Full wwPDB EM Validation Report

Nov 29, 2022 – 03:28 AM JST

PDB ID	:	7VRJ
EMDB ID	:	EMD-32100
Title	:	STRUCTURE OF PHOTOSYNTHETIC LH1-RC SUPER-COMPLEX OF Allochromatium tepidum
Authors	:	Tani, K.; Kobayashi, K.; Hosogi, N.; Ji, X.-C.; Nagashima, S.; Nagashima, K.V.P.; Tsukatani, Y.; Kanno, R.; Hall, M.; Yu, L.-J.; Ishikawa, I.; Okura, Y.; Madigan, M.T.; Mizoguchi, A.; Humbel, B.M.; Kimura, Y.; Wang-Otomo, Z.-Y.
Deposited on	:	2021-10-23
Resolution	:	2.81 Å(reported)
Based on initial model	:	5Y5S

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

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

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

The following versions of software and data (see references (1)) were used in the production of this report:

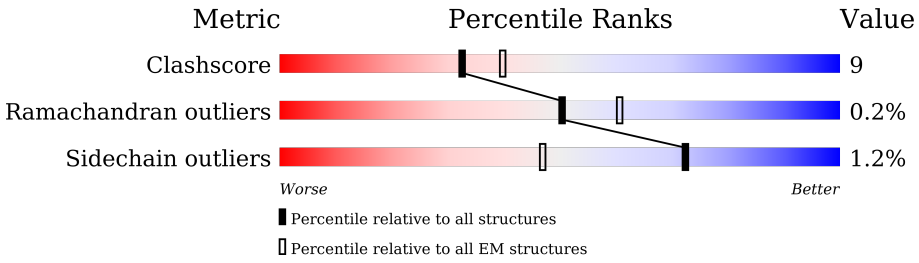
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

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 2.81 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	C	405	73% 5% 23%
2	L	277	90% 10%
3	M	324	88% 9%
4	H	259	6% 86% 14%
5	1	44	5% 75% 23%
5	5	44	7% 82% 16%
5	7	44	9% 80% 18%

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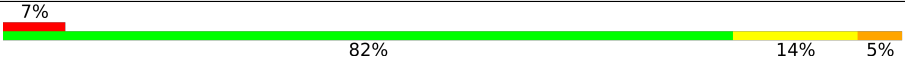
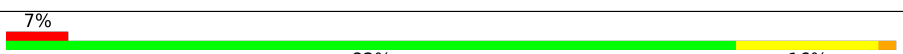
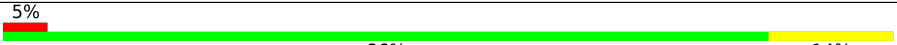
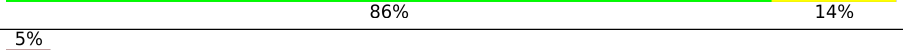
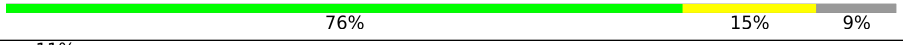
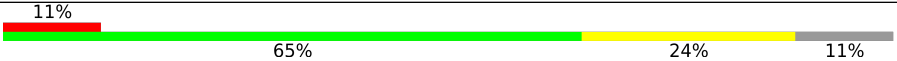
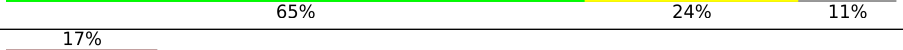
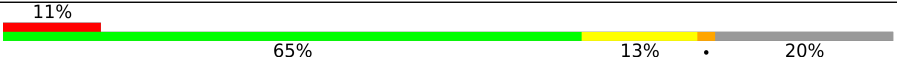
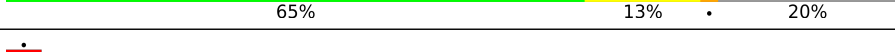
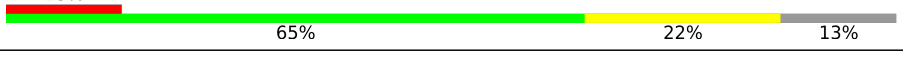
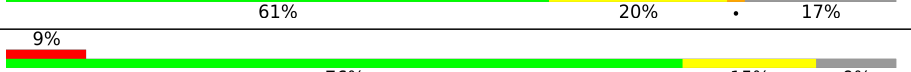
Mol	Chain	Length	Quality of chain
5	9	44	
5	A	44	
5	I	44	
5	K	44	
5	O	44	
5	Q	44	
6	0	46	
6	2	46	
6	4	46	
6	6	46	
6	8	46	
6	B	46	
6	J	46	
6	N	46	
6	P	46	
6	R	46	
7	D	64	
7	F	64	
7	S	64	
7	U	64	
7	W	64	
7	Y	64	
8	E	47	
8	G	47	
8	T	47	

