33
8	2	101	BCL	O2D-CGD	4.96	1.45	1.33
8	4	101	BCL	O2D-CGD	4.95	1.45	1.33
8	E	102	BCL	O2D-CGD	4.94	1.45	1.33
8	2	101	BCL	C3B-C2B	4.91	1.48	1.39
8	R	103	BCL	O2D-CGD	4.90	1.45	1.33
8	Y	102	BCL	O2D-CGD	4.88	1.45	1.33
8	V	102	BCL	O2D-CGD	4.88	1.45	1.33
8	N	101	BCL	O2D-CGD	4.87	1.45	1.33
8	J	103	BCL	O2D-CGD	4.86	1.45	1.33
8	G	102	BCL	O2D-CGD	4.83	1.45	1.33
8	A	101	BCL	O2D-CGD	4.83	1.45	1.33
8	T	102	BCL	C3B-C2B	4.83	1.48	1.39
8	C	100	BCL	O2D-CGD	4.82	1.45	1.33
8	A	102	BCL	O2D-CGD	4.82	1.45	1.33
8	J	102	BCL	O2D-CGD	4.81	1.44	1.33
8	V	101	BCL	O2D-CGD	4.80	1.44	1.33
8	M	402	BCL	C3B-C2B	4.80	1.48	1.39
8	D	104	BCL	O2D-CGD	4.79	1.44	1.33
8	N	102	BCL	O2D-CGD	4.79	1.44	1.33
8	G	103	BCL	O2D-CGD	4.77	1.44	1.33
8	M	407	BCL	C3B-C2B	4.75	1.47	1.39
8	L	402	BCL	C3B-C2B	4.74	1.47	1.39
8	P	101	BCL	O2D-CGD	4.74	1.44	1.33
8	T	102	BCL	O2D-CGD	4.74	1.44	1.33
8	Y	101	BCL	O2D-CGD	4.72	1.44	1.33
8	T	101	BCL	O2D-CGD	4.70	1.44	1.33
8	R	104	BCL	O2D-CGD	4.70	1.44	1.33
8	P	103	BCL	O2D-CGD	4.69	1.44	1.33
8	3	101	BCL	C3B-C2B	4.69	1.47	1.39
8	1	101	BCL	O2D-CGD	4.67	1.44	1.33
8	1	101	BCL	C3B-C2B	4.67	1.47	1.39
8	P	101	BCL	C3B-C2B	4.67	1.47	1.39
8	L	401	BCL	O2D-CGD	4.66	1.44	1.33
8	V	102	BCL	C3B-C2B	4.65	1.47	1.39
8	4	101	BCL	C3B-C2B	4.65	1.47	1.39
8	E	103	BCL	O2D-CGD	4.64	1.44	1.33
8	G	102	BCL	C3B-C2B	4.63	1.47	1.39
8	J	103	BCL	C3B-C2B	4.62	1.47	1.39
8	5	102	BCL	OBD-CAD	4.62	1.28	1.22
8	V	101	BCL	C3B-C2B	4.62	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	E	103	BCL	C3B-C2B	4.62	1.47	1.39
8	Y	102	BCL	C3B-C2B	4.61	1.47	1.39
8	N	101	BCL	C3B-C2B	4.60	1.47	1.39
8	Y	101	BCL	C3B-C2B	4.58	1.47	1.39
8	N	102	BCL	C3B-C2B	4.58	1.47	1.39
8	G	103	BCL	C3B-C2B	4.57	1.47	1.39
8	J	102	BCL	C3B-C2B	4.56	1.47	1.39
8	M	407	BCL	O2D-CGD	4.56	1.44	1.33
8	5	101	BCL	C3B-C2B	4.56	1.47	1.39
8	P	103	BCL	C3B-C2B	4.56	1.47	1.39
8	T	101	BCL	C3B-C2B	4.55	1.47	1.39
8	L	401	BCL	OBD-CAD	4.53	1.28	1.22
8	E	102	BCL	C3B-C2B	4.53	1.47	1.39
8	A	102	BCL	O2A-CGA	4.53	1.46	1.33
8	R	104	BCL	C3B-C2B	4.52	1.47	1.39
8	D	104	BCL	C3B-C2B	4.52	1.47	1.39
8	C	100	BCL	C3B-C2B	4.49	1.47	1.39
8	R	103	BCL	C3B-C2B	4.49	1.47	1.39
8	4	101	BCL	OBD-CAD	4.48	1.28	1.22
8	2	101	BCL	OBD-CAD	4.47	1.28	1.22
8	A	102	BCL	C3B-C2B	4.47	1.47	1.39
8	5	102	BCL	C3D-C2D	4.47	1.47	1.39
8	L	401	BCL	C3B-C2B	4.45	1.47	1.39
8	5	102	BCL	C3B-C2B	4.45	1.47	1.39
8	4	101	BCL	C3D-C2D	4.44	1.47	1.39
8	Y	102	BCL	OBD-CAD	4.43	1.28	1.22
8	1	101	BCL	OBD-CAD	4.42	1.28	1.22
8	5	101	BCL	OBD-CAD	4.42	1.28	1.22
8	5	102	BCL	O2A-CGA	4.39	1.46	1.33
8	A	101	BCL	C3B-C2B	4.39	1.47	1.39
8	4	101	BCL	O2A-CGA	4.38	1.46	1.33
8	G	103	BCL	OBD-CAD	4.36	1.28	1.22
8	D	104	BCL	C3D-C2D	4.35	1.47	1.39
8	Y	102	BCL	O2A-CGA	4.32	1.46	1.33
8	M	407	BCL	OBD-CAD	4.31	1.28	1.22
8	R	104	BCL	C3D-C2D	4.30	1.47	1.39
8	G	103	BCL	O2A-CGA	4.30	1.45	1.33
8	2	101	BCL	C3D-C2D	4.29	1.47	1.39
8	J	103	BCL	OBD-CAD	4.29	1.28	1.22
8	E	103	BCL	OBD-CAD	4.28	1.28	1.22
8	R	104	BCL	O2A-CGA	4.28	1.45	1.33
8	L	402	BCL	OBD-CAD	4.28	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	3	101	BCL	OBD-CAD	4.28	1.28	1.22
8	J	103	BCL	C3D-C2D	4.27	1.47	1.39
8	D	104	BCL	O2A-CGA	4.27	1.45	1.33
8	J	102	BCL	OBD-CAD	4.24	1.28	1.22
8	P	103	BCL	OBD-CAD	4.24	1.28	1.22
8	E	103	BCL	O2A-CGA	4.24	1.45	1.33
8	V	102	BCL	C3D-C2D	4.23	1.47	1.39
8	E	103	BCL	C3D-C2D	4.23	1.47	1.39
8	V	102	BCL	OBD-CAD	4.23	1.28	1.22
8	M	407	BCL	O2A-CGA	4.22	1.45	1.33
8	T	102	BCL	O2A-CGA	4.21	1.45	1.33
8	3	101	BCL	O2A-CGA	4.20	1.45	1.33
8	D	104	BCL	OBD-CAD	4.20	1.28	1.22
8	2	101	BCL	O2A-CGA	4.20	1.45	1.33
8	N	102	BCL	OBD-CAD	4.20	1.28	1.22
8	T	102	BCL	C3D-C2D	4.19	1.46	1.39
8	R	103	BCL	OBD-CAD	4.18	1.28	1.22
8	P	103	BCL	C3D-C2D	4.18	1.46	1.39
8	N	102	BCL	C3D-C2D	4.18	1.46	1.39
8	A	102	BCL	OBD-CAD	4.18	1.28	1.22
8	N	102	BCL	O2A-CGA	4.17	1.45	1.33
8	Y	102	BCL	C3D-C2D	4.16	1.46	1.39
8	Y	101	BCL	OBD-CAD	4.16	1.28	1.22
8	V	102	BCL	O2A-CGA	4.16	1.45	1.33
8	T	102	BCL	OBD-CAD	4.15	1.28	1.22
8	T	101	BCL	O2A-CGA	4.15	1.45	1.33
8	G	103	BCL	C3D-C2D	4.14	1.46	1.39
8	3	101	BCL	C3D-C2D	4.13	1.46	1.39
8	R	104	BCL	OBD-CAD	4.13	1.28	1.22
8	M	407	BCL	C3D-C2D	4.13	1.46	1.39
8	N	101	BCL	O2A-CGA	4.13	1.45	1.33
8	R	103	BCL	O2A-CGA	4.12	1.45	1.33
8	A	102	BCL	C3D-C2D	4.11	1.46	1.39
8	L	402	BCL	O2A-CGA	4.11	1.45	1.33
8	V	101	BCL	OBD-CAD	4.10	1.28	1.22
8	N	101	BCL	OBD-CAD	4.10	1.28	1.22
8	E	102	BCL	OBD-CAD	4.09	1.28	1.22
8	G	102	BCL	O2A-CGA	4.09	1.45	1.33
8	R	103	BCL	C3D-C2D	4.09	1.46	1.39
8	V	101	BCL	O2A-CGA	4.09	1.45	1.33
8	Y	101	BCL	O2A-CGA	4.09	1.45	1.33
8	A	101	BCL	O2A-CGA	4.08	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	L	402	BCL	C3D-C2D	4.08	1.46	1.39
8	C	100	BCL	C3D-C2D	4.08	1.46	1.39
8	E	102	BCL	O2A-CGA	4.08	1.45	1.33
8	P	103	BCL	O2A-CGA	4.08	1.45	1.33
8	Y	101	BCL	C3D-C2D	4.08	1.46	1.39
8	C	100	BCL	OBD-CAD	4.08	1.28	1.22
8	T	101	BCL	OBD-CAD	4.08	1.28	1.22
8	M	402	BCL	OBD-CAD	4.07	1.28	1.22
8	J	103	BCL	O2A-CGA	4.07	1.45	1.33
8	5	101	BCL	O2A-CGA	4.07	1.45	1.33
8	V	101	BCL	C3D-C2D	4.06	1.46	1.39
8	L	401	BCL	C3D-C2D	4.05	1.46	1.39
8	C	100	BCL	O2A-CGA	4.04	1.45	1.33
8	A	101	BCL	OBD-CAD	4.03	1.27	1.22
8	T	101	BCL	C3D-C2D	4.03	1.46	1.39
8	J	102	BCL	O2A-CGA	4.02	1.45	1.33
8	G	102	BCL	OBD-CAD	4.02	1.27	1.22
8	G	102	BCL	C3D-C2D	4.02	1.46	1.39
8	L	401	BCL	O2A-CGA	4.01	1.45	1.33
8	M	402	BCL	C3D-C2D	4.01	1.46	1.39
8	P	101	BCL	O2A-CGA	4.00	1.45	1.33
15	2	102	CRT	C9-C7	4.00	1.41	1.35
15	2	102	CRT	C14-C12	3.99	1.41	1.35
8	P	101	BCL	OBD-CAD	3.99	1.27	1.22
8	M	402	BCL	O2A-CGA	3.98	1.45	1.33
8	P	101	BCL	C3D-C2D	3.97	1.46	1.39
8	1	101	BCL	C3D-C2D	3.96	1.46	1.39
8	N	101	BCL	C3D-C2D	3.96	1.46	1.39
8	1	101	BCL	O2A-CGA	3.96	1.44	1.33
8	5	101	BCL	C3D-C2D	3.96	1.46	1.39
8	E	102	BCL	C3D-C2D	3.94	1.46	1.39
15	X	102	CRT	C9-C7	3.94	1.41	1.35
8	A	101	BCL	C3D-C2D	3.92	1.46	1.39
15	3	103	CRT	C27-C28	3.90	1.40	1.35
15	2	102	CRT	C22-C23	3.87	1.40	1.35
15	3	103	CRT	C22-C23	3.87	1.40	1.35
8	J	102	BCL	C3D-C2D	3.81	1.46	1.39
15	X	102	CRT	C22-C23	3.80	1.40	1.35
15	Z	101	CRT	C22-C23	3.79	1.40	1.35
15	2	102	CRT	C27-C28	3.74	1.40	1.35
15	X	102	CRT	C14-C12	3.73	1.40	1.35
15	2	102	CRT	C19-C17	3.72	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	3	103	CRT	C9-C7	3.71	1.40	1.35
15	X	102	CRT	C19-C17	3.71	1.40	1.35
15	Q	103	CRT	C9-C7	3.71	1.40	1.35
15	Z	101	CRT	C9-C7	3.70	1.40	1.35
15	Z	101	CRT	C14-C12	3.66	1.40	1.35
15	Z	101	CRT	C19-C17	3.65	1.40	1.35
15	K	103	CRT	C22-C23	3.65	1.40	1.35
15	3	103	CRT	C19-C17	3.64	1.40	1.35
15	S	103	CRT	C9-C7	3.61	1.40	1.35
15	D	105	CRT	C14-C12	3.61	1.40	1.35
15	D	105	CRT	C9-C7	3.61	1.40	1.35
8	5	101	BCL	C2D-C1D	3.59	1.50	1.42
15	X	102	CRT	C27-C28	3.58	1.40	1.35
8	Y	101	BCL	C2D-C1D	3.54	1.50	1.42
15	2	102	CRT	C32-C33	3.54	1.40	1.35
15	K	103	CRT	C27-C28	3.52	1.40	1.35
15	F	103	CRT	C14-C12	3.51	1.40	1.35
10	M	404	U10	C4-C5	-3.50	1.38	1.48
10	M	404	U10	C3-C2	-3.50	1.38	1.48
8	3	101	BCL	C2D-C1D	3.50	1.50	1.42
15	Q	103	CRT	C14-C12	3.50	1.40	1.35
15	B	103	CRT	C9-C7	3.50	1.40	1.35
8	1	101	BCL	C2D-C1D	3.48	1.50	1.42
8	J	102	BCL	C2D-C1D	3.48	1.50	1.42
8	C	100	BCL	C2D-C1D	3.47	1.50	1.42
15	B	103	CRT	C14-C12	3.47	1.40	1.35
8	G	102	BCL	C2D-C1D	3.46	1.50	1.42
10	L	406	U10	C3-C2	-3.45	1.38	1.48
15	3	103	CRT	C32-C33	3.44	1.40	1.35
15	K	103	CRT	C19-C17	3.44	1.40	1.35
15	R	101	CRT	C9-C7	3.44	1.40	1.35
8	L	401	BCL	C2D-C1D	3.43	1.50	1.42
15	F	103	CRT	C9-C7	3.43	1.40	1.35
8	R	103	BCL	C2D-C1D	3.43	1.50	1.42
10	1	102	U10	C4-C5	-3.42	1.39	1.48
15	O	102	CRT	C22-C23	3.41	1.40	1.35
10	1	102	U10	C3-C2	-3.41	1.39	1.48
15	X	102	CRT	C32-C33	3.41	1.40	1.35
8	5	102	BCL	C2D-C1D	3.40	1.50	1.42
10	L	406	U10	C4-C5	-3.39	1.39	1.48
15	F	103	CRT	C19-C17	3.39	1.40	1.35
15	Z	101	CRT	C27-C28	3.38	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	O	102	CRT	C9-C7	3.37	1.40	1.35
15	O	102	CRT	C27-C28	3.37	1.40	1.35
15	F	103	CRT	C32-C33	3.36	1.40	1.35
15	D	105	CRT	C19-C17	3.35	1.40	1.35
8	N	101	BCL	C2D-C1D	3.35	1.50	1.42
8	V	101	BCL	C2D-C1D	3.35	1.50	1.42
15	3	103	CRT	C14-C12	3.34	1.40	1.35
8	M	407	BCL	C2D-C1D	3.33	1.50	1.42
15	R	101	CRT	C22-C23	3.33	1.40	1.35
15	S	103	CRT	C14-C12	3.32	1.40	1.35
8	Y	102	BCL	C2D-C1D	3.32	1.50	1.42
15	F	103	CRT	C22-C23	3.31	1.40	1.35
15	B	103	CRT	C22-C23	3.31	1.40	1.35
8	T	101	BCL	C2D-C1D	3.30	1.50	1.42
15	D	105	CRT	C27-C28	3.30	1.40	1.35
8	P	101	BCL	C2D-C1D	3.30	1.50	1.42
8	E	102	BCL	C2D-C1D	3.30	1.50	1.42
15	R	101	CRT	C14-C12	3.30	1.40	1.35
15	K	103	CRT	C14-C12	3.28	1.40	1.35
8	A	101	BCL	C2D-C1D	3.28	1.50	1.42
15	Q	103	CRT	C22-C23	3.28	1.40	1.35
15	O	102	CRT	C19-C17	3.27	1.40	1.35
8	J	103	BCL	C2D-C1D	3.27	1.50	1.42
15	R	101	CRT	C19-C17	3.26	1.40	1.35
15	K	103	CRT	C9-C7	3.25	1.40	1.35
8	M	402	BCL	C2D-C1D	3.25	1.49	1.42
15	B	103	CRT	C19-C17	3.25	1.40	1.35
15	K	103	CRT	C32-C33	3.24	1.40	1.35
15	D	105	CRT	C22-C23	3.24	1.40	1.35
8	4	101	BCL	C2D-C1D	3.22	1.49	1.42
15	Q	103	CRT	C19-C17	3.22	1.40	1.35
15	F	103	CRT	C27-C28	3.20	1.40	1.35
15	O	102	CRT	C32-C33	3.20	1.40	1.35
15	O	102	CRT	C14-C12	3.20	1.40	1.35
15	Q	103	CRT	C27-C28	3.18	1.40	1.35
15	S	103	CRT	C22-C23	3.17	1.40	1.35
8	R	104	BCL	C2D-C1D	3.15	1.49	1.42
8	2	101	BCL	C2D-C1D	3.15	1.49	1.42
8	L	402	BCL	C2D-C1D	3.15	1.49	1.42
15	R	101	CRT	C27-C28	3.15	1.40	1.35
8	5	102	BCL	MG-NC	-3.14	1.98	2.06
15	I	103	CRT	C22-C23	3.13	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	E	103	BCL	C2D-C1D	3.12	1.49	1.42
15	I	103	CRT	C14-C12	3.11	1.39	1.35
8	P	103	BCL	C2D-C1D	3.10	1.49	1.42
15	B	103	CRT	C27-C28	3.09	1.39	1.35
15	Z	101	CRT	C32-C33	3.08	1.39	1.35
15	D	105	CRT	C32-C33	3.07	1.39	1.35
8	N	102	BCL	C2D-C1D	3.07	1.49	1.42
8	V	102	BCL	C2D-C1D	3.04	1.49	1.42
8	G	103	BCL	C2D-C1D	3.03	1.49	1.42
9	M	403	BPH	C3A-C2A	-3.02	1.52	1.54
14	F	101	LMT	O3'-C3'	-3.01	1.35	1.43
8	D	104	BCL	C2D-C1D	3.01	1.49	1.42
15	S	103	CRT	C32-C33	3.00	1.39	1.35
14	B	101	LMT	O3'-C3'	-2.99	1.35	1.43
15	I	103	CRT	C27-C28	2.97	1.39	1.35
15	I	103	CRT	C16-C17	-2.96	1.39	1.45
14	L	405	LMT	O3'-C3'	-2.95	1.36	1.43
15	R	101	CRT	C32-C33	2.95	1.39	1.35
15	I	103	CRT	C25-C23	-2.95	1.39	1.45
14	J	101	LMT	O3'-C3'	-2.94	1.36	1.43
15	S	103	CRT	C27-C28	2.94	1.39	1.35
14	O	101	LMT	O3'-C3'	-2.94	1.36	1.43
14	R	102	LMT	O3'-C3'	-2.94	1.36	1.43
15	I	103	CRT	C9-C7	2.93	1.39	1.35
8	A	102	BCL	C2D-C1D	2.93	1.49	1.42
15	I	103	CRT	C30-C28	-2.93	1.39	1.45
15	I	103	CRT	C19-C17	2.90	1.39	1.35
14	4	102	LMT	O3'-C3'	-2.90	1.36	1.43
15	B	103	CRT	C32-C33	2.90	1.39	1.35
15	Z	101	CRT	C30-C28	-2.90	1.39	1.45
15	S	103	CRT	C19-C17	2.90	1.39	1.35
15	I	103	CRT	C11-C12	-2.89	1.39	1.45
14	Q	101	LMT	O3'-C3'	-2.85	1.36	1.43
14	Q	102	LMT	O3'-C3'	-2.84	1.36	1.43
15	S	103	CRT	C30-C28	-2.84	1.39	1.45
15	O	102	CRT	C16-C17	-2.83	1.39	1.45
15	I	103	CRT	C32-C33	2.83	1.39	1.35
8	T	102	BCL	C2D-C1D	2.83	1.49	1.42
15	Z	101	CRT	C35-C33	-2.82	1.39	1.45
15	R	101	CRT	C16-C17	-2.82	1.39	1.45
14	D	101	LMT	O3'-C3'	-2.81	1.36	1.43
15	R	101	CRT	C30-C28	-2.81	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	F	103	CRT	C25-C23	-2.81	1.39	1.45
8	5	102	BCL	MG-NA	-2.80	1.99	2.06
8	4	101	BCL	MG-NA	-2.80	1.99	2.06
8	4	101	BCL	MG-NC	-2.80	1.99	2.06
14	S	101	LMT	O3'-C3'	-2.80	1.36	1.43
15	S	103	CRT	C25-C23	-2.79	1.39	1.45
15	S	103	CRT	C35-C33	-2.79	1.40	1.45
10	M	404	U10	C6-C5	-2.79	1.38	1.46
14	D	102	LMT	O3'-C3'	-2.78	1.36	1.43
15	B	103	CRT	C25-C23	-2.78	1.40	1.45
15	K	103	CRT	C16-C17	-2.77	1.40	1.45
14	U	101	LMT	O3'-C3'	-2.77	1.36	1.43
15	B	103	CRT	C30-C28	-2.77	1.40	1.45
14	B	102	LMT	O3'-C3'	-2.76	1.36	1.43
15	Q	103	CRT	C30-C28	-2.76	1.40	1.45
10	1	102	U10	C6-C5	-2.76	1.38	1.46
14	6	101	LMT	O3'-C3'	-2.75	1.36	1.43
15	B	103	CRT	C35-C33	-2.75	1.40	1.45
8	M	407	BCL	MG-NA	-2.74	1.99	2.06
15	Q	103	CRT	C32-C33	2.74	1.39	1.35
15	I	103	CRT	C35-C33	-2.74	1.40	1.45
15	D	105	CRT	C25-C23	-2.73	1.40	1.45
15	O	102	CRT	C30-C28	-2.72	1.40	1.45
14	I	101	LMT	O3'-C3'	-2.72	1.36	1.43
15	I	103	CRT	C6-C7	-2.72	1.40	1.45
14	L	405	LMT	O2'-C2'	-2.72	1.36	1.43
14	2	103	LMT	O3'-C3'	-2.71	1.36	1.43
15	F	103	CRT	C30-C28	-2.71	1.40	1.45
14	2	104	LMT	O3'-C3'	-2.71	1.36	1.43
15	O	102	CRT	C25-C23	-2.71	1.40	1.45
14	S	102	LMT	O3'-C3'	-2.70	1.36	1.43
14	M	409	LMT	O3'-C3'	-2.70	1.36	1.43
15	F	103	CRT	C16-C17	-2.69	1.40	1.45
15	D	105	CRT	C30-C28	-2.69	1.40	1.45
15	K	103	CRT	C30-C28	-2.69	1.40	1.45
15	B	103	CRT	C16-C17	-2.69	1.40	1.45
15	Z	101	CRT	C25-C23	-2.68	1.40	1.45
15	S	103	CRT	C16-C17	-2.68	1.40	1.45
14	U	102	LMT	O3'-C3'	-2.68	1.36	1.43
15	Q	103	CRT	C16-C17	-2.66	1.40	1.45
14	X	103	LMT	O3'-C3'	-2.66	1.36	1.43
8	L	401	BCL	MG-NA	-2.65	2.00	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	K	101	LMT	O3'-C3'	-2.65	1.36	1.43
14	2	103	LMT	O2'-C2'	-2.65	1.36	1.43
15	K	103	CRT	C35-C33	-2.64	1.40	1.45
14	B	101	LMT	O2B-C2B	-2.64	1.36	1.43
10	L	406	U10	C6-C5	-2.64	1.39	1.46
14	B	101	LMT	O2'-C2'	-2.63	1.36	1.43
15	R	101	CRT	C25-C23	-2.63	1.40	1.45
8	M	402	BCL	MG-NA	-2.63	2.00	2.06
15	D	105	CRT	C16-C17	-2.63	1.40	1.45
14	Z	102	LMT	O3'-C3'	-2.62	1.36	1.43
15	O	102	CRT	C35-C33	-2.62	1.40	1.45
15	B	103	CRT	C11-C12	-2.62	1.40	1.45
15	D	105	CRT	C11-C12	-2.62	1.40	1.45
15	K	103	CRT	C11-C12	-2.62	1.40	1.45
14	F	102	LMT	O3'-C3'	-2.62	1.36	1.43
14	Q	102	LMT	O2B-C2B	-2.60	1.36	1.43
14	I	102	LMT	O3'-C3'	-2.60	1.36	1.43
14	K	101	LMT	O2B-C2B	-2.60	1.36	1.43
14	X	101	LMT	O2B-C2B	-2.59	1.36	1.43
15	F	103	CRT	C11-C12	-2.59	1.40	1.45
14	F	101	LMT	O2'-C2'	-2.59	1.36	1.43
14	K	102	LMT	O3'-C3'	-2.58	1.36	1.43
15	Q	103	CRT	C25-C23	-2.58	1.40	1.45
15	R	101	CRT	C11-C12	-2.58	1.40	1.45
15	K	103	CRT	C25-C23	-2.57	1.40	1.45
14	L	405	LMT	O2B-C2B	-2.57	1.36	1.43
15	X	102	CRT	C30-C28	-2.57	1.40	1.45
15	2	102	CRT	C35-C33	-2.56	1.40	1.45
15	F	103	CRT	C6-C7	-2.56	1.40	1.45
14	Q	101	LMT	O3B-C3B	-2.56	1.37	1.43
15	R	101	CRT	C35-C33	-2.55	1.40	1.45
8	R	104	BCL	MG-NA	-2.55	2.00	2.06
15	3	103	CRT	C30-C28	-2.55	1.40	1.45
15	D	105	CRT	C6-C7	-2.54	1.40	1.45
15	Q	103	CRT	C35-C33	-2.53	1.40	1.45
15	Q	103	CRT	C11-C12	-2.53	1.40	1.45
14	U	102	LMT	O2B-C2B	-2.53	1.37	1.43
15	2	102	CRT	C30-C28	-2.53	1.40	1.45
8	R	103	BCL	MG-NA	-2.53	2.00	2.06
14	2	103	LMT	O2B-C2B	-2.52	1.37	1.43
8	A	101	BCL	MG-NA	-2.52	2.00	2.06
14	D	102	LMT	O2'-C2'	-2.52	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	3	103	CRT	C11-C12	-2.51	1.40	1.45
14	X	101	LMT	O3'-C3'	-2.51	1.37	1.43
14	D	101	LMT	O2B-C2B	-2.51	1.37	1.43
8	2	101	BCL	MG-NC	-2.51	2.00	2.06
15	S	103	CRT	C11-C12	-2.50	1.40	1.45
15	X	102	CRT	C25-C23	-2.50	1.40	1.45
15	F	103	CRT	C35-C33	-2.50	1.40	1.45
8	5	101	BCL	MG-NC	-2.50	2.00	2.06
14	X	101	LMT	O2'-C2'	-2.50	1.37	1.43
15	3	103	CRT	C35-C33	-2.50	1.40	1.45
14	F	102	LMT	O2'-C2'	-2.50	1.37	1.43
9	L	403	BPH	C3A-C2A	-2.49	1.52	1.54
14	F	102	LMT	O2B-C2B	-2.49	1.37	1.43
15	X	102	CRT	C35-C33	-2.49	1.40	1.45
8	V	102	BCL	MG-NC	-2.49	2.00	2.06
14	Q	102	LMT	O2'-C2'	-2.49	1.37	1.43
8	P	103	BCL	MG-NA	-2.48	2.00	2.06
15	D	105	CRT	C35-C33	-2.48	1.40	1.45
14	D	103	LMT	O2B-C2B	-2.48	1.37	1.43
14	R	102	LMT	O2B-C2B	-2.48	1.37	1.43
8	M	402	BCL	C3C-C4C	-2.48	1.48	1.51
15	O	102	CRT	C11-C12	-2.48	1.40	1.45
14	D	103	LMT	O3'-C3'	-2.47	1.37	1.43
10	M	404	U10	C1-C2	-2.47	1.38	1.47
14	M	409	LMT	O2B-C2B	-2.47	1.37	1.43
8	J	103	BCL	MG-NA	-2.46	2.00	2.06
15	3	103	CRT	C6-C7	-2.46	1.40	1.45
15	Q	103	CRT	C6-C7	-2.45	1.40	1.45
14	I	101	LMT	O3B-C3B	-2.45	1.37	1.43
15	X	102	CRT	C16-C17	-2.45	1.40	1.45
15	R	101	CRT	C6-C7	-2.45	1.40	1.45
14	2	104	LMT	O2'-C2'	-2.45	1.37	1.43
14	I	102	LMT	O2B-C2B	-2.44	1.37	1.43
14	O	101	LMT	O2'-C2'	-2.44	1.37	1.43
8	3	101	BCL	MG-NC	-2.44	2.00	2.06
14	Q	101	LMT	O2B-C2B	-2.44	1.37	1.43
10	L	406	U10	C1-C2	-2.44	1.38	1.47
14	S	102	LMT	O2B-C2B	-2.43	1.37	1.43
14	D	103	LMT	O3B-C3B	-2.43	1.37	1.43
15	3	103	CRT	C25-C23	-2.43	1.40	1.45
14	D	101	LMT	O3B-C3B	-2.43	1.37	1.43
14	2	104	LMT	O2B-C2B	-2.43	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	J	101	LMT	O3B-C3B	-2.43	1.37	1.43
14	X	101	LMT	O3B-C3B	-2.43	1.37	1.43
14	X	103	LMT	O2'-C2'	-2.43	1.37	1.43
14	I	102	LMT	O3B-C3B	-2.43	1.37	1.43
14	2	104	LMT	O3B-C3B	-2.42	1.37	1.43
14	Q	102	LMT	O3B-C3B	-2.42	1.37	1.43
14	R	102	LMT	O3B-C3B	-2.42	1.37	1.43
14	I	102	LMT	O2'-C2'	-2.42	1.37	1.43
8	A	101	BCL	MG-NC	-2.42	2.00	2.06
14	R	102	LMT	O4'-C4B	-2.42	1.37	1.43
14	U	102	LMT	O2'-C2'	-2.42	1.37	1.43
8	E	102	BCL	MG-NA	-2.41	2.00	2.06
15	2	102	CRT	C25-C23	-2.41	1.40	1.45
15	S	103	CRT	C6-C7	-2.41	1.40	1.45
14	Z	102	LMT	O3B-C3B	-2.40	1.37	1.43
14	D	102	LMT	O2B-C2B	-2.40	1.37	1.43
14	K	102	LMT	O3B-C3B	-2.40	1.37	1.43
8	1	101	BCL	MG-NC	-2.40	2.00	2.06
14	U	102	LMT	O3B-C3B	-2.40	1.37	1.43
8	Y	102	BCL	MG-NC	-2.40	2.00	2.06
15	O	102	CRT	C6-C7	-2.40	1.40	1.45
8	N	102	BCL	MG-NA	-2.40	2.00	2.06
10	M	404	U10	C6-C1	2.39	1.39	1.35
14	S	101	LMT	O2B-C2B	-2.39	1.37	1.43
14	6	101	LMT	O2B-C2B	-2.39	1.37	1.43
8	A	102	BCL	MG-NC	-2.39	2.00	2.06
8	G	103	BCL	MG-NC	-2.39	2.00	2.06
8	5	101	BCL	MG-NA	-2.38	2.00	2.06
15	K	103	CRT	C6-C7	-2.38	1.40	1.45
8	V	102	BCL	MG-NA	-2.38	2.00	2.06
14	S	101	LMT	O3B-C3B	-2.38	1.37	1.43
8	P	103	BCL	MG-NC	-2.37	2.00	2.06
8	N	102	BCL	MG-NC	-2.37	2.00	2.06
8	D	104	BCL	C3C-C4C	-2.37	1.48	1.51
14	F	102	LMT	O3B-C3B	-2.37	1.37	1.43
8	E	103	BCL	MG-NC	-2.37	2.00	2.06
14	O	101	LMT	O3B-C3B	-2.37	1.37	1.43
15	3	103	CRT	C16-C17	-2.37	1.40	1.45
14	K	102	LMT	O2B-C2B	-2.36	1.37	1.43
14	U	101	LMT	O2'-C2'	-2.36	1.37	1.43
15	Z	101	CRT	C16-C17	-2.36	1.40	1.45
14	4	102	LMT	O3B-C3B	-2.35	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	J	103	BCL	MG-NC	-2.35	2.00	2.06
14	B	102	LMT	O2'-C2'	-2.35	1.37	1.43
14	F	101	LMT	O3B-C3B	-2.35	1.37	1.43
8	R	103	BCL	MG-NC	-2.35	2.00	2.06
8	R	104	BCL	MG-NC	-2.35	2.00	2.06
14	I	101	LMT	O2B-C2B	-2.35	1.37	1.43
14	D	102	LMT	O3B-C3B	-2.35	1.37	1.43
14	S	101	LMT	O2'-C2'	-2.35	1.37	1.43
8	4	101	BCL	C4B-CHC	2.35	1.47	1.41
14	J	101	LMT	O4'-C4B	-2.35	1.37	1.43
15	X	102	CRT	C6-C7	-2.35	1.40	1.45
8	L	401	BCL	MG-NC	-2.34	2.00	2.06
8	2	101	BCL	MG-NA	-2.34	2.00	2.06
8	N	101	BCL	MG-NC	-2.34	2.00	2.06
15	X	102	CRT	C11-C12	-2.33	1.40	1.45
14	U	101	LMT	O3B-C3B	-2.33	1.37	1.43
14	M	409	LMT	O4'-C4B	-2.33	1.37	1.43
8	D	104	BCL	MG-NA	-2.33	2.00	2.06
8	D	104	BCL	MG-NC	-2.33	2.00	2.06
14	B	102	LMT	O3B-C3B	-2.32	1.37	1.43
14	B	101	LMT	O3B-C3B	-2.32	1.37	1.43
8	G	103	BCL	MG-NA	-2.32	2.00	2.06
14	6	101	LMT	O3B-C3B	-2.32	1.37	1.43
8	V	101	BCL	MG-NA	-2.32	2.00	2.06
8	J	102	BCL	MG-NA	-2.32	2.00	2.06
8	E	103	BCL	MG-NA	-2.32	2.00	2.06
14	6	101	LMT	O2'-C2'	-2.32	1.37	1.43
14	L	405	LMT	O3B-C3B	-2.31	1.37	1.43
15	2	102	CRT	C11-C12	-2.31	1.41	1.45
15	B	103	CRT	C6-C7	-2.31	1.41	1.45
14	K	101	LMT	O2'-C2'	-2.31	1.37	1.43
8	T	101	BCL	MG-NC	-2.31	2.00	2.06
8	5	102	BCL	C1B-CHB	2.31	1.47	1.41
8	Y	102	BCL	MG-NA	-2.31	2.00	2.06
14	Z	102	LMT	O2'-C2'	-2.30	1.37	1.43
14	X	103	LMT	O2B-C2B	-2.30	1.37	1.43
14	M	409	LMT	O2'-C2'	-2.30	1.37	1.43
8	A	102	BCL	MG-NA	-2.30	2.00	2.06
14	O	101	LMT	O2B-C2B	-2.30	1.37	1.43
15	Z	101	CRT	C6-C7	-2.30	1.41	1.45
14	4	102	LMT	O2B-C2B	-2.29	1.37	1.43
14	4	102	LMT	O2'-C2'	-2.29	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	X	103	LMT	O3B-C3B	-2.29	1.37	1.43
8	E	102	BCL	MG-NC	-2.29	2.00	2.06
14	2	103	LMT	O3B-C3B	-2.29	1.37	1.43
14	S	102	LMT	O3B-C3B	-2.29	1.37	1.43
14	I	101	LMT	O4'-C4B	-2.29	1.37	1.43
14	M	409	LMT	O1'-C1'	-2.29	1.36	1.40
14	Q	101	LMT	O2'-C2'	-2.28	1.37	1.43
14	B	101	LMT	O1'-C1'	-2.28	1.36	1.40
8	N	101	BCL	MG-NA	-2.28	2.00	2.06
8	Y	101	BCL	MG-NC	-2.28	2.00	2.06
14	M	409	LMT	O3B-C3B	-2.28	1.37	1.43
8	T	102	BCL	MG-NA	-2.28	2.00	2.06
14	Z	102	LMT	O2B-C2B	-2.27	1.37	1.43
10	1	102	U10	C1-C2	-2.27	1.39	1.47
8	L	402	BCL	MG-NC	-2.26	2.00	2.06
14	K	102	LMT	O2'-C2'	-2.26	1.37	1.43
14	D	103	LMT	O5'-C5'	-2.26	1.38	1.44
8	J	102	BCL	MG-NC	-2.26	2.00	2.06
14	K	101	LMT	O3B-C3B	-2.26	1.37	1.43
8	T	101	BCL	MG-NA	-2.25	2.00	2.06
15	Z	101	CRT	C11-C12	-2.25	1.41	1.45
14	D	103	LMT	O4'-C4B	-2.25	1.37	1.43
14	S	102	LMT	O4'-C4B	-2.25	1.37	1.43
8	V	101	BCL	MG-NC	-2.24	2.00	2.06
14	J	101	LMT	O2B-C2B	-2.24	1.37	1.43
8	G	102	BCL	MG-NC	-2.24	2.00	2.06
14	S	101	LMT	O4'-C4B	-2.24	1.37	1.43
8	A	101	BCL	C3C-C4C	-2.24	1.48	1.51
14	B	102	LMT	O2B-C2B	-2.24	1.37	1.43
8	G	102	BCL	MG-NA	-2.23	2.01	2.06
14	F	101	LMT	O4'-C4B	-2.23	1.37	1.43
15	2	102	CRT	C6-C7	-2.23	1.41	1.45
8	E	102	BCL	C3C-C4C	-2.23	1.48	1.51
8	V	102	BCL	C3C-C4C	-2.23	1.48	1.51
14	R	102	LMT	O1'-C1'	-2.22	1.36	1.40
14	X	103	LMT	O4'-C4B	-2.22	1.37	1.43
14	S	102	LMT	O2'-C2'	-2.22	1.37	1.43
14	F	101	LMT	O2B-C2B	-2.22	1.37	1.43
8	P	101	BCL	MG-NC	-2.22	2.01	2.06
8	T	102	BCL	MG-NC	-2.22	2.01	2.06
8	Y	101	BCL	MG-NA	-2.21	2.01	2.06
15	2	102	CRT	C16-C17	-2.21	1.41	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	5	101	BCL	C1B-CHB	2.21	1.47	1.41
8	L	402	BCL	MG-NA	-2.21	2.01	2.06
14	Q	102	LMT	O4'-C4B	-2.21	1.37	1.43
8	3	101	BCL	MG-NA	-2.20	2.01	2.06
14	O	101	LMT	O4'-C4B	-2.20	1.37	1.43
14	L	405	LMT	O4'-C4B	-2.20	1.37	1.43
8	L	402	BCL	C3C-C4C	-2.20	1.48	1.51
8	P	101	BCL	MG-NA	-2.20	2.01	2.06
14	F	101	LMT	O1'-C1'	-2.19	1.36	1.40
14	D	101	LMT	O4'-C4B	-2.18	1.37	1.43
14	F	102	LMT	O4'-C4B	-2.18	1.37	1.43
14	D	103	LMT	O2'-C2'	-2.18	1.37	1.43
8	C	100	BCL	MG-NC	-2.18	2.01	2.06
14	I	101	LMT	O2'-C2'	-2.17	1.37	1.43
8	5	101	BCL	CHD-C4C	2.17	1.47	1.41
8	M	402	BCL	C1B-CHB	2.17	1.47	1.41
14	Q	101	LMT	O4'-C4B	-2.17	1.37	1.43
14	K	102	LMT	O4'-C4B	-2.17	1.37	1.43
8	M	402	BCL	MG-NC	-2.17	2.01	2.06
8	1	101	BCL	MG-NA	-2.17	2.01	2.06
8	4	101	BCL	C1B-CHB	2.17	1.47	1.41
14	4	102	LMT	O1'-C1'	-2.17	1.36	1.40
14	X	101	LMT	O1'-C1'	-2.16	1.36	1.40
8	C	100	BCL	MG-NA	-2.16	2.01	2.06
14	D	101	LMT	O5'-C5'	-2.16	1.39	1.44
14	U	101	LMT	O2B-C2B	-2.15	1.37	1.43
8	M	407	BCL	MG-NC	-2.15	2.01	2.06
14	B	101	LMT	O4'-C4B	-2.15	1.37	1.43
8	5	102	BCL	CHD-C4C	2.15	1.47	1.41
7	M	401	QAK	O-C	-2.15	1.39	1.44
14	6	101	LMT	O4'-C4B	-2.14	1.37	1.43
8	1	101	BCL	C3C-C4C	-2.13	1.48	1.51
14	D	103	LMT	O1'-C1'	-2.13	1.36	1.40
14	R	102	LMT	O2'-C2'	-2.13	1.38	1.43
14	B	102	LMT	O4'-C4B	-2.12	1.38	1.43
9	M	403	BPH	CBD-CGD	-2.12	1.49	1.52
14	U	101	LMT	O4'-C4B	-2.12	1.38	1.43
8	M	407	BCL	C1B-CHB	2.10	1.46	1.41
8	R	104	BCL	C3C-C4C	-2.10	1.49	1.51
14	2	103	LMT	O1'-C1'	-2.09	1.36	1.40
8	L	401	BCL	C1B-CHB	2.09	1.46	1.41
14	Z	102	LMT	O4'-C4B	-2.09	1.38	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	X	103	LMT	O1'-C1'	-2.08	1.36	1.40
8	5	102	BCL	C4B-CHC	2.08	1.46	1.41
8	E	102	BCL	C1B-CHB	2.08	1.46	1.41
10	L	406	U10	C6-C1	2.08	1.39	1.35
14	X	101	LMT	O4'-C4B	-2.07	1.38	1.43
14	X	101	LMT	O5'-C5'	-2.07	1.39	1.44
8	2	101	BCL	C1B-CHB	2.07	1.46	1.41
8	P	103	BCL	C1B-CHB	2.07	1.46	1.41
14	2	103	LMT	O4'-C4B	-2.07	1.38	1.43
8	1	101	BCL	C4B-CHC	2.06	1.46	1.41
14	K	101	LMT	O4'-C4B	-2.06	1.38	1.43
8	4	101	BCL	C4B-NB	-2.05	1.33	1.35
14	X	101	LMT	C3'-C2'	2.05	1.57	1.52
8	4	101	BCL	CHD-C4C	2.05	1.47	1.41
8	T	102	BCL	C4B-NB	-2.05	1.33	1.35
14	I	102	LMT	O4'-C4B	-2.05	1.38	1.43
9	L	403	BPH	CBD-CGD	-2.05	1.49	1.52
14	K	102	LMT	O1'-C1'	-2.04	1.36	1.40
8	V	101	BCL	C3C-C4C	-2.04	1.49	1.51
14	D	101	LMT	O1'-C1'	-2.03	1.36	1.40
8	J	103	BCL	C3C-C4C	-2.03	1.49	1.51
14	U	101	LMT	O5'-C5'	-2.03	1.39	1.44
8	R	104	BCL	C4B-NB	-2.03	1.33	1.35
14	Q	102	LMT	O1'-C1'	-2.03	1.36	1.40
14	I	102	LMT	O1'-C1'	-2.02	1.36	1.40
8	3	101	BCL	C4B-CHC	2.02	1.46	1.41
14	2	104	LMT	O4'-C4B	-2.02	1.38	1.43
8	2	101	BCL	C4B-CHC	2.02	1.46	1.41
8	D	104	BCL	C4B-CHC	2.01	1.46	1.41
14	U	102	LMT	O4'-C4B	-2.01	1.38	1.43
15	I	103	CRT	C31-C32	-2.01	1.37	1.43
8	3	101	BCL	CHD-C4C	2.00	1.47	1.41
8	P	101	BCL	C1B-CHB	2.00	1.46	1.41
8	3	101	BCL	C1B-CHB	2.00	1.46	1.41
8	J	102	BCL	C1B-CHB	2.00	1.46	1.41
14	Z	102	LMT	O1'-C1'	-2.00	1.36	1.40