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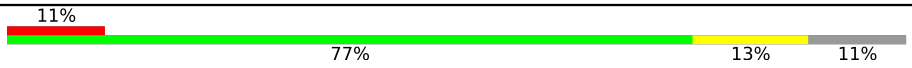
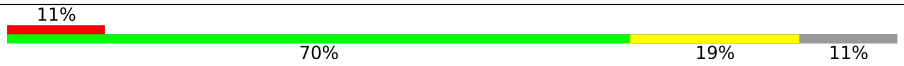
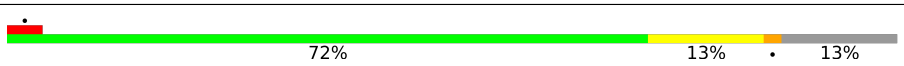
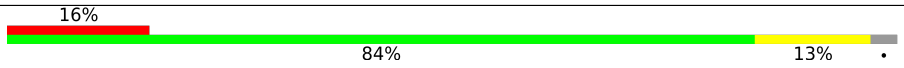
Mol	Chain	Length	Quality of chain
8	V	47	
8	X	47	
8	Z	47	
9	3	67	

2 Entry composition (i)

There are 25 unique types of molecules in this entry. The entry contains 26309 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 Photosynthetic reaction center cytochrome c subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	C	313	Total	C	N	O	S	0	0
			2450	1551	427	455	17		

- Molecule 2 is a protein called Photosynthetic reaction center L subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	L	277	Total	C	N	O	S	0	0
			2212	1491	354	358	9		

- Molecule 3 is a protein called Photosynthetic reaction center M subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	M	318	Total	C	N	O	S	0	0
			2539	1707	409	412	11		

- Molecule 4 is a protein called Photosynthetic reaction center H subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	259	Total	C	N	O	S	1	0
			1989	1280	334	367	8		

- Molecule 5 is a protein called Light-harvesting protein LH1 alpha2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	A	44	Total	C	N	O	S	0	0
			366	251	59	55	1		
5	I	44	Total	C	N	O	S	0	0
			366	251	59	55	1		
5	K	44	Total	C	N	O	S	0	0
			366	251	59	55	1		
5	O	44	Total	C	N	O	S	0	0
			366	251	59	55	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
5	Q	44	Total	C	N	O	S	0	0
			366	251	59	55	1		
5	1	44	Total	C	N	O	S	0	0
			366	251	59	55	1		
5	5	43	Total	C	N	O	S	0	0
			355	245	57	52	1		
5	7	44	Total	C	N	O	S	0	0
			362	248	58	55	1		
5	9	43	Total	C	N	O	S	0	0
			359	248	58	52	1		

- Molecule 6 is a protein called Light-harvesting protein LH1 beta1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	B	44	Total	C	N	O	S	0	0
			359	238	58	61	2		
6	J	40	Total	C	N	O	S	0	0
			331	223	53	54	1		
6	N	38	Total	C	N	O	S	0	0
			320	217	51	51	1		
6	P	42	Total	C	N	O	S	0	0
			345	231	55	57	2		
6	R	41	Total	C	N	O	S	0	0
			339	228	54	55	2		
6	2	41	Total	C	N	O	S	0	0
			339	228	54	55	2		
6	4	42	Total	C	N	O	S	0	0
			345	231	55	57	2		
6	6	38	Total	C	N	O	S	0	0
			320	217	51	51	1		
6	8	37	Total	C	N	O	S	0	0
			312	211	50	50	1		
6	0	42	Total	C	N	O	S	0	0
			345	231	55	57	2		

- Molecule 7 is a protein called Light-harvesting protein LH1 alpha1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	D	50	Total	C	N	O	S	0	0
			411	279	63	67	2		
7	F	49	Total	C	N	O	S	0	0
			401	273	62	65	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
7	S	52	Total	C	N	O	S	0	0
			419	283	65	69	2		
7	U	51	Total	C	N	O	S	0	0
			416	282	64	68	2		
7	W	56	Total	C	N	O	S	0	0
			455	306	72	75	2		
7	Y	63	Total	C	N	O	S	0	0
			510	341	83	84	2		

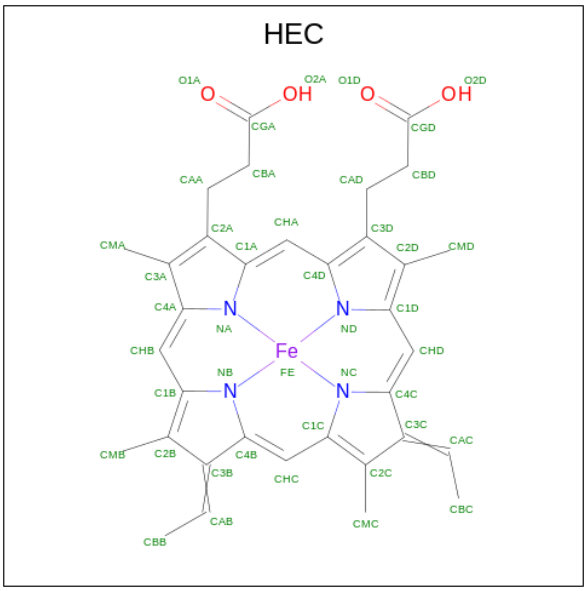
- Molecule 8 is a protein called Light-harvesting protein LH1 beta3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	E	43	Total	C	N	O	S	0	0
			353	236	55	59	3		
8	G	42	Total	C	N	O	S	0	0
			348	233	54	58	3		
8	T	42	Total	C	N	O	S	0	0
			348	233	54	58	3		
8	V	42	Total	C	N	O	S	0	0
			348	233	54	58	3		
8	X	42	Total	C	N	O	S	0	0
			348	233	54	58	3		
8	Z	41	Total	C	N	O	S	0	0
			342	230	53	56	3		

- Molecule 9 is a protein called Light-harvesting protein LH1 alpha3.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	3	65	Total	C	N	O	S	0	0
			499	337	80	79	3		

- Molecule 10 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).

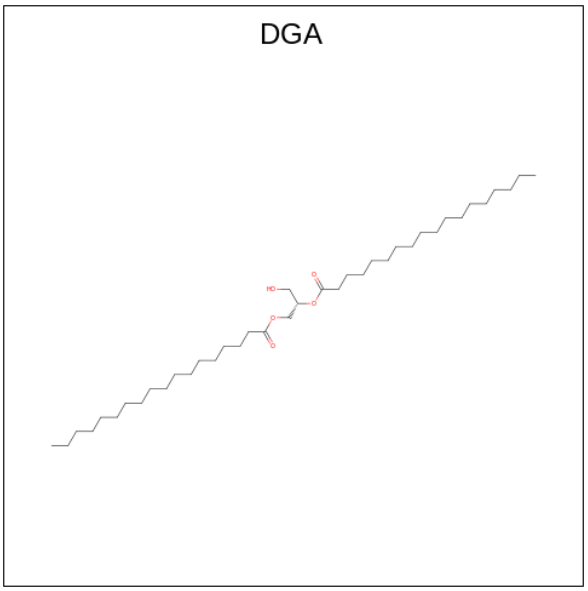


Mol	Chain	Residues	Atoms					AltConf
10	C	1	Total	C	Fe	N	O	0
			172	136	4	16	16	
10	C	1	Total	C	Fe	N	O	0
			172	136	4	16	16	
10	C	1	Total	C	Fe	N	O	0
			172	136	4	16	16	
10	C	1	Total	C	Fe	N	O	0
			172	136	4	16	16	