All (704) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	L	401	BCL	O2D-CGD-CBD	6.01	121.96	111.27
8	M	407	BCL	O2D-CGD-CBD	5.83	121.62	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	M	402	BCL	CHD-C4C-NC	5.25	130.91	125.08
8	5	102	BCL	C4B-CHC-C1C	-5.19	119.84	130.12
8	T	101	BCL	CMB-C2B-C3B	5.08	134.18	124.68
15	2	102	CRT	C20-C21-C22	4.99	133.69	123.47
8	P	101	BCL	O2D-CGD-CBD	4.95	120.06	111.27
8	A	101	BCL	CHD-C4C-NC	4.94	130.57	125.08
8	Y	101	BCL	CMB-C2B-C3B	4.94	133.93	124.68
8	C	100	BCL	O2D-CGD-CBD	4.93	120.04	111.27
8	5	101	BCL	O2D-CGD-CBD	4.93	120.02	111.27
8	M	402	BCL	C3C-C4C-CHD	-4.93	112.87	123.39
8	M	402	BCL	CMB-C2B-C3B	4.91	133.87	124.68
8	T	101	BCL	O2D-CGD-CBD	4.91	119.99	111.27
8	G	103	BCL	CMB-C2B-C3B	4.88	133.81	124.68
8	Y	101	BCL	O2D-CGD-CBD	4.87	119.92	111.27
8	M	407	BCL	CMB-C2B-C3B	4.87	133.78	124.68
8	J	103	BCL	CMB-C2B-C3B	4.85	133.76	124.68
8	E	102	BCL	CHD-C4C-NC	4.82	130.43	125.08
8	1	101	BCL	O2D-CGD-CBD	4.81	119.82	111.27
8	V	102	BCL	CMB-C2B-C3B	4.80	133.65	124.68
8	T	102	BCL	CMB-C2B-C3B	4.79	133.63	124.68
8	P	103	BCL	CMB-C2B-C3B	4.76	133.58	124.68
8	L	401	BCL	CHD-C4C-NC	4.75	130.36	125.08
8	E	102	BCL	O2D-CGD-CBD	4.75	119.70	111.27
8	L	402	BCL	CHD-C4C-NC	4.74	130.34	125.08
8	3	101	BCL	CMB-C2B-C3B	4.72	133.52	124.68
8	3	101	BCL	O2D-CGD-CBD	4.71	119.63	111.27
8	R	103	BCL	CHD-C4C-NC	4.70	130.30	125.08
8	V	101	BCL	CHD-C4C-NC	4.70	130.29	125.08
8	V	101	BCL	CMB-C2B-C3B	4.69	133.46	124.68
8	N	102	BCL	CMB-C2B-C3B	4.69	133.45	124.68
8	1	101	BCL	CMB-C2B-C3B	4.68	133.44	124.68
8	G	102	BCL	O2D-CGD-CBD	4.68	119.58	111.27
8	1	101	BCL	CHD-C4C-NC	4.67	130.26	125.08
8	G	103	BCL	O2D-CGD-CBD	4.67	119.56	111.27
8	R	104	BCL	CMB-C2B-C3B	4.67	133.41	124.68
15	Z	101	CRT	C20-C21-C22	4.66	133.02	123.47
8	M	407	BCL	CHD-C4C-NC	4.64	130.23	125.08
8	L	402	BCL	CMB-C2B-C3B	4.64	133.35	124.68
8	D	104	BCL	CMB-C2B-C3B	4.64	133.35	124.68
8	C	100	BCL	CMB-C2B-C3B	4.64	133.35	124.68
8	R	103	BCL	O2D-CGD-CBD	4.63	119.50	111.27
8	A	101	BCL	O2D-CGD-CBD	4.62	119.48	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	R	104	BCL	O2D-CGD-CBD	4.62	119.47	111.27
8	D	104	BCL	O2D-CGD-CBD	4.62	119.47	111.27
8	E	102	BCL	C3C-C4C-CHD	-4.58	113.60	123.39
8	2	101	BCL	CMB-C2B-C3B	4.58	133.25	124.68
8	3	101	BCL	CHD-C4C-NC	4.58	130.16	125.08
8	L	402	BCL	C3C-C4C-CHD	-4.58	113.61	123.39
8	2	101	BCL	O2D-CGD-CBD	4.57	119.39	111.27
10	1	102	U10	C7-C8-C9	-4.57	119.18	126.79
8	A	102	BCL	CMB-C2B-C3B	4.57	133.23	124.68
8	Y	102	BCL	O2D-CGD-CBD	4.56	119.38	111.27
8	V	101	BCL	O2D-CGD-CBD	4.54	119.33	111.27
8	Y	102	BCL	CMB-C2B-C3B	4.54	133.17	124.68
8	T	101	BCL	CHD-C4C-NC	4.53	130.11	125.08
8	P	101	BCL	CHD-C4C-NC	4.52	130.10	125.08
8	J	103	BCL	O2D-CGD-CBD	4.52	119.30	111.27
8	E	103	BCL	CMB-C2B-C3B	4.51	133.12	124.68
8	V	102	BCL	CHD-C4C-NC	4.51	130.09	125.08
8	R	104	BCL	CHD-C4C-NC	4.50	130.07	125.08
8	P	103	BCL	CHD-C4C-NC	4.50	130.07	125.08
8	A	101	BCL	C3C-C4C-CHD	-4.48	113.81	123.39
8	D	104	BCL	C3C-C4C-CHD	-4.48	113.83	123.39
8	G	102	BCL	CMB-C2B-C3B	4.47	133.04	124.68
15	3	103	CRT	C20-C21-C22	4.46	132.61	123.47
8	N	102	BCL	CHD-C4C-NC	4.45	130.02	125.08
8	J	102	BCL	CHD-C4C-NC	4.45	130.01	125.08
8	D	104	BCL	CHD-C4C-NC	4.43	130.00	125.08
8	N	102	BCL	O2D-CGD-CBD	4.43	119.14	111.27
8	J	102	BCL	O2D-CGD-CBD	4.42	119.12	111.27
8	P	101	BCL	CMB-C2B-C3B	4.42	132.95	124.68
8	G	103	BCL	CHD-C4C-NC	4.41	129.98	125.08
8	V	102	BCL	C3C-C4C-CHD	-4.41	113.97	123.39
8	E	102	BCL	CMB-C2B-C3B	4.41	132.93	124.68
8	N	101	BCL	CHD-C4C-NC	4.40	129.97	125.08
8	J	102	BCL	CMB-C2B-C3B	4.40	132.90	124.68
8	J	103	BCL	CHD-C4C-NC	4.40	129.96	125.08
8	Y	101	BCL	CHD-C4C-NC	4.39	129.95	125.08
8	N	101	BCL	O2D-CGD-CBD	4.38	119.06	111.27
8	1	101	BCL	C3C-C4C-CHD	-4.38	114.03	123.39
8	R	104	BCL	C3C-C4C-CHD	-4.38	114.03	123.39
8	E	103	BCL	O2D-CGD-CBD	4.37	119.03	111.27
8	P	103	BCL	C3C-C4C-CHD	-4.36	114.07	123.39
8	N	102	BCL	C3C-C4C-CHD	-4.34	114.11	123.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	V	101	BCL	C3C-C4C-CHD	-4.34	114.13	123.39
8	4	101	BCL	O2D-CGD-CBD	4.33	118.96	111.27
8	C	100	BCL	CHD-C4C-NC	4.33	129.88	125.08
8	A	102	BCL	O2D-CGD-CBD	4.31	118.92	111.27
8	G	102	BCL	CHD-C4C-NC	4.30	129.85	125.08
8	G	103	BCL	C3C-C4C-CHD	-4.30	114.21	123.39
8	P	101	BCL	C3C-C4C-CHD	-4.29	114.22	123.39
8	5	101	BCL	CHD-C4C-NC	4.29	129.84	125.08
8	L	401	BCL	CMB-C2B-C3B	4.28	132.69	124.68
8	J	103	BCL	C1-C2-C3	-4.26	118.67	126.04
8	M	402	BCL	O2D-CGD-CBD	4.26	118.84	111.27
8	N	101	BCL	CMB-C2B-C3B	4.25	132.64	124.68
8	R	103	BCL	CMB-C2B-C3B	4.25	132.63	124.68
14	J	101	LMT	C3'-C4'-C5'	-4.24	101.22	110.93
8	A	102	BCL	CHD-C4C-NC	4.23	129.77	125.08
8	R	103	BCL	C3C-C4C-CHD	-4.22	114.37	123.39
8	J	103	BCL	C3C-C4C-CHD	-4.22	114.38	123.39
8	3	101	BCL	C3C-C4C-CHD	-4.22	114.38	123.39
15	Z	101	CRT	C6-C7-C9	4.21	125.41	118.94
8	E	103	BCL	CHD-C4C-NC	4.21	129.75	125.08
8	M	407	BCL	C3C-C4C-CHD	-4.20	114.42	123.39
8	C	100	BCL	C3C-C4C-CHD	-4.20	114.43	123.39
8	5	102	BCL	C4C-CHD-C1D	-4.19	119.69	125.88
8	2	101	BCL	CHD-C4C-NC	4.19	129.73	125.08
8	T	102	BCL	O2D-CGD-CBD	4.17	118.68	111.27
15	Z	101	CRT	C8-C7-C9	-4.16	117.09	122.92
8	T	102	BCL	C3C-C4C-CHD	-4.14	114.55	123.39
8	E	103	BCL	C3C-C4C-CHD	-4.12	114.59	123.39
8	L	401	BCL	C3C-C4C-CHD	-4.12	114.60	123.39
8	N	101	BCL	C3C-C4C-CHD	-4.11	114.61	123.39
8	P	103	BCL	O2D-CGD-CBD	4.11	118.57	111.27
8	V	102	BCL	O2D-CGD-CBD	4.06	118.49	111.27
8	Y	101	BCL	C3C-C4C-CHD	-4.06	114.71	123.39
8	G	102	BCL	C3C-C4C-CHD	-4.05	114.73	123.39
8	A	101	BCL	CMB-C2B-C3B	4.05	132.26	124.68
8	T	101	BCL	C3C-C4C-CHD	-4.03	114.78	123.39
8	A	102	BCL	C3C-C4C-CHD	-4.03	114.79	123.39
8	J	102	BCL	C3C-C4C-CHD	-4.02	114.80	123.39
8	4	101	BCL	CHD-C4C-NC	4.02	129.54	125.08
8	2	101	BCL	C3C-C4C-CHD	-4.01	114.82	123.39
8	T	102	BCL	CHD-C4C-NC	4.01	129.53	125.08
8	Y	102	BCL	CHD-C4C-NC	4.00	129.52	125.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	S	103	CRT	C20-C21-C22	4.00	131.66	123.47
15	K	103	CRT	C20-C21-C22	3.96	131.59	123.47
8	5	102	BCL	O2D-CGD-CBD	3.95	118.29	111.27
8	Y	102	BCL	C3C-C4C-CHD	-3.89	115.08	123.39
8	4	101	BCL	C1B-CHB-C4A	-3.86	122.47	130.12
8	R	104	BCL	C1-C2-C3	-3.84	119.40	126.04
15	O	102	CRT	C8-C7-C9	-3.78	117.62	122.92
8	5	101	BCL	CMB-C2B-C3B	3.78	131.75	124.68
8	M	402	BCL	C4A-NA-C1A	3.78	108.40	106.71
14	L	405	LMT	C3'-C4'-C5'	-3.75	102.34	110.93
15	I	103	CRT	C20-C21-C22	3.74	131.13	123.47
8	J	102	BCL	C1-C2-C3	-3.73	119.59	126.04
8	M	402	BCL	C4C-CHD-C1D	-3.72	120.40	125.88
8	D	104	BCL	C1-C2-C3	-3.70	119.64	126.04
8	M	407	BCL	C1-C2-C3	-3.70	119.65	126.04
10	1	102	U10	C10-C9-C11	3.69	121.48	115.27
8	4	101	BCL	C4B-CHC-C1C	-3.67	122.84	130.12
8	N	102	BCL	C4-C3-C5	3.66	121.43	115.27
8	5	102	BCL	C4A-NA-C1A	3.66	108.35	106.71
15	K	103	CRT	C36-C35-C33	3.60	131.34	125.89
15	O	102	CRT	C36-C35-C33	3.60	131.33	125.89
8	5	101	BCL	C3C-C4C-CHD	-3.59	115.72	123.39
8	4	101	BCL	C3C-C4C-CHD	-3.59	115.73	123.39
8	A	102	BCL	O2A-CGA-CBA	3.57	123.10	111.91
15	F	103	CRT	C20-C21-C22	3.56	130.76	123.47
10	M	404	U10	C27-C28-C29	-3.54	119.13	127.66
15	O	102	CRT	C20-C21-C22	3.53	130.71	123.47
8	M	407	BCL	C4C-CHD-C1D	-3.53	120.67	125.88
15	O	102	CRT	C6-C7-C9	3.53	124.36	118.94
10	M	404	U10	C25-C24-C26	3.53	121.20	115.27
8	V	102	BCL	C1-C2-C3	-3.53	119.94	126.04
15	X	102	CRT	C36-C35-C33	3.51	131.20	125.89
15	I	103	CRT	C36-C35-C33	3.51	131.20	125.89
14	S	102	LMT	C3'-C4'-C5'	-3.51	102.88	110.93
14	X	101	LMT	C1'-O5'-C5'	-3.50	106.82	113.69
14	4	102	LMT	C3'-C4'-C5'	-3.50	102.91	110.93
10	M	404	U10	C35-C34-C36	3.49	121.15	115.27
15	X	102	CRT	C20-C21-C22	3.48	130.60	123.47
8	E	102	BCL	C4-C3-C5	3.47	121.10	115.27
15	2	102	CRT	C24-C23-C22	-3.43	118.12	122.92
15	F	103	CRT	C36-C35-C33	3.42	131.06	125.89
8	A	102	BCL	C4C-CHD-C1D	-3.41	120.84	125.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	B	103	CRT	C20-C21-C22	3.39	130.42	123.47
8	T	101	BCL	C4-C3-C5	3.38	120.97	115.27
15	S	103	CRT	C8-C7-C9	-3.38	118.18	122.92
8	N	101	BCL	C1-C2-C3	-3.38	120.20	126.04
15	K	103	CRT	C8-C7-C9	-3.38	118.19	122.92
10	1	102	U10	C32-C31-C29	-3.38	109.10	114.62
10	L	406	U10	C7-C8-C9	-3.37	121.18	126.79
8	5	102	BCL	C1-C2-C3	-3.37	120.21	126.04
8	4	101	BCL	CMB-C2B-C3B	3.36	130.97	124.68
15	Q	103	CRT	C20-C21-C22	3.36	130.36	123.47
8	P	103	BCL	C1-C2-C3	-3.36	120.23	126.04
10	M	404	U10	C22-C23-C24	-3.36	119.58	127.66
8	L	401	BCL	C4C-CHD-C1D	-3.34	120.95	125.88
8	Y	101	BCL	C4-C3-C5	3.34	120.89	115.27
8	C	100	BCL	C4-C3-C5	3.32	120.85	115.27
8	L	402	BCL	O2D-CGD-CBD	3.31	117.14	111.27
8	N	102	BCL	C1-C2-C3	-3.30	120.33	126.04
8	R	104	BCL	C4-C3-C5	3.30	120.82	115.27
8	J	102	BCL	C4C-CHD-C1D	-3.30	121.01	125.88
8	L	402	BCL	O2A-CGA-CBA	3.30	122.25	111.91
15	3	103	CRT	C24-C23-C22	-3.29	118.31	122.92
8	Y	102	BCL	C1-C2-C3	-3.29	120.35	126.04
14	Q	101	LMT	C3'-C4'-C5'	-3.28	103.40	110.93
8	Y	101	BCL	C1-C2-C3	-3.27	120.38	126.04
8	J	103	BCL	C4-C3-C5	3.27	120.77	115.27
14	F	101	LMT	C3'-C4'-C5'	-3.25	103.47	110.93
8	E	102	BCL	C1-C2-C3	-3.25	120.42	126.04
8	G	103	BCL	C4C-CHD-C1D	-3.25	121.09	125.88
8	M	402	BCL	C1-C2-C3	-3.24	120.43	126.04
8	E	102	BCL	C4C-CHD-C1D	-3.24	121.11	125.88
10	1	102	U10	C15-C14-C16	3.22	120.70	115.27
8	J	102	BCL	C4-C3-C5	3.22	120.68	115.27
8	G	102	BCL	C4C-CHD-C1D	-3.21	121.15	125.88
8	P	103	BCL	C4-C3-C5	3.21	120.67	115.27
10	M	404	U10	C17-C18-C19	-3.20	119.95	127.66
8	N	101	BCL	C4C-CHD-C1D	-3.20	121.16	125.88
8	L	402	BCL	C4C-CHD-C1D	-3.20	121.16	125.88
8	N	102	BCL	C4C-CHD-C1D	-3.19	121.18	125.88
8	G	102	BCL	C1-C2-C3	-3.18	120.54	126.04
14	O	101	LMT	C3'-C4'-C5'	-3.17	103.65	110.93
8	T	102	BCL	C4C-CHD-C1D	-3.17	121.21	125.88
14	B	102	LMT	C1'-O5'-C5'	-3.16	107.48	113.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	M	407	BCL	O2D-CGD-O1D	-3.16	117.66	123.84
8	E	103	BCL	C4C-CHD-C1D	-3.16	121.22	125.88
15	Z	101	CRT	C24-C23-C22	-3.15	118.50	122.92
8	P	101	BCL	C4C-CHD-C1D	-3.15	121.23	125.88
8	R	103	BCL	C4C-CHD-C1D	-3.14	121.24	125.88
8	2	101	BCL	C1-C2-C3	-3.14	120.62	126.04
8	2	101	BCL	C4-C3-C5	3.14	120.55	115.27
15	B	103	CRT	C8-C7-C9	-3.14	118.53	122.92
8	C	100	BCL	C1-C2-C3	-3.13	120.63	126.04
14	U	101	LMT	C1'-O5'-C5'	-3.13	107.54	113.69
15	R	101	CRT	C8-C7-C9	-3.13	118.54	122.92
8	T	101	BCL	C1-C2-C3	-3.13	120.63	126.04
8	V	101	BCL	C4C-CHD-C1D	-3.13	121.26	125.88
8	T	101	BCL	C4C-CHD-C1D	-3.13	121.26	125.88
8	A	101	BCL	C4-C3-C5	3.13	120.53	115.27
8	Y	101	BCL	C4C-CHD-C1D	-3.12	121.28	125.88
8	5	101	BCL	O2A-CGA-CBA	3.12	121.70	111.91
15	B	103	CRT	C13-C12-C14	-3.12	118.55	122.92
8	R	103	BCL	CHC-C1C-NC	3.12	128.82	124.51
15	3	103	CRT	C36-C35-C33	3.11	130.59	125.89
15	Z	101	CRT	C36-C35-C33	3.11	130.59	125.89
8	4	101	BCL	O2A-CGA-CBA	3.11	121.66	111.91
8	V	102	BCL	C4-C3-C5	3.10	120.49	115.27
8	Y	102	BCL	C4-C3-C5	3.10	120.48	115.27
8	A	101	BCL	C4C-CHD-C1D	-3.09	121.32	125.88
8	C	100	BCL	O2A-CGA-CBA	3.09	121.61	111.91
8	L	401	BCL	C4-C3-C5	3.09	120.47	115.27
15	Z	101	CRT	C13-C12-C14	-3.09	118.59	122.92
15	X	102	CRT	C24-C23-C22	-3.09	118.59	122.92
14	S	102	LMT	C1'-O5'-C5'	-3.09	107.63	113.69
15	S	103	CRT	C36-C35-C33	3.08	130.55	125.89
8	M	402	BCL	C1C-NC-C4C	-3.08	105.32	106.71
15	I	103	CRT	C8-C7-C9	-3.08	118.61	122.92
15	2	102	CRT	C25-C23-C22	3.06	123.64	118.94
15	X	102	CRT	C8-C7-C9	-3.06	118.64	122.92
10	M	404	U10	C12-C13-C14	-3.06	120.29	127.66
8	G	102	BCL	O2A-CGA-CBA	3.06	121.50	111.91
8	5	101	BCL	C4-C3-C5	3.05	120.40	115.27
8	M	407	BCL	C4A-NA-C1A	3.05	108.08	106.71
8	N	102	BCL	CHB-C4A-NA	3.05	128.72	124.51
8	V	101	BCL	C4-C3-C5	3.04	120.39	115.27
8	5	102	BCL	C4-C3-C5	3.04	120.38	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	E	102	BCL	O2A-CGA-CBA	3.04	121.44	111.91
8	P	101	BCL	C4-C3-C5	3.04	120.38	115.27
15	D	105	CRT	C24-C23-C22	-3.03	118.67	122.92
15	X	102	CRT	C29-C28-C27	-3.03	118.68	122.92
8	Y	102	BCL	CHB-C4A-NA	3.03	128.70	124.51
8	T	102	BCL	C1-C2-C3	-3.03	120.81	126.04
15	Q	103	CRT	C24-C23-C22	-3.02	118.69	122.92
8	V	101	BCL	CHC-C1C-NC	3.02	128.69	124.51
15	F	103	CRT	C24-C23-C22	-3.02	118.69	122.92
8	R	104	BCL	O2D-CGD-O1D	-3.02	117.93	123.84
15	Q	103	CRT	C8-C7-C9	-3.02	118.70	122.92
15	S	103	CRT	C24-C23-C22	-3.02	118.70	122.92
15	D	105	CRT	C20-C21-C22	3.01	129.65	123.47
15	O	102	CRT	C24-C23-C22	-3.01	118.70	122.92
8	Y	101	BCL	O2A-CGA-CBA	3.01	121.36	111.91
8	R	104	BCL	O2A-CGA-CBA	3.00	121.33	111.91
15	K	103	CRT	C24-C23-C22	-3.00	118.72	122.92
10	M	404	U10	C10-C9-C11	3.00	120.32	115.27
8	L	401	BCL	O2D-CGD-O1D	-3.00	117.97	123.84
14	K	102	LMT	C3'-C4'-C5'	-2.99	104.08	110.93
15	2	102	CRT	C13-C12-C14	-2.99	118.74	122.92
15	Z	101	CRT	C5-C6-C7	-2.98	121.38	125.89
14	X	103	LMT	C3'-C4'-C5'	-2.98	104.10	110.93
8	T	101	BCL	O2A-CGA-CBA	2.98	121.25	111.91
8	P	101	BCL	O2A-CGA-CBA	2.97	121.23	111.91
15	S	103	CRT	C13-C12-C14	-2.97	118.77	122.92
8	G	102	BCL	CHC-C1C-NC	2.97	128.62	124.51
8	L	402	BCL	C4-C3-C5	2.96	120.26	115.27
15	S	103	CRT	C6-C7-C9	2.95	123.47	118.94
15	2	102	CRT	C8-C7-C9	-2.95	118.79	122.92
8	R	103	BCL	C1-C2-C3	-2.95	120.94	126.04
10	M	404	U10	C15-C14-C16	2.95	120.23	115.27
8	R	103	BCL	O2A-CGA-CBA	2.95	121.16	111.91
15	I	103	CRT	C24-C23-C22	-2.94	118.80	122.92
8	1	101	BCL	C4C-CHD-C1D	-2.94	121.55	125.88
10	L	406	U10	C10-C9-C11	2.94	119.34	115.98
15	Z	101	CRT	C25-C23-C22	2.93	123.44	118.94
8	R	104	BCL	C4C-CHD-C1D	-2.93	121.55	125.88
8	L	402	BCL	CED-O2D-CGD	2.93	122.56	115.94
8	N	101	BCL	O2A-CGA-CBA	2.93	121.09	111.91
8	5	102	BCL	CMB-C2B-C3B	2.93	130.15	124.68
15	R	101	CRT	C24-C23-C22	-2.93	118.83	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	V	102	BCL	C4C-CHD-C1D	-2.92	121.57	125.88
15	B	103	CRT	C24-C23-C22	-2.92	118.84	122.92
8	D	104	BCL	C4-C3-C5	2.92	120.18	115.27
8	V	101	BCL	C1-C2-C3	-2.92	121.00	126.04
8	G	103	BCL	CHB-C4A-NA	2.92	128.54	124.51
8	Y	102	BCL	O2D-CGD-O1D	-2.91	118.14	123.84
8	A	101	BCL	O2A-CGA-CBA	2.91	121.05	111.91
8	A	102	BCL	CHB-C4A-NA	2.91	128.54	124.51
8	G	103	BCL	O2A-CGA-CBA	2.91	121.04	111.91
10	1	102	U10	C1M-C1-C6	-2.91	119.65	124.40
8	J	102	BCL	CHC-C1C-NC	2.90	128.52	124.51
10	M	404	U10	C32-C33-C34	-2.90	120.68	127.66
8	4	101	BCL	C4C-CHD-C1D	-2.90	121.60	125.88
8	D	104	BCL	C4C-CHD-C1D	-2.90	121.61	125.88
8	D	104	BCL	O2D-CGD-O1D	-2.89	118.18	123.84
14	I	102	LMT	C1'-O5'-C5'	-2.89	108.02	113.69
15	2	102	CRT	C29-C28-C27	-2.89	118.88	122.92
14	S	101	LMT	C3'-C4'-C5'	-2.88	104.32	110.93
15	3	103	CRT	C8-C7-C9	-2.88	118.89	122.92
15	D	105	CRT	C21-C20-C19	2.88	129.38	123.47
8	J	102	BCL	O2A-CGA-CBA	2.88	120.95	111.91
8	E	103	BCL	CHB-C4A-NA	2.87	128.48	124.51
8	2	101	BCL	C4C-CHD-C1D	-2.86	121.66	125.88
8	3	101	BCL	C1-C2-C3	-2.86	121.10	126.04
8	N	101	BCL	CHC-C1C-NC	2.86	128.46	124.51
8	C	100	BCL	CHC-C1C-NC	2.85	128.46	124.51
15	3	103	CRT	C25-C23-C22	2.85	123.32	118.94
15	K	103	CRT	C6-C7-C9	2.85	123.31	118.94
8	D	104	BCL	O2A-CGA-CBA	2.85	120.84	111.91
15	D	105	CRT	C18-C17-C19	-2.84	118.95	122.92
15	Q	103	CRT	C18-C17-C19	-2.84	118.95	122.92
8	G	103	BCL	C4-C3-C5	2.84	120.04	115.27
15	3	103	CRT	C13-C12-C14	-2.84	118.95	122.92
8	E	102	BCL	CHC-C1C-NC	2.83	128.43	124.51
15	Q	103	CRT	C34-C33-C32	-2.83	118.95	122.92
8	E	103	BCL	O2A-CGA-CBA	2.83	120.80	111.91
8	T	102	BCL	O2A-CGA-CBA	2.83	120.79	111.91
8	L	402	BCL	CHC-C1C-NC	2.83	128.43	124.51
8	J	103	BCL	C4C-CHD-C1D	-2.83	121.71	125.88
15	2	102	CRT	C36-C35-C33	2.82	130.16	125.89
15	K	103	CRT	C31-C32-C33	2.82	131.34	127.31
8	L	402	BCL	C1-C2-C3	-2.82	121.17	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	T	101	BCL	CHC-C1C-NC	2.82	128.41	124.51
8	J	103	BCL	O2D-CGD-O1D	-2.82	118.33	123.84
14	Q	102	LMT	C3'-C4'-C5'	-2.82	104.47	110.93
15	R	101	CRT	C34-C33-C32	-2.81	118.98	122.92
15	F	103	CRT	C29-C28-C27	-2.81	118.98	122.92
8	N	101	BCL	C4-C3-C5	2.81	120.00	115.27
15	D	105	CRT	C8-C7-C9	-2.81	118.99	122.92
8	P	103	BCL	C4C-CHD-C1D	-2.81	121.74	125.88
8	V	101	BCL	O2A-CGA-CBA	2.80	120.71	111.91
8	2	101	BCL	O2A-CGA-CBA	2.80	120.71	111.91
15	2	102	CRT	C18-C17-C19	-2.80	119.00	122.92
8	P	101	BCL	CHC-C1C-NC	2.80	128.38	124.51
15	D	105	CRT	C34-C33-C32	-2.80	119.00	122.92
8	M	407	BCL	C4-C3-C5	2.79	119.96	115.27
15	Z	101	CRT	C18-C17-C19	-2.78	119.03	122.92
10	M	404	U10	C30-C29-C31	2.78	119.94	115.27
15	3	103	CRT	C18-C17-C19	-2.77	119.04	122.92
8	3	101	BCL	C4C-CHD-C1D	-2.77	121.79	125.88
15	F	103	CRT	C8-C7-C9	-2.77	119.04	122.92
8	Y	102	BCL	C4C-CHD-C1D	-2.77	121.79	125.88
8	P	101	BCL	C1-C2-C3	-2.77	121.26	126.04
14	Q	102	LMT	C1'-O5'-C5'	-2.76	108.26	113.69
8	R	104	BCL	CHC-C1C-NC	2.76	128.33	124.51
8	R	104	BCL	CHB-C4A-NA	2.76	128.33	124.51
15	S	103	CRT	C31-C32-C33	2.76	131.24	127.31
14	D	103	LMT	C1'-O5'-C5'	-2.76	108.28	113.69
8	5	101	BCL	C4C-CHD-C1D	-2.75	121.82	125.88
15	R	101	CRT	C20-C21-C22	2.75	129.12	123.47
10	1	102	U10	C27-C28-C29	-2.75	121.03	127.66
8	G	103	BCL	C1-C2-C3	-2.75	121.29	126.04
15	B	103	CRT	C18-C17-C19	-2.75	119.08	122.92
15	R	101	CRT	C29-C28-C27	-2.75	119.08	122.92
8	P	101	BCL	O2D-CGD-O1D	-2.74	118.47	123.84
14	X	101	LMT	C2'-C3'-C4'	2.74	115.94	109.68
8	M	402	BCL	O2A-CGA-CBA	2.74	120.51	111.91
8	L	401	BCL	O2A-CGA-CBA	2.74	120.51	111.91
15	Z	101	CRT	C31-C32-C33	2.74	131.22	127.31
8	V	102	BCL	O2A-CGA-CBA	2.74	120.50	111.91
10	M	404	U10	C20-C19-C21	2.74	119.87	115.27
8	D	104	BCL	CHB-C4A-NA	2.73	128.29	124.51
15	O	102	CRT	C13-C12-C14	-2.72	119.11	122.92
8	E	103	BCL	CHC-C1C-NC	2.72	128.27	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	F	103	CRT	C13-C12-C14	-2.72	119.12	122.92
15	K	103	CRT	C15-C14-C12	2.72	131.19	127.31
8	P	103	BCL	CHB-C4A-NA	2.71	128.26	124.51
8	G	102	BCL	C4-C3-C5	2.71	119.83	115.27
8	G	103	BCL	O2D-CGD-O1D	-2.71	118.54	123.84
8	R	103	BCL	CHB-C4A-NA	2.71	128.26	124.51
8	C	100	BCL	CHB-C4A-NA	2.71	128.26	124.51
8	E	103	BCL	C4-C3-C5	2.70	119.82	115.27
15	Q	103	CRT	C13-C12-C14	-2.70	119.14	122.92
15	R	101	CRT	C18-C17-C19	-2.70	119.14	122.92
14	2	103	LMT	C1'-O5'-C5'	-2.70	108.39	113.69
8	3	101	BCL	C4-C3-C5	2.69	119.80	115.27
15	D	105	CRT	C29-C28-C27	-2.69	119.15	122.92
10	1	102	U10	C22-C23-C24	-2.69	121.18	127.66
15	Z	101	CRT	C29-C28-C27	-2.69	119.16	122.92
8	1	101	BCL	CAC-C3C-C4C	-2.69	106.62	112.58
8	P	101	BCL	CHB-C4A-NA	2.69	128.22	124.51
15	O	102	CRT	C31-C32-C33	2.69	131.14	127.31
8	A	101	BCL	CHC-C1C-NC	2.68	128.22	124.51
8	N	101	BCL	CHB-C4A-NA	2.68	128.21	124.51
8	E	103	BCL	O2D-CGD-O1D	-2.68	118.61	123.84
8	Y	102	BCL	O2A-CGA-CBA	2.68	120.30	111.91
8	A	102	BCL	O2D-CGD-O1D	-2.67	118.61	123.84
8	L	401	BCL	C1-C2-C3	-2.67	121.42	126.04
15	F	103	CRT	C34-C33-C32	-2.67	119.18	122.92
8	5	101	BCL	CAD-C3D-C4D	2.67	109.96	108.47
14	M	409	LMT	C1'-O5'-C5'	-2.67	108.45	113.69
8	M	407	BCL	C4B-CHC-C1C	-2.67	124.83	130.12
8	R	103	BCL	C4-C3-C5	2.67	119.76	115.27
8	N	102	BCL	O2D-CGD-O1D	-2.66	118.63	123.84
8	1	101	BCL	CHC-C1C-NC	2.66	128.19	124.51
15	X	102	CRT	C18-C17-C19	-2.66	119.20	122.92
15	X	102	CRT	C13-C12-C14	-2.65	119.21	122.92
8	5	102	BCL	O2A-CGA-CBA	2.65	120.23	111.91
8	J	102	BCL	CAD-C3D-C4D	2.65	109.95	108.47
15	K	103	CRT	C18-C17-C19	-2.65	119.22	122.92
14	Z	102	LMT	C1'-O5'-C5'	-2.64	108.50	113.69
8	C	100	BCL	C4C-CHD-C1D	-2.64	121.98	125.88
7	M	401	QAK	CD2-CE2-CZ2	2.64	113.75	110.75
15	X	102	CRT	C21-C20-C19	2.64	128.88	123.47
14	S	101	LMT	C1'-O5'-C5'	-2.64	108.51	113.69
15	X	102	CRT	C6-C7-C9	2.64	122.98	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	J	103	BCL	CHB-C4A-NA	2.63	128.15	124.51
8	T	102	BCL	CHB-C4A-NA	2.63	128.15	124.51
8	T	101	BCL	O2D-CGD-O1D	-2.63	118.70	123.84
15	R	101	CRT	C21-C20-C19	2.63	128.85	123.47
14	2	104	LMT	C3'-C4'-C5'	-2.62	104.92	110.93
15	X	102	CRT	C34-C33-C32	-2.61	119.26	122.92
8	M	402	BCL	C4-C3-C5	2.61	119.66	115.27
8	1	101	BCL	C1-C2-C3	-2.61	121.53	126.04
15	R	101	CRT	C13-C12-C14	-2.61	119.27	122.92
8	E	103	BCL	C1-C2-C3	-2.61	121.53	126.04
15	B	103	CRT	C11-C12-C14	2.61	122.94	118.94
8	P	103	BCL	C2A-C1A-CHA	-2.61	119.30	123.86
8	5	101	BCL	CHC-C1C-NC	2.61	128.12	124.51
8	Y	101	BCL	CHC-C1C-NC	2.60	128.11	124.51
8	T	102	BCL	C4-C3-C5	2.60	119.65	115.27
10	1	102	U10	C25-C24-C26	2.60	119.65	115.27
15	S	103	CRT	C29-C28-C27	-2.60	119.28	122.92
8	N	102	BCL	CHC-C1C-NC	2.60	128.11	124.51
8	V	102	BCL	CHC-C1C-NC	2.60	128.10	124.51
8	J	103	BCL	CHC-C1C-NC	2.60	128.10	124.51
8	J	102	BCL	CHB-C4A-NA	2.59	128.10	124.51
15	3	103	CRT	C34-C33-C32	-2.59	119.29	122.92
15	B	103	CRT	C31-C32-C33	2.59	131.01	127.31
14	2	103	LMT	C3'-C4'-C5'	-2.59	104.99	110.93
14	Z	102	LMT	O5B-C5B-C4B	2.59	114.39	109.69
8	3	101	BCL	O2A-CGA-CBA	2.59	120.03	111.91
15	K	103	CRT	C29-C28-C27	-2.59	119.30	122.92
15	3	103	CRT	C31-C32-C33	2.59	131.00	127.31
15	O	102	CRT	C29-C28-C27	-2.58	119.30	122.92
15	2	102	CRT	C34-C33-C32	-2.58	119.31	122.92
8	1	101	BCL	CHB-C4A-NA	2.58	128.08	124.51
8	G	103	BCL	CHC-C1C-NC	2.58	128.08	124.51
15	D	105	CRT	C13-C12-C14	-2.58	119.31	122.92
8	1	101	BCL	O2A-CGA-CBA	2.58	120.00	111.91
8	T	102	BCL	O2D-CGD-O1D	-2.58	118.80	123.84
14	Q	101	LMT	O5'-C1'-C2'	2.57	115.80	110.35
14	L	405	LMT	O1B-C4'-C3'	2.57	114.13	107.28
15	F	103	CRT	C18-C17-C19	-2.57	119.32	122.92
15	S	103	CRT	C18-C17-C19	-2.57	119.32	122.92
8	C	100	BCL	C2A-C1A-CHA	-2.57	119.37	123.86
8	3	101	BCL	CHC-C1C-NC	2.57	128.06	124.51
15	X	102	CRT	C25-C23-C22	2.57	122.88	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	A	102	BCL	CHC-C1C-NC	2.57	128.06	124.51
15	3	103	CRT	C29-C28-C27	-2.56	119.33	122.92
15	I	103	CRT	C18-C17-C19	-2.56	119.33	122.92
8	C	100	BCL	O2D-CGD-O1D	-2.56	118.82	123.84
8	M	402	BCL	CHC-C1C-NC	2.56	128.06	124.51
8	M	407	BCL	CHC-C1C-NC	2.56	128.05	124.51
8	V	102	BCL	CHB-C4A-NA	2.56	128.05	124.51
8	Y	101	BCL	O2D-CGD-O1D	-2.56	118.84	123.84
14	D	103	LMT	C2'-C3'-C4'	2.56	115.52	109.68
8	M	407	BCL	CHB-C4A-NA	2.56	128.05	124.51
8	P	103	BCL	CHC-C1C-NC	2.55	128.04	124.51
14	D	103	LMT	C1'-C2'-C3'	2.55	115.31	110.00
15	O	102	CRT	C18-C17-C19	-2.54	119.36	122.92
15	2	102	CRT	C6-C7-C9	2.54	122.83	118.94
8	2	101	BCL	O2D-CGD-O1D	-2.54	118.88	123.84
9	M	403	BPH	CMA-C3A-C4A	-2.53	108.83	114.38
8	E	102	BCL	O2D-CGD-O1D	-2.53	118.89	123.84
8	T	102	BCL	CHC-C1C-NC	2.53	128.01	124.51
8	R	103	BCL	O2D-CGD-O1D	-2.51	118.92	123.84
8	L	401	BCL	CHB-C4A-NA	2.51	127.99	124.51
15	X	102	CRT	C31-C32-C33	2.51	130.89	127.31
15	B	103	CRT	C34-C33-C32	-2.51	119.41	122.92
8	E	102	BCL	CAC-C3C-C4C	-2.51	107.02	112.58
14	S	102	LMT	O5B-C5B-C4B	2.50	114.23	109.69
8	P	103	BCL	O2D-CGD-O1D	-2.50	118.95	123.84
8	L	402	BCL	CHB-C4A-NA	2.49	127.96	124.51
8	N	102	BCL	C2A-C1A-CHA	-2.49	119.51	123.86
15	I	103	CRT	C29-C28-C27	-2.49	119.44	122.92
8	J	102	BCL	O2D-CGD-O1D	-2.48	118.98	123.84
15	Q	103	CRT	C29-C28-C27	-2.48	119.45	122.92
9	L	403	BPH	C1-C2-C3	-2.48	121.76	126.04
14	B	102	LMT	O1'-C1'-C2'	2.47	112.16	108.30
14	D	101	LMT	C2'-C3'-C4'	2.47	115.32	109.68
8	A	101	BCL	O2D-CGD-O1D	-2.47	119.01	123.84
15	I	103	CRT	C13-C12-C14	-2.47	119.47	122.92
15	R	101	CRT	C6-C7-C9	2.47	122.73	118.94
8	D	104	BCL	CHC-C1C-NC	2.46	127.92	124.51
14	X	103	LMT	C1'-O5'-C5'	-2.46	108.85	113.69
15	R	101	CRT	C15-C14-C12	2.46	130.83	127.31
8	G	102	BCL	CHB-C4A-NA	2.45	127.90	124.51
8	A	102	BCL	O2A-CGA-O1A	-2.45	117.41	123.59
8	T	101	BCL	CHB-C4A-NA	2.45	127.90	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	L	401	BCL	C4B-CHC-C1C	-2.44	125.28	130.12
8	Y	102	BCL	CHC-C1C-NC	2.44	127.89	124.51
15	X	102	CRT	C15-C14-C12	2.44	130.79	127.31
8	4	101	BCL	C1C-NC-C4C	2.44	107.80	106.71
8	D	104	BCL	C2A-C1A-CHA	-2.44	119.59	123.86
8	G	102	BCL	O2D-CGD-O1D	-2.43	119.08	123.84
15	B	103	CRT	C29-C28-C27	-2.43	119.52	122.92
8	P	101	BCL	C2A-C1A-CHA	-2.43	119.62	123.86
15	O	102	CRT	C34-C33-C32	-2.43	119.53	122.92
8	A	101	BCL	CAC-C3C-C4C	-2.42	107.20	112.58
8	Y	102	BCL	C2A-C1A-CHA	-2.42	119.63	123.86
14	I	101	LMT	C3'-C4'-C5'	-2.42	105.39	110.93
8	N	101	BCL	O2D-CGD-O1D	-2.41	119.12	123.84
8	L	402	BCL	O2A-CGA-O1A	-2.41	117.51	123.59
15	2	102	CRT	C31-C32-C33	2.40	130.74	127.31
15	K	103	CRT	C13-C12-C14	-2.40	119.57	122.92
8	1	101	BCL	O2D-CGD-O1D	-2.40	119.15	123.84
10	1	102	U10	C30-C29-C31	2.40	119.30	115.27
15	O	102	CRT	C25-C23-C22	2.39	122.61	118.94
15	I	103	CRT	C34-C33-C32	-2.39	119.58	122.92
15	2	102	CRT	C11-C12-C14	2.38	122.60	118.94
15	F	103	CRT	C25-C23-C22	2.38	122.60	118.94
8	J	103	BCL	C2A-C1A-CHA	-2.38	119.69	123.86
14	F	102	LMT	O5'-C5'-C6'	2.38	112.36	106.44
15	Z	101	CRT	C34-C33-C32	-2.38	119.59	122.92
8	E	102	BCL	C2A-C1A-CHA	-2.37	119.71	123.86
15	D	105	CRT	C25-C23-C22	2.37	122.58	118.94
10	1	102	U10	C12-C13-C14	-2.37	121.94	127.66
15	K	103	CRT	C25-C23-C22	2.37	122.58	118.94
14	B	101	LMT	C1'-O5'-C5'	-2.37	109.03	113.69
8	J	102	BCL	C2A-C1A-CHA	-2.37	119.71	123.86
8	1	101	BCL	CAD-C3D-C4D	2.37	109.79	108.47
15	B	103	CRT	C6-C7-C9	2.37	122.58	118.94
14	D	102	LMT	O5'-C5'-C4'	2.37	114.74	109.75
14	6	101	LMT	C3'-C4'-C5'	-2.37	105.50	110.93
15	K	103	CRT	C34-C33-C32	-2.37	119.61	122.92
8	1	101	BCL	C2A-C1A-CHA	-2.36	119.73	123.86
15	D	105	CRT	C15-C14-C12	2.36	130.68	127.31
8	L	401	BCL	C11-C10-C8	-2.36	108.29	115.92
8	G	102	BCL	C2A-C1A-CHA	-2.35	119.75	123.86
15	I	103	CRT	C31-C32-C33	2.35	130.66	127.31
8	Y	101	BCL	C2A-C1A-CHA	-2.35	119.75	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	D	105	CRT	C31-C32-C33	2.34	130.66	127.31
15	B	103	CRT	C26-C27-C28	2.34	130.65	127.31
15	R	101	CRT	C31-C32-C33	2.34	130.65	127.31
8	N	101	BCL	C2A-C1A-CHA	-2.34	119.76	123.86
8	R	104	BCL	C2A-C1A-CHA	-2.34	119.77	123.86
8	5	101	BCL	C1B-CHB-C4A	-2.34	125.49	130.12
15	Q	103	CRT	C6-C7-C9	2.33	122.52	118.94
14	K	102	LMT	C1'-O5'-C5'	-2.33	109.11	113.69
15	O	102	CRT	C15-C14-C12	2.33	130.64	127.31
15	F	103	CRT	C15-C14-C12	2.33	130.64	127.31
15	Z	101	CRT	C11-C12-C14	2.33	122.52	118.94
8	3	101	BCL	CAC-C3C-C4C	-2.33	107.41	112.58
8	P	103	BCL	C1-O2A-CGA	2.33	122.55	116.44
8	A	101	BCL	CHB-C4A-NA	2.33	127.73	124.51
8	5	101	BCL	O2A-CGA-O1A	-2.32	117.73	123.59
9	L	403	BPH	CMA-C3A-C4A	-2.32	109.30	114.38
15	2	102	CRT	C20-C19-C17	2.32	130.62	127.31
8	M	402	BCL	CAA-C2A-C3A	-2.32	106.43	112.78
8	1	101	BCL	C4-C3-C5	2.32	119.17	115.27
8	V	101	BCL	O2D-CGD-O1D	-2.31	119.32	123.84
15	I	103	CRT	C6-C7-C9	2.31	122.48	118.94
8	N	102	BCL	C1C-NC-C4C	-2.30	105.67	106.71
14	I	101	LMT	C1'-O5'-C5'	-2.30	109.18	113.69
15	S	103	CRT	C25-C23-C22	2.30	122.46	118.94
8	E	102	BCL	CHB-C4A-NA	2.29	127.68	124.51
14	B	102	LMT	O5B-C5B-C4B	2.29	113.85	109.69
14	D	101	LMT	C1'-C2'-C3'	2.29	114.76	110.00
15	3	103	CRT	C10-C9-C7	2.29	130.57	127.31
8	T	102	BCL	C1C-NC-C4C	-2.29	105.68	106.71
8	2	101	BCL	CHB-C4A-NA	2.28	127.67	124.51
8	4	101	BCL	O2D-CGD-O1D	-2.28	119.38	123.84
8	5	101	BCL	CMD-C2D-C3D	-2.28	120.41	124.68
8	2	101	BCL	C4B-CHC-C1C	-2.28	125.60	130.12
8	P	103	BCL	O2A-CGA-CBA	2.28	119.06	111.91
15	I	103	CRT	C15-C14-C12	2.28	130.56	127.31
8	5	102	BCL	CHB-C4A-NA	2.28	127.66	124.51
8	M	407	BCL	C1-O2A-CGA	2.27	122.41	116.44
15	X	102	CRT	C30-C28-C27	2.27	122.43	118.94
8	5	102	BCL	C1B-CHB-C4A	-2.27	125.62	130.12
15	Q	103	CRT	C25-C23-C22	2.27	122.42	118.94
8	3	101	BCL	O2D-CGD-O1D	-2.27	119.40	123.84
15	S	103	CRT	C34-C33-C32	-2.27	119.75	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	N	101	BCL	CAD-C3D-C4D	2.26	109.73	108.47
8	D	104	BCL	CAC-C3C-C4C	-2.26	107.56	112.58
10	1	102	U10	C17-C18-C19	-2.26	122.22	127.66
8	3	101	BCL	C1B-CHB-C4A	-2.26	125.65	130.12
8	4	101	BCL	C4-C3-C5	2.25	119.06	115.27
8	L	402	BCL	CAD-C3D-C4D	2.25	109.73	108.47
8	N	102	BCL	CAD-C3D-C4D	2.25	109.73	108.47
8	M	402	BCL	CED-O2D-CGD	2.25	121.03	115.94
8	V	102	BCL	O2D-CGD-O1D	-2.25	119.44	123.84
14	R	102	LMT	C1'-O5'-C5'	-2.25	109.28	113.69
14	F	102	LMT	O5'-C5'-C4'	2.23	114.46	109.75
8	V	101	BCL	CHB-C4A-NA	2.23	127.59	124.51
15	2	102	CRT	C30-C28-C27	2.23	122.36	118.94
8	C	100	BCL	CAA-C2A-C3A	-2.22	106.69	112.78
10	L	406	U10	C1M-C1-C6	-2.22	120.78	124.40
15	R	101	CRT	C25-C23-C22	2.22	122.34	118.94
14	K	101	LMT	C1'-O5'-C5'	-2.21	109.34	113.69
15	I	103	CRT	C25-C23-C22	2.21	122.33	118.94
8	L	401	BCL	CHC-C1C-NC	2.21	127.56	124.51
8	E	103	BCL	C2A-C1A-CHA	-2.20	120.01	123.86
8	V	102	BCL	C2A-C1A-CHA	-2.20	120.01	123.86
14	M	409	LMT	O1'-C1'-C2'	2.20	111.74	108.30
15	F	103	CRT	C31-C32-C33	2.20	130.45	127.31
8	Y	101	BCL	CAA-CBA-CGA	-2.20	106.84	113.25
14	2	104	LMT	C1'-O5'-C5'	-2.20	109.38	113.69
14	J	101	LMT	O5'-C5'-C6'	2.20	111.89	106.44
8	G	102	BCL	CAA-CBA-CGA	-2.19	106.85	113.25
15	3	103	CRT	C6-C7-C9	2.19	122.30	118.94
8	L	401	BCL	C4-C3-C2	-2.18	118.08	123.68
8	T	102	BCL	C2A-C1A-CHA	-2.18	120.05	123.86
8	T	101	BCL	CMB-C2B-C1B	-2.18	125.11	128.46
15	Q	103	CRT	C31-C32-C33	2.18	130.42	127.31
8	5	102	BCL	O2D-CGD-O1D	-2.18	119.58	123.84
8	G	103	BCL	C2A-C1A-CHA	-2.17	120.06	123.86
15	F	103	CRT	C10-C9-C7	2.17	130.41	127.31
15	K	103	CRT	C21-C20-C19	2.17	127.91	123.47
14	K	102	LMT	O5B-C5B-C4B	2.16	113.62	109.69
8	A	102	BCL	C1-O2A-CGA	2.16	122.11	116.44
8	L	401	BCL	CAD-C3D-C4D	2.16	109.67	108.47
8	L	401	BCL	O1D-CGD-CBD	-2.16	120.07	124.48
8	T	101	BCL	C2A-C1A-CHA	-2.16	120.09	123.86
14	X	101	LMT	C1'-C2'-C3'	2.16	114.49	110.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	A	101	BCL	C1-C2-C3	-2.15	122.33	126.04
15	Q	103	CRT	C15-C14-C12	2.15	130.38	127.31
15	D	105	CRT	C10-C9-C7	2.15	130.37	127.31
8	M	407	BCL	O2A-CGA-CBA	2.14	118.63	111.91
8	L	402	BCL	C1C-NC-C4C	-2.14	105.74	106.71
14	4	102	LMT	O5'-C1'-O1'	-2.14	104.91	109.97
8	5	101	BCL	O2D-CGD-O1D	-2.14	119.66	123.84
8	Y	101	BCL	CHB-C4A-NA	2.14	127.47	124.51
14	M	409	LMT	O5B-C5B-C4B	2.14	113.57	109.69
8	J	103	BCL	O2A-CGA-CBA	2.13	118.60	111.91
8	M	402	BCL	CHB-C4A-NA	2.13	127.46	124.51
14	Q	102	LMT	O5B-C5B-C4B	2.13	113.56	109.69
8	P	101	BCL	O2A-CGA-O1A	-2.13	118.22	123.59
10	1	102	U10	C20-C19-C21	2.13	118.85	115.27
8	E	102	BCL	CAA-CBA-CGA	-2.13	107.04	113.25
8	P	103	BCL	CAD-C3D-C4D	2.12	109.65	108.47
8	G	102	BCL	C6-C7-C8	-2.12	109.07	115.92
8	A	101	BCL	O2A-CGA-O1A	-2.12	118.25	123.59
15	B	103	CRT	C25-C23-C22	2.12	122.19	118.94
14	U	101	LMT	C2'-C3'-C4'	2.11	114.51	109.68
8	A	101	BCL	C2A-C1A-CHA	-2.11	120.16	123.86
8	Y	102	BCL	CAD-C3D-C4D	2.11	109.65	108.47
15	Q	103	CRT	C26-C27-C28	2.10	130.31	127.31
10	M	404	U10	C41-C39-C40	2.10	119.24	114.60
7	M	401	QAK	CD2-CE3-CZ3	-2.10	115.24	125.81
14	O	101	LMT	C3B-C4B-C5B	-2.10	106.50	110.24
8	J	103	BCL	C1-O2A-CGA	2.10	121.94	116.44
10	M	404	U10	C37-C38-C39	-2.09	120.59	127.75
10	1	102	U10	C10-C9-C8	-2.09	118.31	123.68
8	M	402	BCL	O2D-CGD-O1D	-2.09	119.75	123.84
15	B	103	CRT	C21-C20-C19	2.09	127.75	123.47
8	V	101	BCL	CAC-C3C-C4C	-2.09	107.95	112.58
14	I	101	LMT	O5B-C5B-C4B	2.08	113.48	109.69
15	B	103	CRT	C36-C35-C33	2.08	129.04	125.89
8	3	101	BCL	C2A-C1A-CHA	-2.07	120.24	123.86
8	C	100	BCL	CAA-CBA-CGA	-2.07	107.21	113.25
14	Z	102	LMT	O1'-C1'-C2'	2.07	111.53	108.30
8	E	102	BCL	C1C-NC-C4C	-2.06	105.78	106.71
8	C	100	BCL	O2A-CGA-O1A	-2.06	118.39	123.59
15	S	103	CRT	C11-C12-C14	2.06	122.10	118.94
8	5	101	BCL	C2A-C3A-C4A	-2.05	98.55	101.87
8	T	101	BCL	O2A-CGA-O1A	-2.05	118.41	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	D	105	CRT	C6-C7-C9	2.05	122.09	118.94
15	F	103	CRT	C21-C20-C19	2.05	127.67	123.47
8	M	402	BCL	C11-C10-C8	-2.05	109.29	115.92
14	U	102	LMT	O1'-C1'-C2'	2.05	111.50	108.30
8	V	101	BCL	C2A-C1A-CHA	-2.05	120.28	123.86
14	U	102	LMT	O5B-C5B-C6B	2.05	111.52	106.44
8	N	102	BCL	C1-O2A-CGA	2.05	121.81	116.44
14	D	102	LMT	O5'-C5'-C6'	2.04	111.52	106.44
8	5	101	BCL	C1-C2-C3	-2.04	122.51	126.04
8	2	101	BCL	C1B-CHB-C4A	-2.04	126.07	130.12
8	A	101	BCL	C4B-CHC-C1C	-2.04	126.07	130.12
15	2	102	CRT	C10-C9-C7	2.04	130.22	127.31
14	U	102	LMT	O5B-C5B-C4B	2.04	113.40	109.69
15	D	105	CRT	C26-C27-C28	2.04	130.22	127.31
8	5	101	BCL	O1D-CGD-CBD	-2.04	120.32	124.48
8	A	102	BCL	C4-C3-C2	-2.03	118.47	123.68
15	S	103	CRT	C15-C14-C12	2.03	130.21	127.31
14	Q	101	LMT	C1'-C2'-C3'	2.03	114.22	110.00
15	Q	103	CRT	C21-C20-C19	2.03	127.63	123.47
14	4	102	LMT	C1'-O5'-C5'	-2.02	109.72	113.69
8	A	101	BCL	C1B-CHB-C4A	-2.02	126.12	130.12
8	4	101	BCL	O2A-CGA-O1A	-2.02	118.50	123.59
14	X	101	LMT	O5B-C5B-C4B	2.02	113.36	109.69
8	R	103	BCL	C2A-C1A-CHA	-2.01	120.34	123.86
8	M	402	BCL	CAC-C3C-C4C	-2.01	108.11	112.58
8	M	402	BCL	C11-C12-C13	-2.01	109.41	115.92
14	L	405	LMT	O5B-C5B-C4B	2.01	113.35	109.69
15	3	103	CRT	C26-C27-C28	2.01	130.18	127.31
15	K	103	CRT	C26-C27-C28	2.01	130.18	127.31
14	D	101	LMT	C1'-O5'-C5'	-2.00	109.76	113.69