- Molecule 11 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

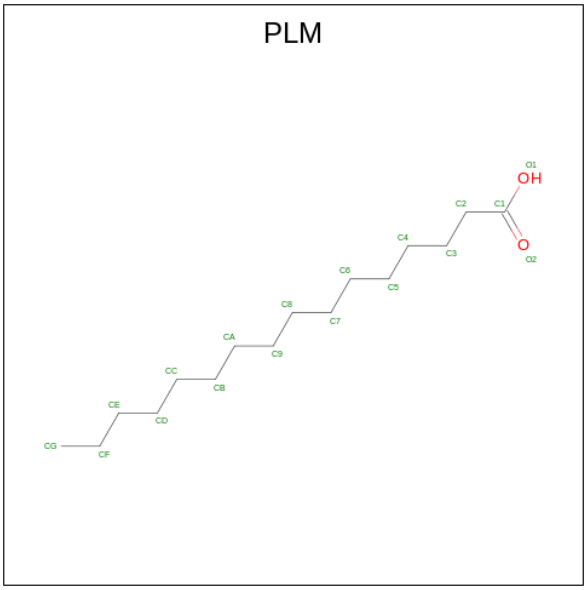
Mol	Chain	Residues	Atoms		AltConf
11	C	1	Total	Mg	0
			1	1	

- Molecule 12 is DIACYL GLYCEROL (three-letter code: DGA) (formula: $C_{39}H_{76}O_5$).



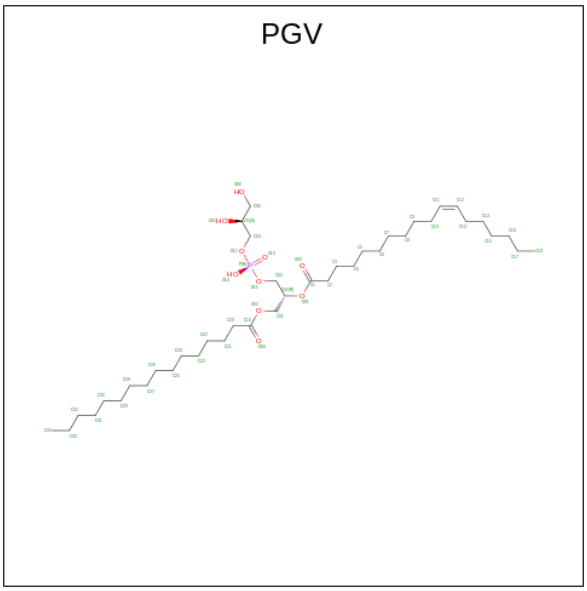
Mol	Chain	Residues	Atoms			AltConf
12	C	1	Total	C	O	0
			17	13	4	

- Molecule 13 is PALMITIC ACID (three-letter code: PLM) (formula: $C_{16}H_{32}O_2$).



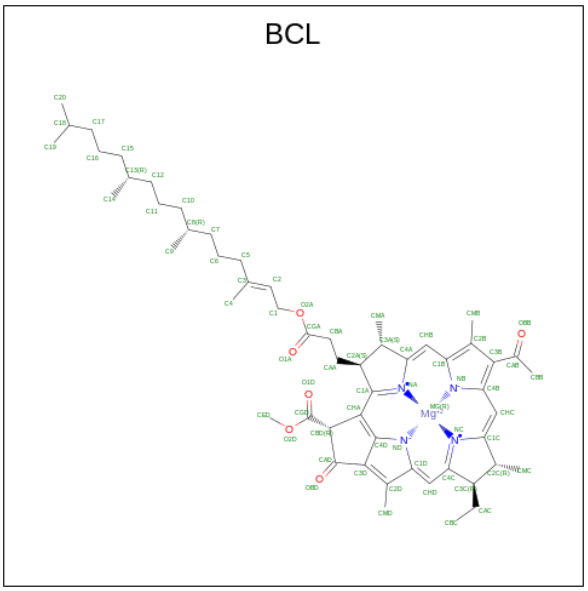
Mol	Chain	Residues	Atoms			AltConf
13	C	1	Total	C	O	0
			12	11	1	

- Molecule 14 is (1R)-2-{[{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (three-letter code: PGV) (formula: $C_{40}H_{77}O_{10}P$).