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	M	401	QAK	CE2
9	M	403	BPH	C8
9	M	403	BPH	C13
9	L	403	BPH	C8
9	L	403	BPH	C13

All (1012) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	M	401	QAK	CE3-CD2-CE2-CZ2
7	M	401	QAK	CE3-CD2-CE2-C39
7	M	401	QAK	C37-C14-C15-C16
7	M	401	QAK	C22-C23-C24-C25
8	M	407	BCL	C4C-C3C-CAC-CBC
8	L	401	BCL	C1A-C2A-CAA-CBA
8	2	101	BCL	C1A-C2A-CAA-CBA
8	2	101	BCL	C3A-C2A-CAA-CBA
8	2	101	BCL	C2C-C3C-CAC-CBC
8	2	101	BCL	C4C-C3C-CAC-CBC
8	2	101	BCL	C4-C3-C5-C6
8	5	101	BCL	C4C-C3C-CAC-CBC
8	5	102	BCL	C2-C3-C5-C6
8	5	102	BCL	C4-C3-C5-C6
8	Y	101	BCL	C4C-C3C-CAC-CBC
8	Y	101	BCL	C4-C3-C5-C6
8	Y	102	BCL	C1A-C2A-CAA-CBA
8	Y	102	BCL	C4C-C3C-CAC-CBC
8	V	101	BCL	C2-C3-C5-C6
8	V	101	BCL	C4-C3-C5-C6
8	V	102	BCL	C1A-C2A-CAA-CBA
8	V	102	BCL	C3A-C2A-CAA-CBA
8	V	102	BCL	C4-C3-C5-C6
8	T	101	BCL	C4C-C3C-CAC-CBC
8	T	102	BCL	C1A-C2A-CAA-CBA
8	T	102	BCL	C3A-C2A-CAA-CBA
8	T	102	BCL	C2C-C3C-CAC-CBC
8	T	102	BCL	C4C-C3C-CAC-CBC
8	A	101	BCL	C11-C10-C8-C9
8	A	102	BCL	C2C-C3C-CAC-CBC
8	A	102	BCL	C4C-C3C-CAC-CBC
8	A	102	BCL	C2-C3-C5-C6
8	A	102	BCL	C4-C3-C5-C6
8	C	100	BCL	C1A-C2A-CAA-CBA
8	C	100	BCL	C3A-C2A-CAA-CBA
8	C	100	BCL	C2C-C3C-CAC-CBC
8	C	100	BCL	C4C-C3C-CAC-CBC
8	C	100	BCL	C4-C3-C5-C6
8	D	104	BCL	C1A-C2A-CAA-CBA
8	D	104	BCL	C2-C3-C5-C6
8	D	104	BCL	C4-C3-C5-C6
8	R	103	BCL	C1A-C2A-CAA-CBA
8	R	103	BCL	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
8	R	103	BCL	C4C-C3C-CAC-CBC
8	R	103	BCL	C2-C3-C5-C6
8	R	103	BCL	C4-C3-C5-C6
8	R	104	BCL	C1A-C2A-CAA-CBA
8	R	104	BCL	C3A-C2A-CAA-CBA
8	R	104	BCL	C2C-C3C-CAC-CBC
8	R	104	BCL	C4C-C3C-CAC-CBC
8	P	101	BCL	C1A-C2A-CAA-CBA
8	P	101	BCL	C3A-C2A-CAA-CBA
8	P	101	BCL	C4C-C3C-CAC-CBC
8	P	101	BCL	C2-C3-C5-C6
8	P	101	BCL	C4-C3-C5-C6
8	P	103	BCL	C1A-C2A-CAA-CBA
8	N	101	BCL	C2C-C3C-CAC-CBC
8	N	101	BCL	C4C-C3C-CAC-CBC
8	N	102	BCL	C1A-C2A-CAA-CBA
8	N	102	BCL	C3A-C2A-CAA-CBA
8	J	102	BCL	C4C-C3C-CAC-CBC
8	J	102	BCL	C2-C3-C5-C6
8	J	102	BCL	C4-C3-C5-C6
8	J	103	BCL	C1A-C2A-CAA-CBA
8	J	103	BCL	C3A-C2A-CAA-CBA
8	J	103	BCL	C2C-C3C-CAC-CBC
8	J	103	BCL	C4C-C3C-CAC-CBC
8	G	102	BCL	C2C-C3C-CAC-CBC
8	G	102	BCL	C4C-C3C-CAC-CBC
8	G	102	BCL	C11-C10-C8-C7
8	G	103	BCL	C2C-C3C-CAC-CBC
8	G	103	BCL	C4C-C3C-CAC-CBC
8	G	103	BCL	C2-C3-C5-C6
8	G	103	BCL	C4-C3-C5-C6
8	G	103	BCL	C11-C12-C13-C14
8	E	102	BCL	C11-C10-C8-C9
8	E	103	BCL	C1A-C2A-CAA-CBA
8	E	103	BCL	C2C-C3C-CAC-CBC
8	E	103	BCL	C4C-C3C-CAC-CBC
10	1	102	U10	C14-C16-C17-C18
10	1	102	U10	C19-C21-C22-C23
11	H	301	6PL	C4-O4P-P-O3P
11	H	301	6PL	C4-O4P-P-O1P
11	H	301	6PL	C4-O4P-P-O2P
11	H	301	6PL	C5-C4-O4P-P

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Mol	Chain	Res	Type	Atoms
12	M	406	CDL	CA2-OA2-PA1-OA3
12	M	406	CDL	OA9-CA7-OA8-CA6
12	M	406	CDL	C31-CA7-OA8-CA6
12	M	406	CDL	CB3-OB5-PB2-OB2
12	M	406	CDL	CB4-CB3-OB5-PB2
12	3	102	CDL	C1-CB2-OB2-PB2
12	3	102	CDL	CB2-OB2-PB2-OB5
12	G	101	CDL	CA3-OA5-PA1-OA3
12	G	101	CDL	OA7-CA5-OA6-CA4
12	G	101	CDL	C11-CA5-OA6-CA4
12	G	101	CDL	OA9-CA7-OA8-CA6
12	G	101	CDL	C31-CA7-OA8-CA6
12	G	101	CDL	CB3-OB5-PB2-OB3
12	G	101	CDL	OB9-CB7-OB8-CB6
12	G	101	CDL	C71-CB7-OB8-CB6
12	G	104	CDL	CA2-OA2-PA1-OA3
12	G	104	CDL	CA3-OA5-PA1-OA3
12	G	104	CDL	CA3-OA5-PA1-OA4
14	L	405	LMT	C2'-C1'-O1'-C1
14	L	405	LMT	O5'-C1'-O1'-C1
14	2	104	LMT	C2-C1-O1'-C1'
14	X	101	LMT	O5'-C1'-O1'-C1
14	X	101	LMT	C2-C1-O1'-C1'
14	X	103	LMT	O5'-C1'-O1'-C1
14	U	102	LMT	C2'-C1'-O1'-C1
14	U	102	LMT	O5'-C1'-O1'-C1
14	U	102	LMT	C2-C1-O1'-C1'
14	B	101	LMT	O5'-C1'-O1'-C1
14	D	101	LMT	O5'-C1'-O1'-C1
14	D	102	LMT	C2'-C1'-O1'-C1
14	R	102	LMT	O5B-C1B-O1B-C4'
14	R	102	LMT	O5'-C1'-O1'-C1
14	S	101	LMT	C2'-C1'-O1'-C1
14	S	101	LMT	O5'-C1'-O1'-C1
14	S	102	LMT	O5'-C1'-O1'-C1
14	Q	101	LMT	C2'-C1'-O1'-C1
14	Q	101	LMT	O5'-C1'-O1'-C1
14	Q	102	LMT	C2-C1-O1'-C1'
14	O	101	LMT	C2'-C1'-O1'-C1
14	O	101	LMT	O5'-C1'-O1'-C1
14	O	101	LMT	C2-C1-O1'-C1'
14	J	101	LMT	O5'-C1'-O1'-C1

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Mol	Chain	Res	Type	Atoms
14	K	101	LMT	C2'-C1'-O1'-C1
14	K	101	LMT	O5'-C1'-O1'-C1
14	K	102	LMT	C2'-C1'-O1'-C1
14	K	102	LMT	O5'-C1'-O1'-C1
14	F	101	LMT	C2'-C1'-O1'-C1
14	F	101	LMT	O5'-C1'-O1'-C1
14	F	102	LMT	C2'-C1'-O1'-C1
14	F	102	LMT	O5'-C1'-O1'-C1
15	2	102	CRT	C36-C37-C38-C39
15	2	102	CRT	C36-C37-C38-C40
15	2	102	CRT	C36-C37-C38-O2
15	3	103	CRT	C1-C4-C5-C6
16	P	102	PGT	C4-O4P-P-O1P
14	2	103	LMT	C3'-C4'-O1B-C1B
14	M	409	LMT	O5B-C1B-O1B-C4'
14	S	102	LMT	O5B-C1B-O1B-C4'
8	5	102	BCL	CBD-CGD-O2D-CED
14	U	101	LMT	O5B-C1B-O1B-C4'
14	L	405	LMT	C3'-C4'-O1B-C1B
14	B	102	LMT	O5B-C1B-O1B-C4'
10	M	404	U10	C37-C38-C39-C40
10	M	404	U10	C37-C38-C39-C41
8	M	402	BCL	CBD-CGD-O2D-CED
8	4	101	BCL	CBD-CGD-O2D-CED
14	K	102	LMT	O5B-C1B-O1B-C4'
8	J	103	BCL	C5-C6-C7-C8
14	S	102	LMT	C2B-C1B-O1B-C4'
14	M	409	LMT	O5'-C5'-C6'-O6'
14	D	103	LMT	O5B-C1B-O1B-C4'
14	6	101	LMT	C4B-C5B-C6B-O6B
8	1	101	BCL	C3-C5-C6-C7
8	4	101	BCL	C3-C5-C6-C7
8	Y	102	BCL	C3-C5-C6-C7
8	T	102	BCL	C3-C5-C6-C7
8	5	102	BCL	O1D-CGD-O2D-CED
14	K	101	LMT	O5'-C5'-C6'-O6'
14	R	102	LMT	O5B-C5B-C6B-O6B
14	F	102	LMT	O5'-C5'-C6'-O6'
8	G	102	BCL	C4-C3-C5-C6
8	Y	101	BCL	C2-C3-C5-C6
8	C	100	BCL	C2-C3-C5-C6
8	G	102	BCL	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
14	X	101	LMT	C3'-C4'-O1B-C1B
8	E	102	BCL	C3-C5-C6-C7
8	N	101	BCL	CBA-CGA-O2A-C1
14	6	101	LMT	O5B-C5B-C6B-O6B
14	X	101	LMT	O5'-C5'-C6'-O6'
14	Z	102	LMT	C3'-C4'-O1B-C1B
10	1	102	U10	C17-C18-C19-C20
10	1	102	U10	C27-C28-C29-C30
10	1	102	U10	C17-C18-C19-C21
14	L	405	LMT	C4'-C5'-C6'-O6'
14	B	101	LMT	C4'-C5'-C6'-O6'
14	I	101	LMT	C4B-C5B-C6B-O6B
8	N	101	BCL	O1A-CGA-O2A-C1
14	2	104	LMT	O5B-C5B-C6B-O6B
14	O	101	LMT	O5'-C5'-C6'-O6'
12	M	406	CDL	O1-C1-CB2-OB2
8	V	102	BCL	C3-C5-C6-C7
8	R	104	BCL	C3-C5-C6-C7
14	D	102	LMT	O5B-C5B-C6B-O6B
14	S	102	LMT	O5B-C5B-C6B-O6B
11	E	101	6PL	C32-C31-O2-C2
12	L	404	CDL	C11-CA5-OA6-CA4
12	H	302	CDL	C11-CA5-OA6-CA4
14	I	101	LMT	C5'-C4'-O1B-C1B
14	6	101	LMT	O5B-C1B-O1B-C4'
8	L	401	BCL	CBD-CGD-O2D-CED
14	U	102	LMT	O5B-C5B-C6B-O6B
14	M	409	LMT	C4'-C5'-C6'-O6'
14	K	101	LMT	O5B-C1B-O1B-C4'
14	6	101	LMT	C2B-C1B-O1B-C4'
14	B	101	LMT	O5'-C5'-C6'-O6'
14	F	101	LMT	C3'-C4'-O1B-C1B
8	M	402	BCL	C3-C5-C6-C7
8	2	101	BCL	C3-C5-C6-C7
14	L	405	LMT	O5'-C5'-C6'-O6'
14	Q	102	LMT	O5'-C5'-C6'-O6'
14	K	101	LMT	C4'-C5'-C6'-O6'
16	P	102	PGT	C5-C4-O4P-P
10	1	102	U10	C29-C31-C32-C33
14	I	101	LMT	O5B-C5B-C6B-O6B
8	T	101	BCL	C4-C3-C5-C6
8	N	102	BCL	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
8	E	103	BCL	C4-C3-C5-C6
8	2	101	BCL	C2-C3-C5-C6
8	V	102	BCL	C2-C3-C5-C6
8	T	101	BCL	C2-C3-C5-C6
8	N	102	BCL	C2-C3-C5-C6
8	G	102	BCL	C2-C3-C5-C6
8	E	103	BCL	C2-C3-C5-C6
8	C	100	BCL	CBD-CGD-O2D-CED
14	D	103	LMT	O5'-C5'-C6'-O6'
14	D	102	LMT	O5'-C1'-O1'-C1
14	Q	102	LMT	O5'-C1'-O1'-C1
10	M	404	U10	C29-C31-C32-C33
10	M	404	U10	C34-C36-C37-C38
14	R	102	LMT	O5'-C5'-C6'-O6'
14	X	101	LMT	C4'-C5'-C6'-O6'
14	D	101	LMT	C4'-C5'-C6'-O6'
14	K	102	LMT	C4B-C5B-C6B-O6B
7	M	401	QAK	C15-C16-C17-C18
14	2	103	LMT	C4'-C5'-C6'-O6'
14	Q	101	LMT	C4'-C5'-C6'-O6'
14	I	102	LMT	C4B-C5B-C6B-O6B
14	D	103	LMT	C4'-C5'-C6'-O6'
8	L	401	BCL	CBA-CGA-O2A-C1
8	5	102	BCL	CBA-CGA-O2A-C1
8	N	102	BCL	CBA-CGA-O2A-C1
14	Q	101	LMT	C2B-C1B-O1B-C4'
14	R	102	LMT	C4B-C5B-C6B-O6B
14	Q	101	LMT	O5'-C5'-C6'-O6'
14	D	102	LMT	C4B-C5B-C6B-O6B
14	Q	101	LMT	O5B-C1B-O1B-C4'
14	S	102	LMT	C4B-C5B-C6B-O6B
14	O	101	LMT	C4'-C5'-C6'-O6'
14	F	102	LMT	C4'-C5'-C6'-O6'
8	L	401	BCL	C5-C6-C7-C8
8	3	101	BCL	C8-C10-C11-C12
8	V	101	BCL	C13-C15-C16-C17
8	E	103	BCL	C10-C11-C12-C13
8	E	103	BCL	C13-C15-C16-C17
12	G	104	CDL	O1-C1-CA2-OA2
14	4	102	LMT	C2'-C1'-O1'-C1
14	D	101	LMT	C2'-C1'-O1'-C1
14	R	102	LMT	C2'-C1'-O1'-C1

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Mol	Chain	Res	Type	Atoms
7	M	401	QAK	C17-C18-C19-C20
7	M	401	QAK	C27-C28-C29-C30
8	M	402	BCL	C6-C7-C8-C9
8	L	401	BCL	C6-C7-C8-C9
8	2	101	BCL	C6-C7-C8-C9
8	5	102	BCL	C11-C10-C8-C9
8	Y	102	BCL	C11-C10-C8-C9
8	V	102	BCL	C6-C7-C8-C9
8	V	102	BCL	C11-C10-C8-C9
8	R	104	BCL	C6-C7-C8-C9
8	R	104	BCL	C11-C10-C8-C9
8	P	103	BCL	C6-C7-C8-C9
8	P	103	BCL	C11-C10-C8-C9
8	N	102	BCL	C11-C12-C13-C14
8	J	102	BCL	C14-C13-C15-C16
8	J	103	BCL	C14-C13-C15-C16
8	G	103	BCL	C6-C7-C8-C9
14	K	101	LMT	C3'-C4'-O1B-C1B
14	6	101	LMT	O5'-C5'-C6'-O6'
14	S	101	LMT	C4B-C5B-C6B-O6B
8	N	102	BCL	O1A-CGA-O2A-C1
8	M	407	BCL	C15-C16-C17-C18
8	1	101	BCL	C5-C6-C7-C8
8	N	101	BCL	C8-C10-C11-C12
8	E	103	BCL	C5-C6-C7-C8
14	L	405	LMT	O5B-C5B-C6B-O6B
14	Q	102	LMT	C4'-C5'-C6'-O6'
8	4	101	BCL	O1D-CGD-O2D-CED
8	5	102	BCL	C3-C5-C6-C7
8	5	101	BCL	C5-C6-C7-C8
8	A	101	BCL	C8-C10-C11-C12
14	B	101	LMT	C3'-C4'-O1B-C1B
8	L	402	BCL	C15-C16-C17-C18
8	V	102	BCL	C15-C16-C17-C18
8	T	101	BCL	C5-C6-C7-C8
8	C	100	BCL	C8-C10-C11-C12
8	C	100	BCL	C10-C11-C12-C13
8	N	101	BCL	C13-C15-C16-C17
8	N	101	BCL	C15-C16-C17-C18
8	V	102	BCL	C8-C10-C11-C12
14	B	102	LMT	O5'-C5'-C6'-O6'
10	1	102	U10	C27-C28-C29-C31

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Mol	Chain	Res	Type	Atoms
14	X	101	LMT	O1'-C1-C2-C3
7	M	401	QAK	C11-C12-C13-C14
8	T	102	BCL	C5-C6-C7-C8
8	N	102	BCL	C10-C11-C12-C13
12	G	101	CDL	C39-C40-C41-C42
7	M	401	QAK	C29-C31-CB-CA
8	5	101	BCL	C11-C10-C8-C7
8	3	101	BCL	C6-C7-C8-C10
8	3	101	BCL	C12-C13-C15-C16
8	E	103	BCL	C11-C10-C8-C7
8	5	101	BCL	C2A-CAA-CBA-CGA
8	J	102	BCL	C2A-CAA-CBA-CGA
8	E	102	BCL	C2A-CAA-CBA-CGA
8	M	402	BCL	O1D-CGD-O2D-CED
8	Y	101	BCL	C8-C10-C11-C12
8	P	103	BCL	C8-C10-C11-C12
12	G	104	CDL	C39-C40-C41-C42
8	L	401	BCL	O1A-CGA-O2A-C1
8	5	102	BCL	O1A-CGA-O2A-C1
8	V	102	BCL	C10-C11-C12-C13
10	M	404	U10	C24-C26-C27-C28
10	1	102	U10	C9-C11-C12-C13
16	P	102	PGT	O4P-C4-C5-O5
11	E	101	6PL	O31-C31-O2-C2
12	H	302	CDL	OA7-CA5-OA6-CA4
8	V	101	BCL	C5-C6-C7-C8
8	A	102	BCL	C10-C11-C12-C13
8	N	101	BCL	C10-C11-C12-C13
8	N	102	BCL	C13-C15-C16-C17
7	M	401	QAK	C3-C4-CZ2-CE2
14	U	101	LMT	C5'-C4'-O1B-C1B
8	Y	101	BCL	C15-C16-C17-C18
8	T	101	BCL	C8-C10-C11-C12
8	A	101	BCL	C10-C11-C12-C13
8	R	104	BCL	C15-C16-C17-C18
14	2	103	LMT	O5'-C5'-C6'-O6'
7	M	401	QAK	C26-C27-C28-C29
8	1	101	BCL	C15-C16-C17-C18
8	5	101	BCL	C13-C15-C16-C17
8	J	103	BCL	C10-C11-C12-C13
8	E	102	BCL	C8-C10-C11-C12
11	H	301	6PL	C1-O3P-P-O4P

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Mol	Chain	Res	Type	Atoms
12	M	406	CDL	CB2-OB2-PB2-OB5
12	G	101	CDL	CA3-OA5-PA1-OA2
12	G	104	CDL	CA3-OA5-PA1-OA2
14	U	102	LMT	C4'-C5'-C6'-O6'
7	M	401	QAK	C35-C-CA-CB
8	L	402	BCL	CBD-CGD-O2D-CED
8	J	102	BCL	C8-C10-C11-C12
14	X	103	LMT	O5'-C5'-C6'-O6'
14	D	101	LMT	O5'-C5'-C6'-O6'
16	P	102	PGT	O4P-C4-C5-C6
12	L	404	CDL	OA7-CA5-OA6-CA4
8	Y	102	BCL	C4-C3-C5-C6
8	2	101	BCL	C15-C16-C17-C18
8	5	102	BCL	C13-C15-C16-C17
8	Y	101	BCL	C2A-CAA-CBA-CGA
14	X	103	LMT	O5B-C5B-C6B-O6B
14	Q	101	LMT	O5B-C5B-C6B-O6B
8	V	101	BCL	CBA-CGA-O2A-C1
14	K	102	LMT	O1'-C1-C2-C3
14	D	103	LMT	C5'-C4'-O1B-C1B
8	T	102	BCL	C13-C15-C16-C17
14	U	101	LMT	C5-C6-C7-C8
11	H	301	6PL	C19-C20-C21-C22
14	X	101	LMT	C11-C10-C9-C8
14	B	101	LMT	C11-C10-C9-C8
8	V	101	BCL	C16-C17-C18-C19
14	2	103	LMT	C7-C8-C9-C10
14	4	102	LMT	C3-C4-C5-C6
12	G	104	CDL	C38-C39-C40-C41
12	G	101	CDL	CA4-CA3-OA5-PA1
14	2	104	LMT	C4B-C5B-C6B-O6B
14	Z	102	LMT	O1'-C1-C2-C3
14	S	102	LMT	O1'-C1-C2-C3
14	B	101	LMT	C2'-C1'-O1'-C1
8	T	102	BCL	C10-C11-C12-C13
8	R	103	BCL	C16-C17-C18-C19
8	J	103	BCL	C16-C17-C18-C19
14	Q	101	LMT	C4-C5-C6-C7
14	F	102	LMT	C5-C6-C7-C8
7	M	401	QAK	C20-C19-C21-C22
8	P	101	BCL	C14-C13-C15-C16
14	2	103	LMT	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
7	M	401	QAK	C21-C22-C23-C24
8	Y	102	BCL	C13-C15-C16-C17
8	G	103	BCL	C8-C10-C11-C12
14	I	102	LMT	O5B-C5B-C6B-O6B
14	S	102	LMT	O5'-C5'-C6'-O6'
8	5	102	BCL	C15-C16-C17-C18
8	Y	102	BCL	C8-C10-C11-C12
14	2	103	LMT	C2-C3-C4-C5
14	Z	102	LMT	C7-C8-C9-C10
8	1	101	BCL	C13-C15-C16-C17
10	1	102	U10	C24-C26-C27-C28
14	U	102	LMT	O5'-C5'-C6'-O6'
14	K	101	LMT	C5'-C4'-O1B-C1B
14	K	101	LMT	C11-C10-C9-C8
14	K	102	LMT	C6-C7-C8-C9
8	J	103	BCL	C13-C15-C16-C17
14	S	102	LMT	C4-C5-C6-C7
8	5	101	BCL	C3A-C2A-CAA-CBA
8	5	102	BCL	C3A-C2A-CAA-CBA
8	4	101	BCL	C3A-C2A-CAA-CBA
8	Y	101	BCL	C3A-C2A-CAA-CBA
8	Y	102	BCL	C3A-C2A-CAA-CBA
8	V	101	BCL	C3A-C2A-CAA-CBA
8	T	101	BCL	C3A-C2A-CAA-CBA
8	A	101	BCL	C3A-C2A-CAA-CBA
8	D	104	BCL	C3A-C2A-CAA-CBA
8	P	103	BCL	C3A-C2A-CAA-CBA
8	J	102	BCL	C3A-C2A-CAA-CBA
8	G	102	BCL	C3A-C2A-CAA-CBA
8	G	103	BCL	C3A-C2A-CAA-CBA
8	E	102	BCL	C3A-C2A-CAA-CBA
8	E	103	BCL	C3A-C2A-CAA-CBA
8	G	103	BCL	C10-C11-C12-C13
14	D	103	LMT	C2-C1-O1'-C1'
14	S	101	LMT	C2-C1-O1'-C1'
14	Q	101	LMT	C2-C1-O1'-C1'
14	J	101	LMT	C2-C1-O1'-C1'
14	K	102	LMT	C2-C1-O1'-C1'
14	I	101	LMT	C2-C1-O1'-C1'
14	F	102	LMT	C2-C1-O1'-C1'
14	L	405	LMT	C6-C7-C8-C9
14	S	102	LMT	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
8	T	101	BCL	CBD-CGD-O2D-CED
14	S	101	LMT	C11-C10-C9-C8
14	F	101	LMT	O1'-C1-C2-C3
14	F	102	LMT	C11-C10-C9-C8
8	L	401	BCL	C3-C5-C6-C7
8	E	103	BCL	C3-C5-C6-C7
14	D	101	LMT	C1-C2-C3-C4
14	B	101	LMT	O1'-C1-C2-C3
14	S	101	LMT	O1'-C1-C2-C3
14	U	102	LMT	C7-C8-C9-C10
14	F	101	LMT	C5'-C4'-O1B-C1B
14	F	102	LMT	O1'-C1-C2-C3
8	2	101	BCL	C10-C11-C12-C13
14	J	101	LMT	C7-C8-C9-C10
8	R	103	BCL	C16-C17-C18-C20
8	J	103	BCL	C16-C17-C18-C20
14	F	101	LMT	C3-C4-C5-C6
14	K	102	LMT	O5B-C5B-C6B-O6B
14	6	101	LMT	C2-C3-C4-C5
14	F	102	LMT	C6-C7-C8-C9
8	V	101	BCL	O1A-CGA-O2A-C1
14	B	101	LMT	C5'-C4'-O1B-C1B
14	Q	102	LMT	O1'-C1-C2-C3
14	K	101	LMT	O5B-C5B-C6B-O6B
14	I	101	LMT	C3-C4-C5-C6
8	V	101	BCL	C15-C16-C17-C18
14	B	102	LMT	C4-C5-C6-C7
14	Q	101	LMT	C7-C8-C9-C10
10	M	404	U10	C35-C34-C36-C37
8	L	402	BCL	C11-C10-C8-C7
8	5	102	BCL	C11-C10-C8-C7
8	V	102	BCL	C11-C10-C8-C7
8	T	102	BCL	C11-C10-C8-C7
8	D	104	BCL	C11-C10-C8-C7
8	P	101	BCL	C12-C13-C15-C16
8	G	103	BCL	C11-C12-C13-C15
8	M	402	BCL	C5-C6-C7-C8
8	J	102	BCL	C5-C6-C7-C8
8	L	401	BCL	O1D-CGD-O2D-CED
8	C	100	BCL	O1D-CGD-O2D-CED
14	U	102	LMT	C11-C10-C9-C8
14	B	101	LMT	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
8	C	100	BCL	CBA-CGA-O2A-C1
8	T	101	BCL	C16-C17-C18-C19
14	4	102	LMT	O5'-C1'-O1'-C1
14	Z	102	LMT	O5'-C1'-O1'-C1
8	4	101	BCL	C5-C6-C7-C8
8	Y	101	BCL	C10-C11-C12-C13
14	Q	101	LMT	C5-C6-C7-C8
16	P	102	PGT	C20-C21-C22-C23
12	L	404	CDL	C51-CB5-OB6-CB4
16	P	102	PGT	C32-C31-O2-C2
16	P	102	PGT	O31-C31-O2-C2
8	L	402	BCL	C3-C5-C6-C7
14	M	409	LMT	O1'-C1-C2-C3
12	3	102	CDL	C53-C54-C55-C56
14	U	101	LMT	C3'-C4'-O1B-C1B
14	D	102	LMT	C5-C6-C7-C8
14	2	104	LMT	O5'-C5'-C6'-O6'
7	M	401	QAK	C14-C15-C16-C17
8	Y	102	BCL	C2-C3-C5-C6
10	M	404	U10	C33-C34-C36-C37
8	L	402	BCL	C11-C10-C8-C9
8	5	101	BCL	C11-C10-C8-C9
8	3	101	BCL	C14-C13-C15-C16
8	4	101	BCL	C11-C10-C8-C9
8	T	102	BCL	C11-C10-C8-C9
8	D	104	BCL	C11-C10-C8-C9
8	P	101	BCL	C11-C10-C8-C9
8	N	101	BCL	C6-C7-C8-C9
8	P	101	BCL	C2A-CAA-CBA-CGA
14	S	101	LMT	O5'-C5'-C6'-O6'
8	L	401	BCL	C15-C16-C17-C18
8	R	103	BCL	C8-C10-C11-C12
14	O	101	LMT	C5-C6-C7-C8
8	5	101	BCL	C1A-C2A-CAA-CBA
8	4	101	BCL	C1A-C2A-CAA-CBA
8	Y	101	BCL	C1A-C2A-CAA-CBA
8	T	101	BCL	C1A-C2A-CAA-CBA
8	A	101	BCL	C1A-C2A-CAA-CBA
8	J	102	BCL	C1A-C2A-CAA-CBA
8	G	102	BCL	C1A-C2A-CAA-CBA
8	G	103	BCL	C1A-C2A-CAA-CBA
8	E	102	BCL	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
8	A	102	BCL	C16-C17-C18-C20
12	G	101	CDL	C21-C22-C23-C24
14	X	103	LMT	C5-C6-C7-C8
14	U	102	LMT	C4B-C5B-C6B-O6B
8	3	101	BCL	C5-C6-C7-C8
8	3	101	BCL	C15-C16-C17-C18
14	4	102	LMT	C1-C2-C3-C4
12	M	406	CDL	CA3-OA5-PA1-OA2
14	Z	102	LMT	C5'-C4'-O1B-C1B
14	2	104	LMT	O5B-C1B-O1B-C4'
14	L	405	LMT	C3-C4-C5-C6
8	5	101	BCL	C3-C5-C6-C7
14	S	102	LMT	C2-C3-C4-C5
8	5	101	BCL	C2C-C3C-CAC-CBC
8	Y	101	BCL	C2C-C3C-CAC-CBC
8	Y	102	BCL	C2C-C3C-CAC-CBC
8	T	101	BCL	C2C-C3C-CAC-CBC
8	D	104	BCL	C2C-C3C-CAC-CBC
8	R	103	BCL	C2C-C3C-CAC-CBC
8	P	101	BCL	C2C-C3C-CAC-CBC
8	N	102	BCL	C2C-C3C-CAC-CBC
8	J	102	BCL	C2C-C3C-CAC-CBC
8	5	101	BCL	C16-C17-C18-C19
8	V	101	BCL	C16-C17-C18-C20
8	A	102	BCL	C16-C17-C18-C19
12	H	302	CDL	CA3-CA4-CA6-OA8
14	2	104	LMT	C3-C4-C5-C6
8	Y	102	BCL	C15-C16-C17-C18
10	1	102	U10	C1-C6-C7-C8
12	H	302	CDL	C53-C54-C55-C56
14	Q	102	LMT	C3-C4-C5-C6
8	A	102	BCL	CAA-CBA-CGA-O2A
14	D	103	LMT	O1'-C1-C2-C3
14	D	103	LMT	C3'-C4'-O1B-C1B
8	L	401	BCL	C10-C11-C12-C13
14	M	409	LMT	O5B-C5B-C6B-O6B
8	1	101	BCL	C4-C3-C5-C6
14	S	101	LMT	C3-C4-C5-C6
14	J	101	LMT	O5'-C5'-C6'-O6'
8	J	102	BCL	C3-C5-C6-C7
14	K	102	LMT	C9-C10-C11-C12
8	A	101	BCL	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
8	1	101	BCL	C16-C17-C18-C20
8	T	101	BCL	C16-C17-C18-C20
14	F	102	LMT	C1-C2-C3-C4
8	L	402	BCL	O1D-CGD-O2D-CED
8	C	100	BCL	O1A-CGA-O2A-C1
7	M	401	QAK	C11-C10-CZ3-CE3
14	X	101	LMT	C2'-C1'-O1'-C1
14	J	101	LMT	C2'-C1'-O1'-C1
14	F	102	LMT	C9-C10-C11-C12
15	X	102	CRT	C36-C37-C38-C39
15	X	102	CRT	C36-C37-C38-C40
15	O	102	CRT	C36-C37-C38-C40
15	F	103	CRT	C36-C37-C38-C39
15	F	103	CRT	C36-C37-C38-C40
12	G	104	CDL	C75-C76-C77-C78
14	X	101	LMT	C4-C5-C6-C7
10	M	404	U10	C30-C29-C31-C32
8	A	102	BCL	C15-C16-C17-C18
7	M	401	QAK	C27-C28-C29-C31
8	M	402	BCL	C6-C7-C8-C10
8	M	402	BCL	C11-C10-C8-C7
8	L	401	BCL	C6-C7-C8-C10
8	1	101	BCL	C2-C3-C5-C6
8	2	101	BCL	C6-C7-C8-C10
8	4	101	BCL	C6-C7-C8-C10
8	4	101	BCL	C11-C10-C8-C7
8	Y	102	BCL	C11-C10-C8-C7
8	T	102	BCL	C6-C7-C8-C10
8	A	101	BCL	C6-C7-C8-C10
8	A	101	BCL	C11-C10-C8-C7
8	A	101	BCL	C11-C12-C13-C15
8	R	104	BCL	C6-C7-C8-C10
8	P	103	BCL	C6-C7-C8-C10
8	P	103	BCL	C11-C12-C13-C15
8	N	101	BCL	C6-C7-C8-C10
8	G	103	BCL	C6-C7-C8-C10
8	M	402	BCL	C11-C10-C8-C9
8	V	101	BCL	C6-C7-C8-C9
8	A	102	BCL	C11-C10-C8-C9
8	N	102	BCL	C5-C6-C7-C8
8	R	104	BCL	C16-C17-C18-C19
14	X	101	LMT	C5'-C4'-O1B-C1B

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Mol	Chain	Res	Type	Atoms
14	D	101	LMT	C4B-C5B-C6B-O6B
14	B	102	LMT	C11-C10-C9-C8
8	3	101	BCL	C10-C11-C12-C13
8	Y	101	BCL	C5-C6-C7-C8
8	Y	102	BCL	C5-C6-C7-C8
8	R	104	BCL	C16-C17-C18-C20
8	V	101	BCL	C10-C11-C12-C13
8	E	102	BCL	C5-C6-C7-C8
14	I	102	LMT	C2-C3-C4-C5
8	4	101	BCL	C8-C10-C11-C12
10	M	404	U10	C28-C29-C31-C32
12	G	101	CDL	C16-C17-C18-C19
12	L	404	CDL	OB7-CB5-OB6-CB4
14	S	101	LMT	O5B-C5B-C6B-O6B
14	2	104	LMT	C2-C3-C4-C5
14	I	102	LMT	C7-C8-C9-C10
8	R	104	BCL	CBA-CGA-O2A-C1
8	P	101	BCL	CBA-CGA-O2A-C1
11	H	301	6PL	C2-C1-O3P-P
12	3	102	CDL	C1-CA2-OA2-PA1
12	G	104	CDL	CB4-CB3-OB5-PB2
8	L	401	BCL	C3A-C2A-CAA-CBA
12	G	101	CDL	C15-C16-C17-C18
14	D	101	LMT	C2-C1-O1'-C1'
14	D	102	LMT	C2-C1-O1'-C1'
8	5	101	BCL	C16-C17-C18-C20
12	3	102	CDL	C71-CB7-OB8-CB6
8	P	103	BCL	C5-C6-C7-C8
14	4	102	LMT	C5-C6-C7-C8
12	G	104	CDL	C41-C42-C43-C44
14	2	103	LMT	C9-C10-C11-C12
14	K	102	LMT	C1-C2-C3-C4
14	S	101	LMT	C5-C6-C7-C8
8	1	101	BCL	C16-C17-C18-C19
12	G	104	CDL	CA2-OA2-PA1-OA5
14	B	102	LMT	C9-C10-C11-C12
14	Q	102	LMT	C7-C8-C9-C10
14	B	101	LMT	C3-C4-C5-C6
14	M	409	LMT	C6-C7-C8-C9
8	A	101	BCL	O1A-CGA-O2A-C1
14	U	101	LMT	C2-C3-C4-C5
10	M	404	U10	C5-C4-O4-C4M

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Mol	Chain	Res	Type	Atoms
14	2	104	LMT	C5-C6-C7-C8
12	M	406	CDL	CA2-C1-CB2-OB2
14	4	102	LMT	O5B-C5B-C6B-O6B
14	L	405	LMT	C2-C3-C4-C5
8	3	101	BCL	C2-C1-O2A-CGA
8	T	101	BCL	C2-C1-O2A-CGA
8	R	103	BCL	C2-C1-O2A-CGA
8	G	103	BCL	C14-C13-C15-C16
8	R	103	BCL	CBA-CGA-O2A-C1
14	L	405	LMT	C4B-C5B-C6B-O6B
8	N	101	BCL	C2A-CAA-CBA-CGA
8	N	102	BCL	C4C-C3C-CAC-CBC
8	T	101	BCL	C10-C11-C12-C13
8	J	103	BCL	C15-C16-C17-C18
14	6	101	LMT	C3'-C4'-O1B-C1B
14	I	101	LMT	C3'-C4'-O1B-C1B
14	U	102	LMT	C3-C4-C5-C6
14	K	101	LMT	C3-C4-C5-C6
7	M	401	QAK	C13-C14-C15-C16
7	M	401	QAK	C22-C23-C24-C26
8	1	101	BCL	C11-C10-C8-C7
8	3	101	BCL	C11-C10-C8-C7
8	Y	102	BCL	C6-C7-C8-C10
8	V	101	BCL	C6-C7-C8-C10
8	T	101	BCL	C6-C7-C8-C10
8	A	102	BCL	C11-C10-C8-C7
8	P	103	BCL	C11-C10-C8-C7
8	J	103	BCL	C11-C10-C8-C7
8	G	103	BCL	C12-C13-C15-C16
8	E	102	BCL	C11-C10-C8-C7
14	U	101	LMT	C1-C2-C3-C4
12	M	406	CDL	C39-C40-C41-C42
14	Z	102	LMT	C6-C7-C8-C9
11	H	301	6PL	C12-C11-O3-C3
14	I	101	LMT	C4-C5-C6-C7
8	M	402	BCL	CAD-CBD-CGD-O2D
8	1	101	BCL	CAD-CBD-CGD-O2D
9	L	403	BPH	CAD-CBD-CGD-O2D
8	P	103	BCL	C4-C3-C5-C6
14	2	103	LMT	O5'-C1'-O1'-C1
14	I	102	LMT	O5'-C1'-O1'-C1
10	L	406	U10	C5-C4-O4-C4M

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Mol	Chain	Res	Type	Atoms
11	E	101	6PL	C1-C2-C3-O3
12	H	302	CDL	C1-CB2-OB2-PB2
12	H	302	CDL	CB3-CB4-CB6-OB8
11	M	405	6PL	O3P-C1-C2-O2
12	H	302	CDL	OA5-CA3-CA4-OA6
8	1	101	BCL	C8-C10-C11-C12
12	G	104	CDL	CB2-C1-CA2-OA2
8	P	101	BCL	O1A-CGA-O2A-C1
12	L	404	CDL	C43-C44-C45-C46
11	M	405	6PL	O2-C2-C3-O3
11	E	101	6PL	O2-C2-C3-O3
12	L	404	CDL	OA6-CA4-CA6-OA8
14	S	101	LMT	C7-C8-C9-C10
8	Y	101	BCL	C13-C15-C16-C17
8	T	102	BCL	C16-C17-C18-C19
14	U	102	LMT	C9-C10-C11-C12
8	R	104	BCL	O1A-CGA-O2A-C1
12	G	104	CDL	C16-C17-C18-C19
8	1	101	BCL	C11-C10-C8-C9
8	Y	102	BCL	C6-C7-C8-C9
8	J	102	BCL	C6-C7-C8-C9
8	G	102	BCL	C11-C10-C8-C9
8	R	103	BCL	O1A-CGA-O2A-C1
8	2	101	BCL	C16-C17-C18-C19
8	Y	101	BCL	C16-C17-C18-C19
14	Z	102	LMT	C9-C10-C11-C12
14	J	101	LMT	O1'-C1-C2-C3
14	I	101	LMT	C2B-C1B-O1B-C4'
7	M	401	QAK	C40-C2-C3-C4
8	5	102	BCL	C1A-C2A-CAA-CBA
8	V	101	BCL	C1A-C2A-CAA-CBA
8	4	101	BCL	C13-C15-C16-C17
14	S	101	LMT	C1-C2-C3-C4
12	H	302	CDL	CB2-OB2-PB2-OB5
14	S	101	LMT	C9-C10-C11-C12
14	M	409	LMT	C7-C8-C9-C10
12	3	102	CDL	CB4-CB3-OB5-PB2
14	L	405	LMT	C5'-C4'-O1B-C1B
14	X	101	LMT	C7-C8-C9-C10
11	H	301	6PL	C1-O3P-P-O1P
12	M	406	CDL	CB2-OB2-PB2-OB3
12	M	406	CDL	CB2-OB2-PB2-OB4

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Mol	Chain	Res	Type	Atoms
12	M	406	CDL	CB3-OB5-PB2-OB4
12	3	102	CDL	CB2-OB2-PB2-OB4
12	G	101	CDL	CA3-OA5-PA1-OA4
15	F	103	CRT	C33-C35-C36-C37
8	L	401	BCL	C16-C17-C18-C19
11	M	405	6PL	O3P-C1-C2-C3
12	H	302	CDL	OA5-CA3-CA4-CA6
14	I	102	LMT	C5'-C4'-O1B-C1B
14	M	409	LMT	C11-C10-C9-C8
11	E	101	6PL	C5-C4-O4P-P
11	H	301	6PL	O11-C11-O3-C3
12	G	101	CDL	CB7-C71-C72-C73
14	F	102	LMT	C7-C8-C9-C10
7	M	401	QAK	C17-C18-C19-C21
8	Y	101	BCL	C6-C7-C8-C10
8	R	104	BCL	C11-C10-C8-C7
8	P	101	BCL	C6-C7-C8-C10
8	J	102	BCL	C6-C7-C8-C10
8	J	103	BCL	C6-C7-C8-C10
8	J	103	BCL	C12-C13-C15-C16
8	G	103	BCL	C11-C10-C8-C7
8	E	102	BCL	C6-C7-C8-C10
11	E	101	6PL	C36-C37-C38-C39
14	R	102	LMT	C11-C10-C9-C8
14	F	101	LMT	C2-C1-O1'-C1'
14	K	101	LMT	O1'-C1-C2-C3
12	G	104	CDL	C77-C78-C79-C80
8	V	102	BCL	C13-C15-C16-C17
8	4	101	BCL	C16-C17-C18-C19
14	R	102	LMT	C4'-C5'-C6'-O6'
12	M	406	CDL	C34-C35-C36-C37
16	P	102	PGT	O2-C31-C32-C33
11	E	101	6PL	O4P-C4-C5-N
12	L	404	CDL	CA3-CA4-CA6-OA8
12	G	104	CDL	CB3-CB4-CB6-OB8
12	H	302	CDL	OA6-CA4-CA6-OA8
12	H	302	CDL	OB6-CB4-CB6-OB8
12	G	104	CDL	OB6-CB4-CB6-OB8
9	L	403	BPH	O2A-C1-C2-C3
14	I	102	LMT	O1'-C1-C2-C3
14	S	102	LMT	C9-C10-C11-C12
14	X	103	LMT	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
8	3	101	BCL	C6-C7-C8-C9
8	3	101	BCL	C11-C10-C8-C9
8	3	101	BCL	C11-C12-C13-C14
8	T	101	BCL	C6-C7-C8-C9
8	D	104	BCL	C6-C7-C8-C9
8	P	103	BCL	C14-C13-C15-C16
8	E	103	BCL	C11-C10-C8-C9
12	3	102	CDL	OB9-CB7-OB8-CB6
14	I	101	LMT	O5B-C1B-O1B-C4'
8	M	407	BCL	C13-C15-C16-C17
7	M	401	QAK	C38-C10-CZ3-CE3
12	G	101	CDL	CA7-C31-C32-C33
12	L	404	CDL	C71-CB7-OB8-CB6
14	Z	102	LMT	C3-C4-C5-C6
12	M	406	CDL	CA5-C11-C12-C13
8	J	103	BCL	C8-C10-C11-C12
14	X	101	LMT	O5B-C5B-C6B-O6B
11	H	301	6PL	O3-C11-C12-C13
14	M	409	LMT	C9-C10-C11-C12
8	L	402	BCL	C2-C1-O2A-CGA
8	Y	102	BCL	C2-C1-O2A-CGA
8	C	100	BCL	C2-C1-O2A-CGA
8	G	103	BCL	C2-C1-O2A-CGA
14	D	101	LMT	C2-C3-C4-C5
8	T	102	BCL	C16-C17-C18-C20
8	G	103	BCL	O1A-CGA-O2A-C1
11	H	301	6PL	C32-C31-O2-C2
8	L	401	BCL	C2A-CAA-CBA-CGA
14	U	102	LMT	C1-C2-C3-C4
12	M	406	CDL	C11-C12-C13-C14
8	G	103	BCL	CBA-CGA-O2A-C1
12	M	406	CDL	CA2-OA2-PA1-OA5
12	L	404	CDL	CA3-OA5-PA1-OA2
12	L	404	CDL	CB3-OB5-PB2-OB2
12	3	102	CDL	CA3-OA5-PA1-OA2
12	3	102	CDL	CB3-OB5-PB2-OB2
12	G	104	CDL	CB2-OB2-PB2-OB5
16	P	102	PGT	C1-O3P-P-O4P
16	P	102	PGT	C4-O4P-P-O3P
12	G	101	CDL	C71-C72-C73-C74
8	J	102	BCL	C16-C17-C18-C19
15	D	105	CRT	C36-C37-C38-C40

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Mol	Chain	Res	Type	Atoms
12	G	101	CDL	C59-C60-C61-C62
8	J	103	BCL	O1D-CGD-O2D-CED
7	M	401	QAK	C18-C19-C21-C22
8	1	101	BCL	C6-C7-C8-C10
8	J	102	BCL	C12-C13-C15-C16
8	4	101	BCL	C6-C7-C8-C9
8	T	102	BCL	C6-C7-C8-C9
8	A	101	BCL	C6-C7-C8-C9
8	A	101	BCL	C11-C12-C13-C14
8	P	103	BCL	C11-C12-C13-C14
8	J	103	BCL	C11-C10-C8-C9
14	X	103	LMT	C1-C2-C3-C4
8	2	101	BCL	C16-C17-C18-C20
8	Y	101	BCL	C16-C17-C18-C20
10	1	102	U10	C5-C4-O4-C4M
8	A	102	BCL	CAA-CBA-CGA-O1A
14	Z	102	LMT	C1-C2-C3-C4
8	A	101	BCL	C2A-CAA-CBA-CGA
14	X	101	LMT	C2-C3-C4-C5
12	H	302	CDL	C1-CA2-OA2-PA1
14	Q	102	LMT	C4B-C5B-C6B-O6B
8	P	103	BCL	C2-C3-C5-C6
8	L	401	BCL	C16-C17-C18-C20
8	J	103	BCL	CBD-CGD-O2D-CED
8	L	402	BCL	C2A-CAA-CBA-CGA
14	X	103	LMT	C2B-C1B-O1B-C4'
8	2	101	BCL	C2-C1-O2A-CGA
8	A	101	BCL	C2-C1-O2A-CGA
8	D	104	BCL	C2-C1-O2A-CGA
8	E	103	BCL	C2-C1-O2A-CGA
14	2	103	LMT	C1-C2-C3-C4
8	A	102	BCL	C2A-CAA-CBA-CGA
11	H	301	6PL	C21-C22-C23-C24
14	2	104	LMT	C2B-C1B-O1B-C4'
14	2	103	LMT	C6-C7-C8-C9
14	J	101	LMT	C6-C7-C8-C9
10	1	102	U10	C25-C24-C26-C27
8	4	101	BCL	C11-C12-C13-C14
8	V	102	BCL	C14-C13-C15-C16
8	C	100	BCL	C11-C10-C8-C9
8	D	104	BCL	C14-C13-C15-C16
8	P	101	BCL	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
8	N	102	BCL	C11-C10-C8-C9
14	X	103	LMT	C9-C10-C11-C12
16	P	102	PGT	C36-C37-C38-C39
14	Z	102	LMT	C5-C6-C7-C8
8	C	100	BCL	C2A-CAA-CBA-CGA
8	R	103	BCL	C2A-CAA-CBA-CGA
14	Q	101	LMT	C11-C10-C9-C8
8	4	101	BCL	C16-C17-C18-C20
14	X	103	LMT	O5B-C1B-O1B-C4'
11	H	301	6PL	C3-C2-O2-C31
12	H	302	CDL	CA6-CA4-OA6-CA5
8	L	401	BCL	C11-C12-C13-C15
8	N	102	BCL	C11-C12-C13-C15
8	G	102	BCL	C11-C12-C13-C15
12	L	404	CDL	OB9-CB7-OB8-CB6
8	5	101	BCL	O1D-CGD-O2D-CED
9	L	403	BPH	C8-C10-C11-C12
7	M	401	QAK	O-C-CA-CB
14	U	102	LMT	C2-C3-C4-C5
12	G	101	CDL	C57-C58-C59-C60
14	6	101	LMT	C5'-C4'-O1B-C1B
14	F	102	LMT	O5B-C1B-O1B-C4'
14	S	102	LMT	C3-C4-C5-C6
8	M	402	BCL	C4-C3-C5-C6
14	B	101	LMT	C2-C3-C4-C5
14	U	101	LMT	C3-C4-C5-C6
16	P	102	PGT	C42-C43-C44-C45
11	M	405	6PL	C41-C42-C43-C44
11	H	301	6PL	O31-C31-O2-C2
12	G	104	CDL	C32-C31-CA7-OA8
11	E	101	6PL	C13-C14-C15-C16
14	D	103	LMT	O5'-C1'-O1'-C1
8	R	103	BCL	C5-C6-C7-C8
8	5	101	BCL	C4-C3-C5-C6
10	1	102	U10	C12-C11-C9-C10
8	V	101	BCL	C2-C1-O2A-CGA
8	T	102	BCL	C2-C1-O2A-CGA
8	E	102	BCL	C2-C1-O2A-CGA
8	A	102	BCL	C13-C15-C16-C17
8	D	104	BCL	C11-C12-C13-C14
14	D	102	LMT	C3-C4-C5-C6
8	5	101	BCL	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
8	M	402	BCL	C15-C16-C17-C18
14	2	103	LMT	C4-C5-C6-C7
8	G	103	BCL	C16-C17-C18-C20
14	U	101	LMT	C4-C5-C6-C7
14	L	405	LMT	C4-C5-C6-C7
8	T	101	BCL	C2A-CAA-CBA-CGA
8	N	102	BCL	C3-C5-C6-C7
8	A	101	BCL	C16-C17-C18-C19
14	F	102	LMT	C2B-C1B-O1B-C4'
8	V	101	BCL	C11-C10-C8-C7
8	C	100	BCL	C6-C7-C8-C10
8	C	100	BCL	C11-C10-C8-C7
10	1	102	U10	C23-C24-C26-C27
8	T	101	BCL	CBA-CGA-O2A-C1
14	D	102	LMT	C4-C5-C6-C7
9	L	403	BPH	C1-C2-C3-C4
8	T	102	BCL	O1A-CGA-O2A-C1
8	J	102	BCL	C15-C16-C17-C18
12	H	302	CDL	C31-CA7-OA8-CA6
8	L	402	BCL	C4-C3-C5-C6
14	I	102	LMT	C3'-C4'-O1B-C1B
8	M	402	BCL	C2-C3-C5-C6
8	5	101	BCL	C2-C3-C5-C6
8	L	401	BCL	C11-C12-C13-C14
8	Y	101	BCL	C6-C7-C8-C9
8	C	100	BCL	C6-C7-C8-C9
8	R	103	BCL	C11-C10-C8-C9
8	G	102	BCL	C11-C12-C13-C14
8	G	103	BCL	C11-C10-C8-C9
8	E	102	BCL	C6-C7-C8-C9
8	E	102	BCL	C11-C12-C13-C14
9	M	403	BPH	C6-C7-C8-C9
9	L	403	BPH	C11-C12-C13-C14
8	T	101	BCL	O1A-CGA-O2A-C1
8	L	401	BCL	CAD-CBD-CGD-O2D
8	L	402	BCL	CAD-CBD-CGD-O2D
8	5	102	BCL	CAD-CBD-CGD-O2D
8	3	101	BCL	CAD-CBD-CGD-O2D
8	4	101	BCL	CAD-CBD-CGD-O2D
9	M	403	BPH	CAD-CBD-CGD-O2D
12	3	102	CDL	CB3-CB4-OB6-CB5
14	6	101	LMT	C2-C1-O1'-C1'

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Mol	Chain	Res	Type	Atoms
8	L	401	BCL	C13-C15-C16-C17
8	C	100	BCL	C15-C16-C17-C18
10	1	102	U10	C30-C29-C31-C32
8	1	101	BCL	CAA-CBA-CGA-O2A
8	T	102	BCL	CBA-CGA-O2A-C1
12	H	302	CDL	C31-C32-C33-C34
8	L	401	BCL	O2A-C1-C2-C3
8	1	101	BCL	O2A-C1-C2-C3
12	3	102	CDL	CB5-C51-C52-C53
11	M	405	6PL	C22-C23-C24-C25
8	T	101	BCL	O1D-CGD-O2D-CED
8	M	407	BCL	CHA-CBD-CGD-O2D
14	D	103	LMT	O5B-C5B-C6B-O6B
16	P	102	PGT	C40-C41-C42-C43
12	M	406	CDL	C12-C11-CA5-OA6
8	V	102	BCL	O1D-CGD-O2D-CED
8	N	101	BCL	CAA-CBA-CGA-O2A
12	M	406	CDL	C40-C41-C42-C43
7	M	401	QAK	C-CA-CB-C31
9	L	403	BPH	CHA-CBD-CGD-O1D
15	D	105	CRT	C36-C37-C38-C39
8	G	102	BCL	C16-C17-C18-C20
8	J	103	BCL	C6-C7-C8-C9
14	2	103	LMT	C5'-C4'-O1B-C1B
14	6	101	LMT	C4'-C5'-C6'-O6'
8	Y	102	BCL	CBA-CGA-O2A-C1
8	G	102	BCL	C5-C6-C7-C8
12	H	302	CDL	C52-C51-CB5-OB6
12	G	104	CDL	C54-C55-C56-C57
8	L	401	BCL	CAA-CBA-CGA-O2A
8	3	101	BCL	C13-C15-C16-C17
8	E	102	BCL	CBA-CGA-O2A-C1
12	G	104	CDL	C36-C37-C38-C39
8	M	402	BCL	C1A-C2A-CAA-CBA
14	Q	101	LMT	C1-C2-C3-C4
8	1	101	BCL	CAA-CBA-CGA-O1A
8	P	101	BCL	C2-C1-O2A-CGA
14	F	101	LMT	C4-C5-C6-C7
11	M	405	6PL	C1-C2-C3-O3
8	E	102	BCL	O1A-CGA-O2A-C1
12	M	406	CDL	C32-C31-CA7-OA8
12	M	406	CDL	CA3-OA5-PA1-OA3

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Mol	Chain	Res	Type	Atoms
12	3	102	CDL	CA3-OA5-PA1-OA3
12	G	101	CDL	CA2-OA2-PA1-OA3
12	G	104	CDL	CB2-OB2-PB2-OB3
14	D	101	LMT	C4-C5-C6-C7
8	A	102	BCL	C3-C5-C6-C7
14	B	102	LMT	C4'-C5'-C6'-O6'
12	G	101	CDL	C36-C37-C38-C39
8	J	103	BCL	CAA-CBA-CGA-O2A
12	G	101	CDL	C32-C31-CA7-OA8
11	E	101	6PL	C33-C34-C35-C36
8	N	102	BCL	O1D-CGD-O2D-CED
12	M	406	CDL	CB3-CB4-OB6-CB5
12	M	406	CDL	CB6-CB4-OB6-CB5
16	P	102	PGT	C1-C2-O2-C31
16	P	102	PGT	C3-C2-O2-C31
8	Y	102	BCL	O1A-CGA-O2A-C1
8	Y	102	BCL	C11-C12-C13-C14
8	C	100	BCL	C11-C12-C13-C14
12	G	104	CDL	C58-C59-C60-C61
8	N	101	BCL	CAA-CBA-CGA-O1A
12	M	406	CDL	C12-C11-CA5-OA7
12	M	406	CDL	C32-C31-CA7-OA9
8	5	102	BCL	C16-C17-C18-C19
12	H	302	CDL	C59-C60-C61-C62
8	1	101	BCL	C10-C11-C12-C13
8	3	101	BCL	C11-C12-C13-C15
8	D	104	BCL	C6-C7-C8-C10
8	P	103	BCL	C2C-C3C-CAC-CBC
8	G	102	BCL	C6-C7-C8-C10
9	L	403	BPH	C11-C12-C13-C15
10	1	102	U10	C12-C11-C9-C8
12	L	404	CDL	C12-C11-CA5-OA6
15	Q	103	CRT	C5-C6-C7-C9
14	Z	102	LMT	C2-C1-O1'-C1'
14	B	101	LMT	C2-C1-O1'-C1'
8	P	103	BCL	CAA-CBA-CGA-O2A
12	H	302	CDL	C72-C71-CB7-OB8
14	B	102	LMT	C5'-C4'-O1B-C1B
8	L	401	BCL	CAA-CBA-CGA-O1A
11	H	301	6PL	O2-C31-C32-C33
12	3	102	CDL	C72-C71-CB7-OB8
12	H	302	CDL	C52-C51-CB5-OB7

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Mol	Chain	Res	Type	Atoms
8	T	101	BCL	C15-C16-C17-C18
12	G	101	CDL	C32-C31-CA7-OA9
8	L	401	BCL	C8-C10-C11-C12

There are no ring outliers.

88 monomers are involved in 368 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	O	102	CRT	3	0
8	E	103	BCL	5	0
15	K	103	CRT	6	0
15	B	103	CRT	3	0
14	U	101	LMT	2	0
15	3	103	CRT	5	0
8	L	402	BCL	1	0
12	G	101	CDL	13	0
8	P	103	BCL	4	0
15	2	102	CRT	7	0
8	J	103	BCL	9	0
8	V	102	BCL	7	0
11	H	301	6PL	9	0
14	F	101	LMT	5	0
8	M	407	BCL	3	0
14	D	102	LMT	3	0
14	S	101	LMT	3	0
9	L	403	BPH	6	0
8	Y	102	BCL	9	0
12	G	104	CDL	8	0
14	F	102	LMT	1	0
14	I	101	LMT	2	0
8	A	101	BCL	8	0
12	M	406	CDL	12	0
8	Y	101	BCL	8	0
8	V	101	BCL	2	0
14	I	102	LMT	2	0
14	O	101	LMT	3	0
12	H	302	CDL	12	0
8	J	102	BCL	7	0
8	3	101	BCL	6	0
14	M	409	LMT	2	0
8	G	102	BCL	3	0
8	D	104	BCL	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	K	102	LMT	1	0
15	X	102	CRT	8	0
8	G	103	BCL	8	0
14	2	104	LMT	2	0
14	X	101	LMT	3	0
14	K	101	LMT	3	0
14	4	102	LMT	1	0
14	U	102	LMT	1	0
15	R	101	CRT	2	0
12	3	102	CDL	10	0
14	Q	101	LMT	2	0
11	M	405	6PL	5	0
8	1	101	BCL	11	0
16	P	102	PGT	3	0
8	R	103	BCL	6	0
8	N	102	BCL	7	0
14	X	103	LMT	2	0
12	L	404	CDL	9	0
8	E	102	BCL	8	0
10	L	406	U10	1	0
8	5	102	BCL	6	0
9	M	403	BPH	6	0
14	Z	102	LMT	3	0
14	R	102	LMT	4	0
14	D	101	LMT	6	0
8	P	101	BCL	2	0
15	Z	101	CRT	13	0
8	M	402	BCL	6	0
14	6	101	LMT	3	0
10	M	404	U10	6	0
8	5	101	BCL	9	0
14	S	102	LMT	1	0
8	T	102	BCL	8	0
14	B	101	LMT	3	0
8	R	104	BCL	4	0
14	2	103	LMT	3	0
15	I	103	CRT	5	0
14	J	101	LMT	2	0
14	D	103	LMT	2	0
15	F	103	CRT	6	0
8	N	101	BCL	10	0
8	L	401	BCL	6	0

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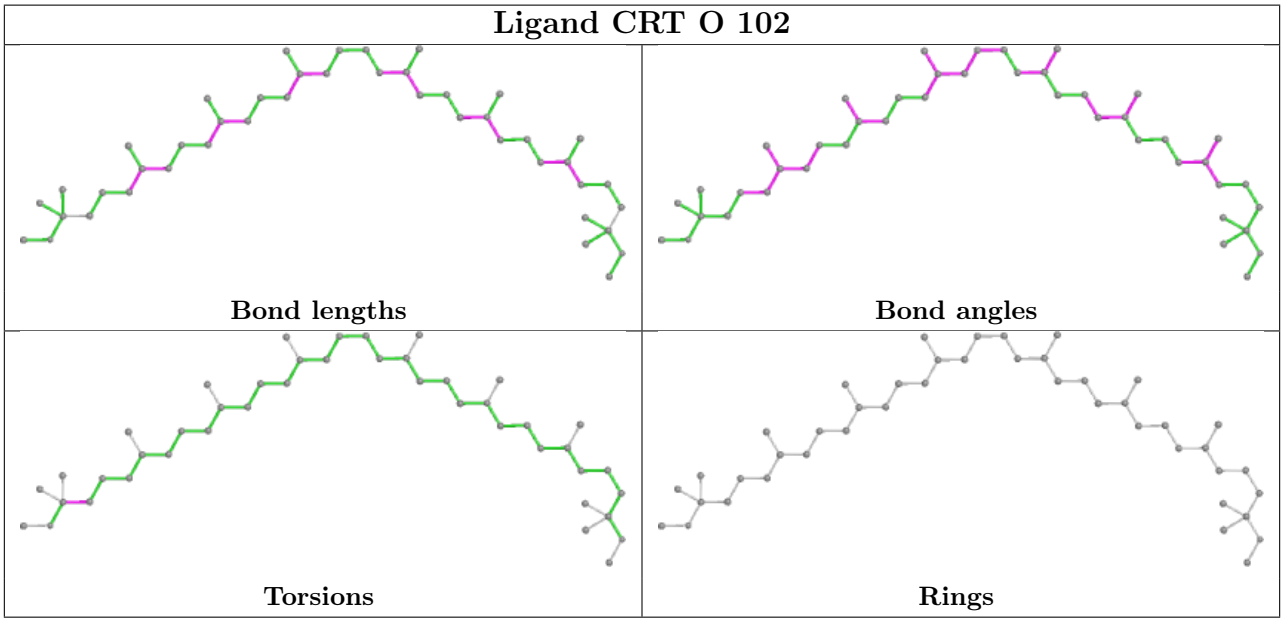
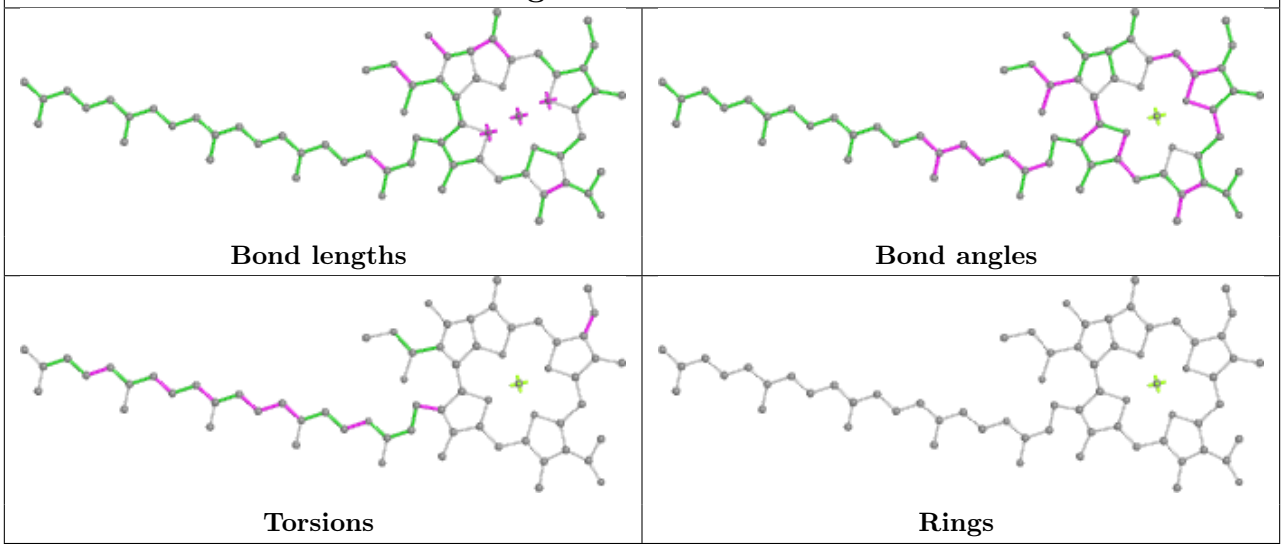
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	E	101	6PL	9	0
15	D	105	CRT	1	0
15	S	103	CRT	1	0
8	C	100	BCL	5	0
10	1	102	U10	2	0
15	Q	103	CRT	2	0
8	4	101	BCL	5	0
8	T	101	BCL	2	0
14	B	102	LMT	3	0
8	A	102	BCL	11	0
14	L	405	LMT	3	0
8	2	101	BCL	5	0

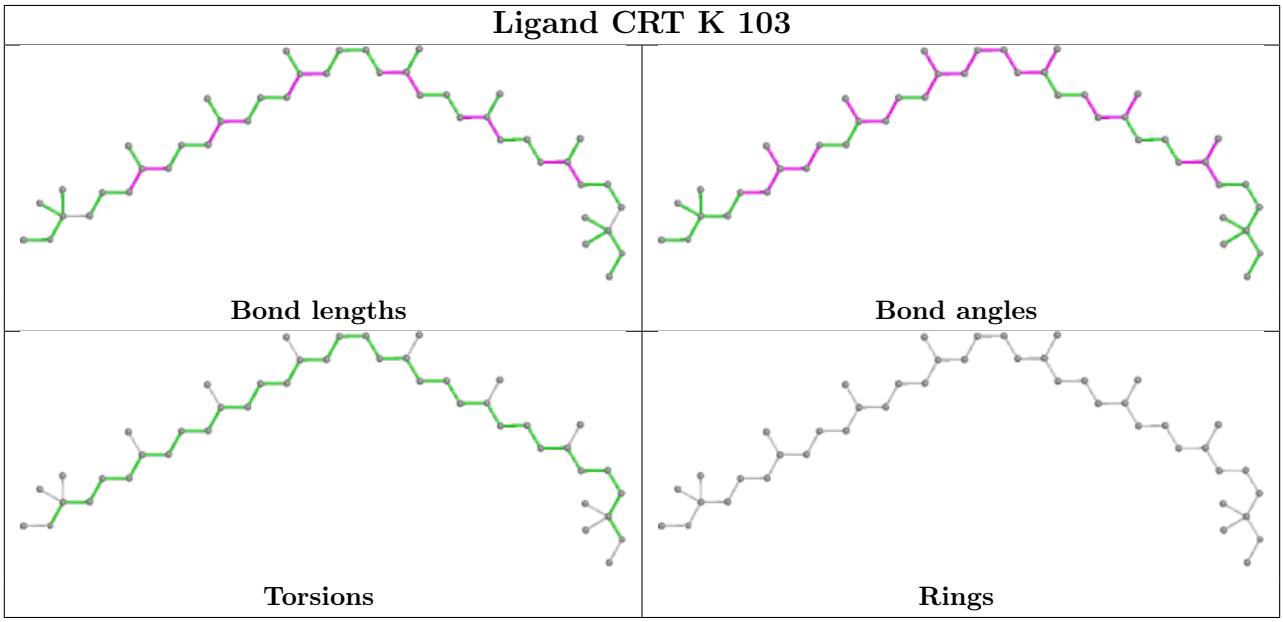
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