Mol	Chain	Residues	Atoms				AltConf
14	C	1	Total 31	C 20	O 10	P 1	0
14	L	1	Total 118	C 76	O 38	P 4	0
14	L	1	Total 118	C 76	O 38	P 4	0
14	L	1	Total 118	C 76	O 38	P 4	0
14	L	1	Total 118	C 76	O 38	P 4	0
14	M	1	Total 104	C 73	O 28	P 3	0
14	M	1	Total 104	C 73	O 28	P 3	0
14	M	1	Total 104	C 73	O 28	P 3	0
14	H	1	Total 36	C 25	O 10	P 1	0
14	D	1	Total 35	C 24	O 10	P 1	0
14	1	1	Total 27	C 18	O 8	P 1	0
14	5	1	Total 44	C 33	O 10	P 1	0

- Molecule 15 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
15	L	1	Total	C	Mg	N	O	0
			198	165	3	12	18	
15	L	1	Total	C	Mg	N	O	0
			198	165	3	12	18	
15	L	1	Total	C	Mg	N	O	0
			198	165	3	12	18	
15	M	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
15	A	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
15	B	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
15	D	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
15	E	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
15	F	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
15	G	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
15	I	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
15	J	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
15	K	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
15	N	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
15	O	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
15	P	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
15	Q	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
15	R	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
15	S	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
15	T	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
15	U	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
15	V	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
15	W	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
15	X	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
15	Y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
15	Z	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
15	1	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
15	2	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
15	3	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
15	4	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
15	5	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
15	6	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
15	7	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
15	8	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
15	9	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

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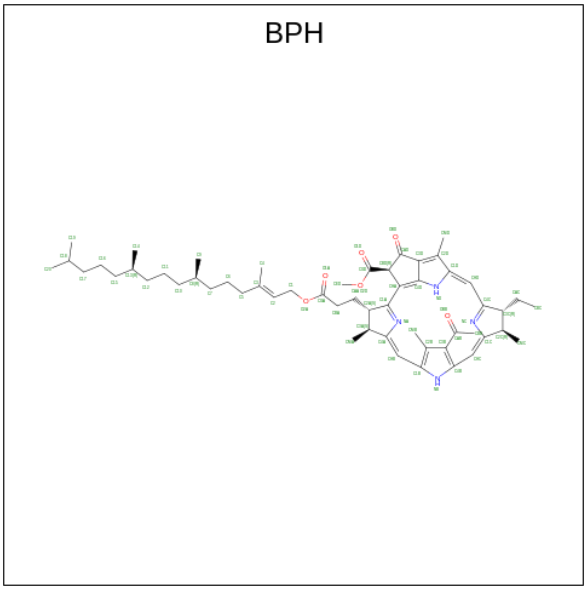
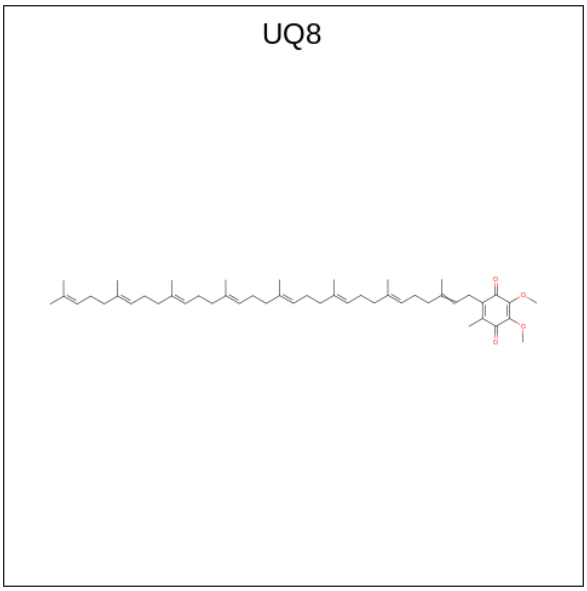
Mol	Chain	Residues	Atoms					AltConf
15	0	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

- Molecule 16 is BACTERIOPHEOPHYTIN A (three-letter code: BPH) (formula: $C_{55}H_{76}N_4O_6$).