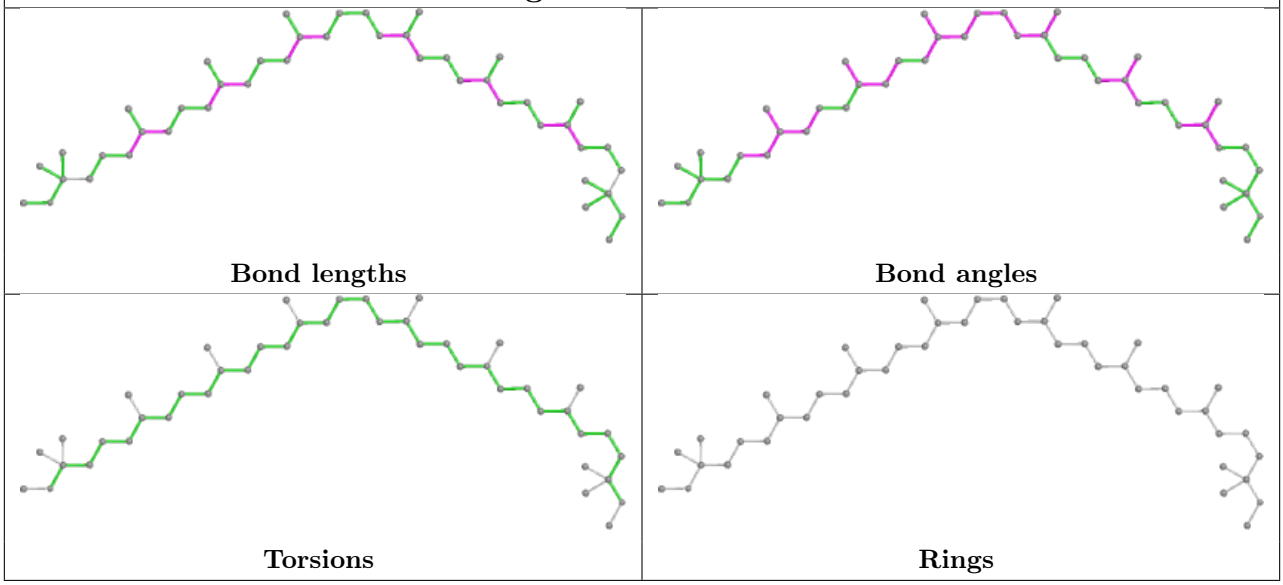
Ligand BCL E 103



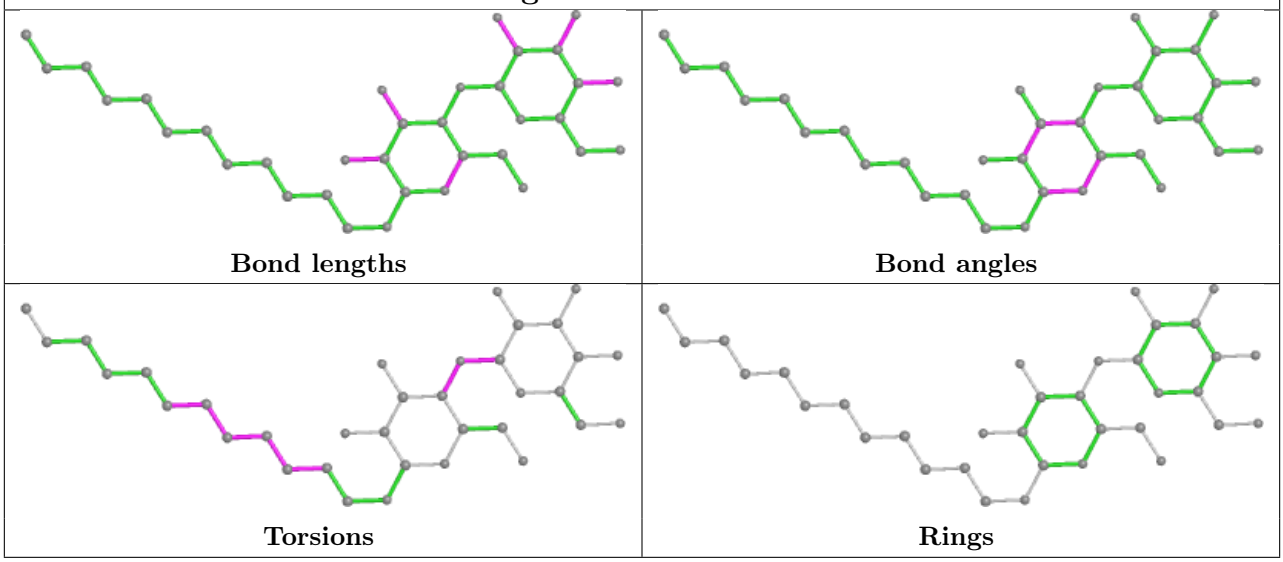
Ligand CRT K 103



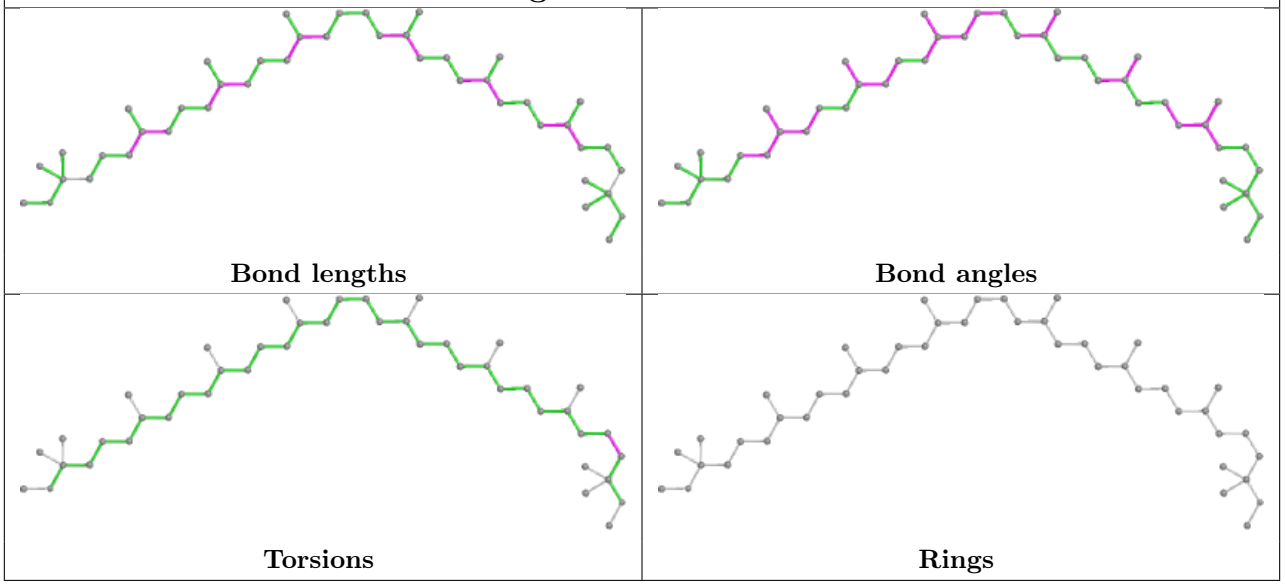
Ligand CRT B 103



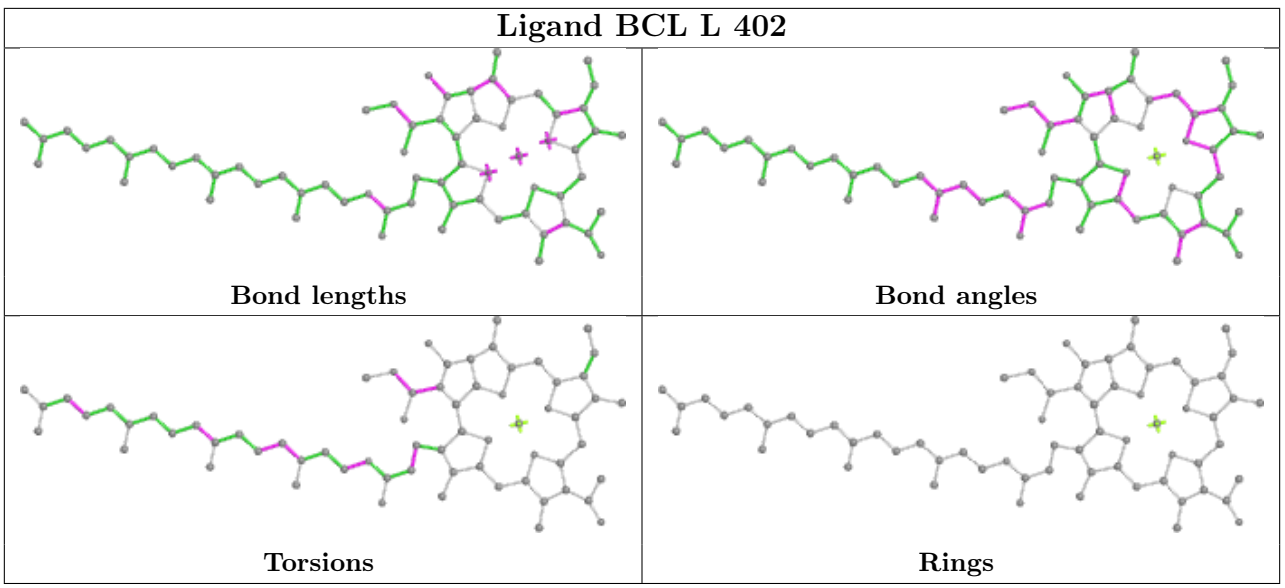
Ligand LMT U 101



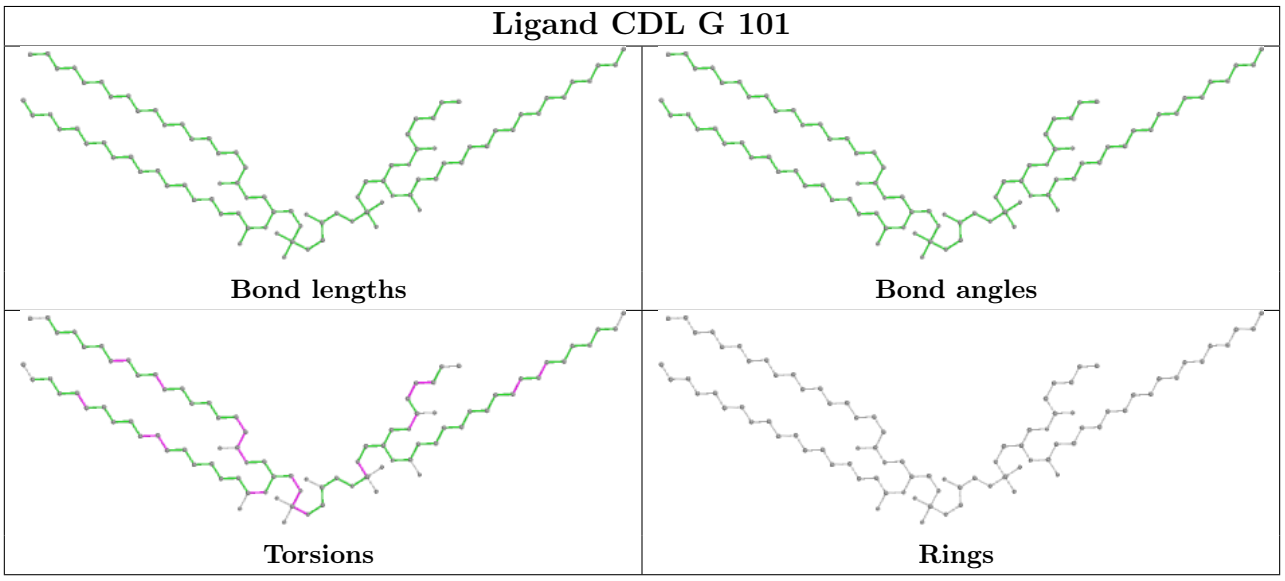
Ligand CRT 3 103



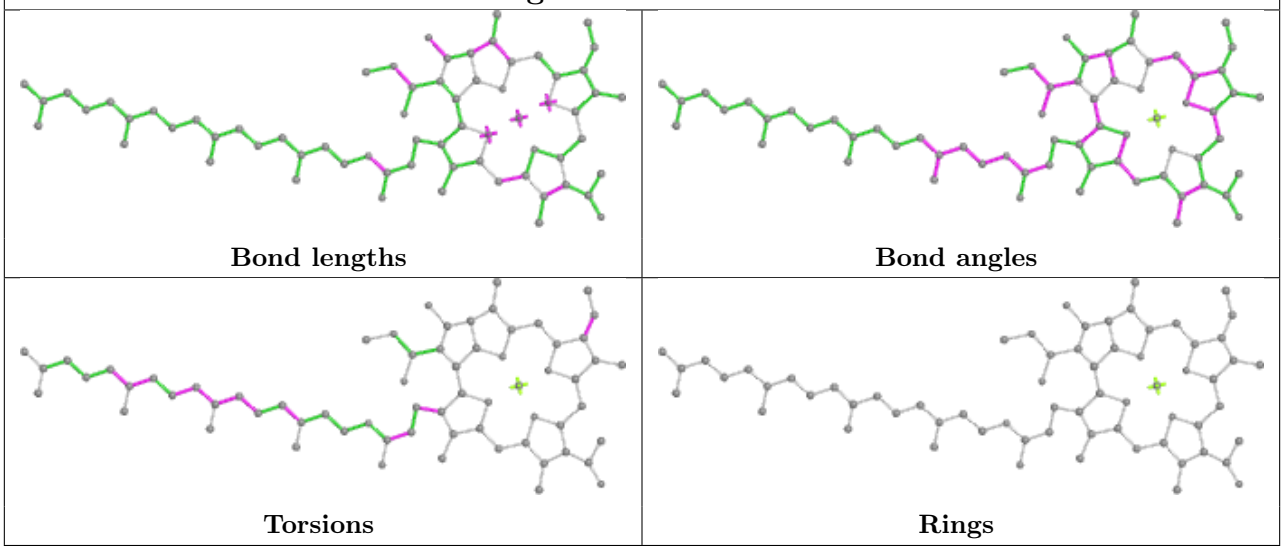
Ligand BCL L 402



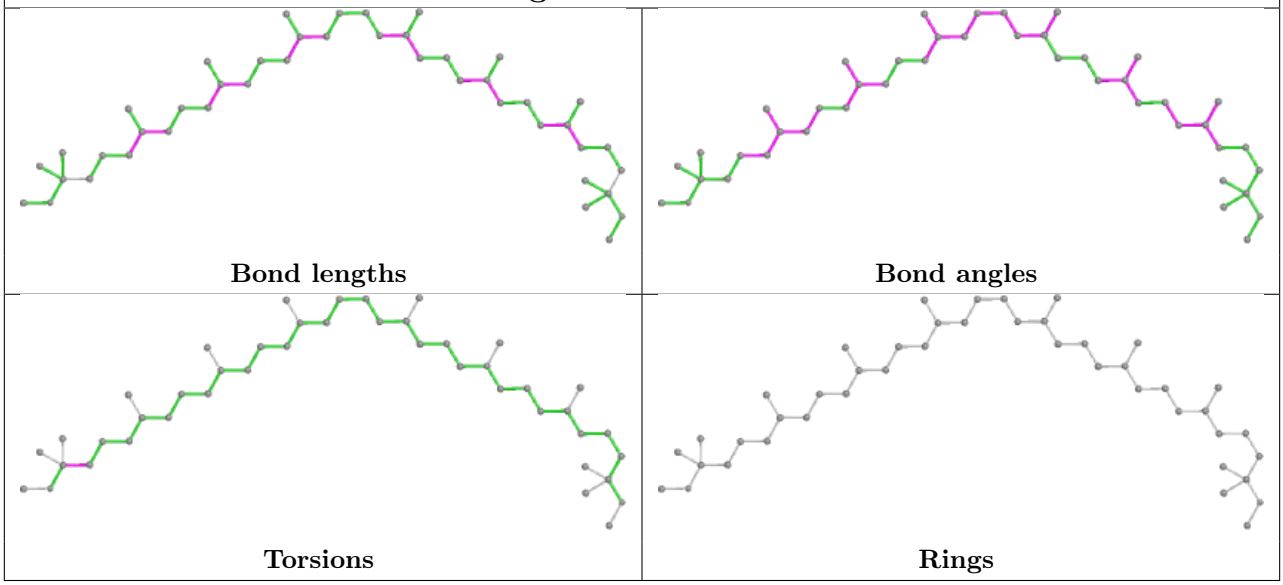
Ligand CDL G 101



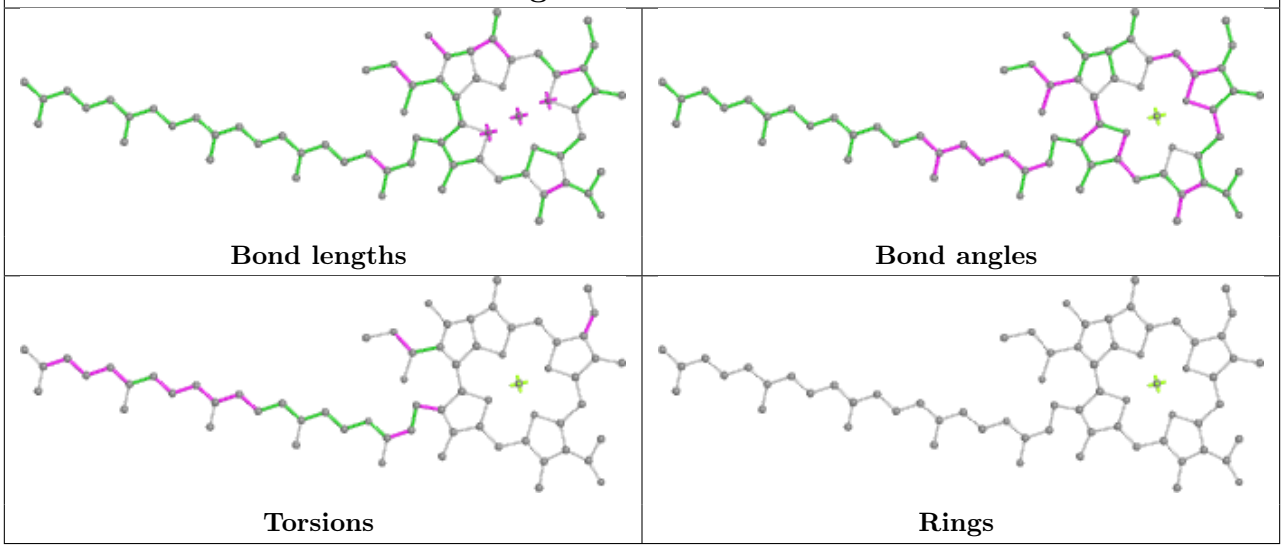
Ligand BCL P 103



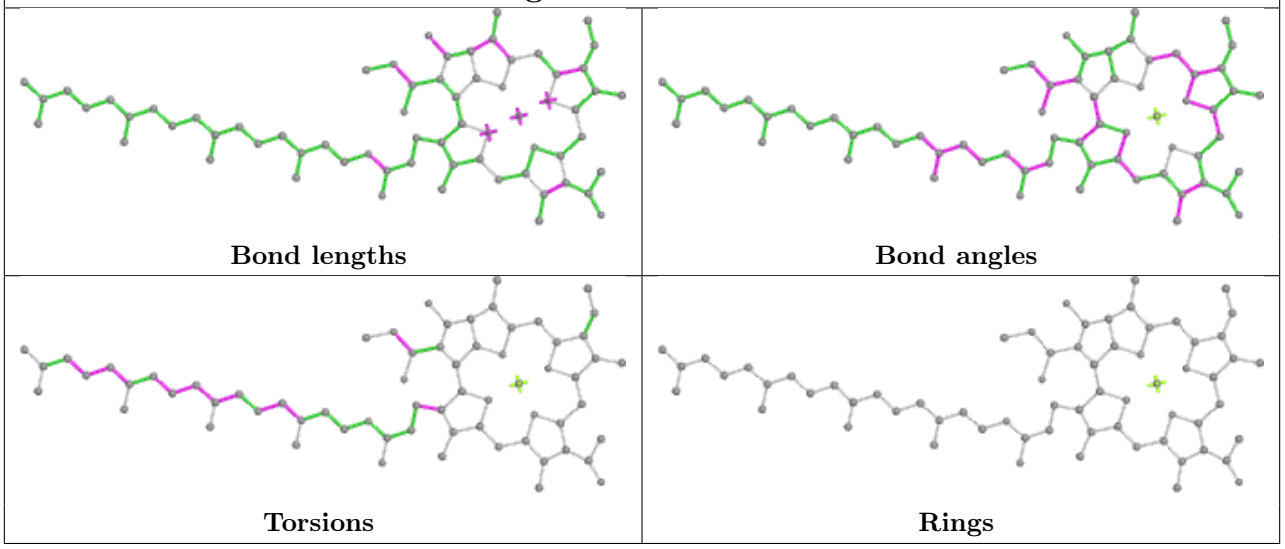
Ligand CRT 2 102



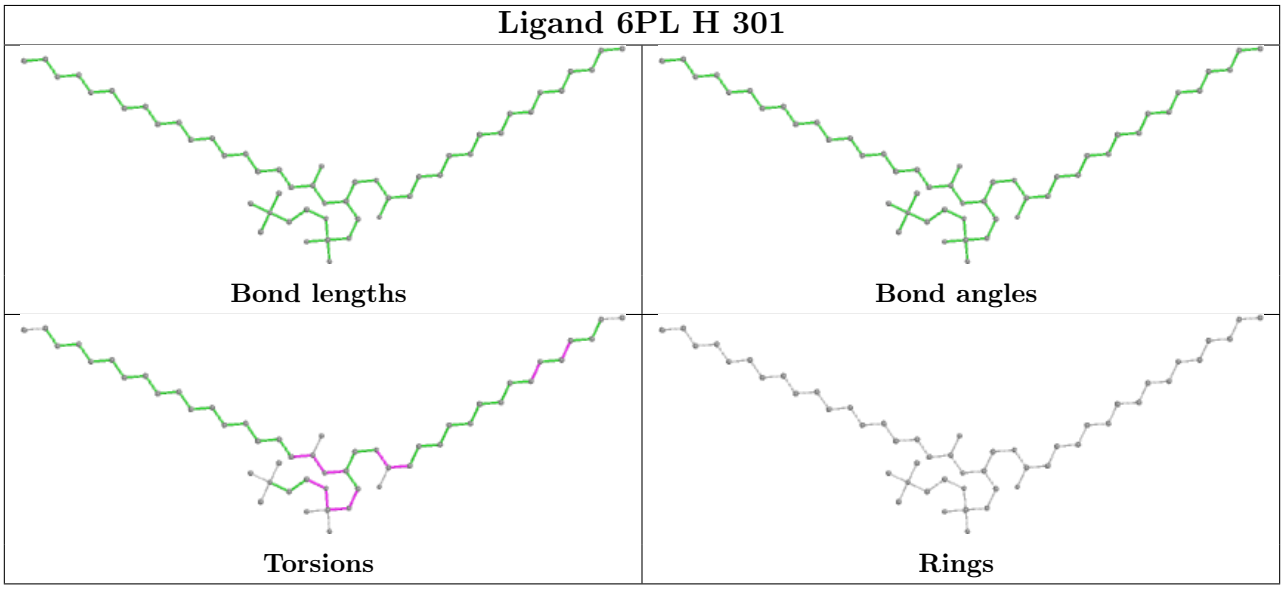
Ligand BCL J 103



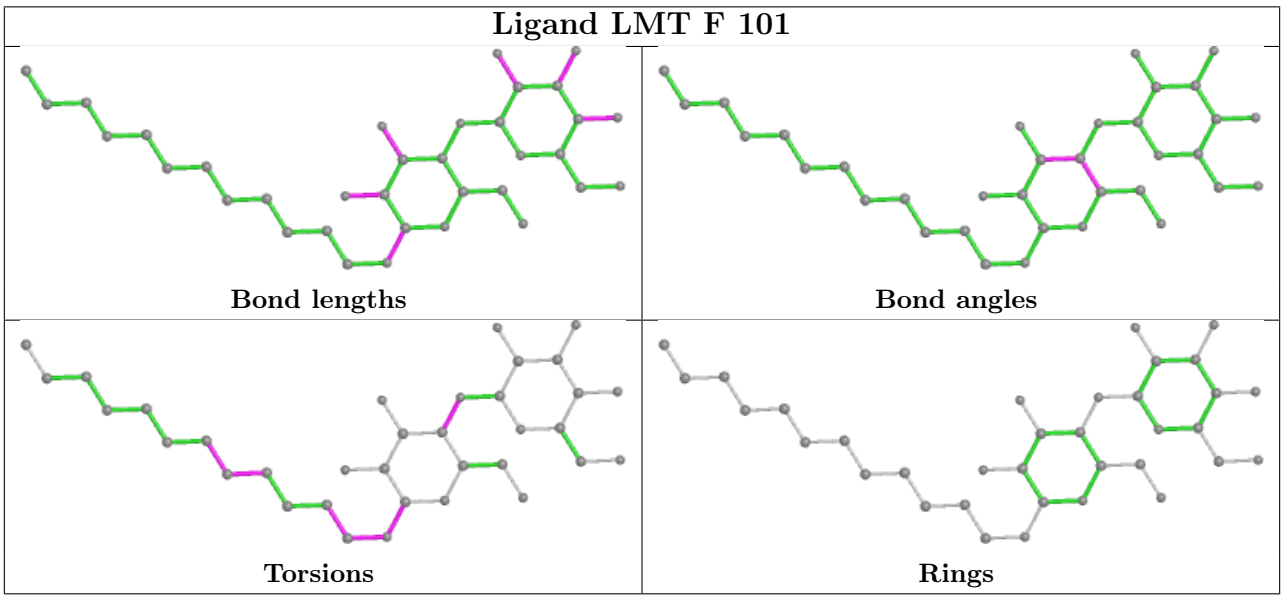
Ligand BCL V 102



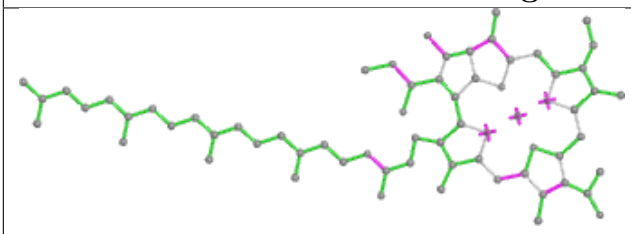
Ligand 6PL H 301



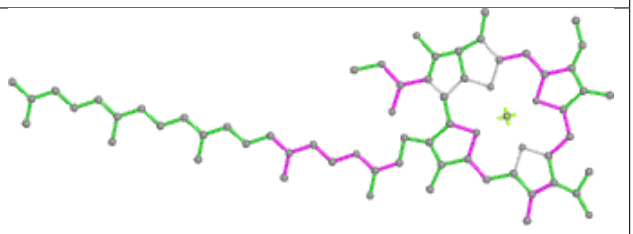
Ligand LMT F 101



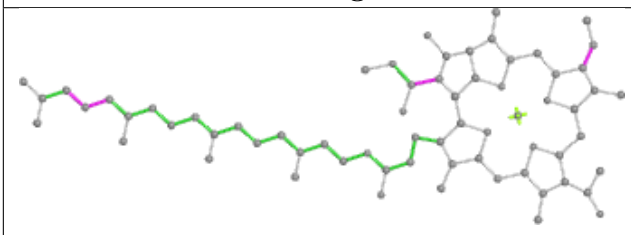
Ligand BCL M 407



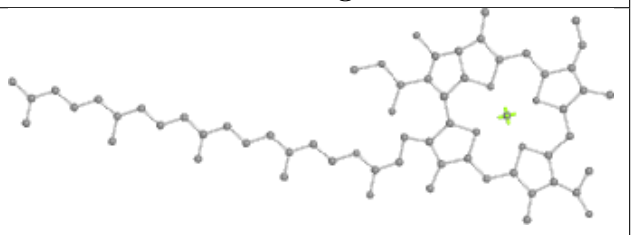
Bond lengths



Bond angles

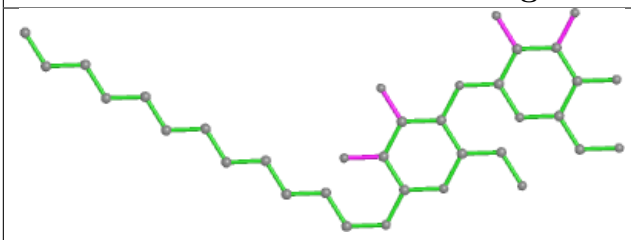


Torsions

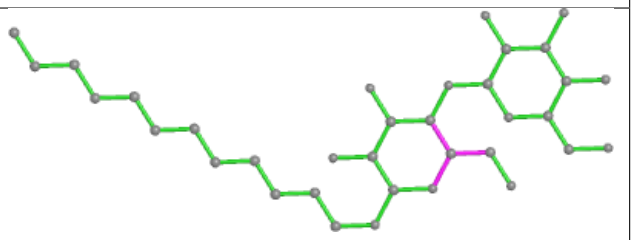


Rings

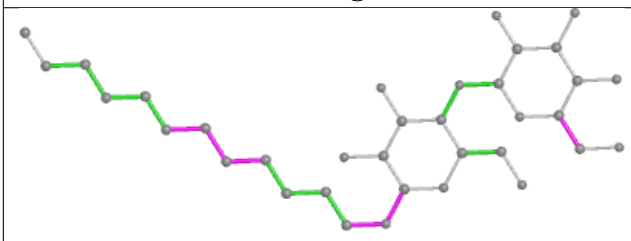
Ligand LMT D 102



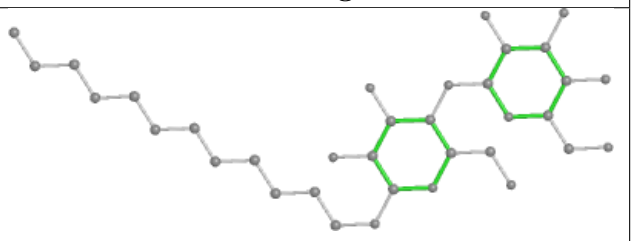
Bond lengths



Bond angles

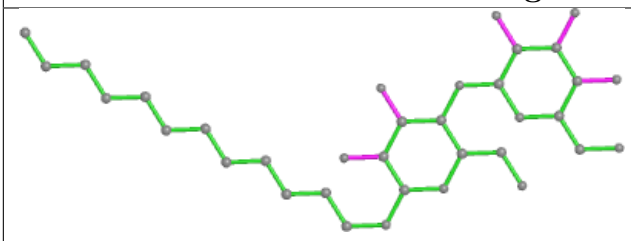


Torsions

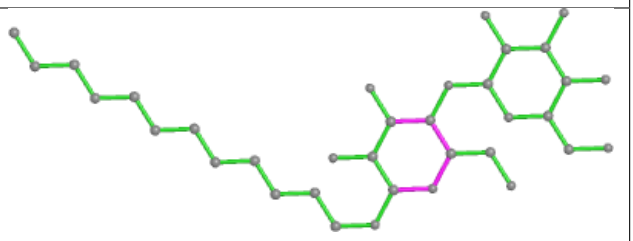


Rings

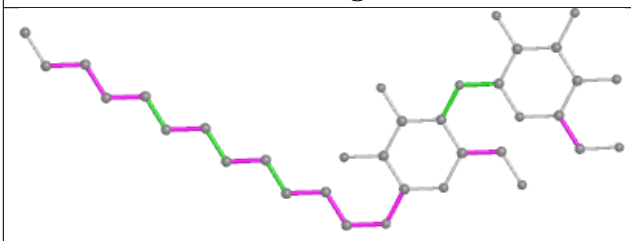
Ligand LMT S 101



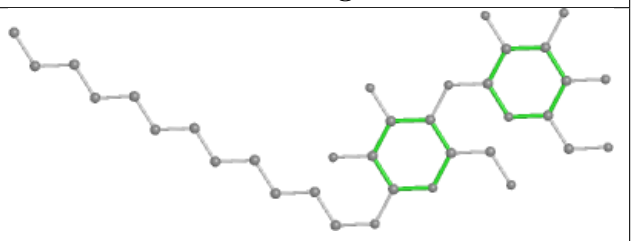
Bond lengths



Bond angles

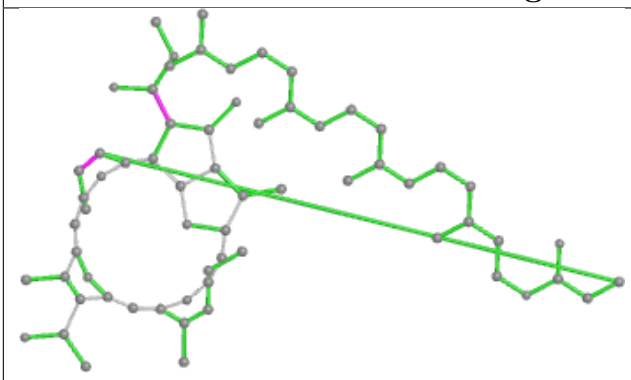


Torsions

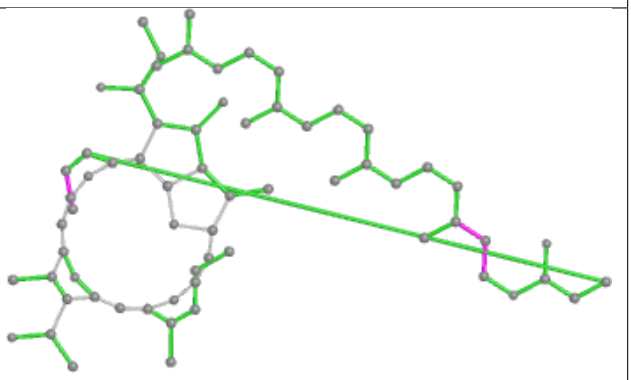


Rings

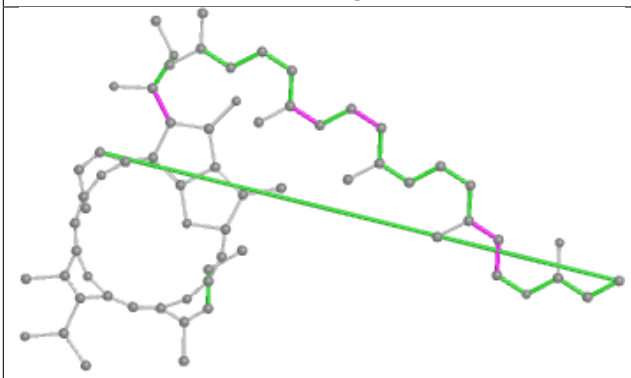
Ligand BPH L 403



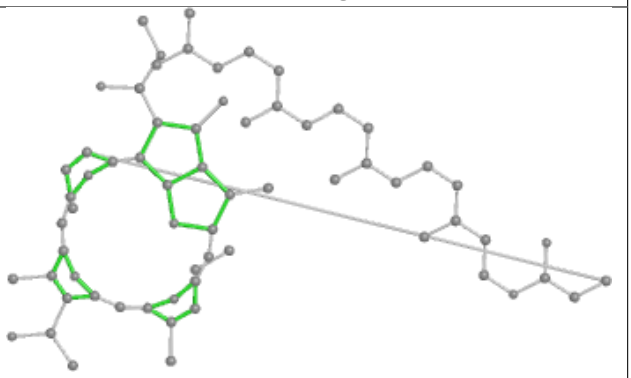
Bond lengths



Bond angles

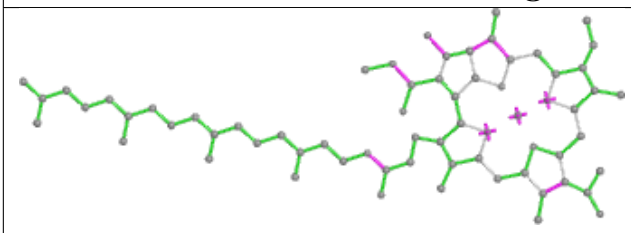


Torsions

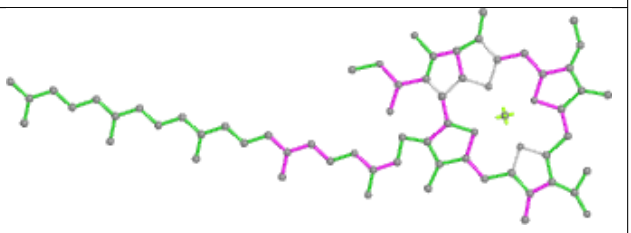


Rings

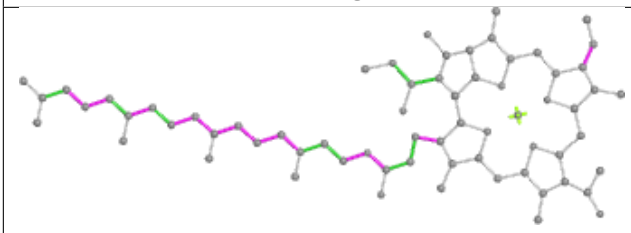
Ligand BCL Y 102



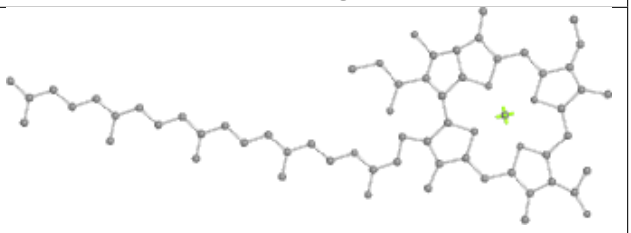
Bond lengths



Bond angles

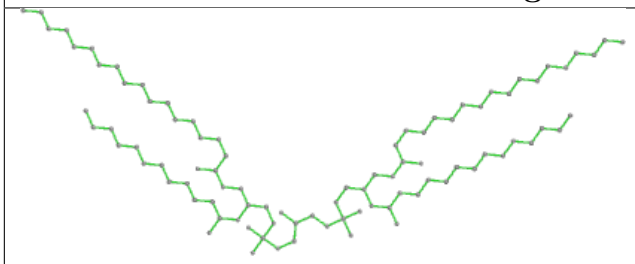


Torsions

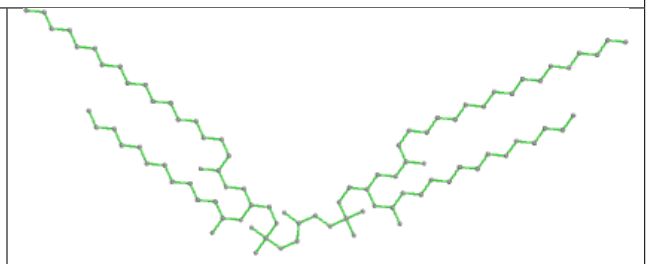


Rings

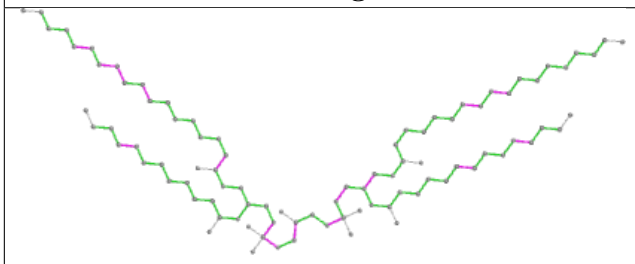
Ligand CDL G 104



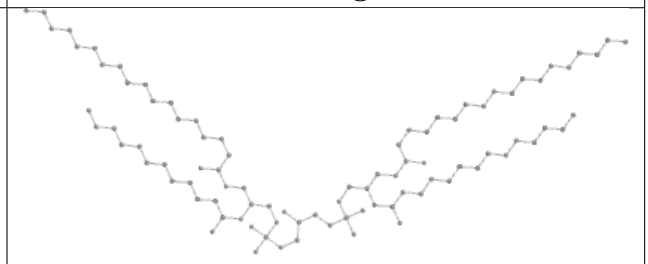
Bond lengths



Bond angles

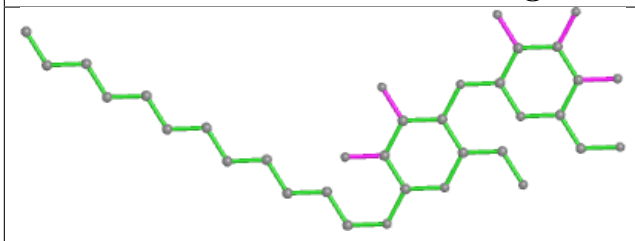


Torsions

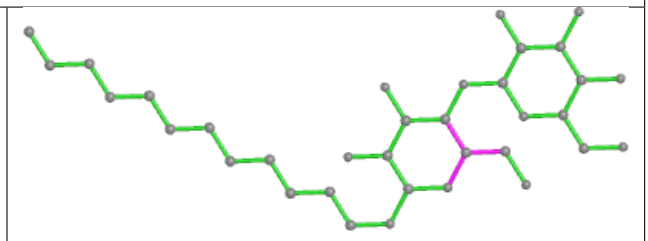


Rings

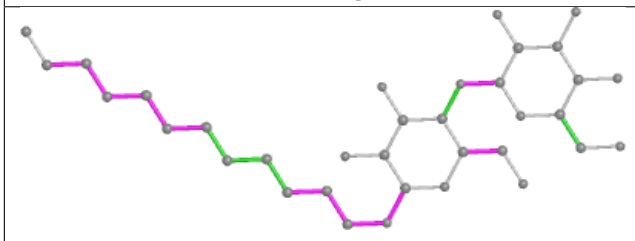
Ligand LMT F 102



Bond lengths



Bond angles



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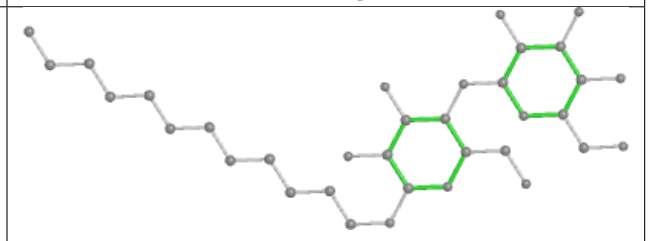
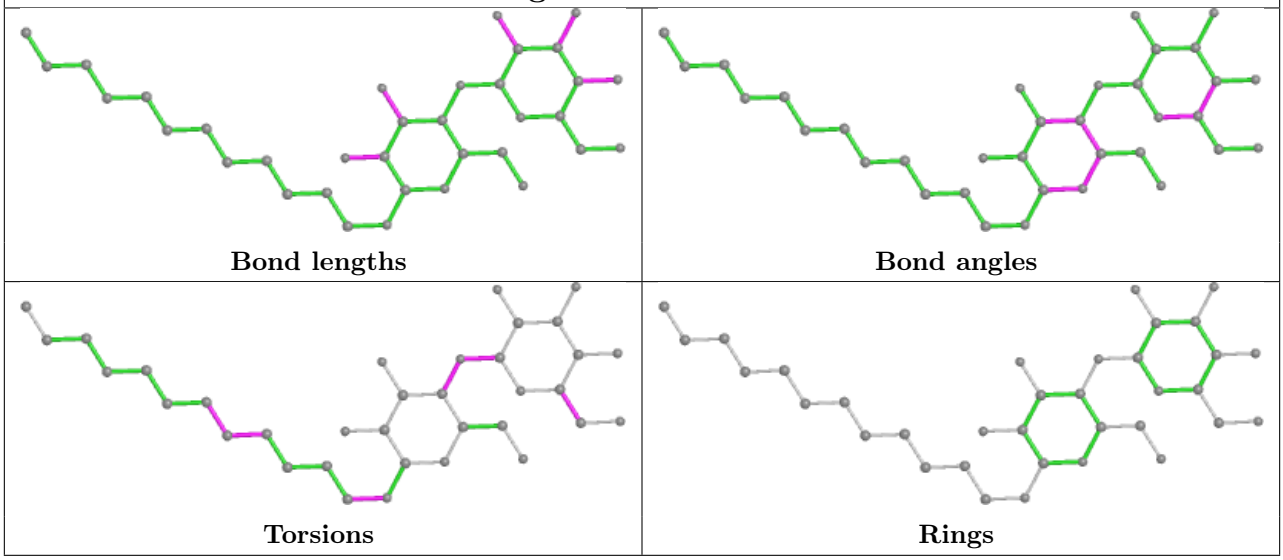
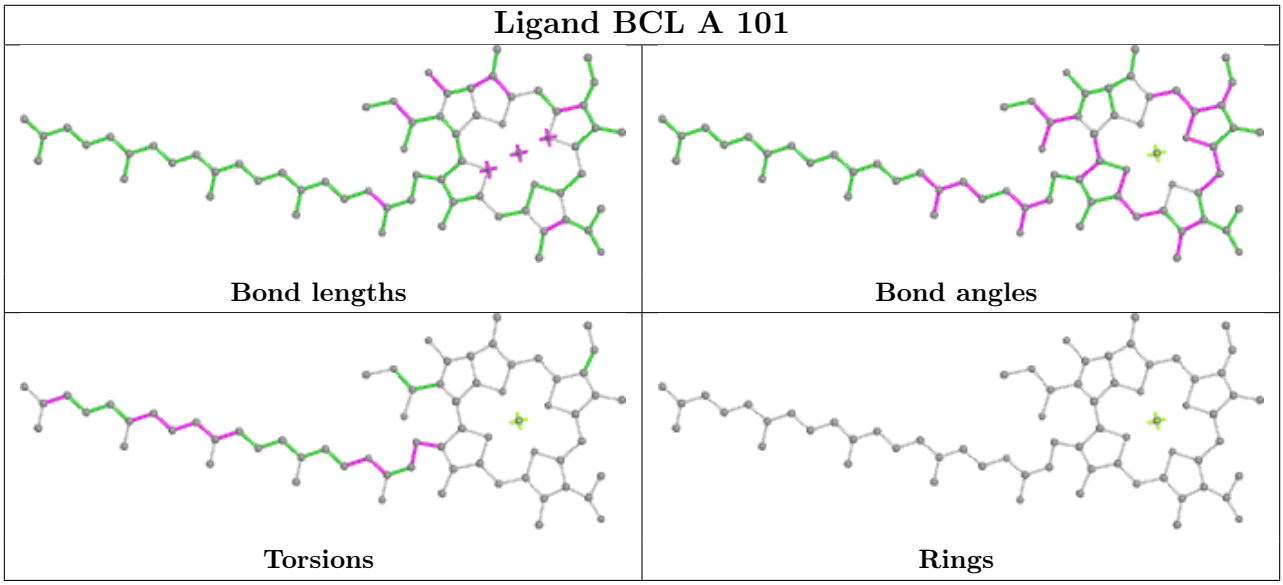


Rings

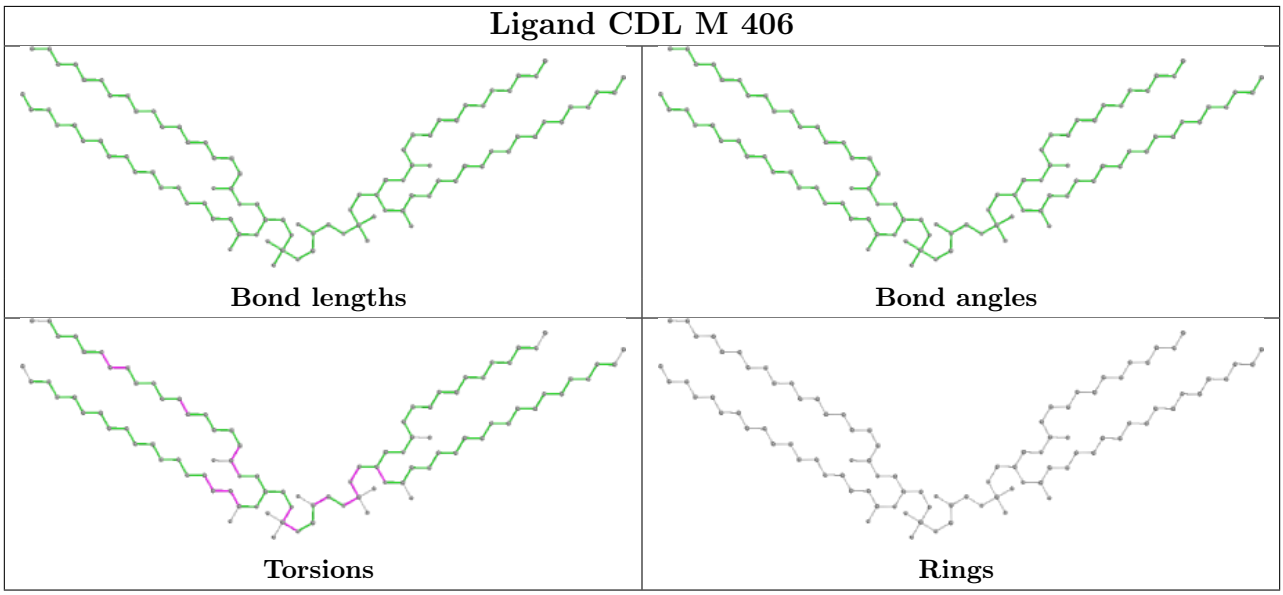
Ligand LMT I 101



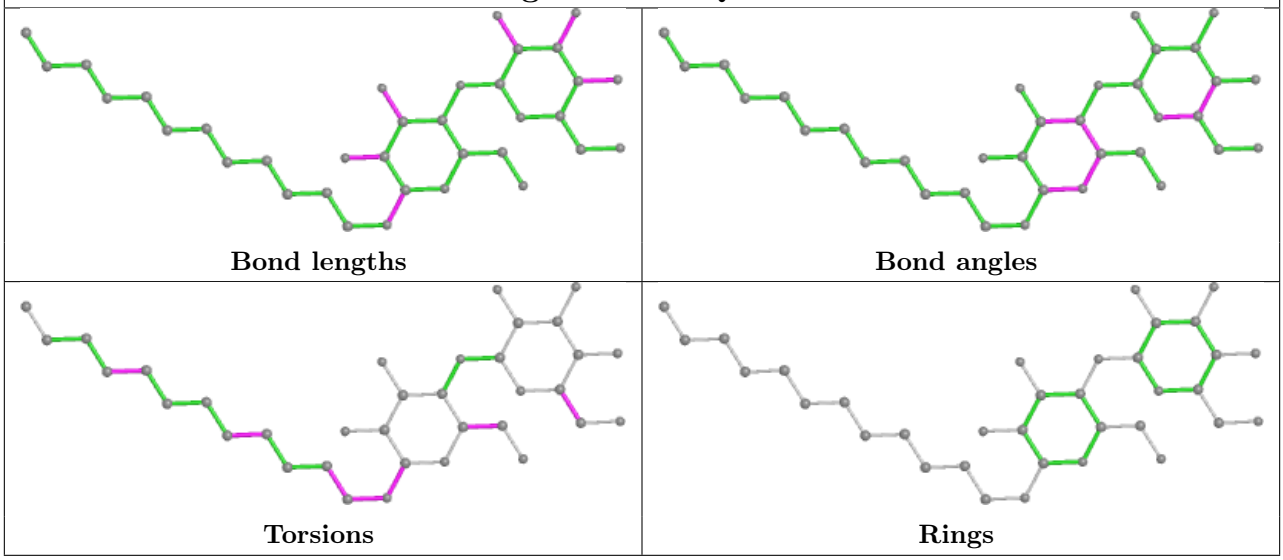
Ligand BCL A 101



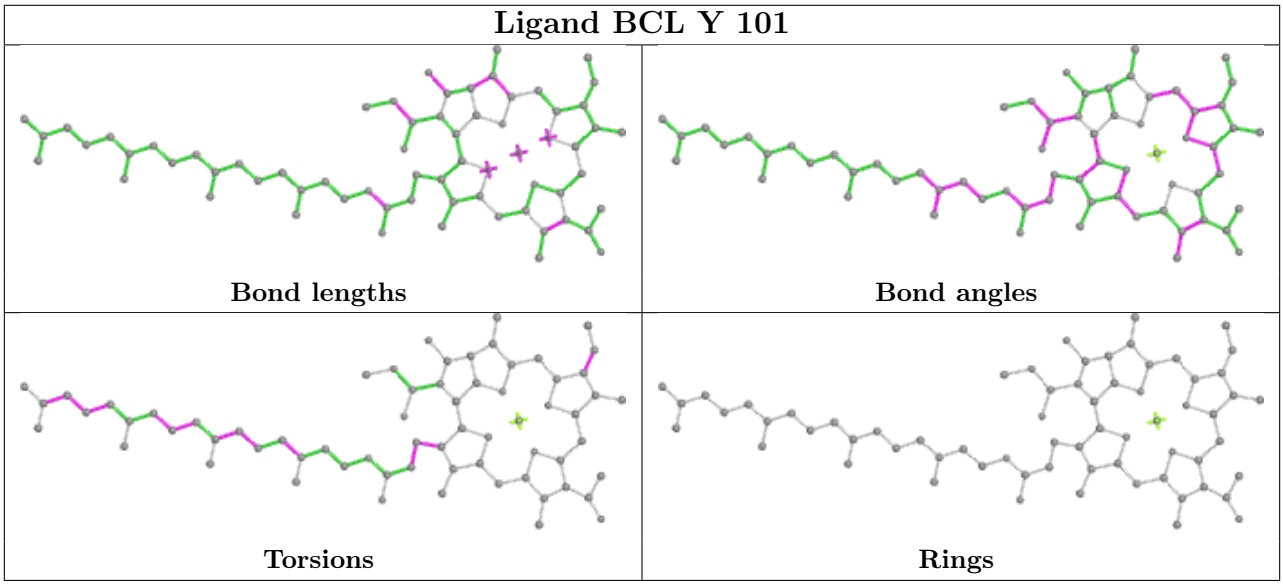
Ligand CDL M 406



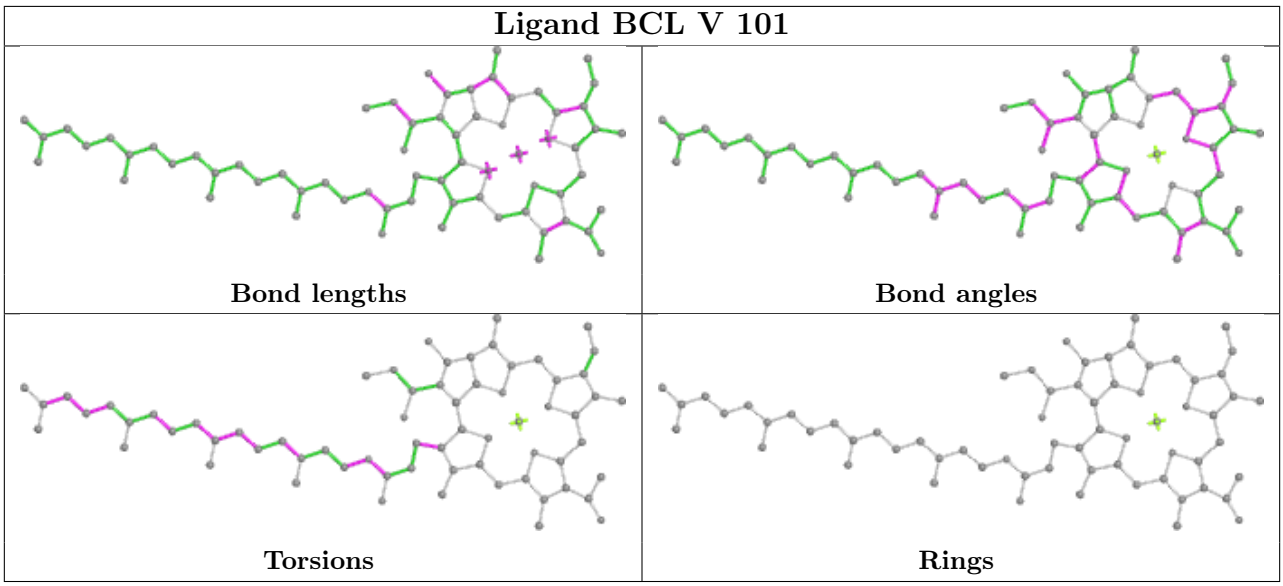
Ligand LMT Q 102

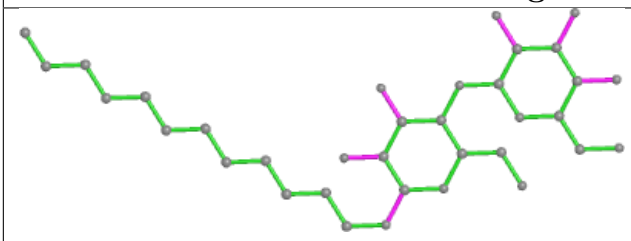
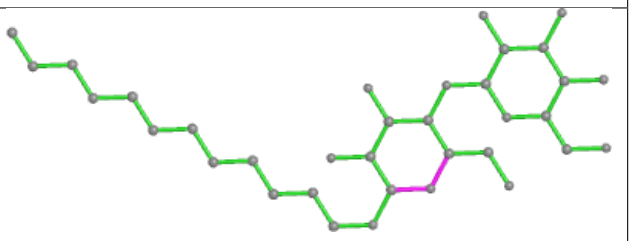
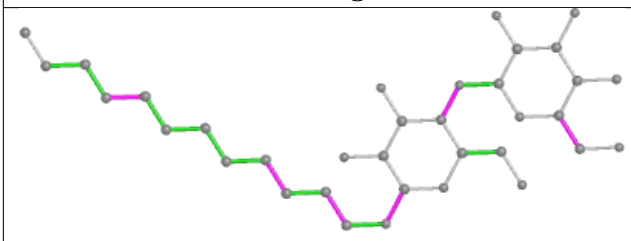
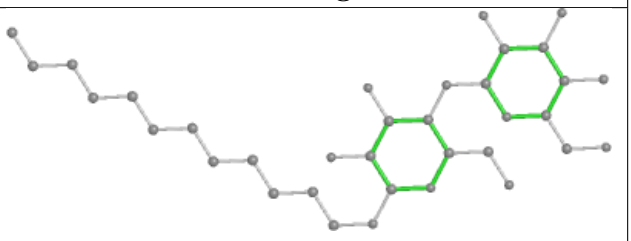


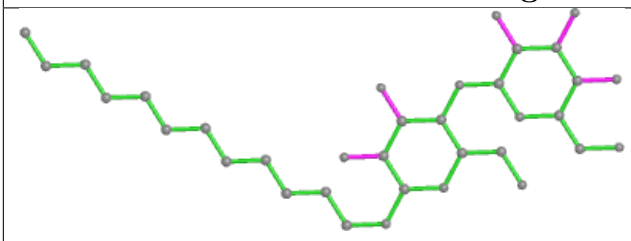
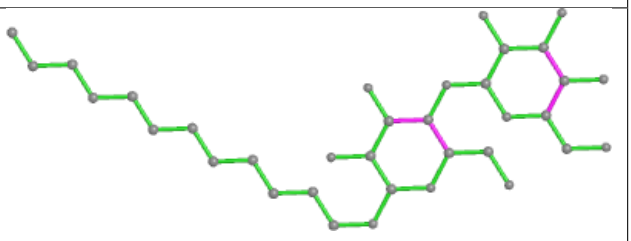
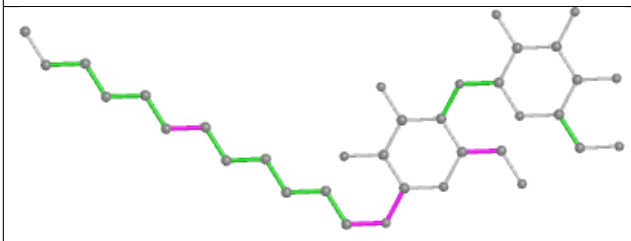
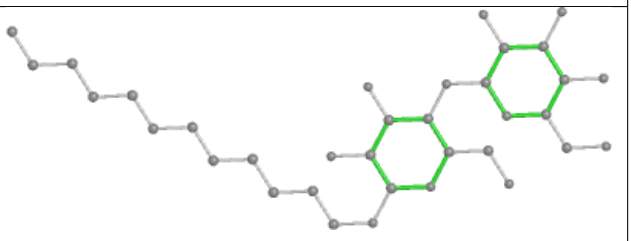
Ligand BCL Y 101



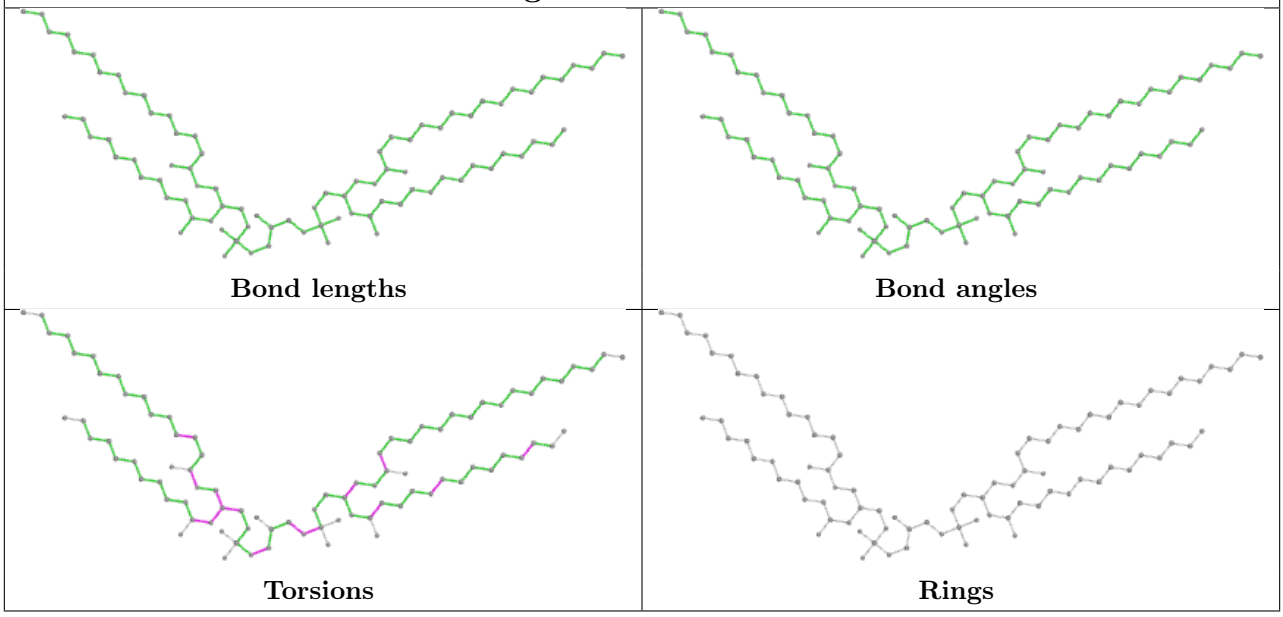
Ligand BCL V 101



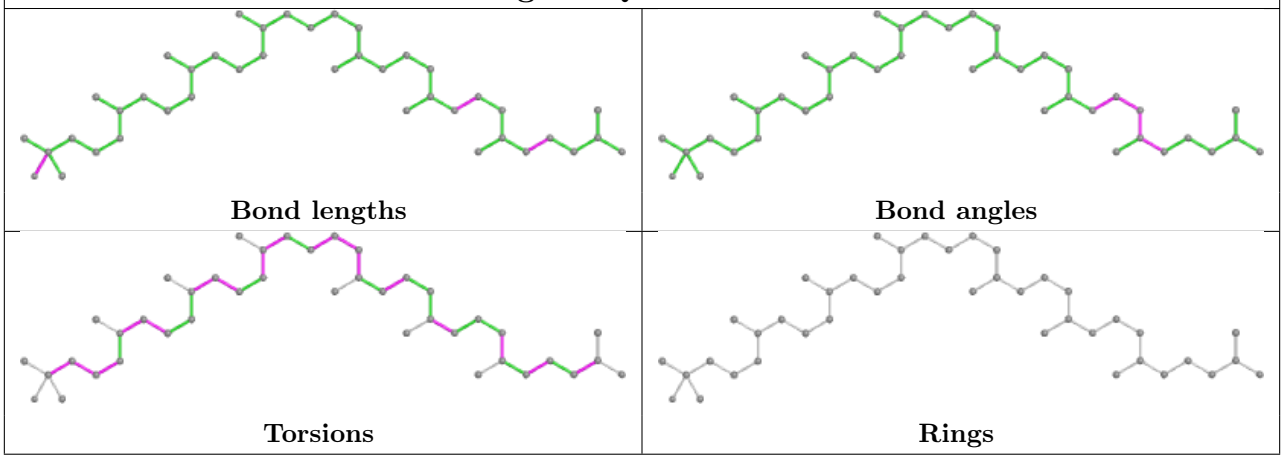
Ligand LMT I 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LMT O 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

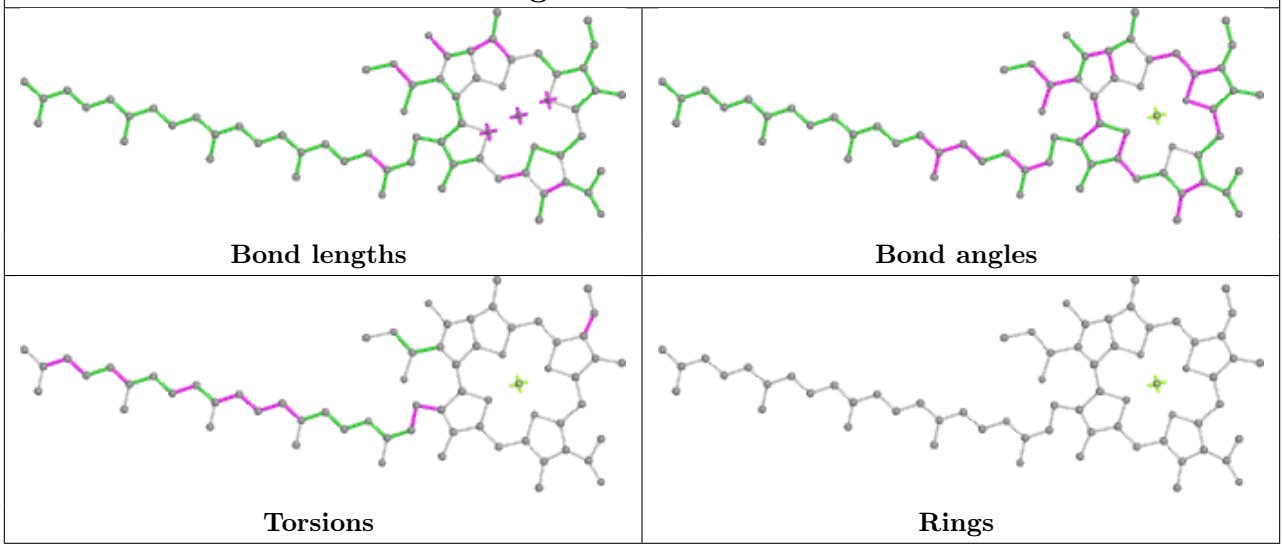
Ligand CDL H 302



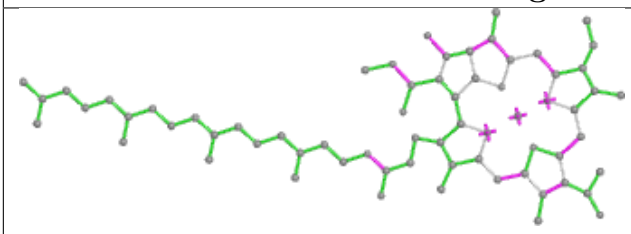
Ligand QAK M 401



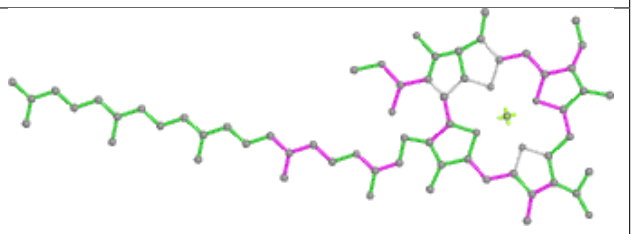
Ligand BCL J 102



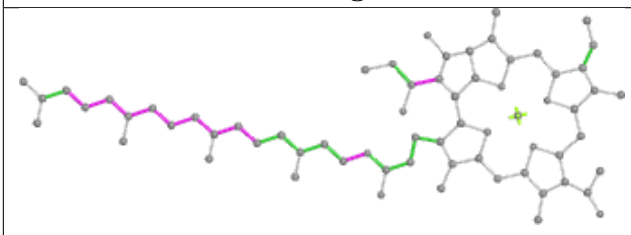
Ligand BCL 3 101



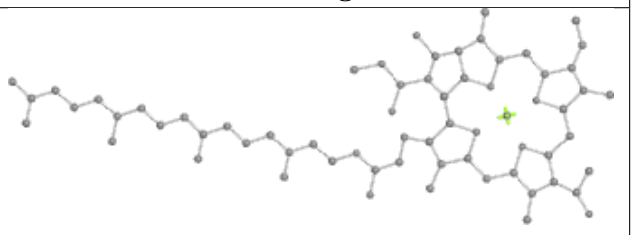
Bond lengths



Bond angles

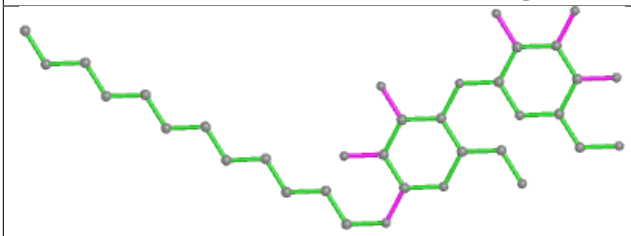


Torsions

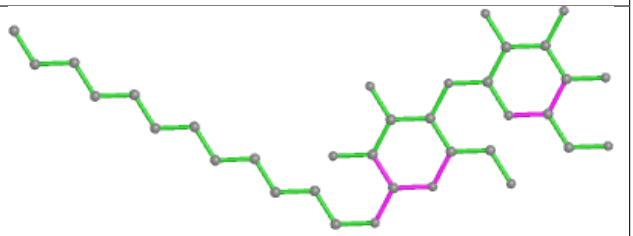


Rings

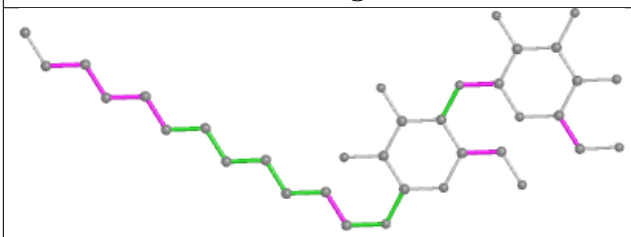
Ligand LMT M 409



Bond lengths



Bond angles



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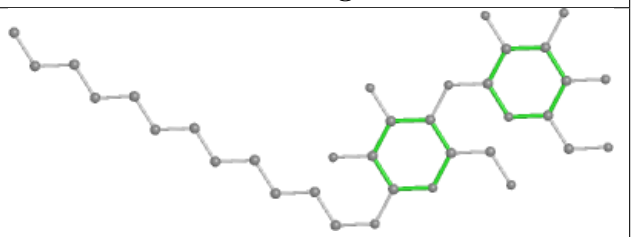
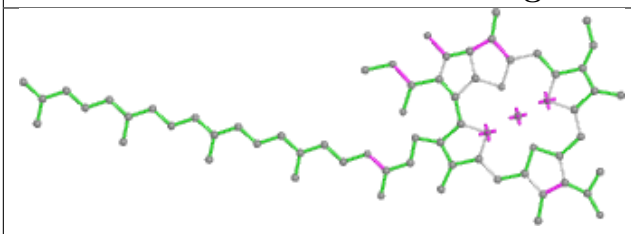
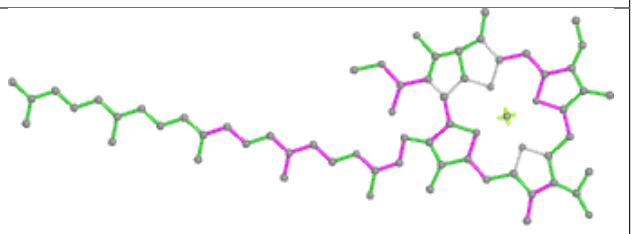


Rings

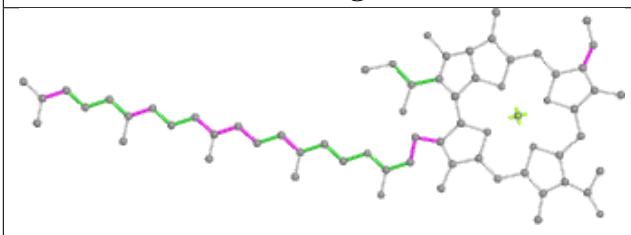
Ligand BCL G 102



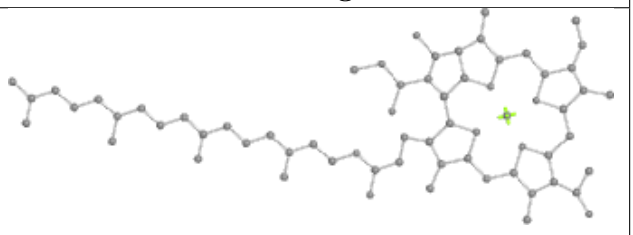
Bond lengths



Bond angles

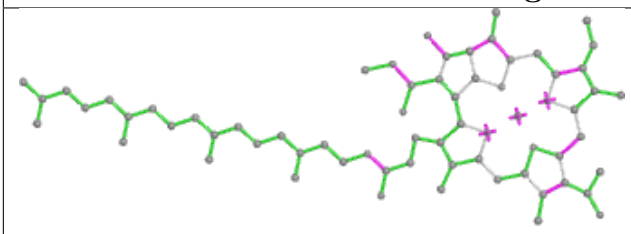


Torsions

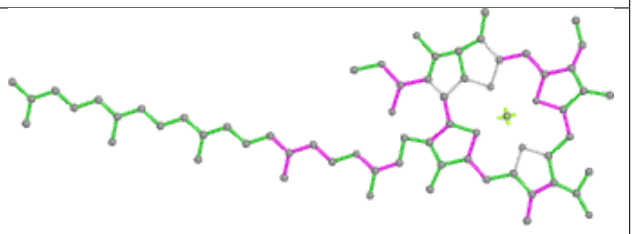


Rings

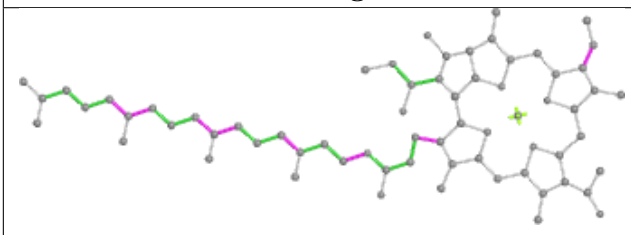
Ligand BCL D 104



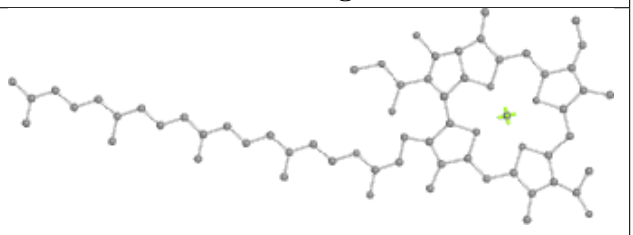
Bond lengths



Bond angles

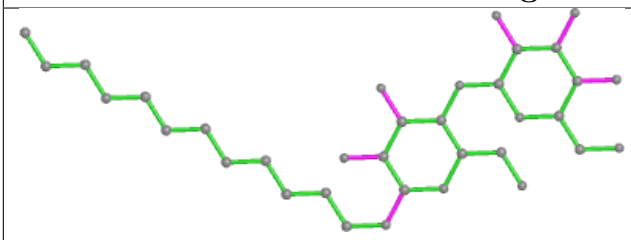


Torsions

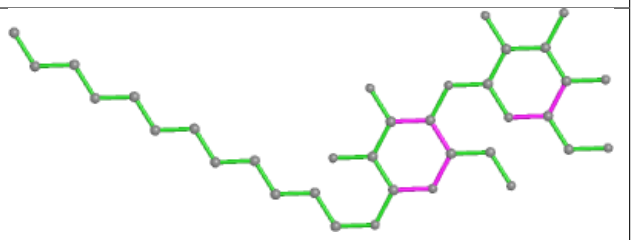


Rings

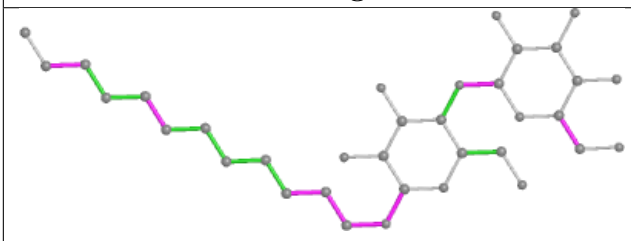
Ligand LMT K 102



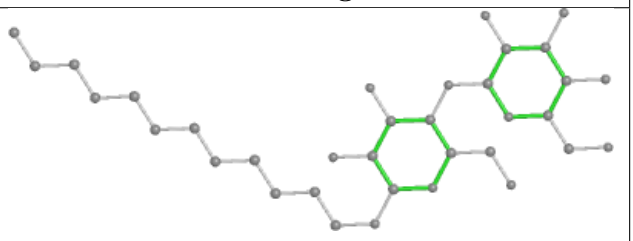
Bond lengths



Bond angles

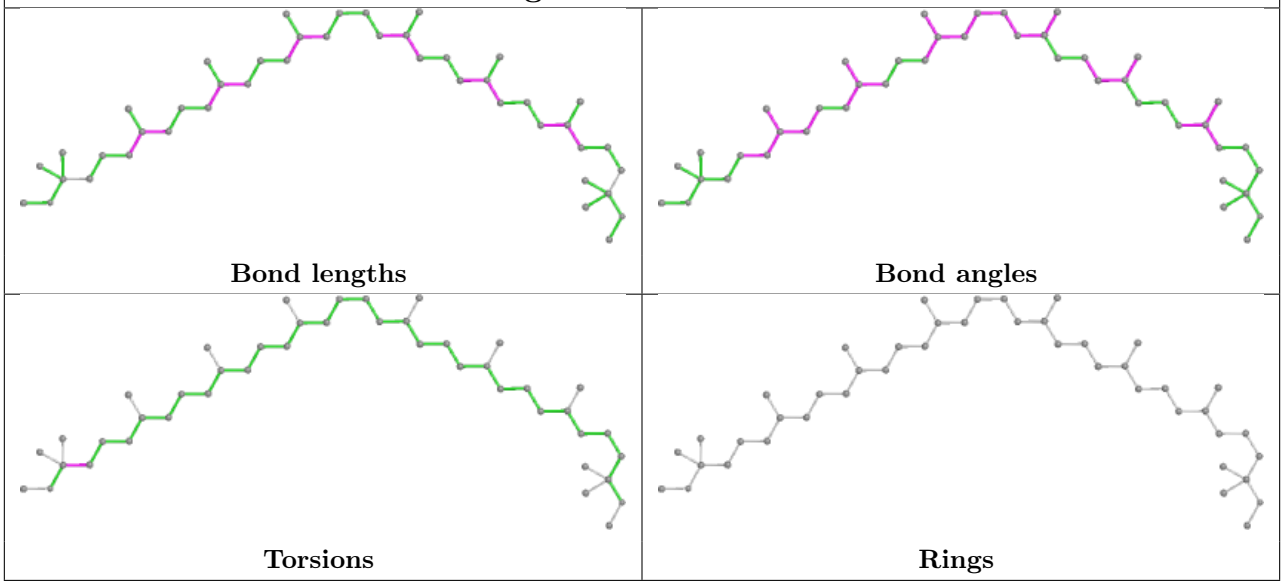


Torsions

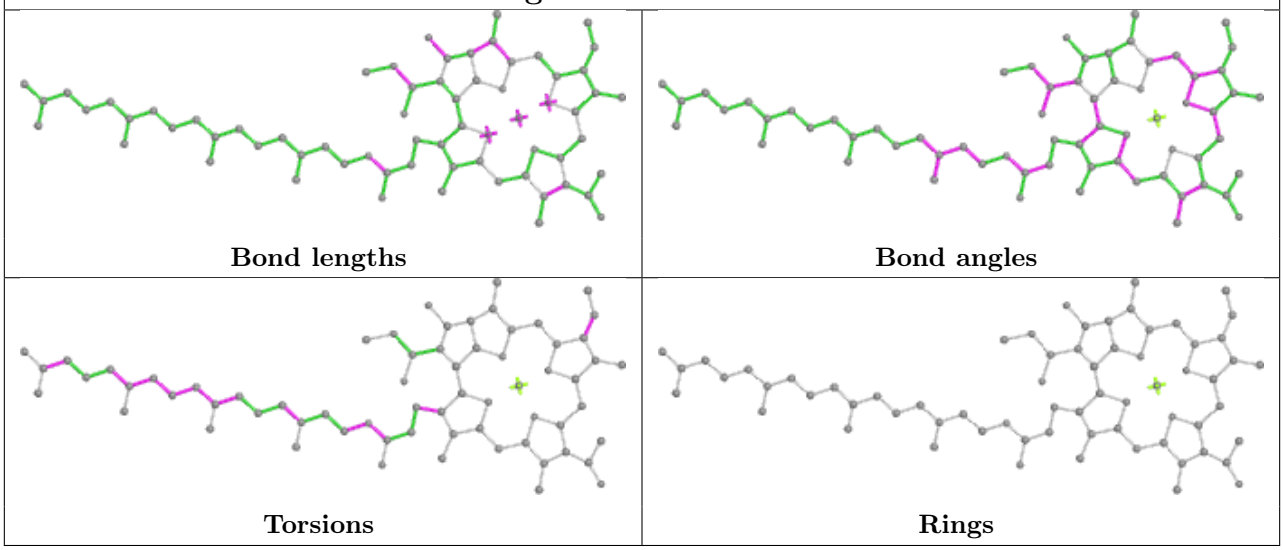


Rings

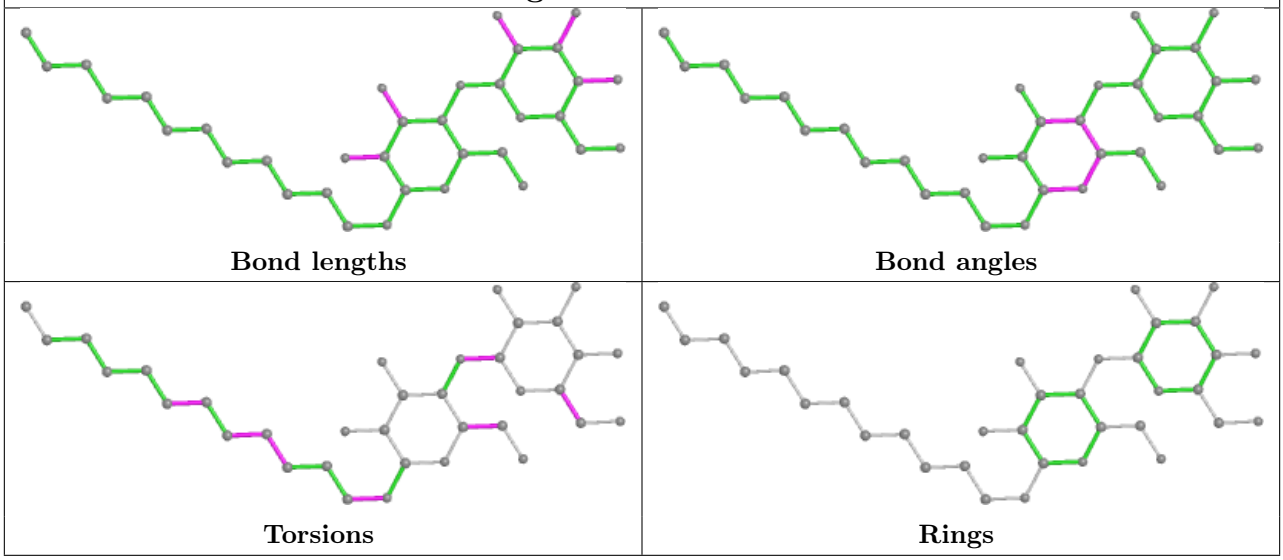
Ligand CRT X 102



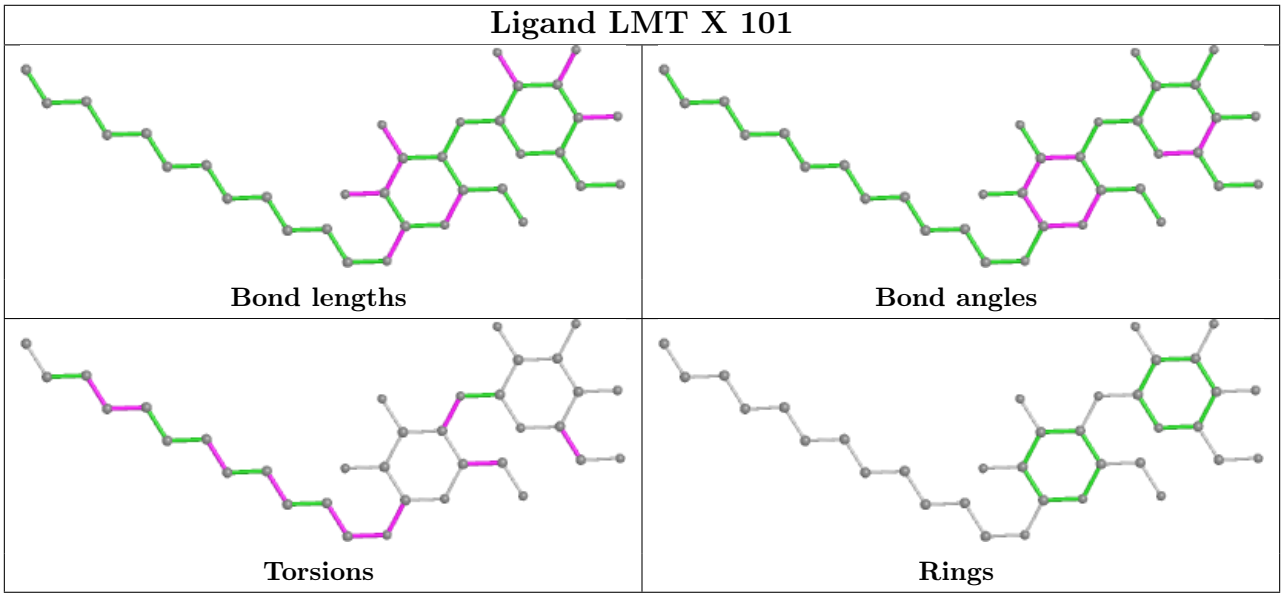
Ligand BCL G 103



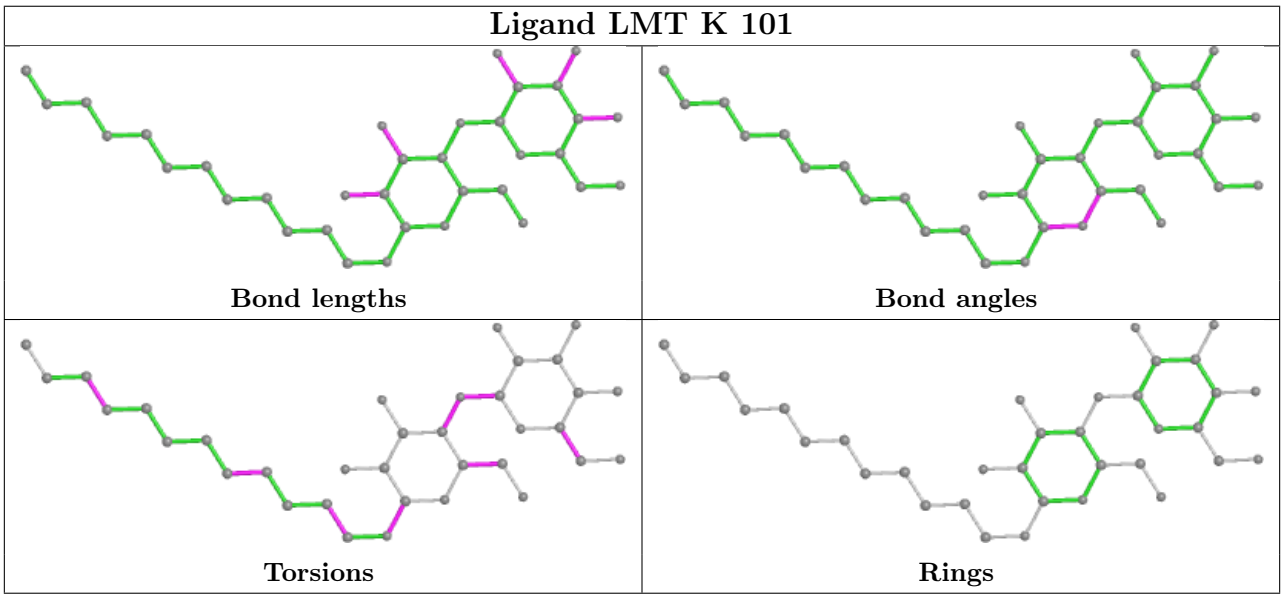
Ligand LMT 2 104

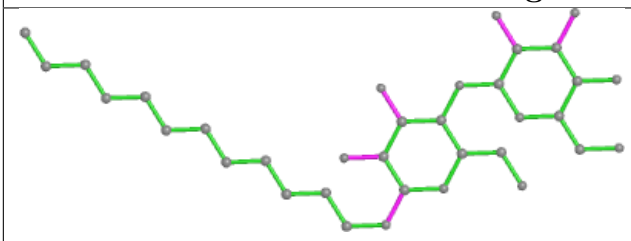
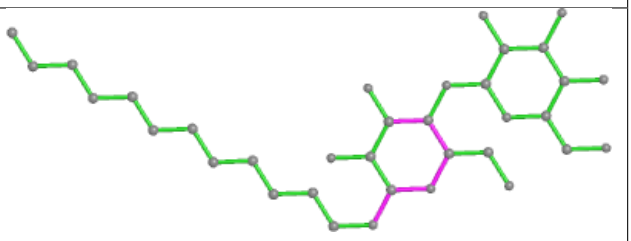
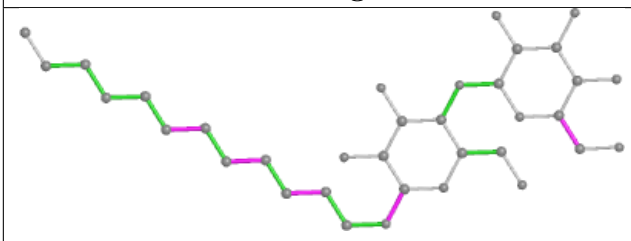
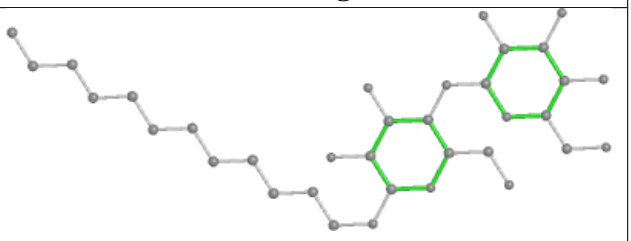


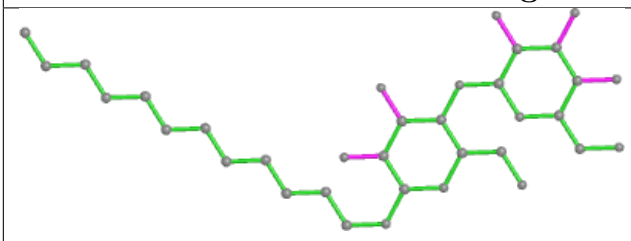
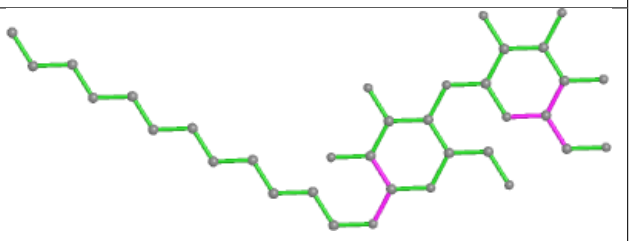
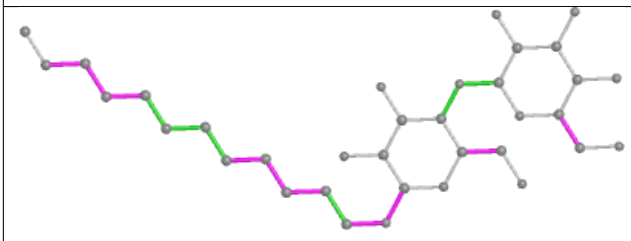
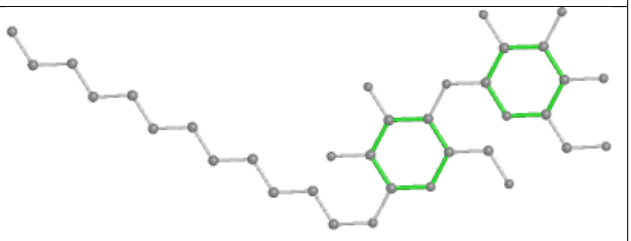
Ligand LMT X 101



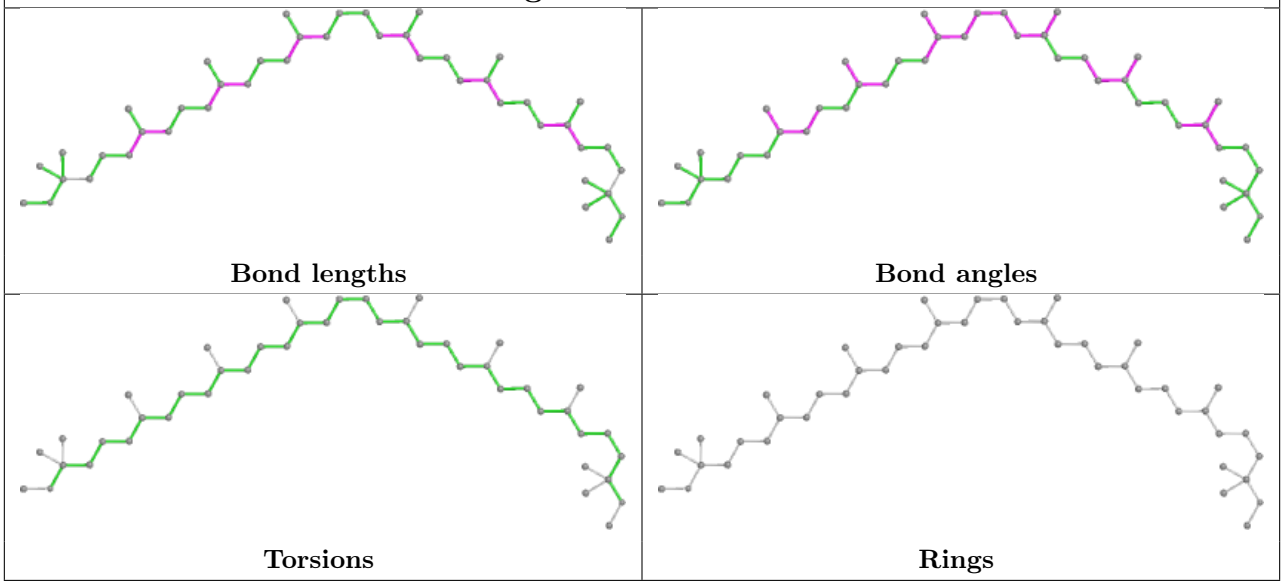
Ligand LMT K 101



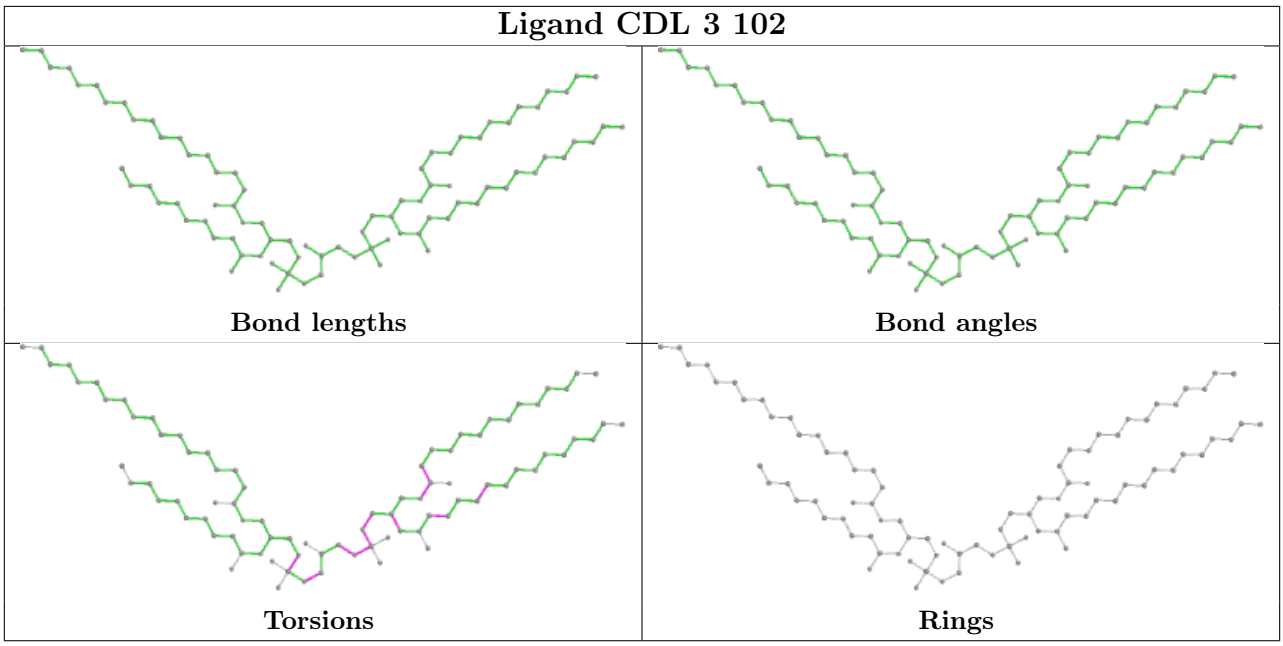
Ligand LMT 4 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LMT U 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

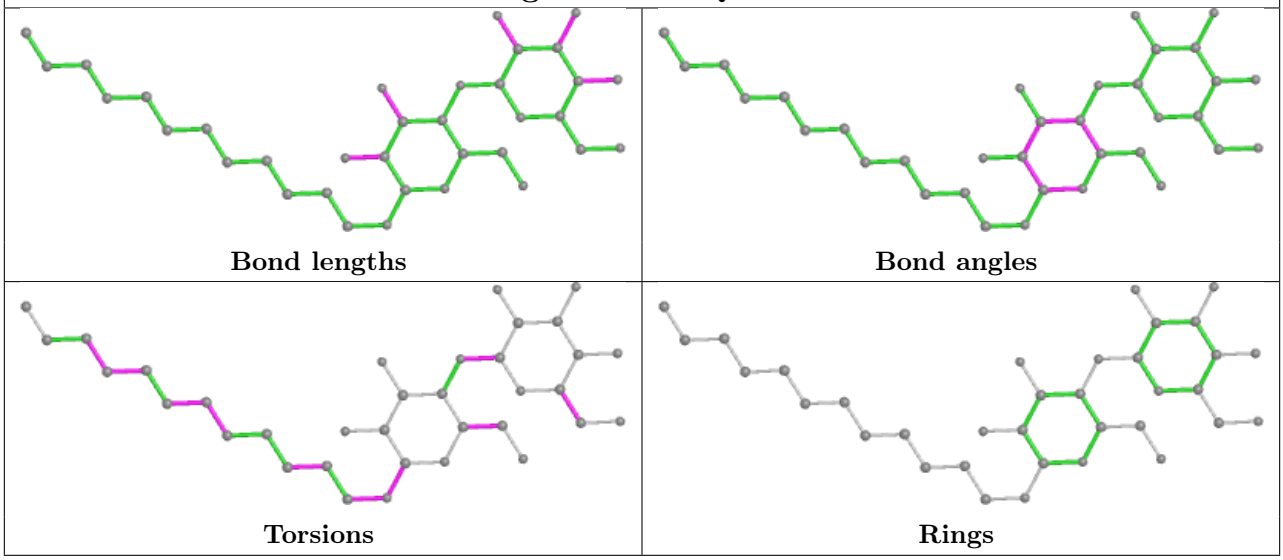
Ligand CRT R 101



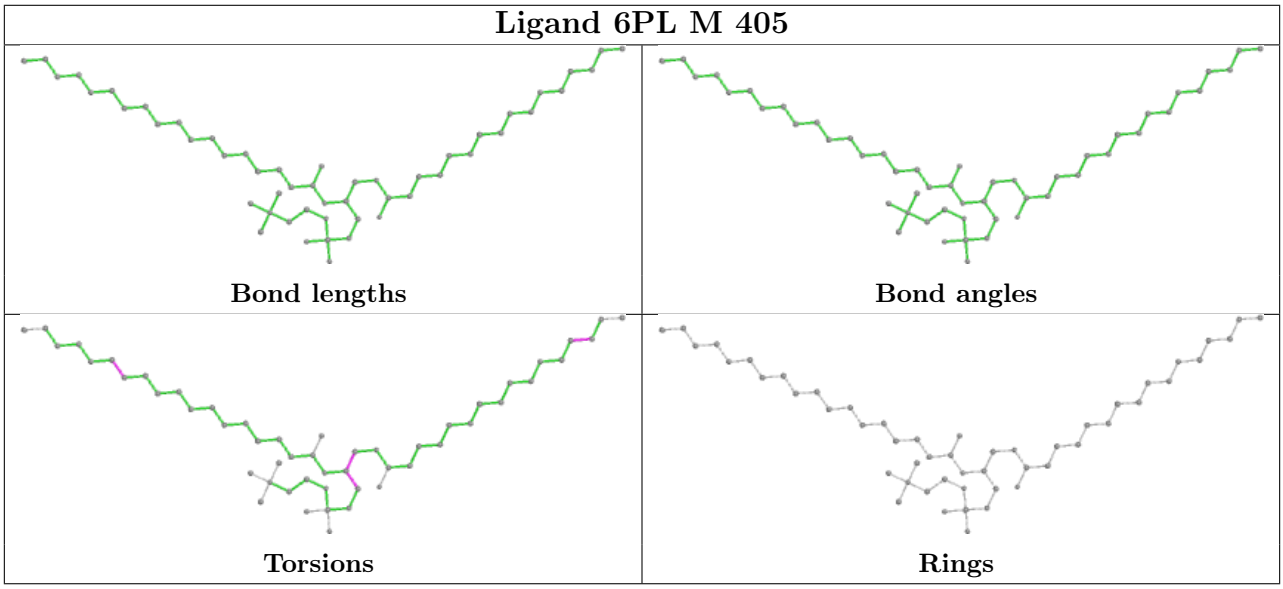
Ligand CDL 3 102



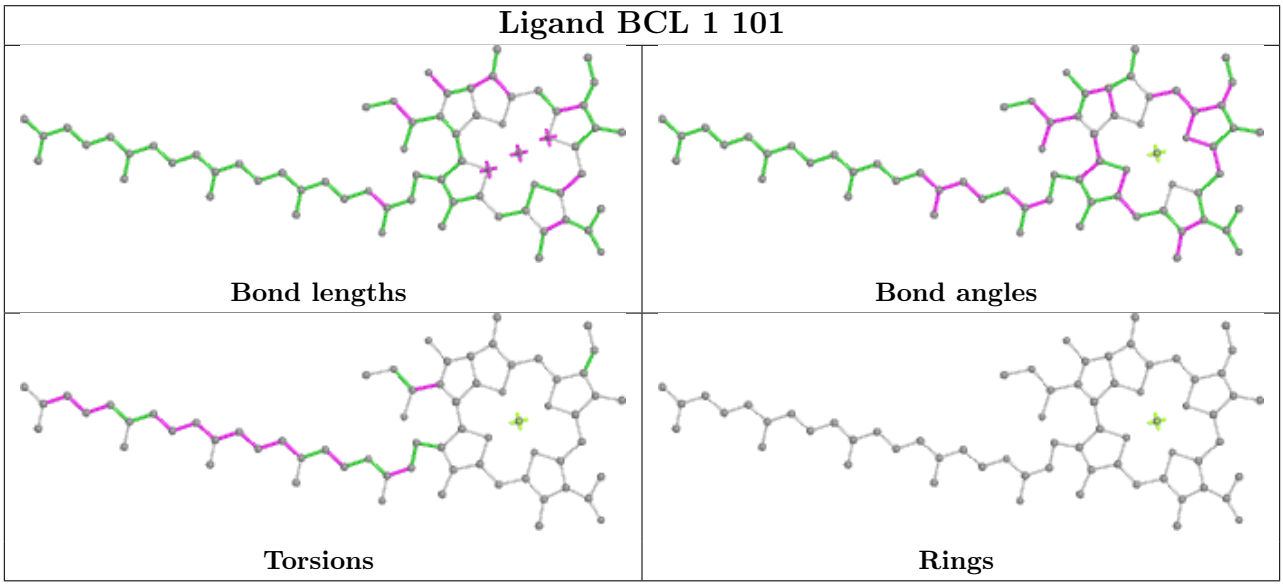
Ligand LMT Q 101



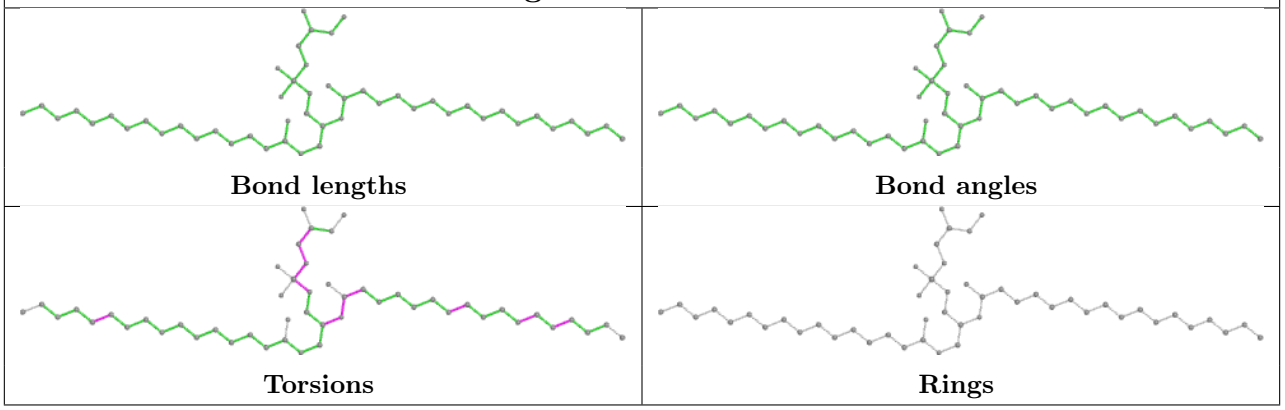
Ligand 6PL M 405



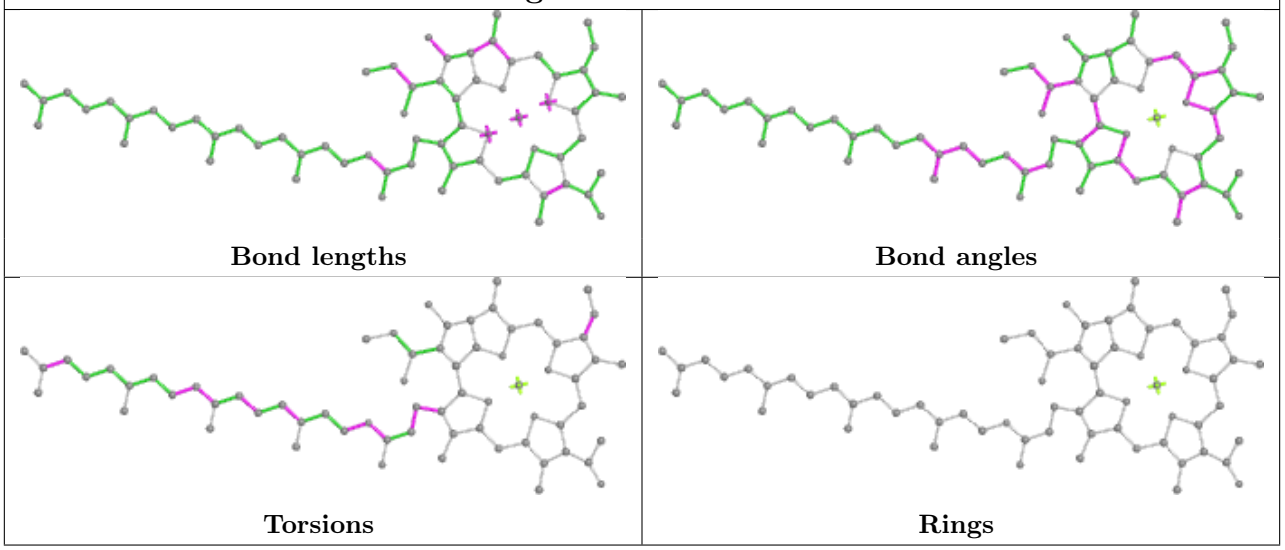
Ligand BCL 1 101



Ligand PGT P 102



Ligand BCL R 103



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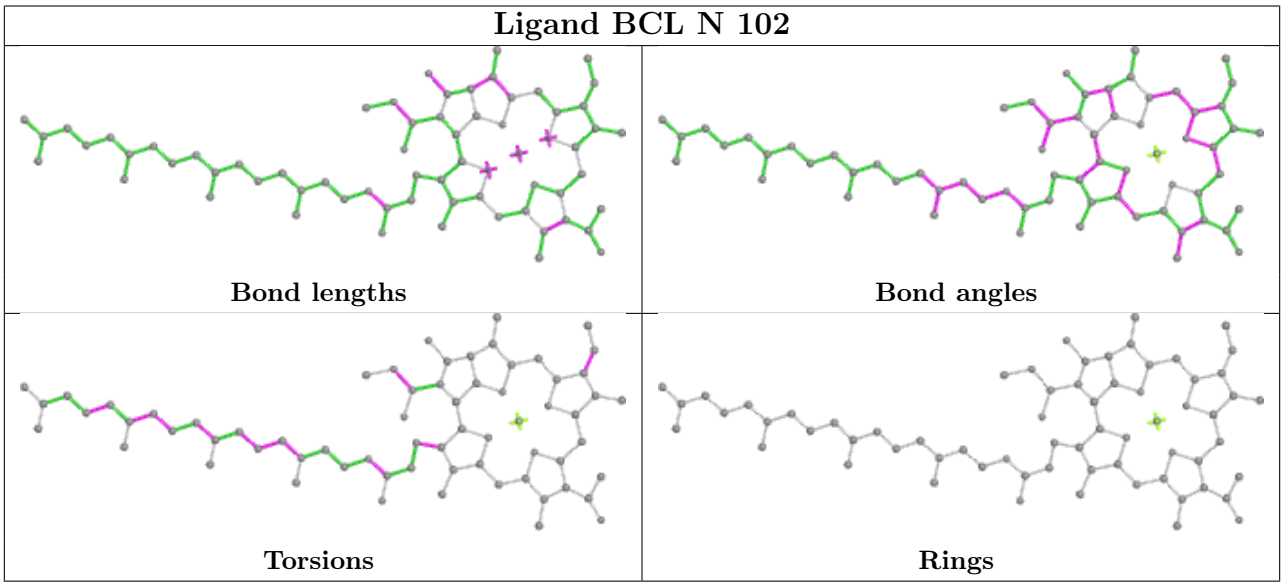
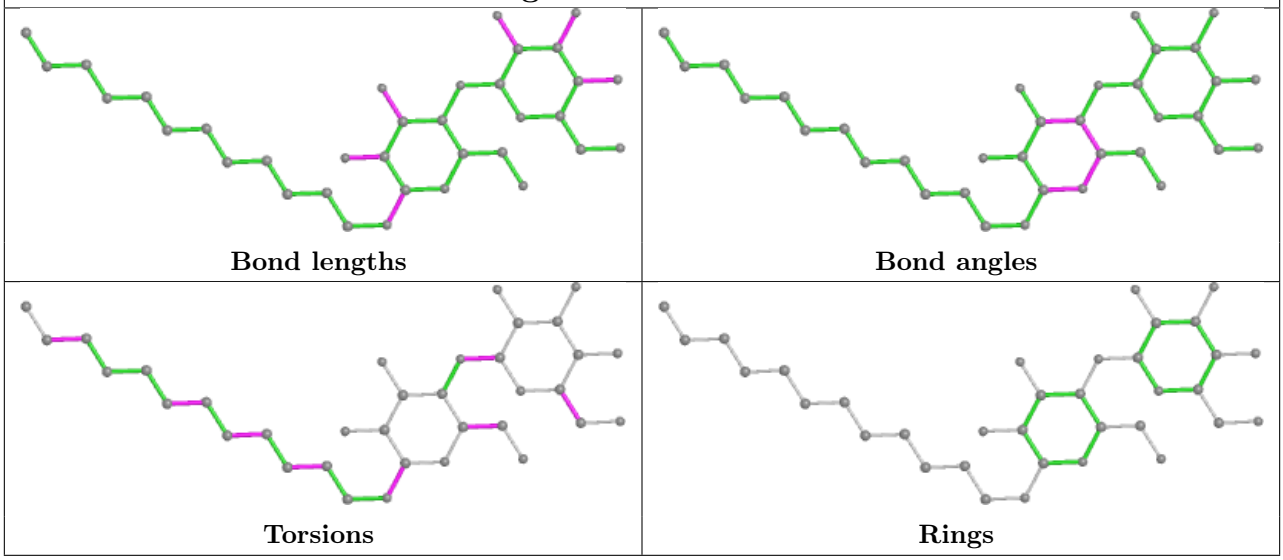
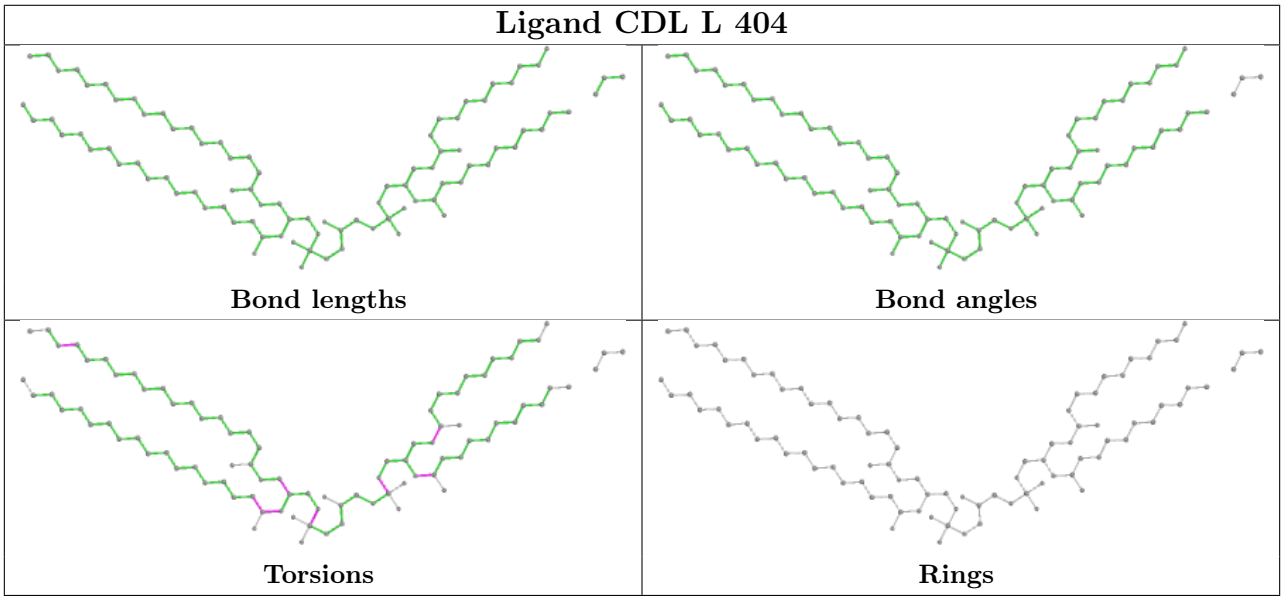


Ligand LMT X 103



Ligand CDL L 404



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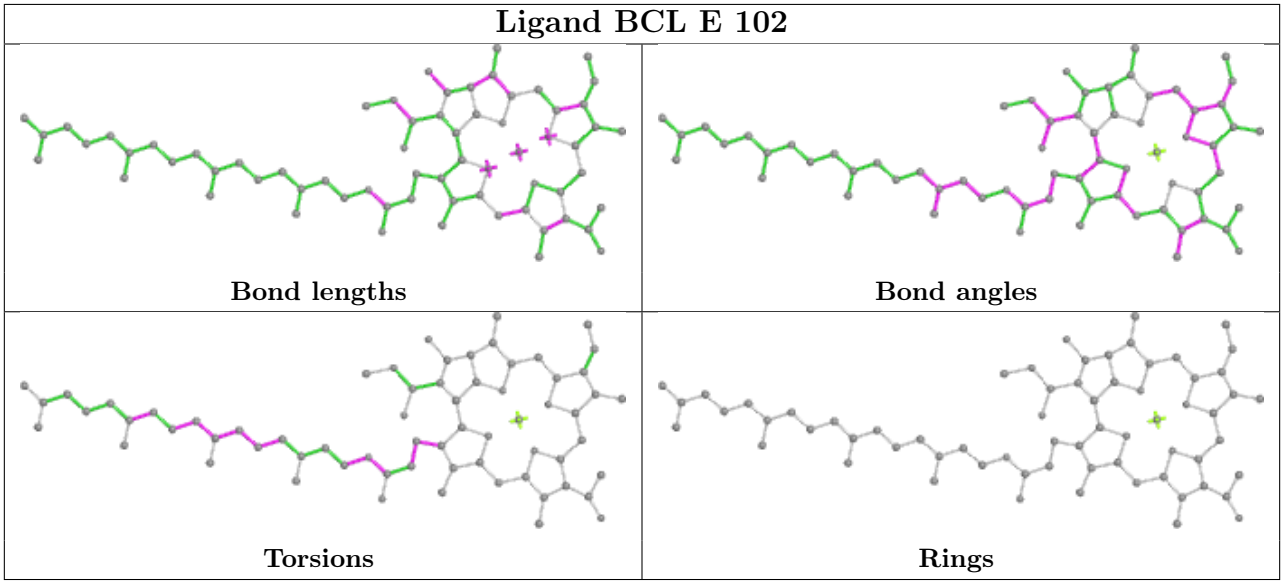
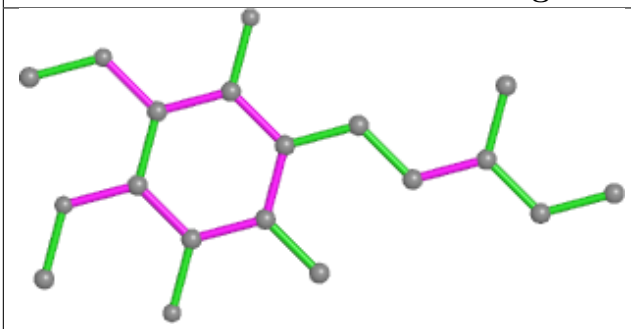
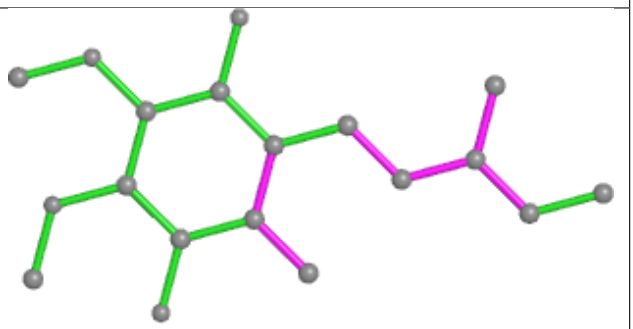