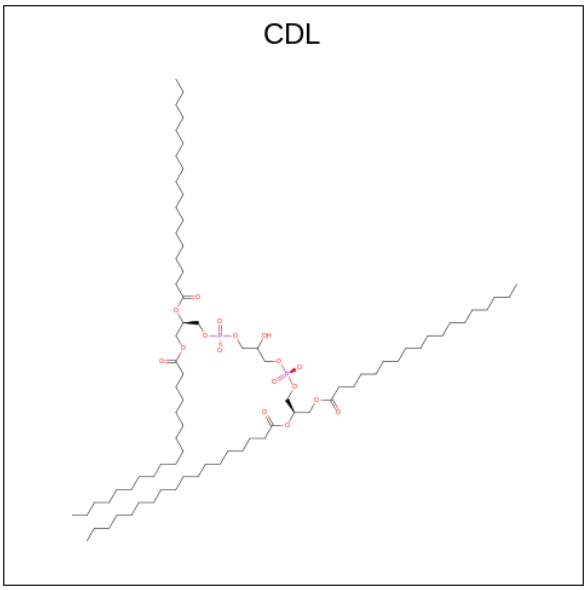
Mol	Chain	Residues	Atoms				AltConf
16	L	1	Total	C	N	O	0
			65	55	4	6	
16	M	1	Total	C	N	O	0
			65	55	4	6	

- Molecule 17 is Ubiquinone-8 (three-letter code: UQ8) (formula: $C_{49}H_{74}O_4$).



Mol	Chain	Residues	Atoms			AltConf
17	L	1	Total 119	C 107	O 12	0
17	L	1	Total 119	C 107	O 12	0
17	L	1	Total 119	C 107	O 12	0

- Molecule 18 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



Mol	Chain	Residues	Atoms				AltConf
18	L	1	Total 84	C 65	O 17	P 2	0

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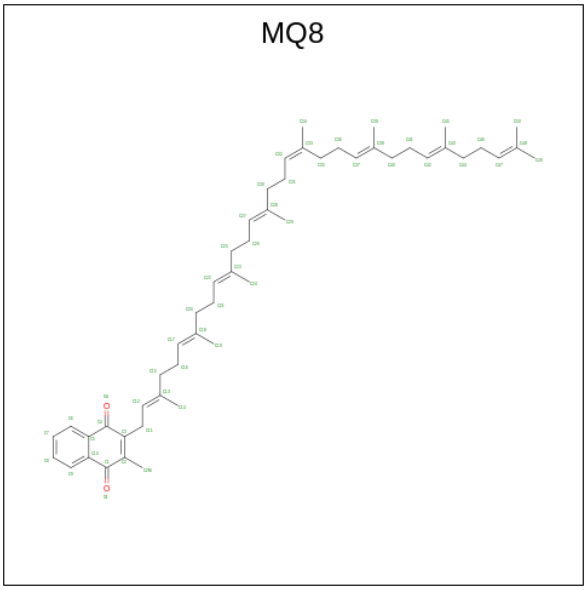
Mol	Chain	Residues	Atoms				AltConf
18	M	1	Total	C	O	P	0
			134	97	33	4	
18	M	1	Total	C	O	P	0
			134	97	33	4	
18	H	1	Total	C	O	P	0
			114	78	32	4	
18	H	1	Total	C	O	P	0
			114	78	32	4	
18	D	1	Total	C	O	P	0
			58	39	17	2	
18	I	1	Total	C	O	P	0
			51	32	17	2	
18	S	1	Total	C	O	P	0
			65	46	17	2	

- Molecule 19 is FE (III) ION (three-letter code: FE) (formula: Fe).

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

- Molecule 20 is MENAQUINONE 8 (three-letter code: MQ8) (formula: $C_{51}H_{72}O_2$).