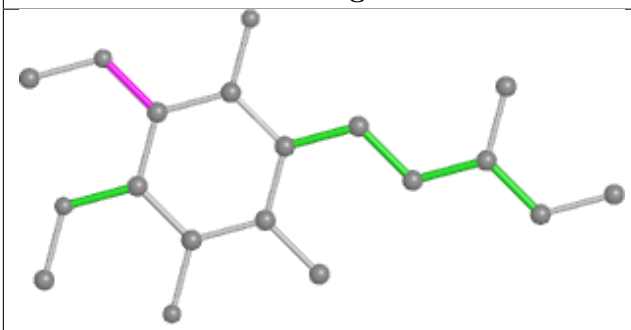
Ligand U10 L 406



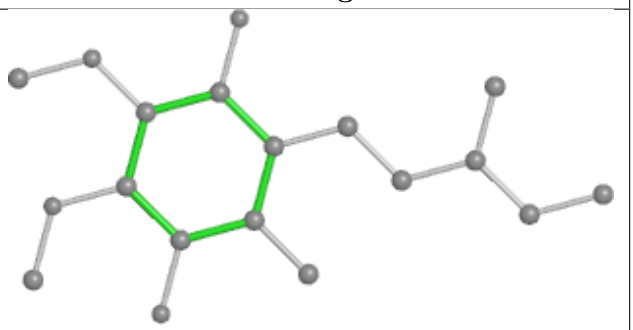
Bond lengths



Bond angles

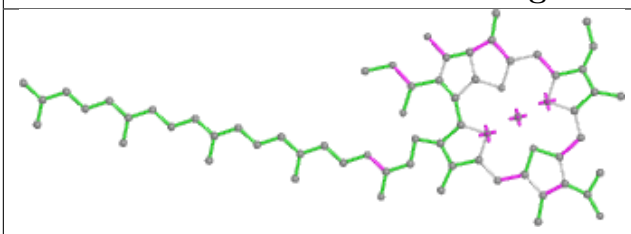


Torsions

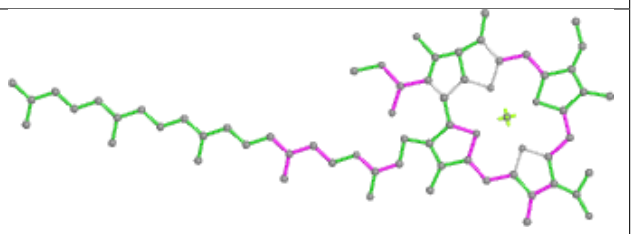


Rings

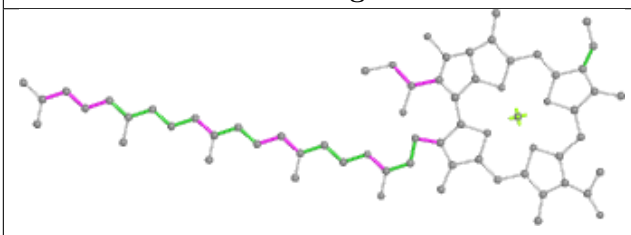
Ligand BCL 5 102



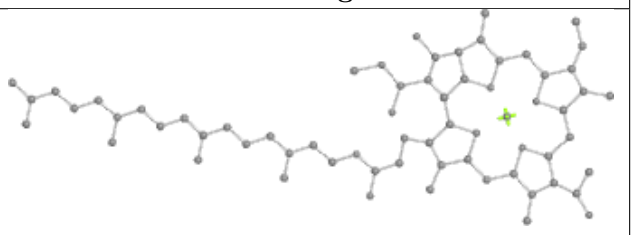
Bond lengths



Bond angles

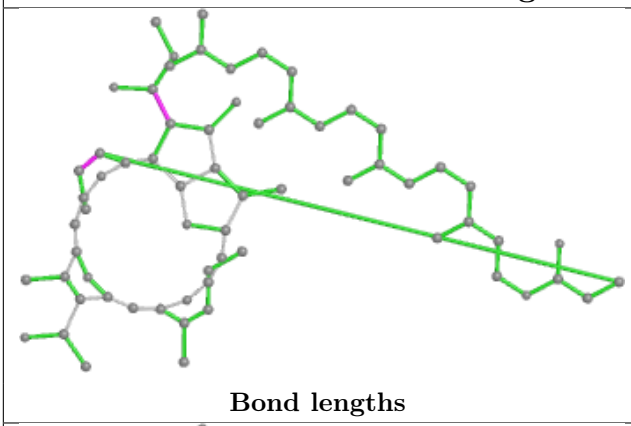


Torsions

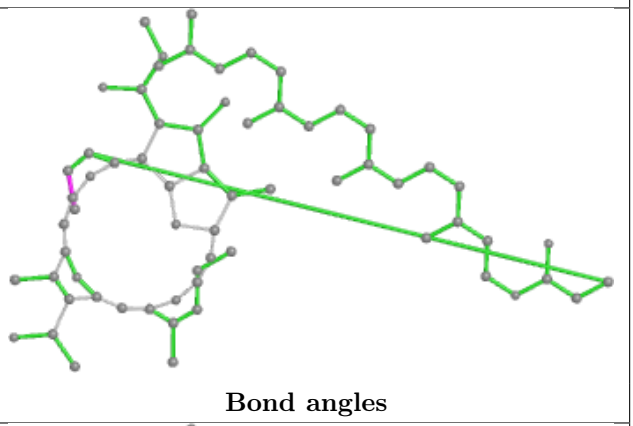


Rings

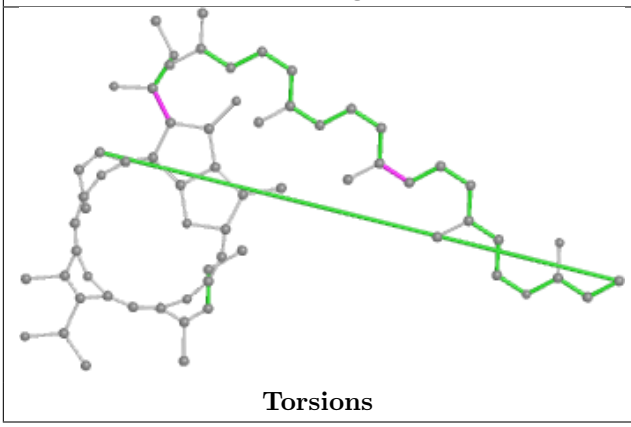
Ligand BPH M 403



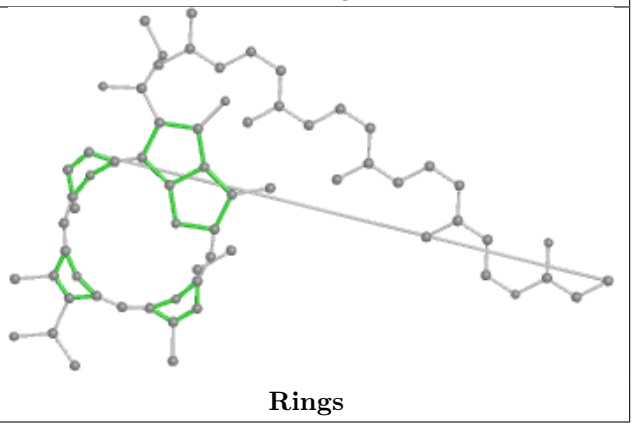
Bond lengths



Bond angles

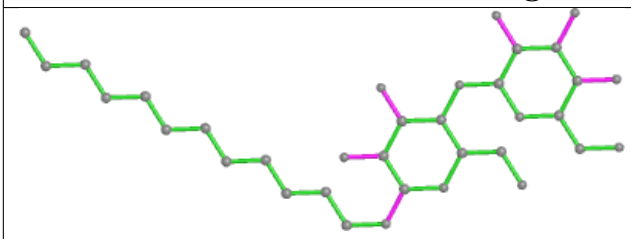


Torsions

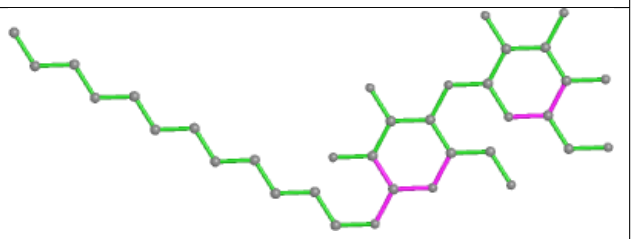


Rings

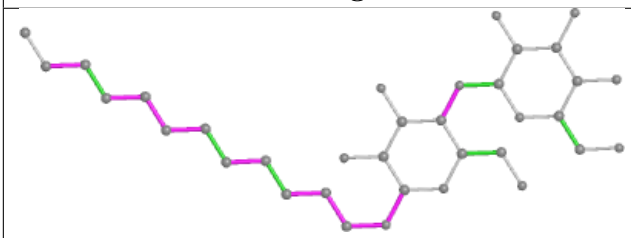
Ligand LMT Z 102



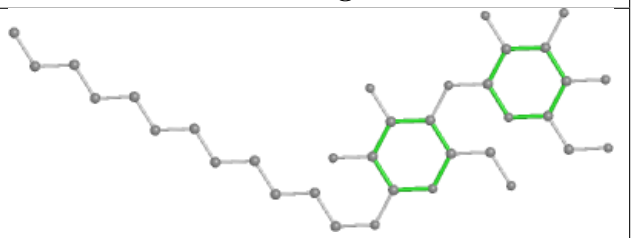
Bond lengths



Bond angles

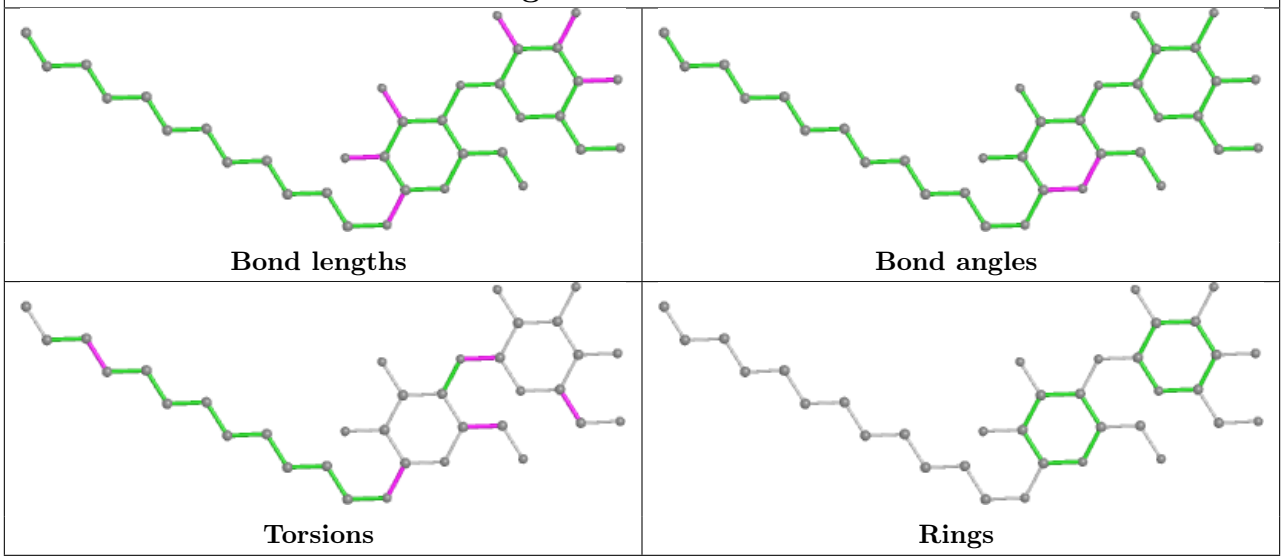


Torsions

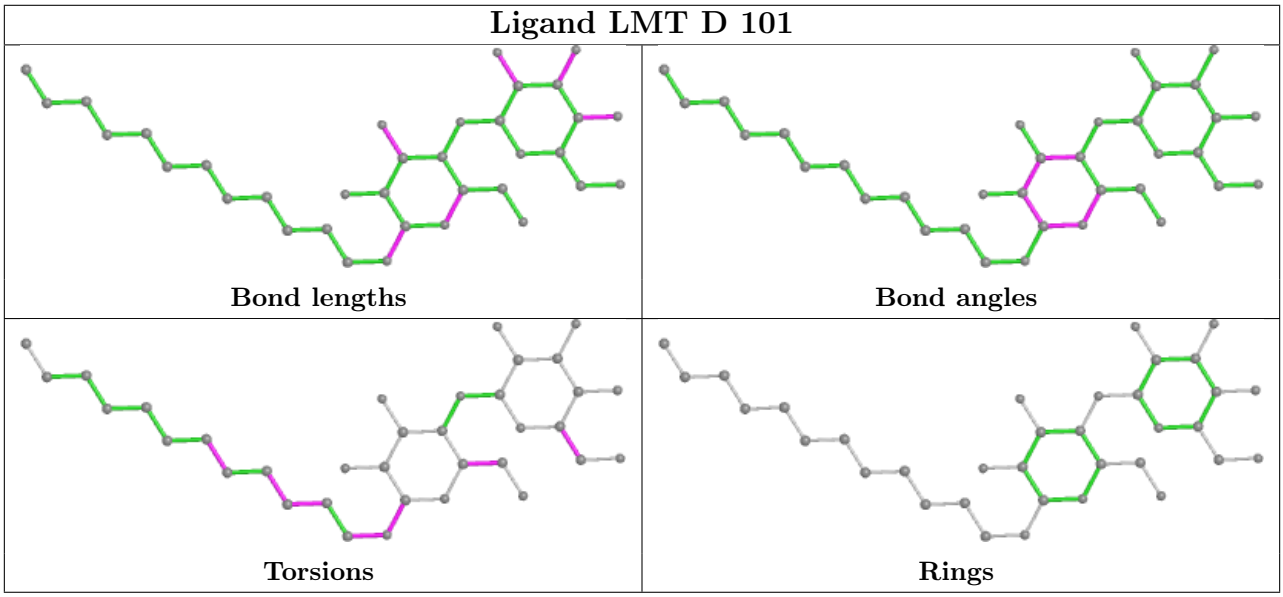


Rings

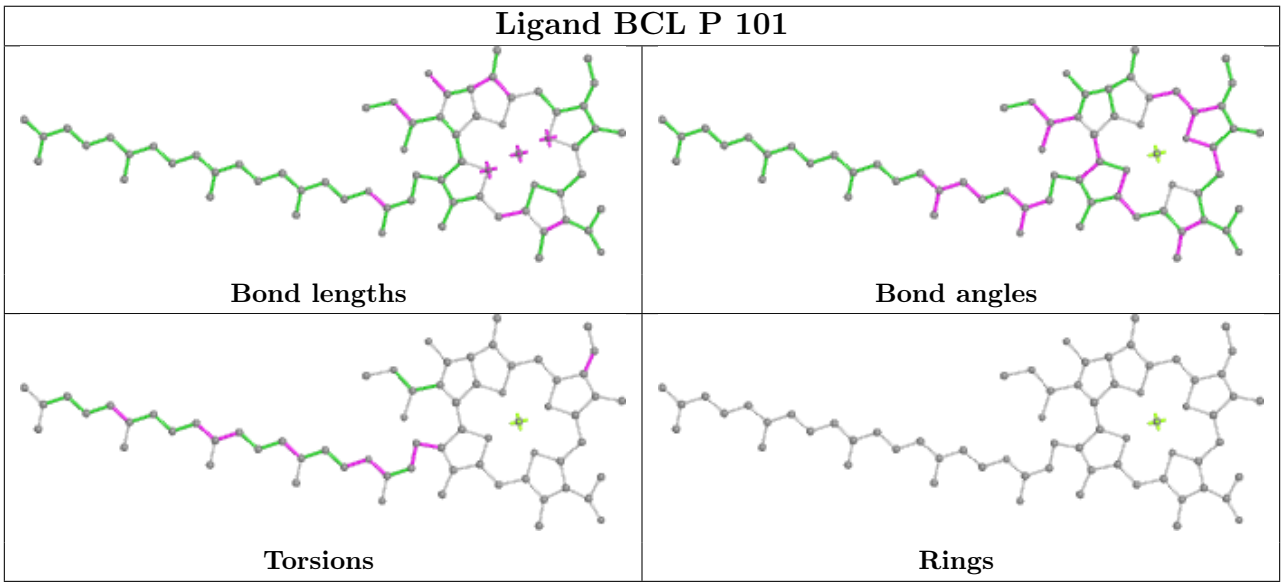
Ligand LMT R 102



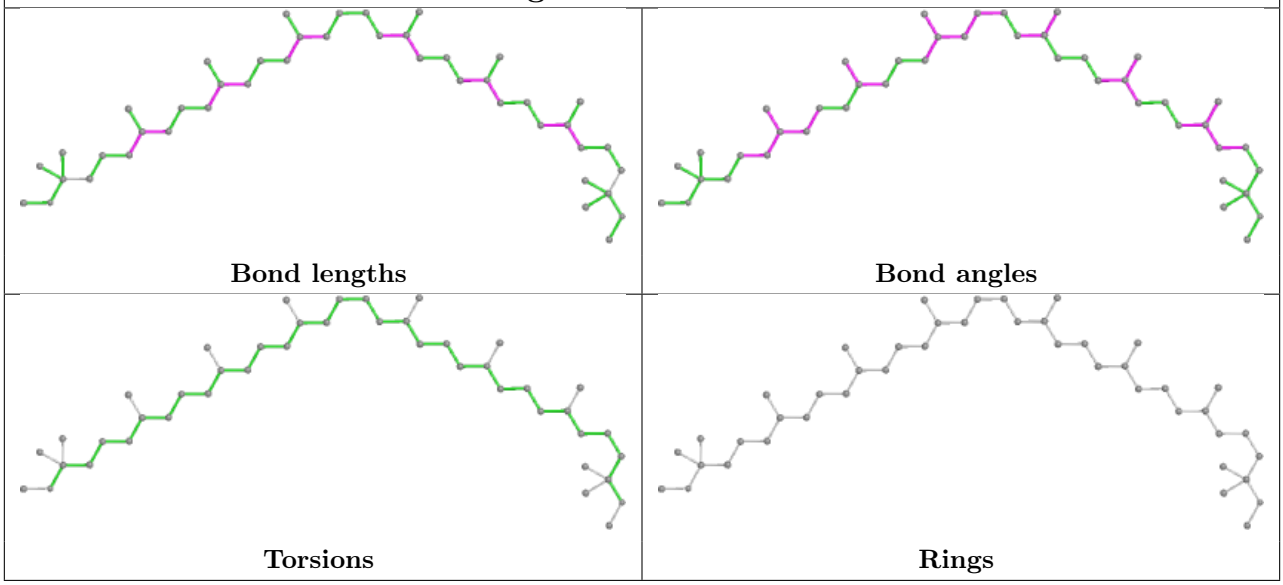
Ligand LMT D 101



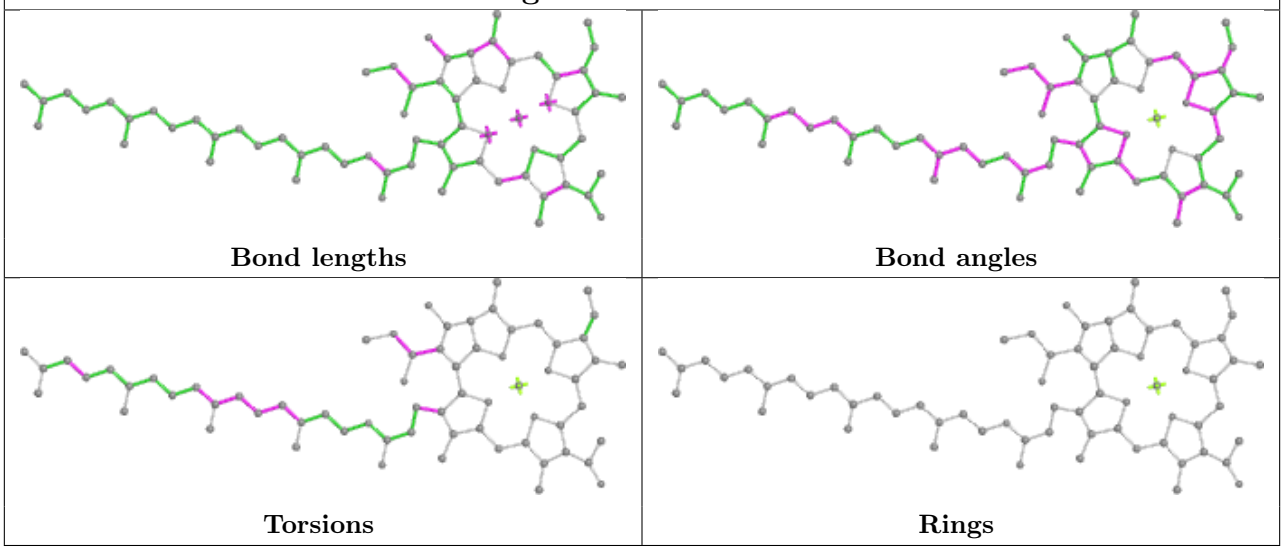
Ligand BCL P 101



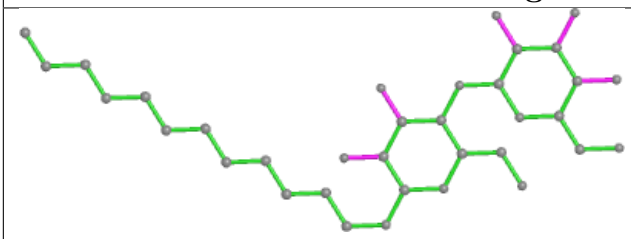
Ligand CRT Z 101



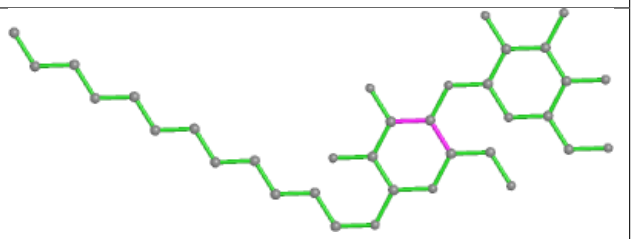
Ligand BCL M 402



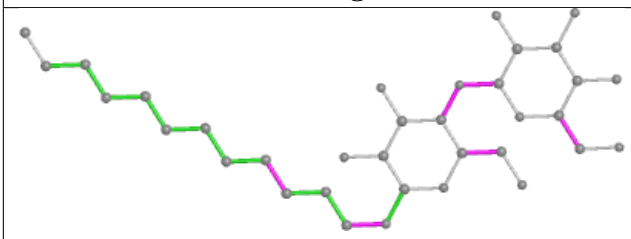
Ligand LMT 6 101



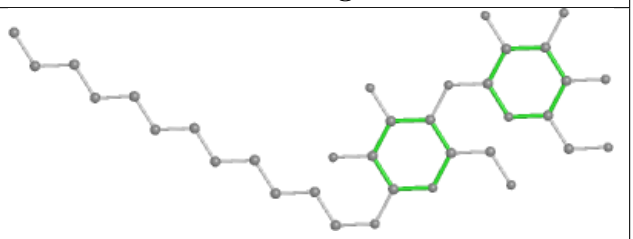
Bond lengths



Bond angles

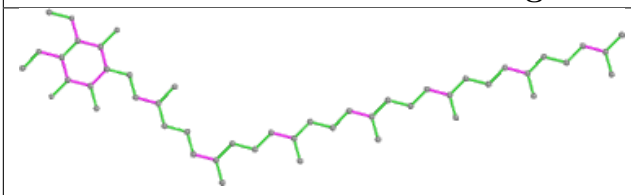


Torsions

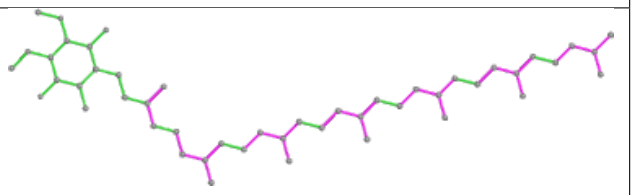


Rings

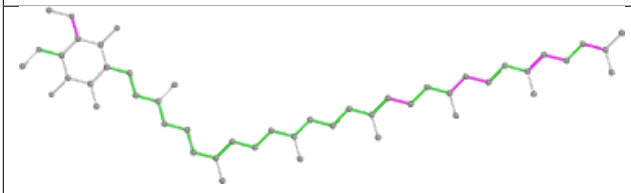
Ligand U10 M 404



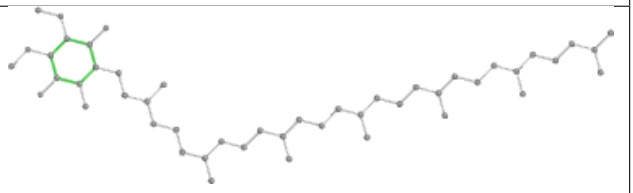
Bond lengths



Bond angles

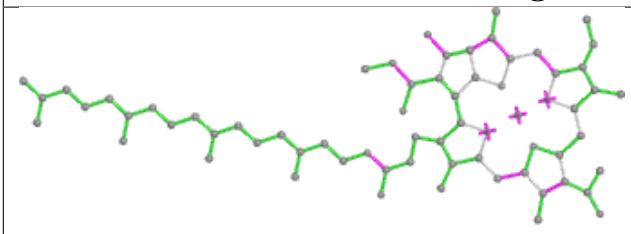


Torsions

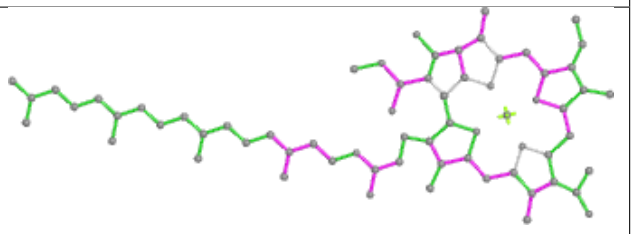


Rings

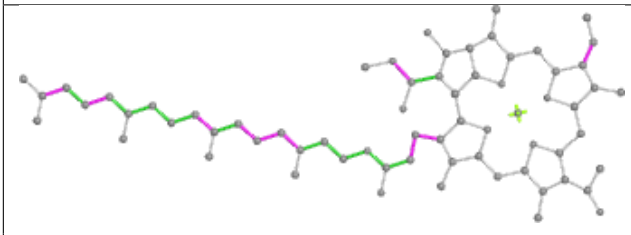
Ligand BCL 5 101



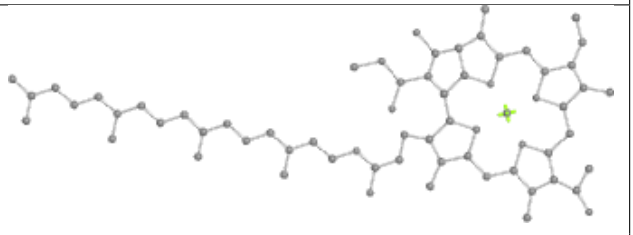
Bond lengths



Bond angles

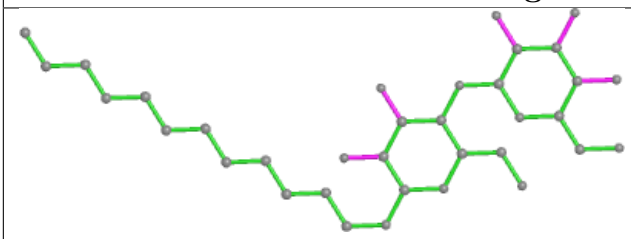


Torsions

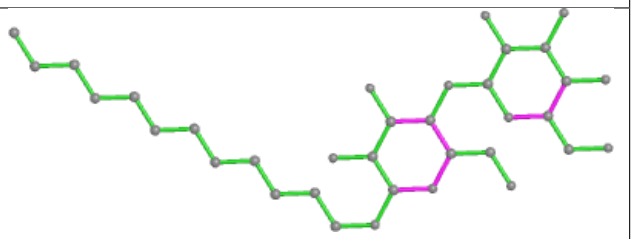


Rings

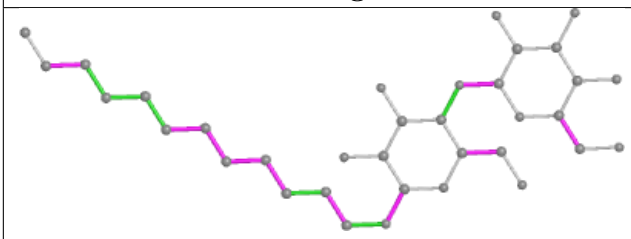
Ligand LMT S 102



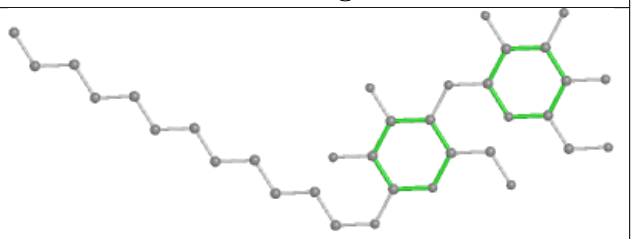
Bond lengths



Bond angles

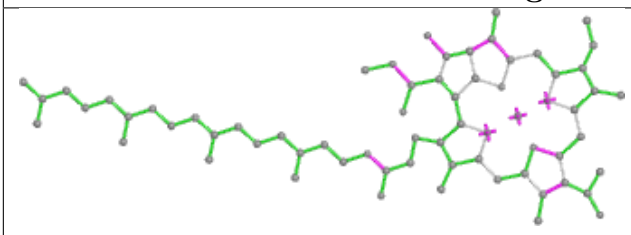


Torsions

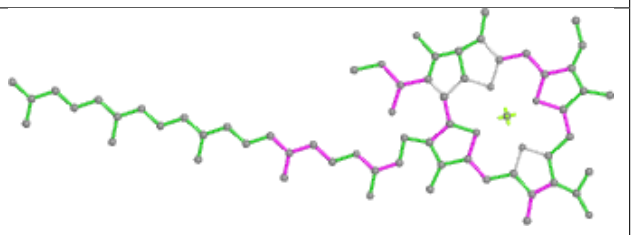


Rings

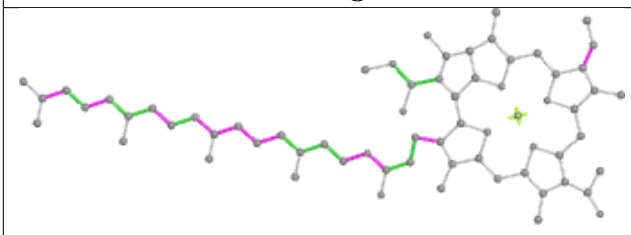
Ligand BCL T 102



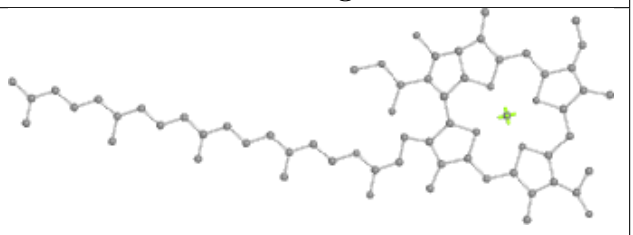
Bond lengths



Bond angles

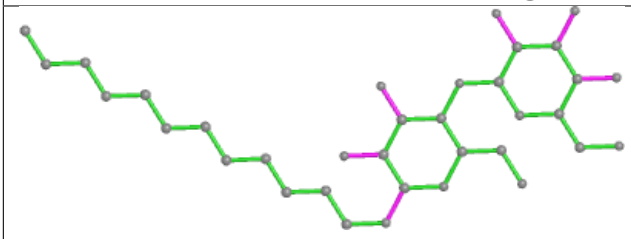


Torsions

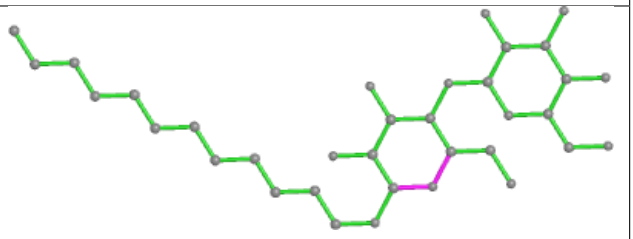


Rings

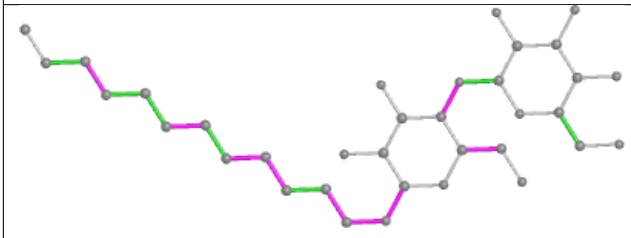
Ligand LMT B 101



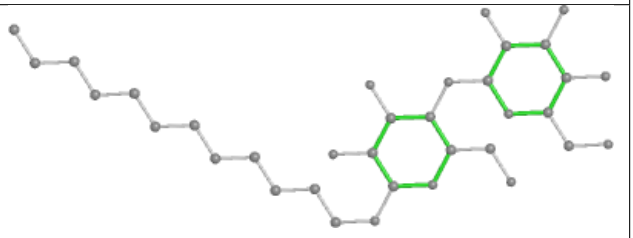
Bond lengths



Bond angles

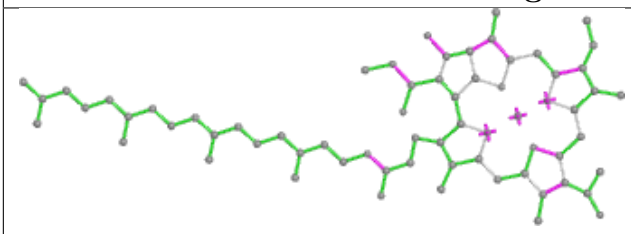


Torsions

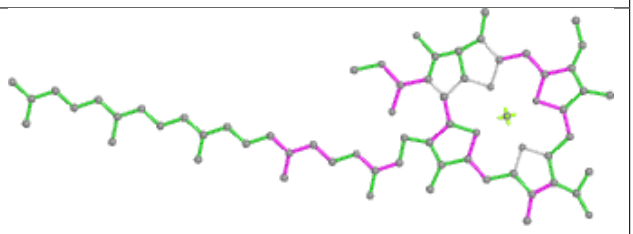


Rings

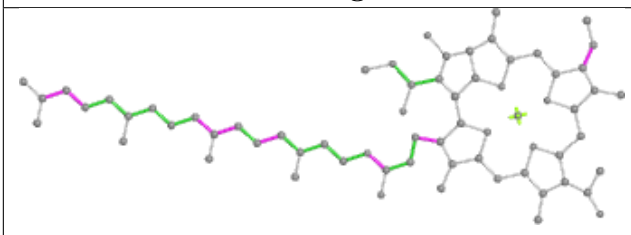
Ligand BCL R 104



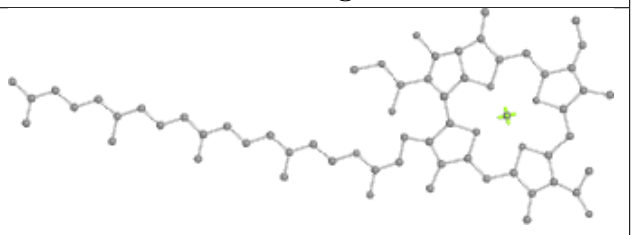
Bond lengths



Bond angles

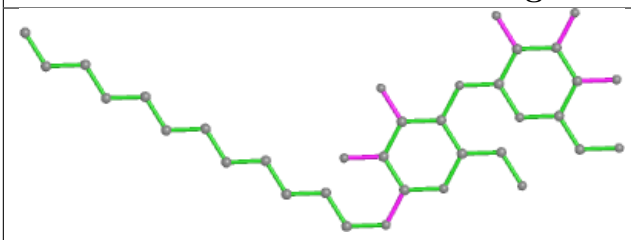


Torsions

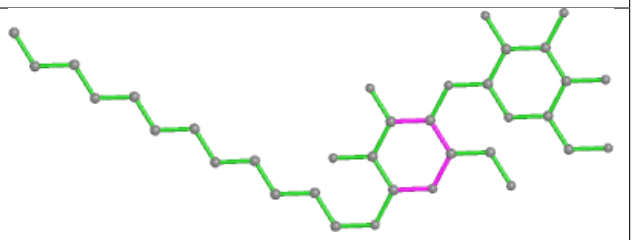


Rings

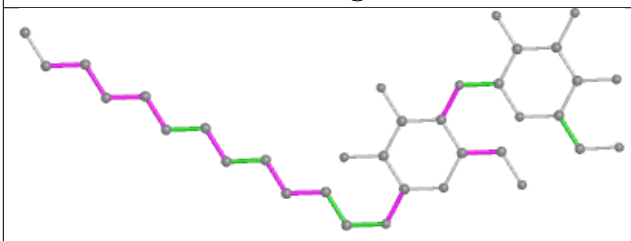
Ligand LMT 2 103



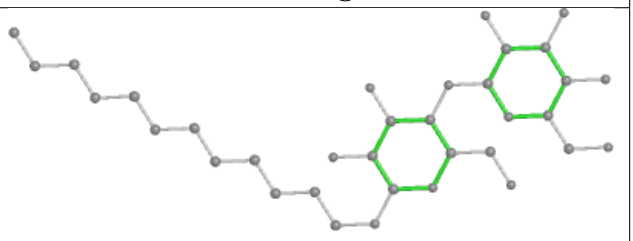
Bond lengths



Bond angles

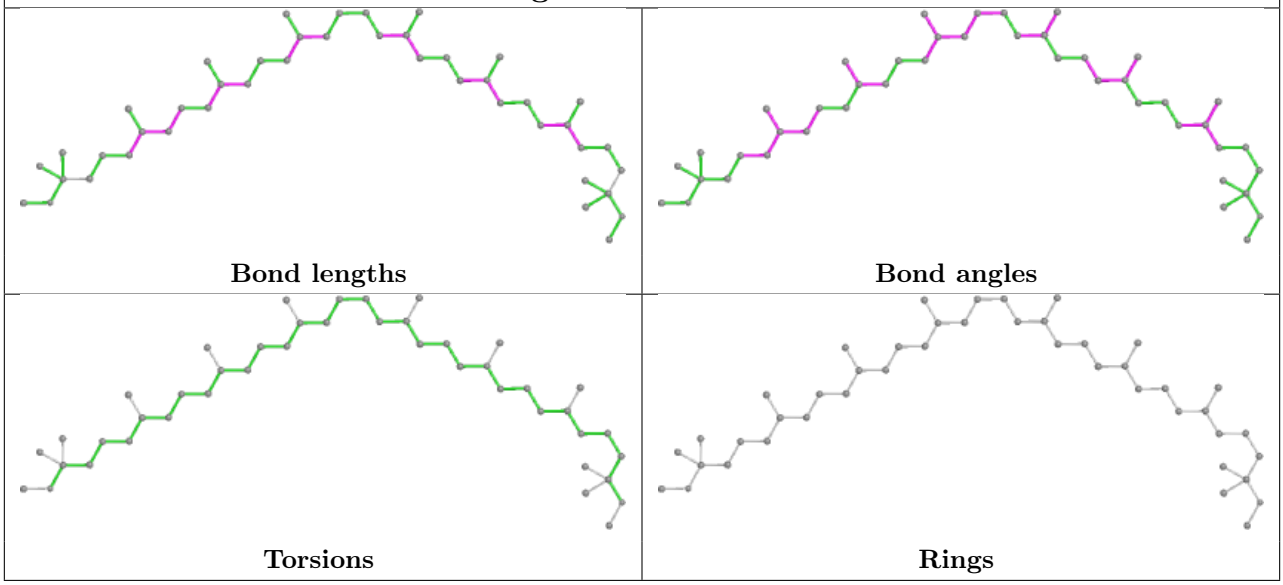


Torsions

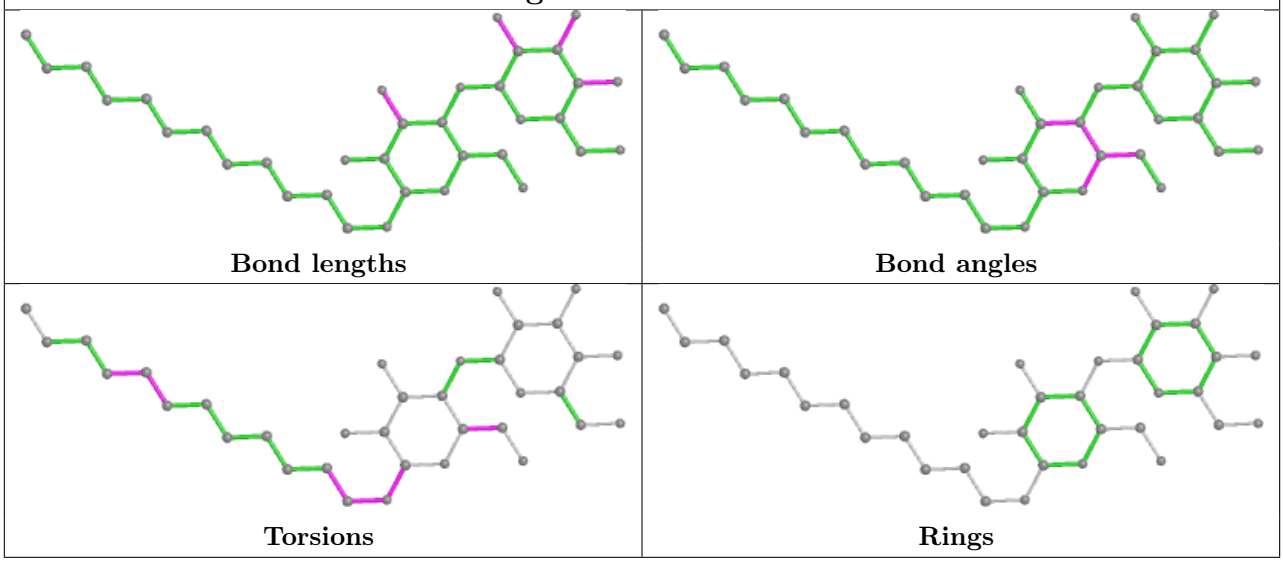


Rings

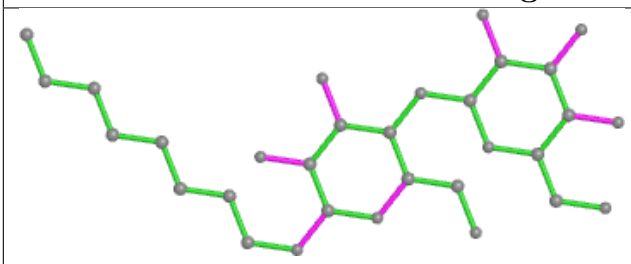
Ligand CRT I 103



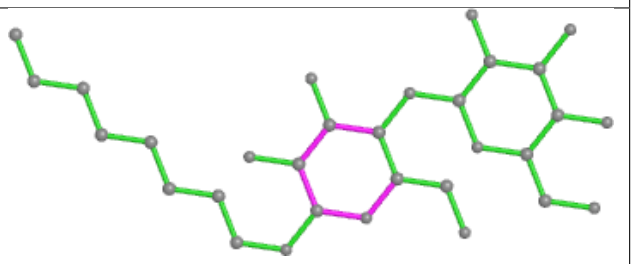
Ligand LMT J 101



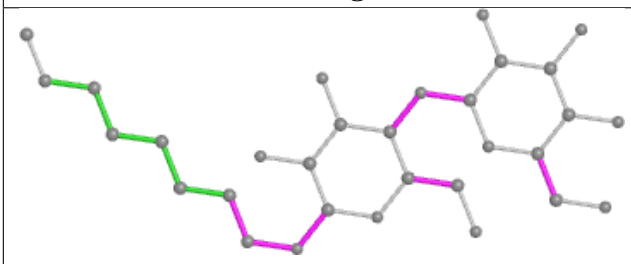
Ligand LMT D 103



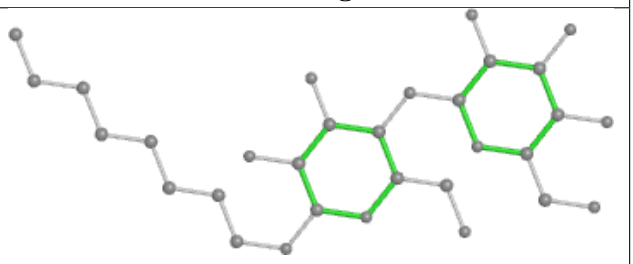
Bond lengths



Bond angles

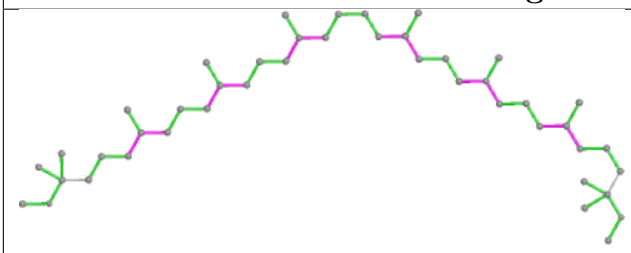


Torsions

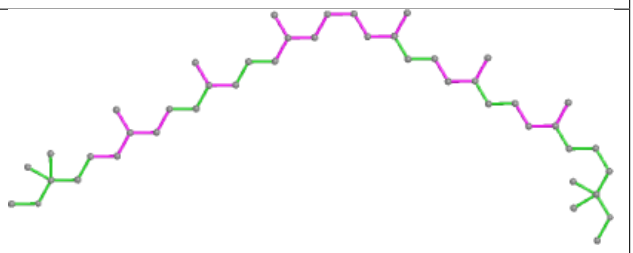


Rings

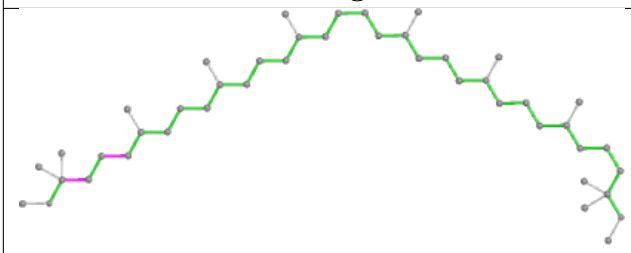
Ligand CRT F 103



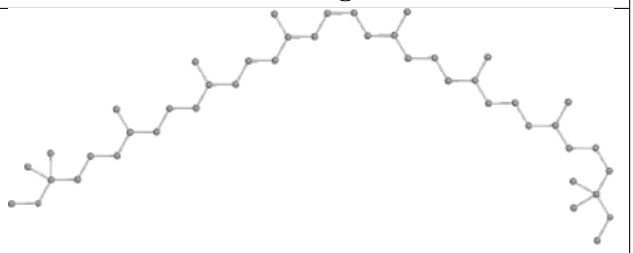
Bond lengths



Bond angles

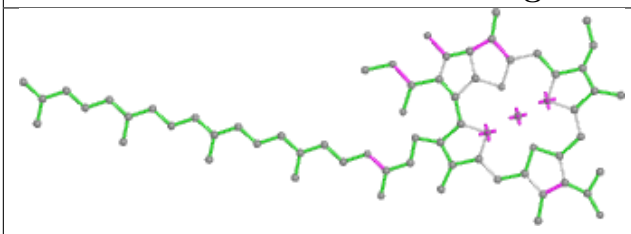


Torsions

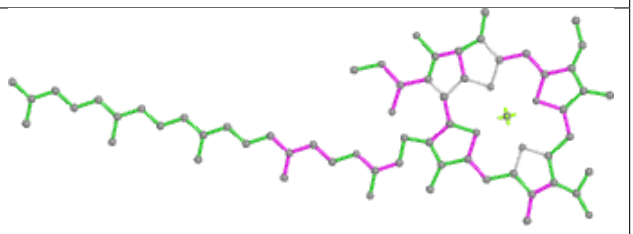


Rings

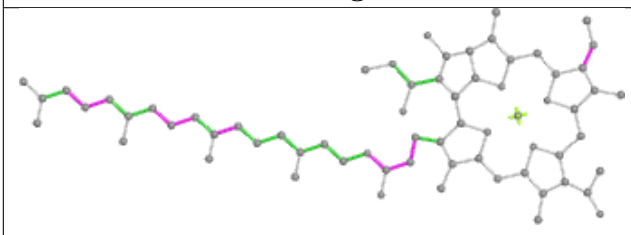
Ligand BCL N 101



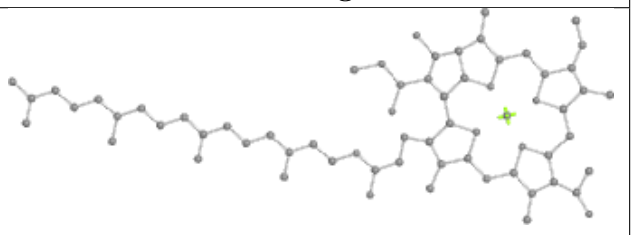
Bond lengths



Bond angles

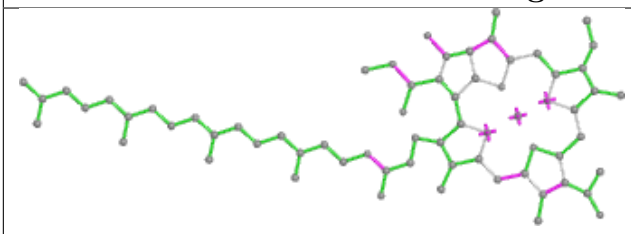


Torsions

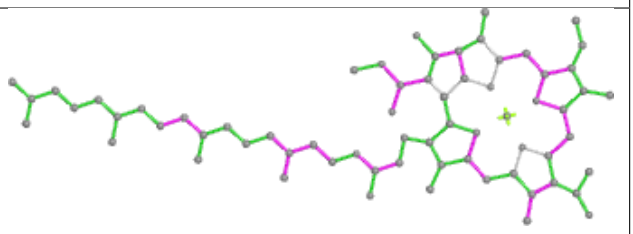


Rings

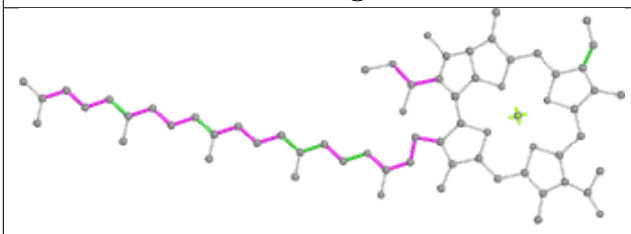
Ligand BCL L 401



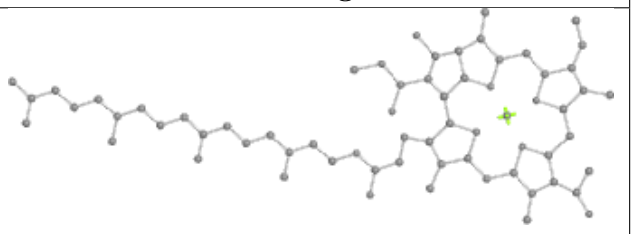
Bond lengths



Bond angles

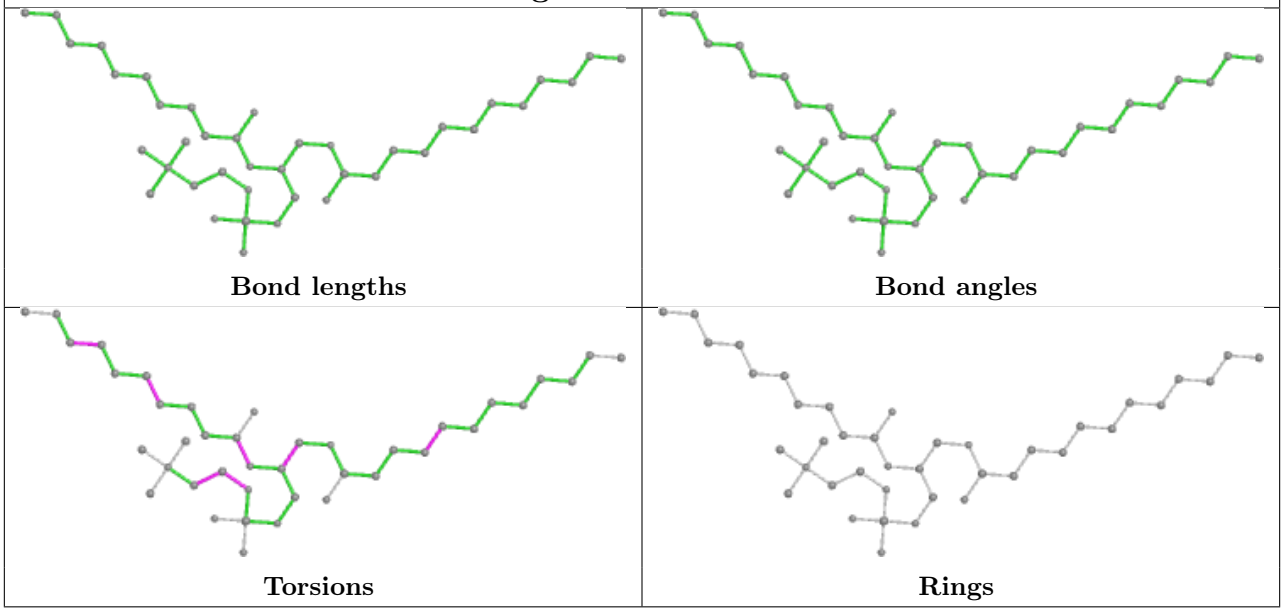


Torsions

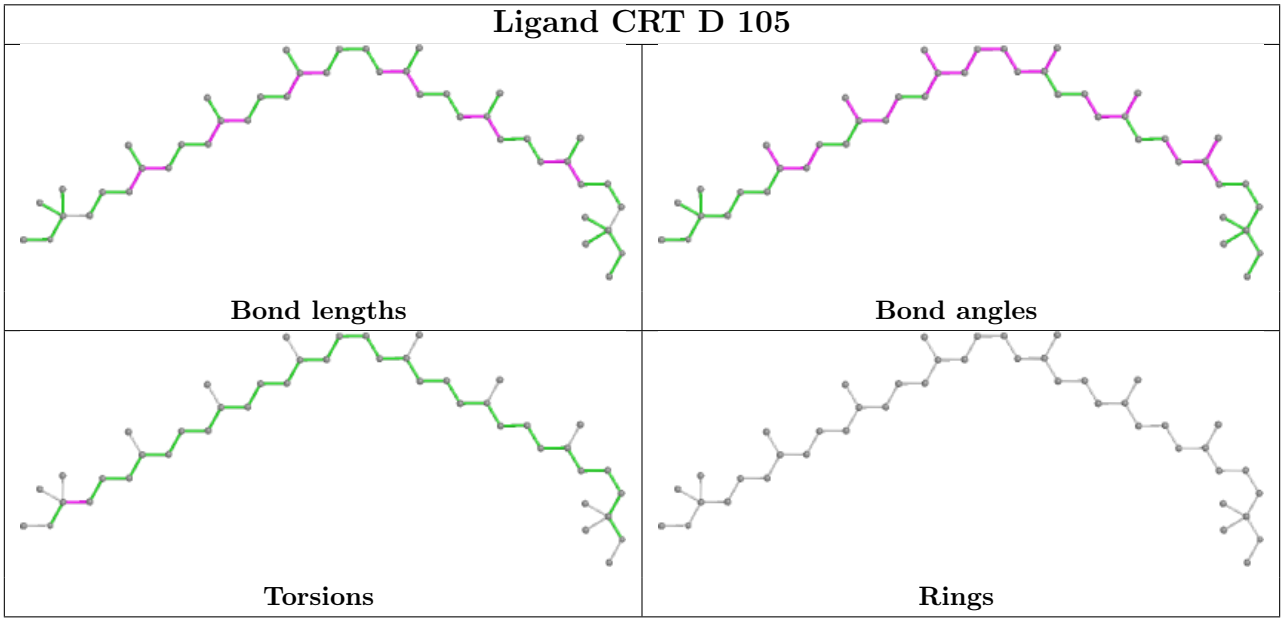


Rings

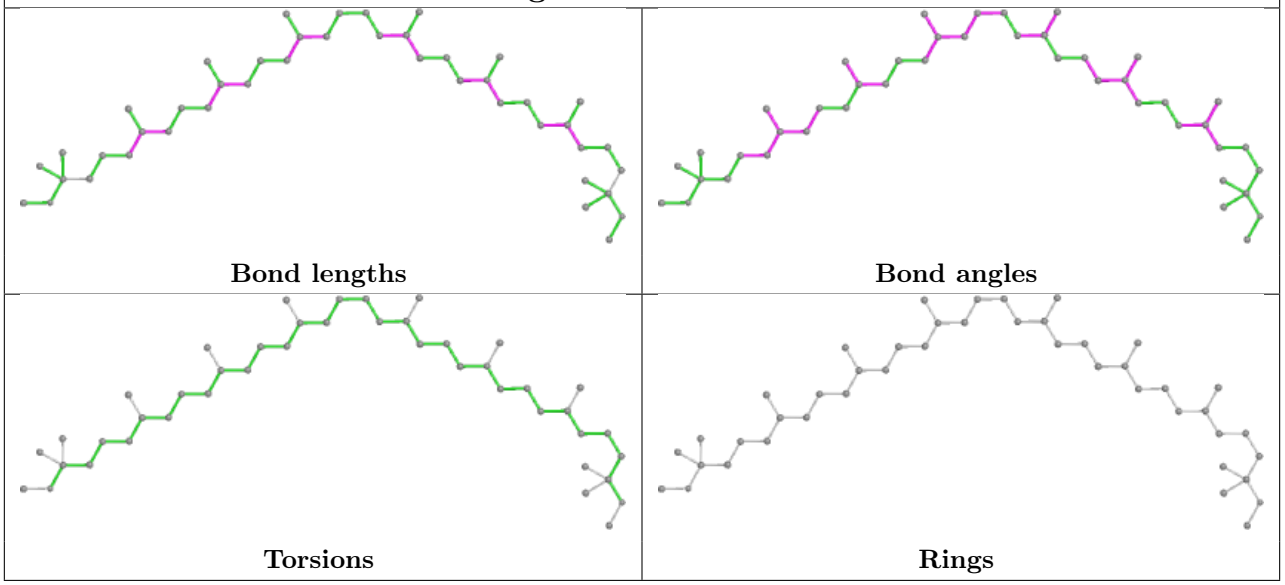
Ligand 6PL E 101



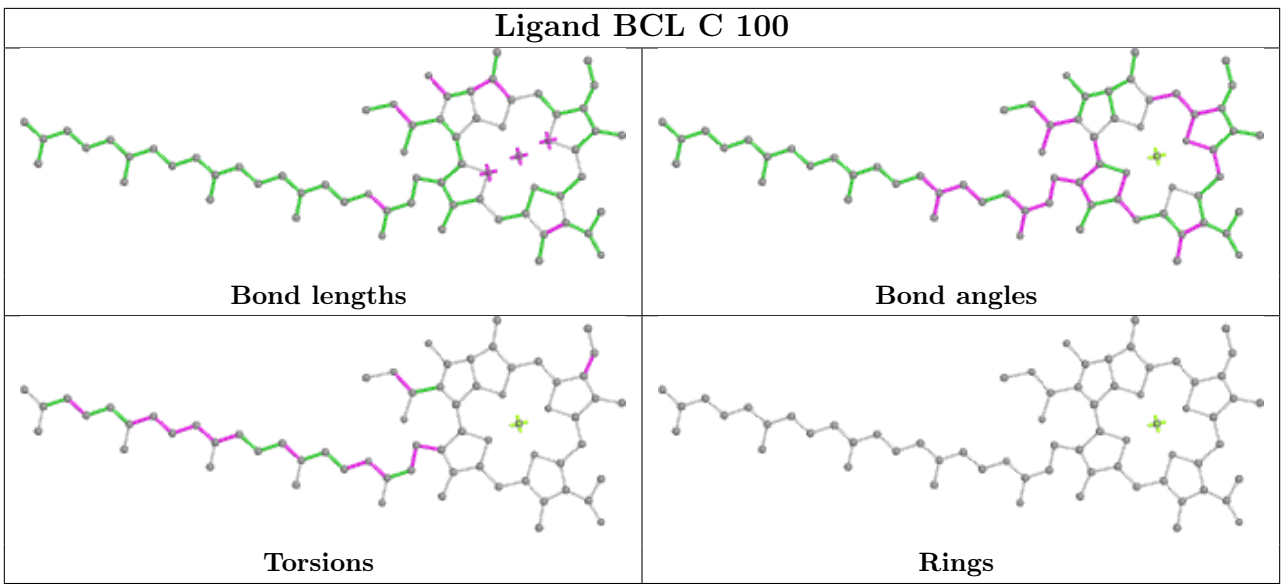
Ligand CRT D 105



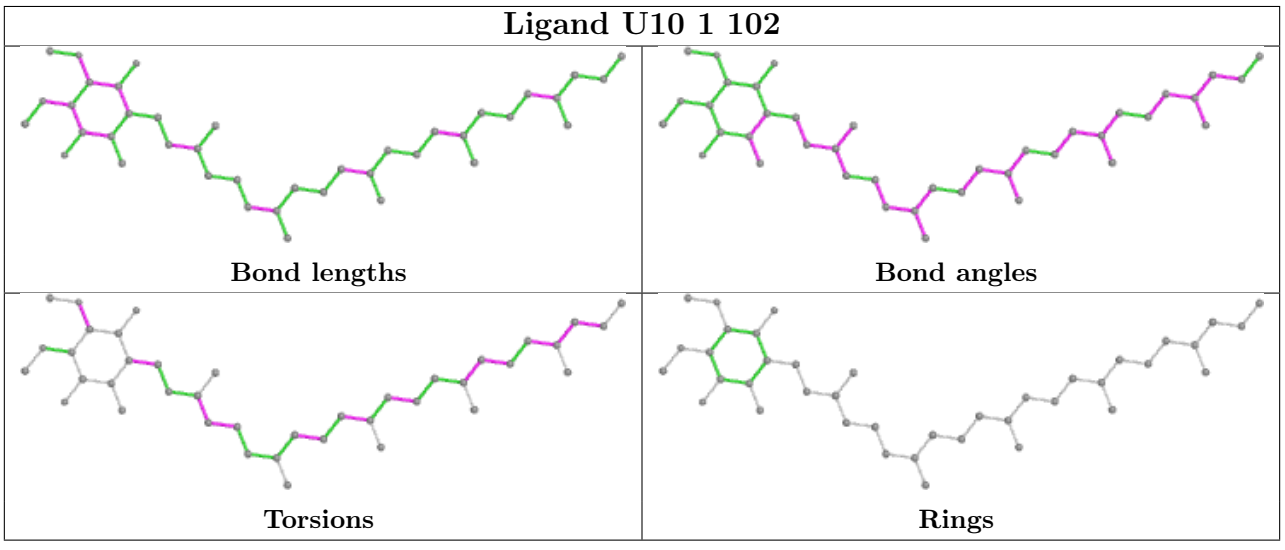
Ligand CRT S 103



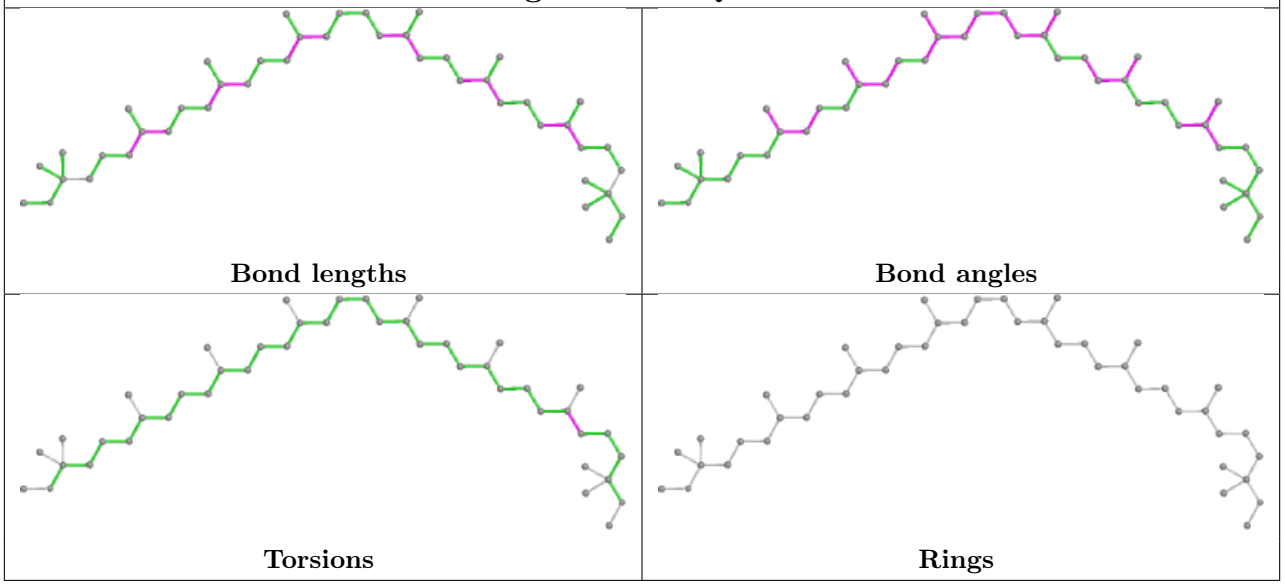
Ligand BCL C 100



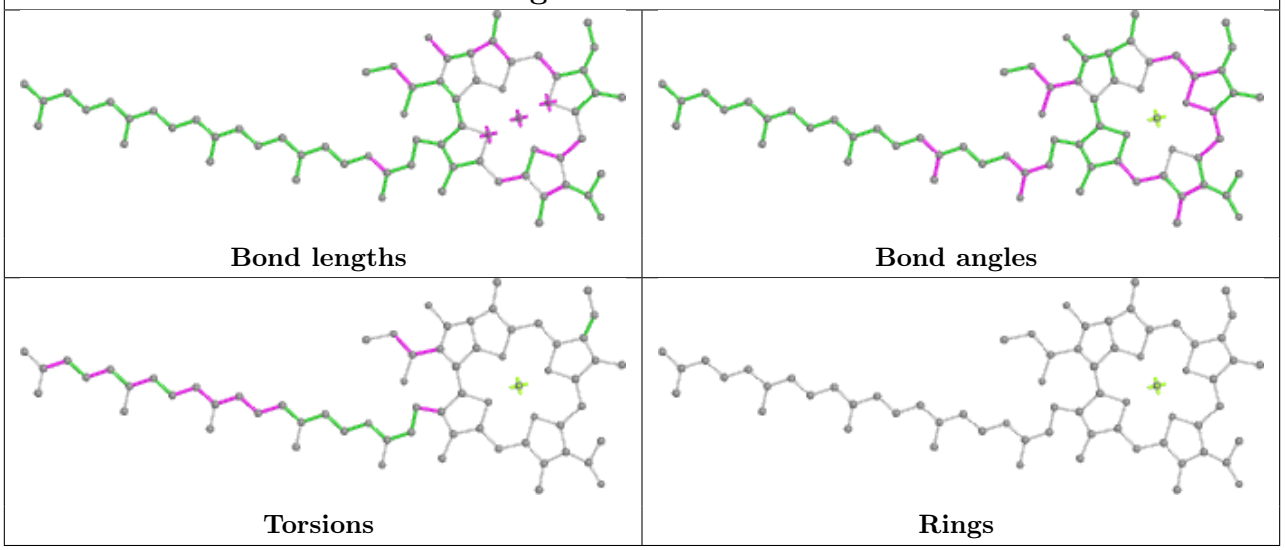
Ligand U10 1 102



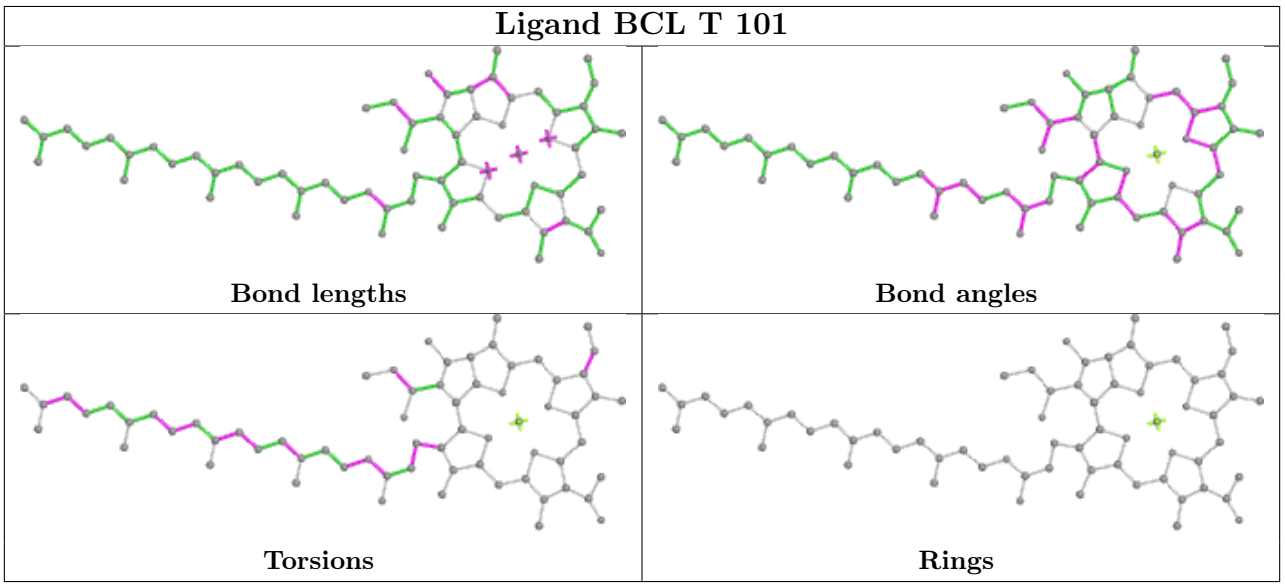
Ligand CRT Q 103



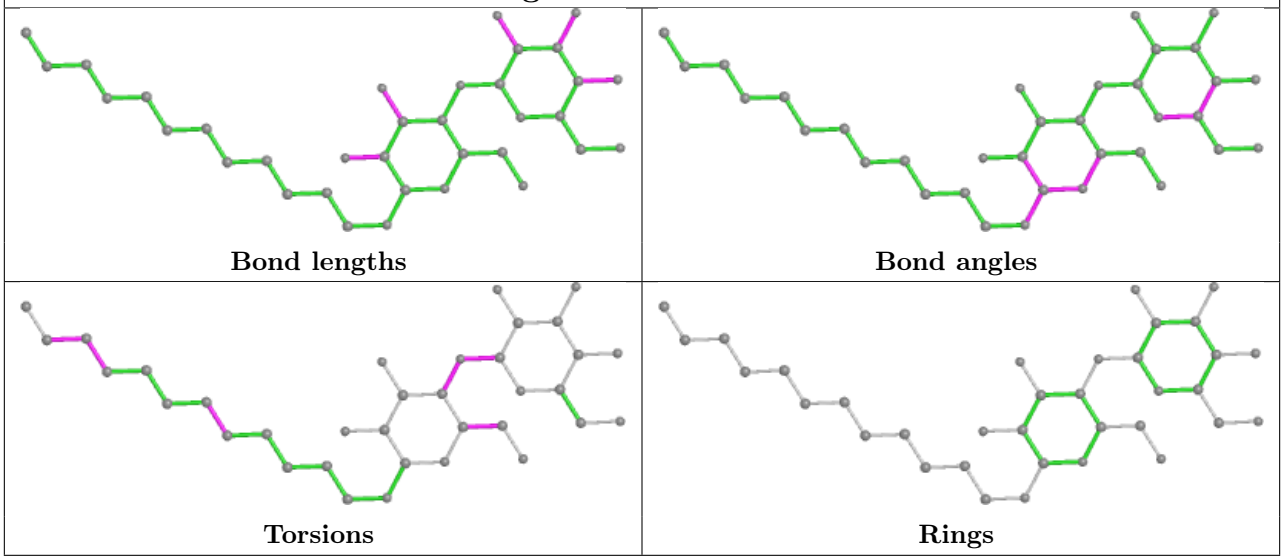
Ligand BCL 4 101



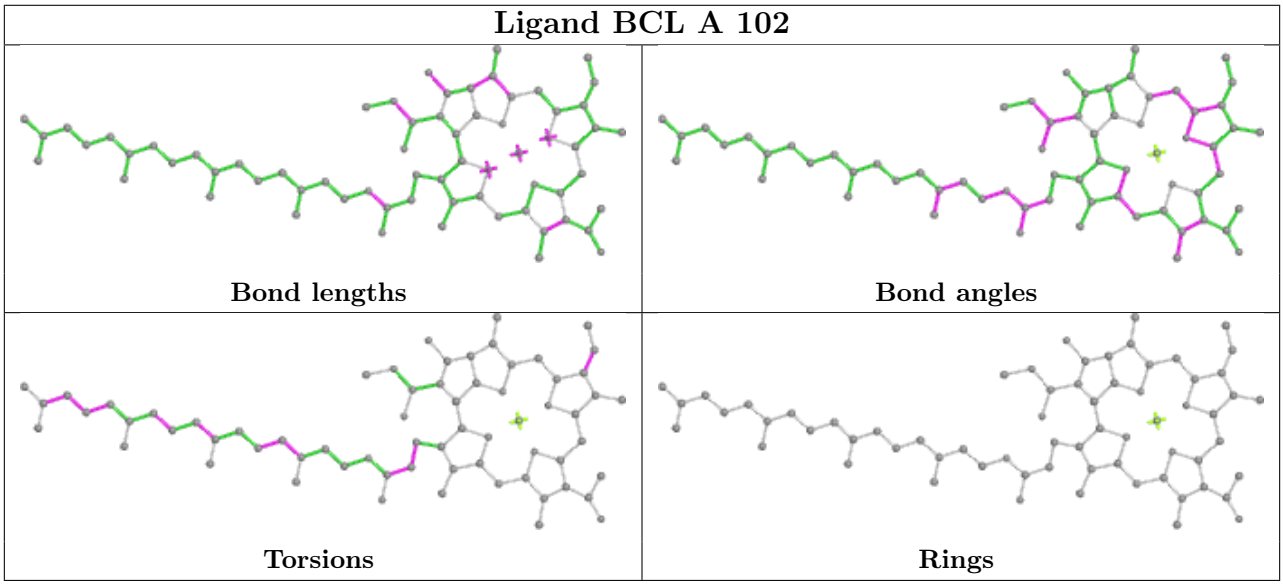
Ligand BCL T 101



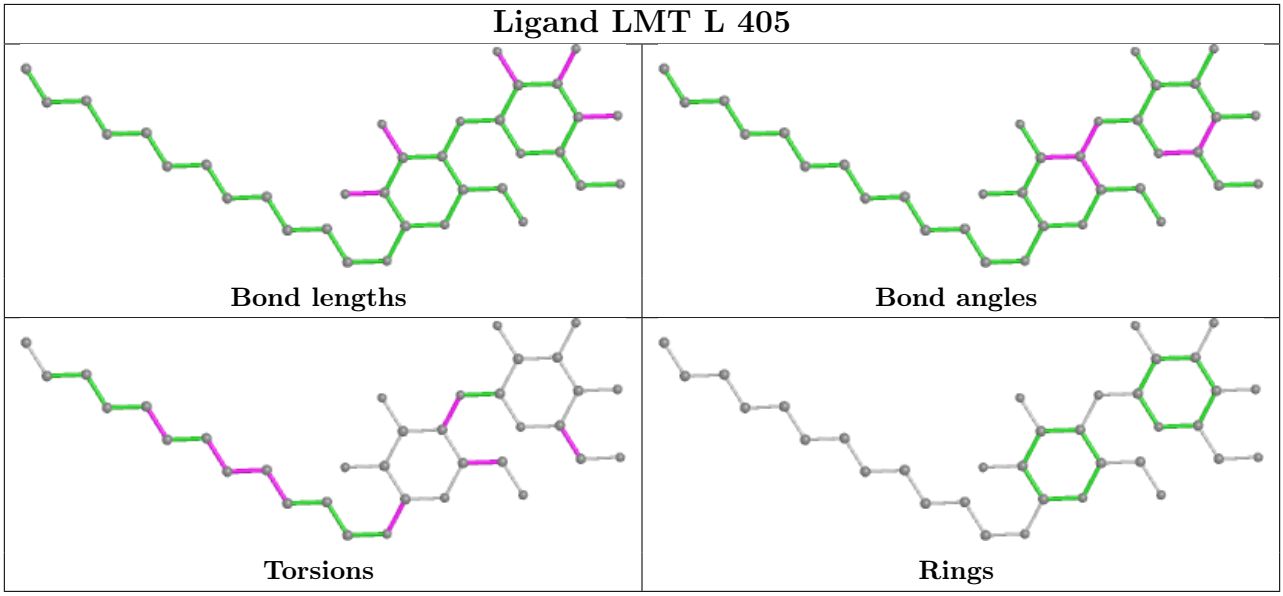
Ligand LMT B 102



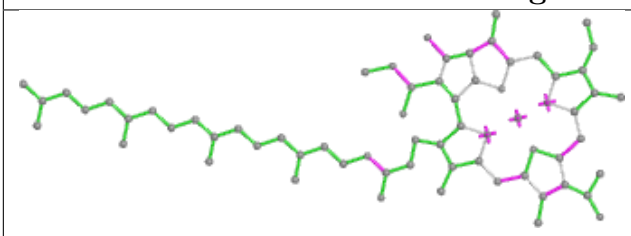
Ligand BCL A 102



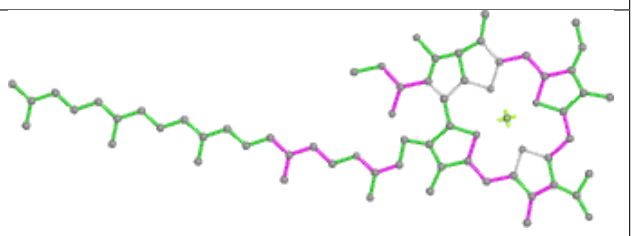
Ligand LMT L 405



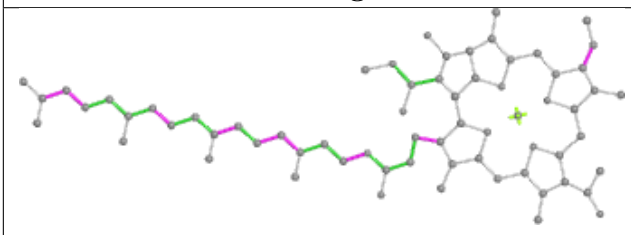
Ligand BCL 2 101



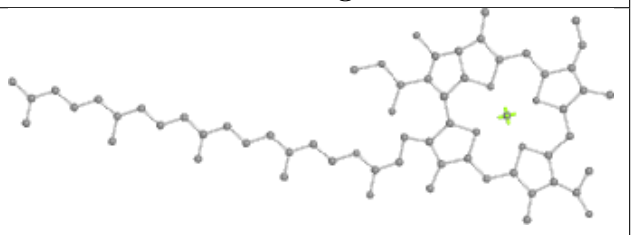
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

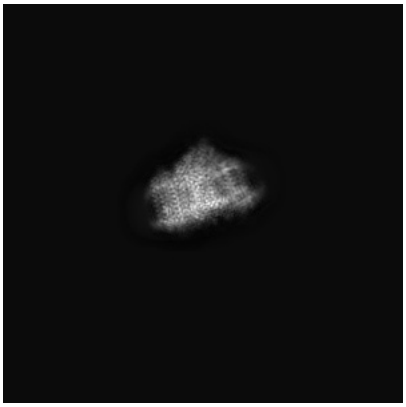
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-11081. These allow visual inspection of the internal detail of the map and identification of artifacts.

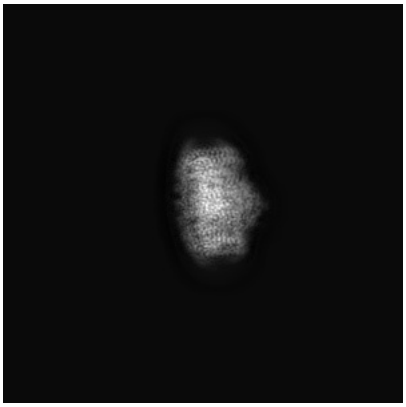
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

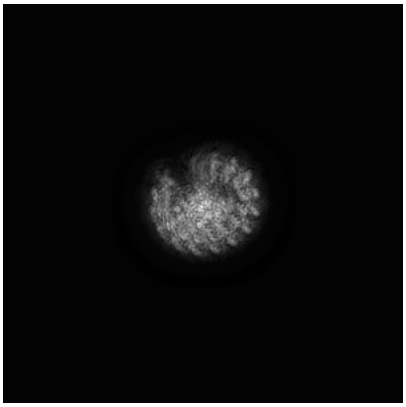
6.1.1 Primary map



X



Y



Z

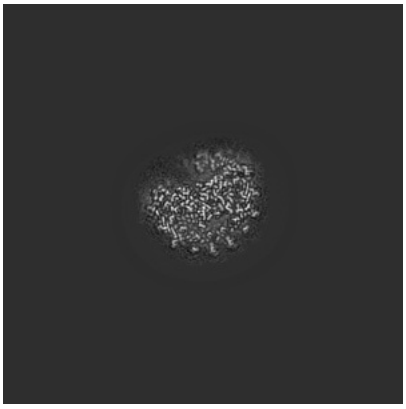
The images above show the map projected in three orthogonal directions.

6.2 Central slices

6.2.1 Primary map

X Index: 200

Y Index: 200



Z Index: 200

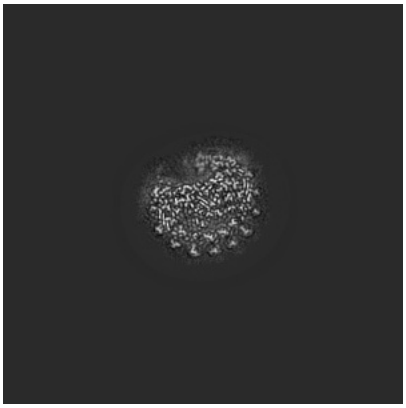
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 199

Y Index: 193

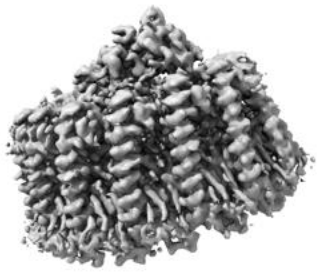


Z Index: 202

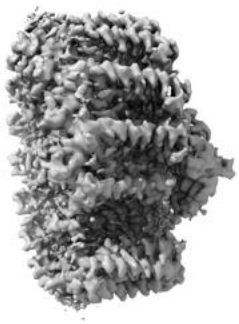
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

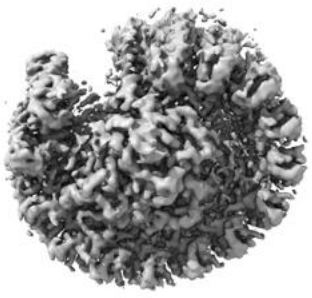
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.15. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

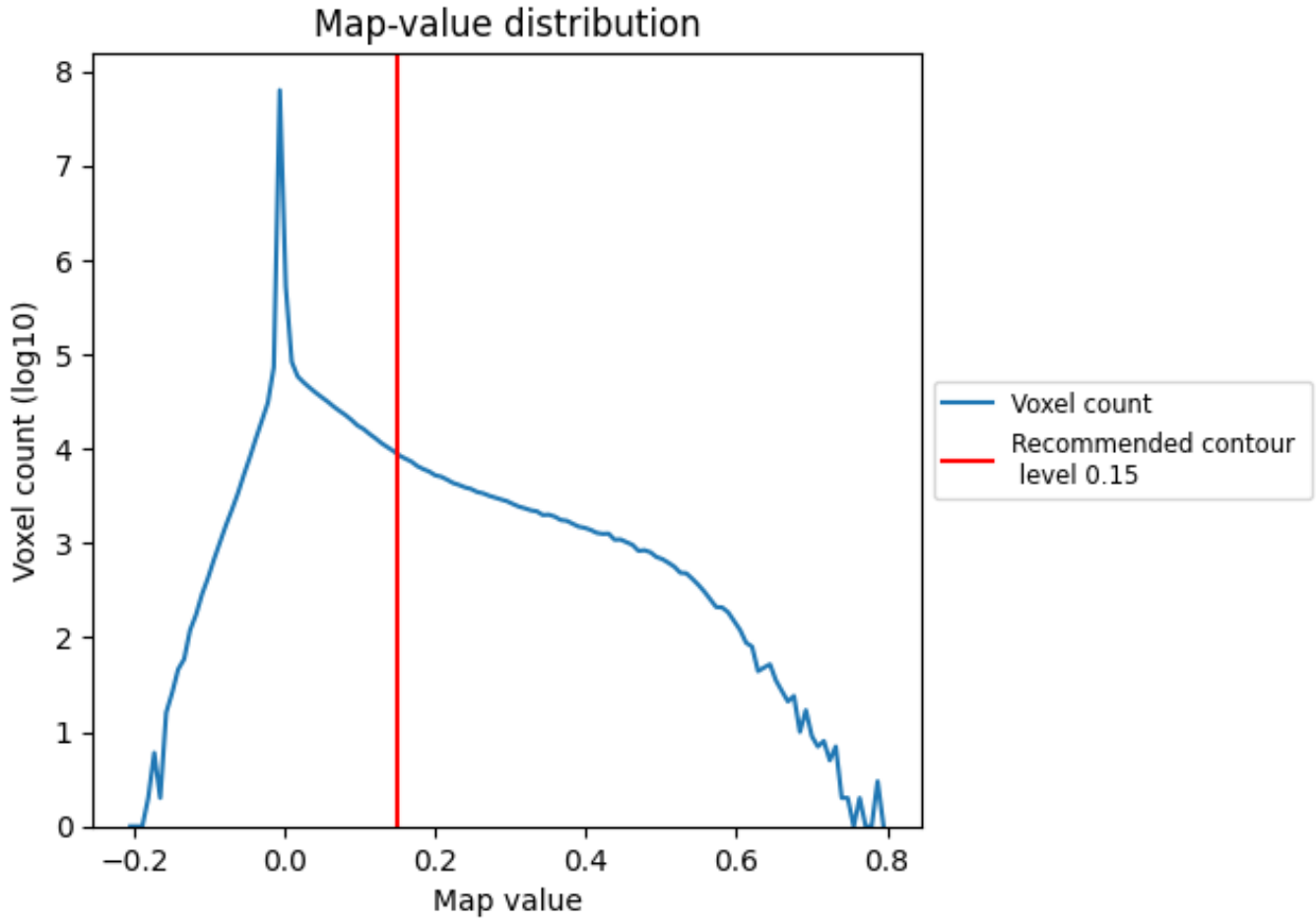
6.5 Mask visualisation (i)

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

7 Map analysis

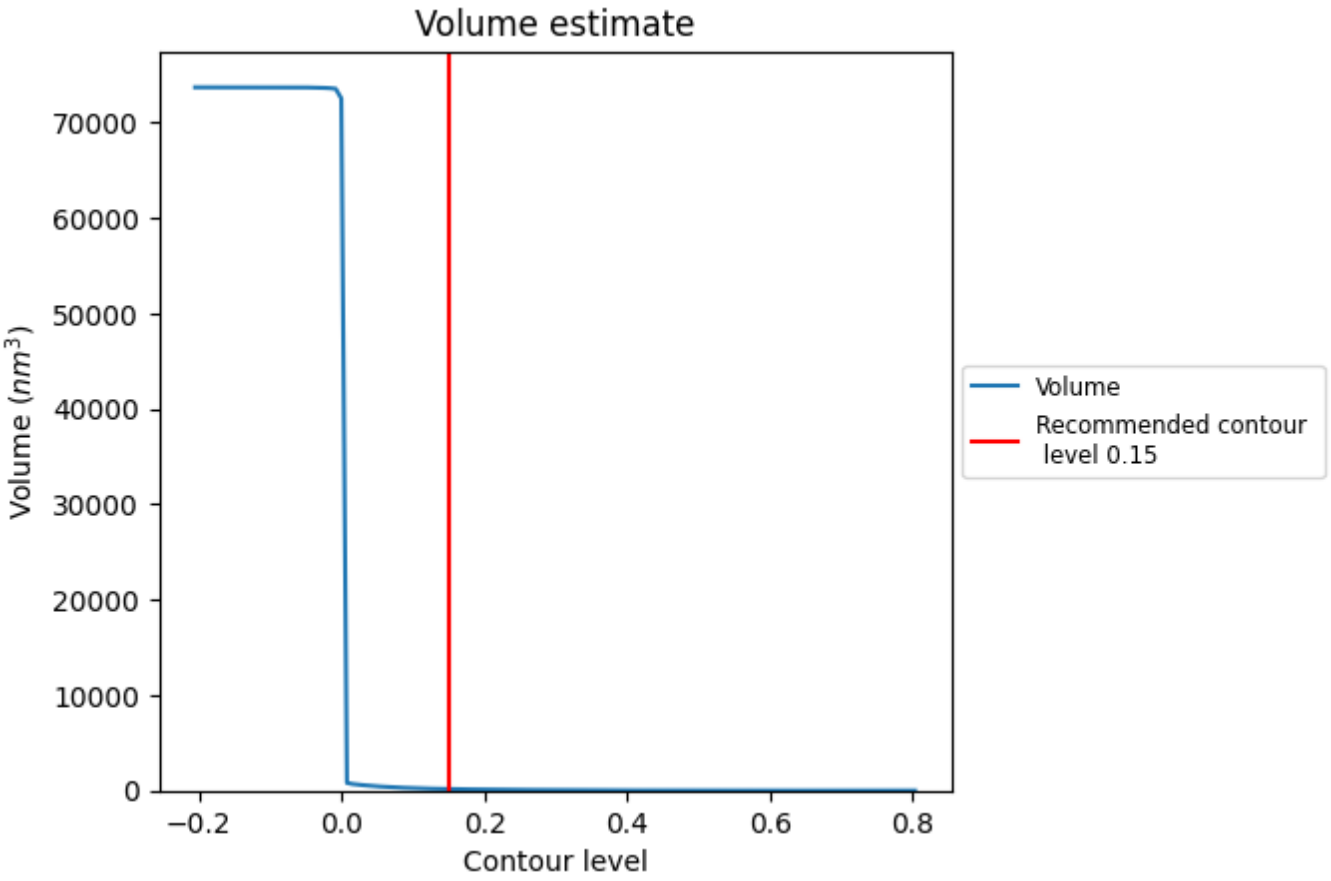
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

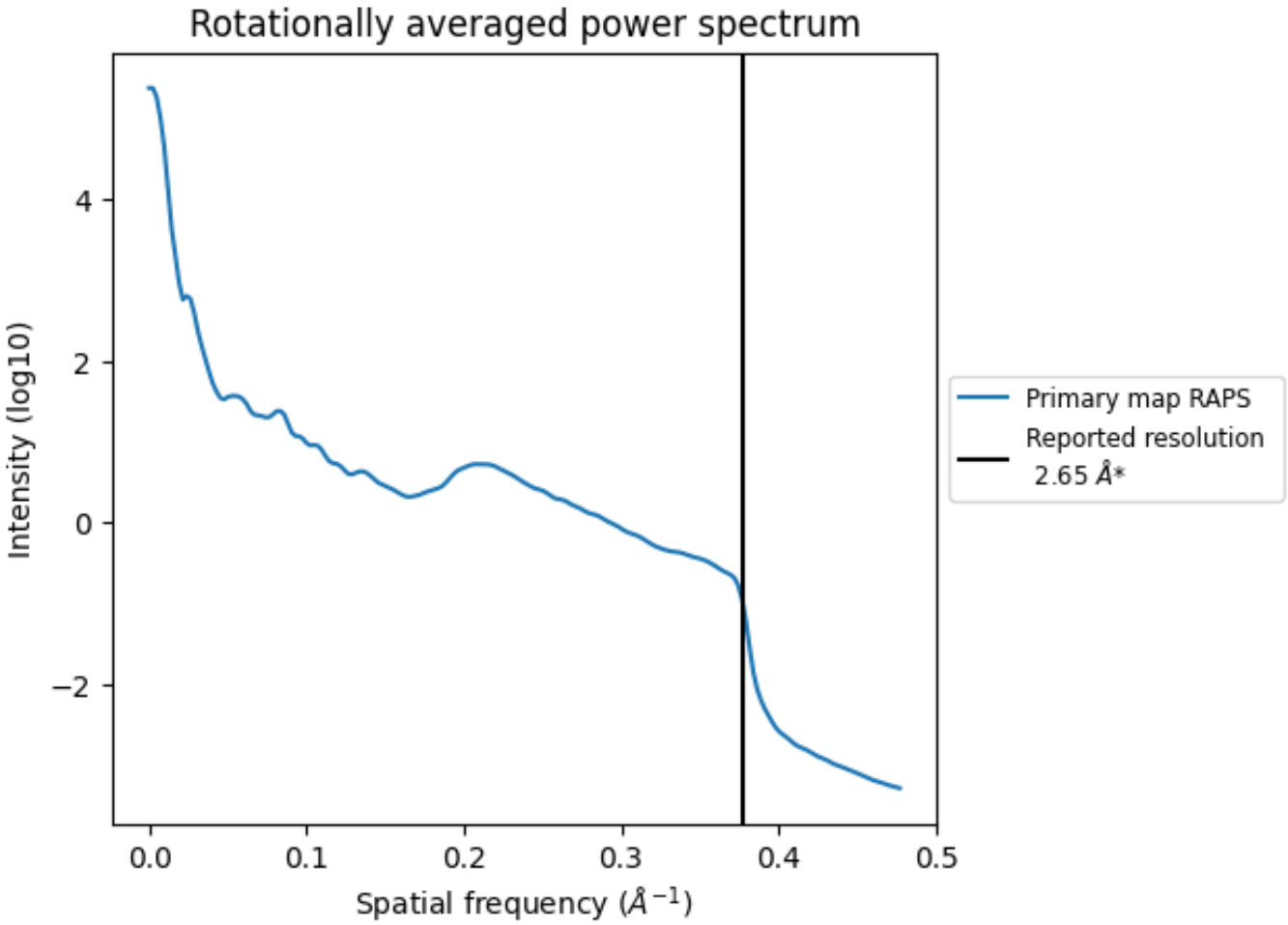
7.2 Volume estimate



The volume at the recommended contour level is 159 nm^3; this corresponds to an approximate mass of 143 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)

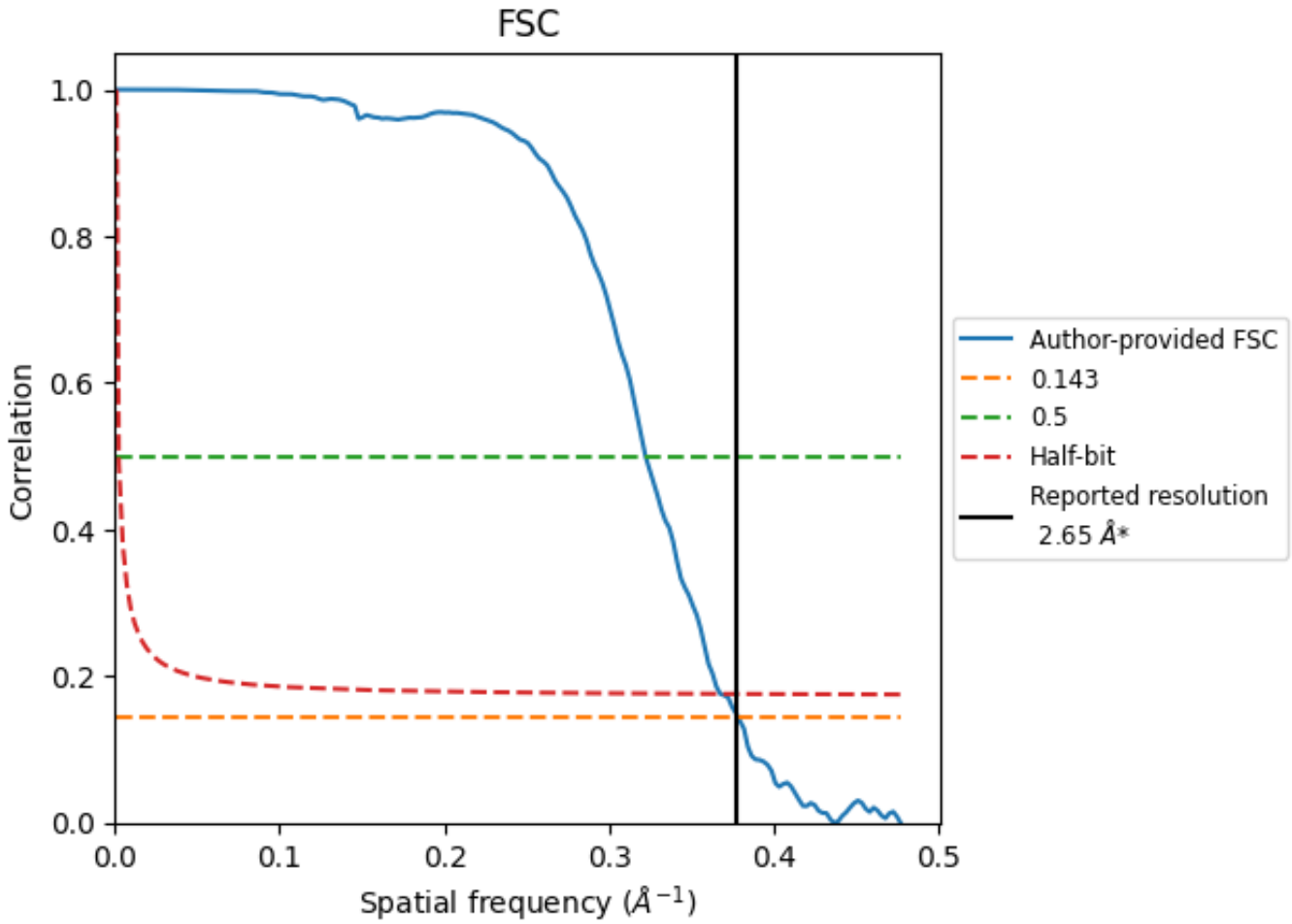


*Reported resolution corresponds to spatial frequency of 0.377 $Å^{-1}$

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.377 Å^{-1}

8.2 Resolution estimates (i)

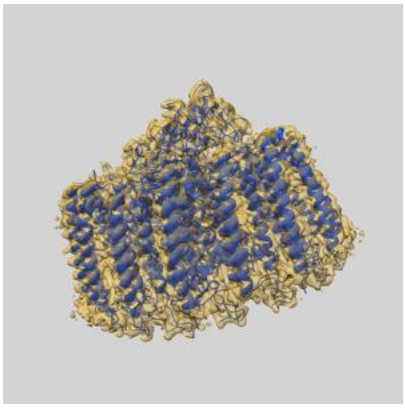
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.65	-	-
Author-provided FSC curve	2.64	3.11	2.72
Unmasked-calculated*	-	-	-

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

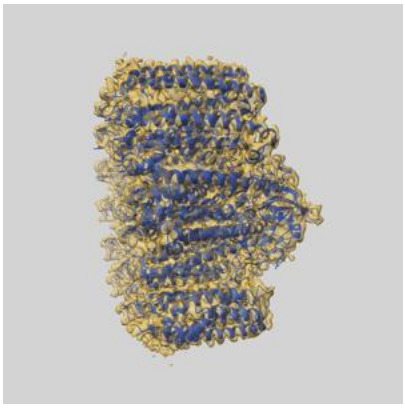
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-11081 and PDB model 6Z5S. Per-residue inclusion information can be found in section 3 on page 17.

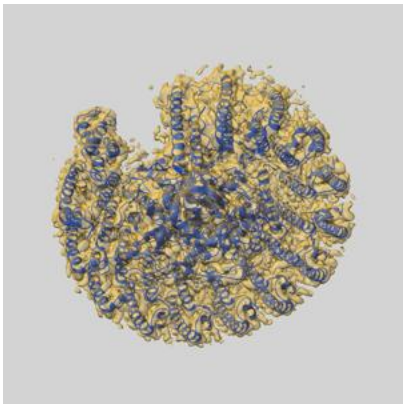
9.1 Map-model overlay



X



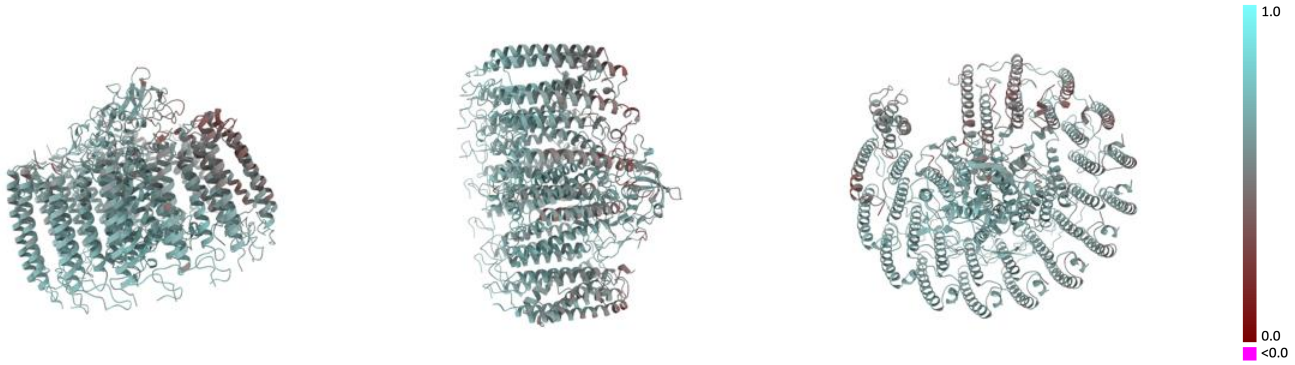
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.15 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.

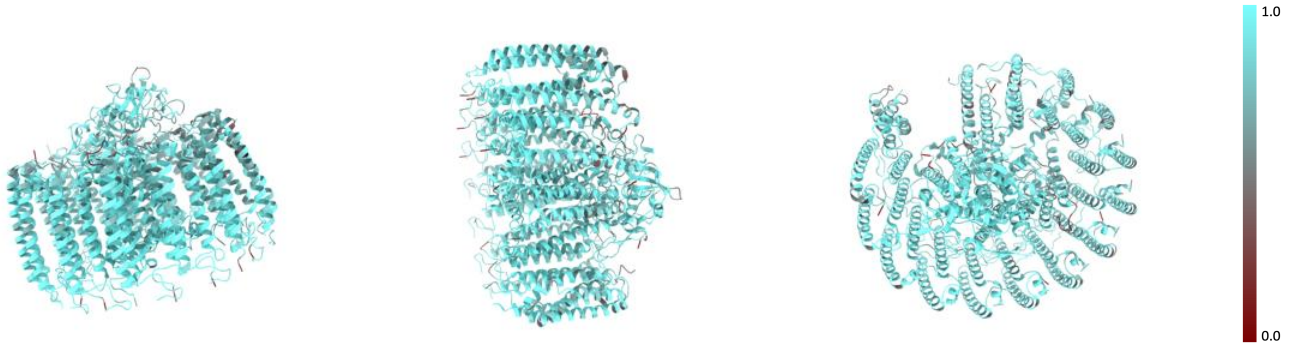
9.2 Q-score mapped to coordinate model (i)



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.

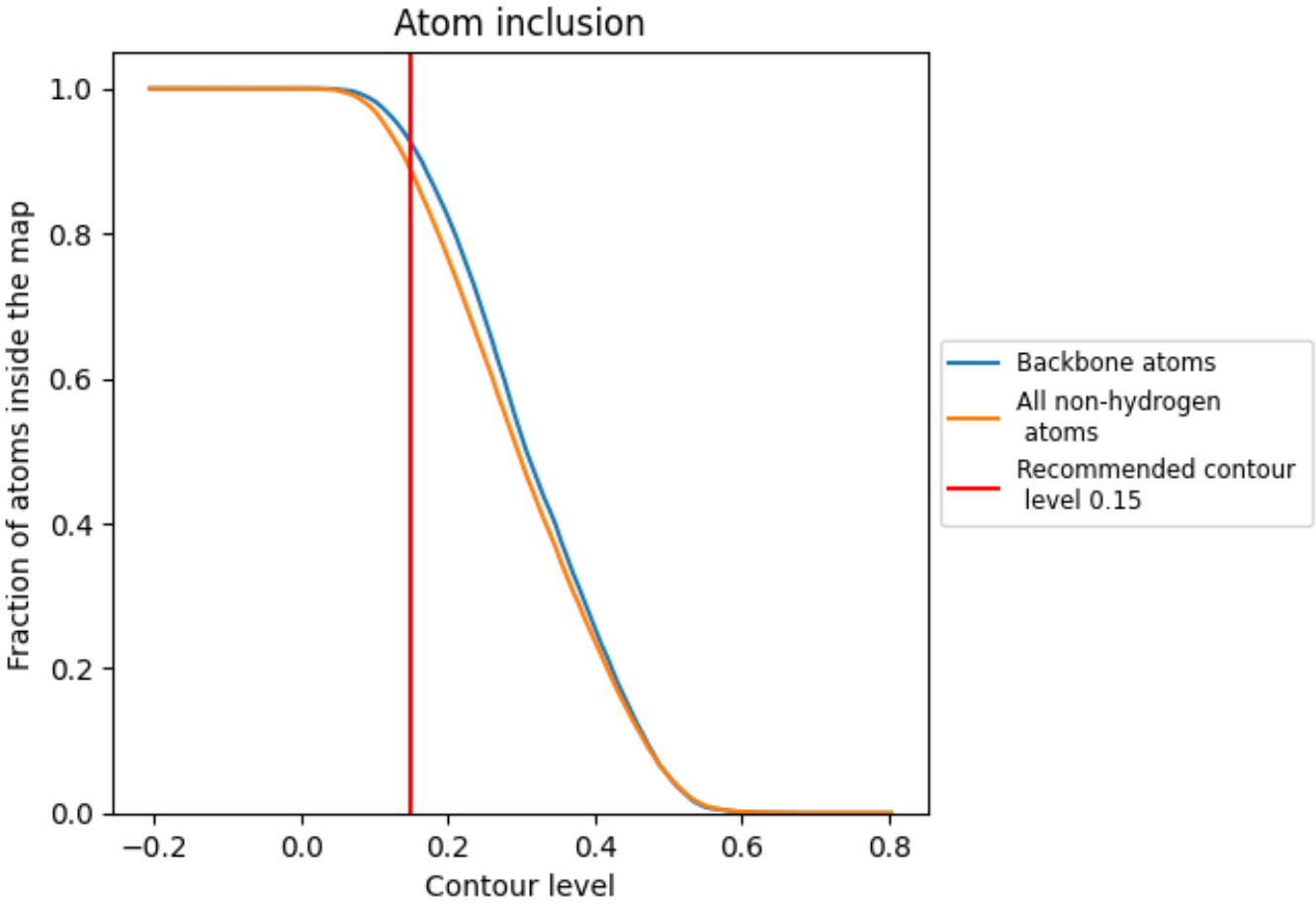
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.15).

9.4 Atom inclusion (i)



At the recommended contour level, 92% of all backbone atoms, 89% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8863	0.5930
1	0.8580	0.5470
2	0.7337	0.4980
3	0.7617	0.5030
4	0.7699	0.4670
5	0.7598	0.5030
6	0.7467	0.4680
A	0.9118	0.5960
B	0.8204	0.5510
C	0.9776	0.6390
D	0.8625	0.6160
E	0.9434	0.6270
F	0.8649	0.6060
G	0.9446	0.6200
H	0.9116	0.5870
I	0.8816	0.6100
J	0.9405	0.6220
K	0.8735	0.6110
L	0.9733	0.6500
M	0.9303	0.6330
N	0.9409	0.6280
O	0.9024	0.6050
P	0.9391	0.6170
Q	0.8548	0.5960
R	0.9302	0.6160
S	0.8327	0.5840
T	0.9173	0.6080
U	0.8386	0.5890
V	0.8917	0.5980
W	0.7746	0.5000
X	0.8184	0.5560
Y	0.8740	0.5790
Z	0.8176	0.5360