Mol	Chain	Residues	Atoms			AltConf
20	M	1	Total	C	O	0
			106	102	4	

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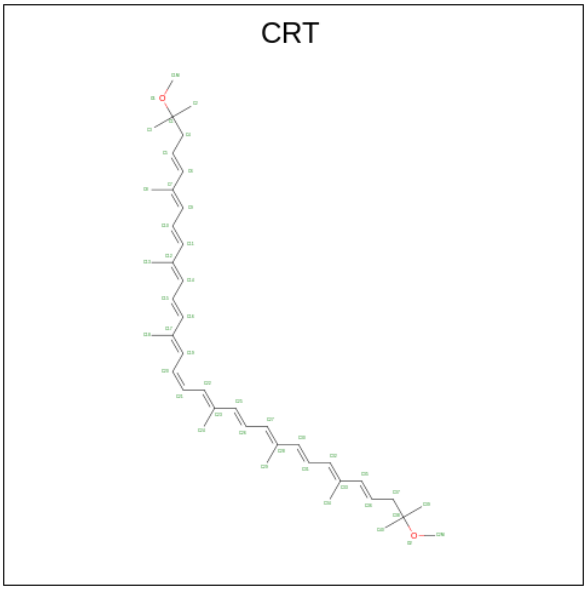
Mol	Chain	Residues	Atoms			AltConf
20	M	1	Total 106	C 102	O 4	0

- Molecule 21 is SPIRILLOXANTHIN (three-letter code: CRT) (formula: $C_{42}H_{60}O_2$).



Mol	Chain	Residues	Atoms			AltConf
21	M	1	Total 44	C 42	O 2	0
21	B	1	Total 44	C 42	O 2	0
21	E	1	Total 44	C 42	O 2	0
21	G	1	Total 44	C 42	O 2	0
21	J	1	Total 44	C 42	O 2	0
21	N	1	Total 44	C 42	O 2	0
21	P	1	Total 44	C 42	O 2	0
21	Q	1	Total 44	C 42	O 2	0
21	R	1	Total 44	C 42	O 2	0
21	S	1	Total 44	C 42	O 2	0

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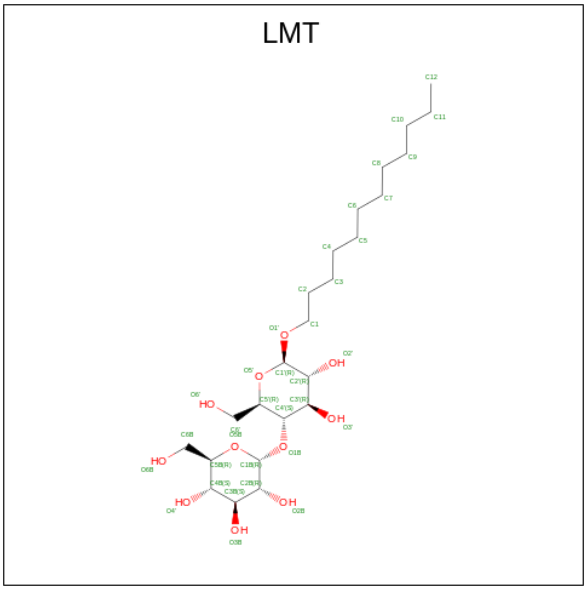
Mol	Chain	Residues	Atoms	AltConf
21	X	1	Total C O 44 42 2	0
21	1	1	Total C O 44 42 2	0
21	2	1	Total C O 44 42 2	0
21	4	1	Total C O 44 42 2	0
21	6	1	Total C O 44 42 2	0
21	7	1	Total C O 44 42 2	0
21	8	1	Total C O 44 42 2	0

- Molecule 22 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms	AltConf
22	H	1	Total C O 35 24 11	0
22	B	1	Total C O 35 24 11	0
22	E	1	Total C O 35 24 11	0
22	G	1	Total C O 35 24 11	0

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Mol	Chain	Residues	Atoms	AltConf
22	J	1	Total C O 70 48 22	0
22	J	1	Total C O 70 48 22	0
22	K	1	Total C O 35 24 11	0
22	N	1	Total C O 35 24 11	0
22	P	1	Total C O 35 24 11	0
22	T	1	Total C O 35 24 11	0
22	V	1	Total C O 35 24 11	0
22	X	1	Total C O 35 24 11	0
22	Z	1	Total C O 35 24 11	0
22	2	1	Total C O 35 24 11	0
22	4	1	Total C O 70 48 22	0
22	4	1	Total C O 70 48 22	0
22	8	1	Total C O 35 24 11	0
22	0	1	Total C O 35 24 11	0

- Molecule 23 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	AltConf
23	D	1	Total Ca 1 1	0
23	F	1	Total Ca 1 1	0
23	S	1	Total Ca 1 1	0
23	U	1	Total Ca 1 1	0
23	W	1	Total Ca 1 1	0

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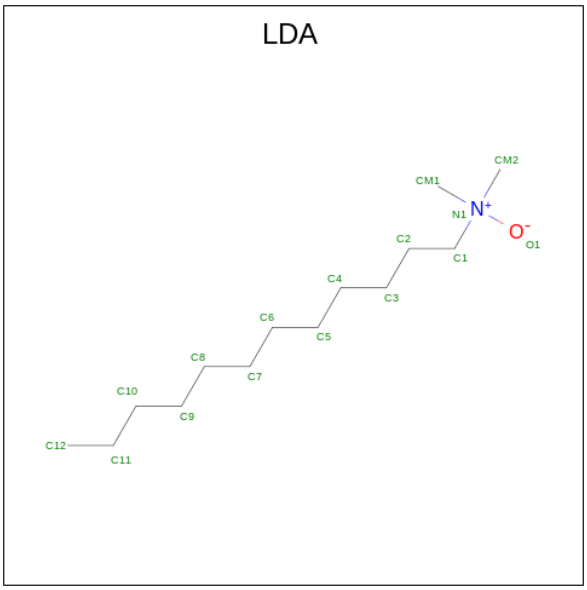
Mol	Chain	Residues	Atoms	AltConf
23	Y	1	Total Ca 1 1	0

- Molecule 24 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula: $C_{14}H_{31}NO$).



Mol	Chain	Residues	Atoms	AltConf
24	K	1	Total C N O 16 14 1 1	0
24	O	1	Total C N O 16 14 1 1	0

- Molecule 25 is water.

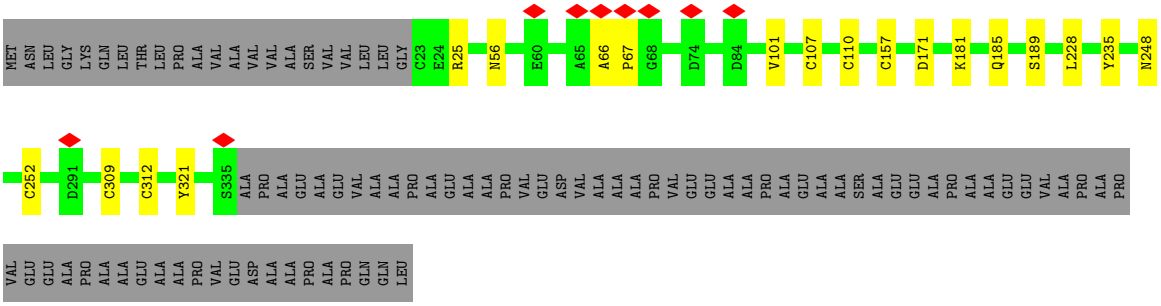
Mol	Chain	Residues	Atoms	AltConf
25	C	18	Total O 18 18	0
25	L	13	Total O 13 13	0
25	M	15	Total O 15 15	0
25	Y	1	Total O 1 1	0
25	3	1	Total O 1 1	0

3 Residue-property plots (i)

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

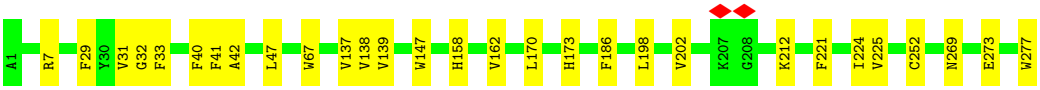
• Molecule 1: Photosynthetic reaction center cytochrome c subunit

Chain C:



• Molecule 2: Photosynthetic reaction center L subunit

Chain L:

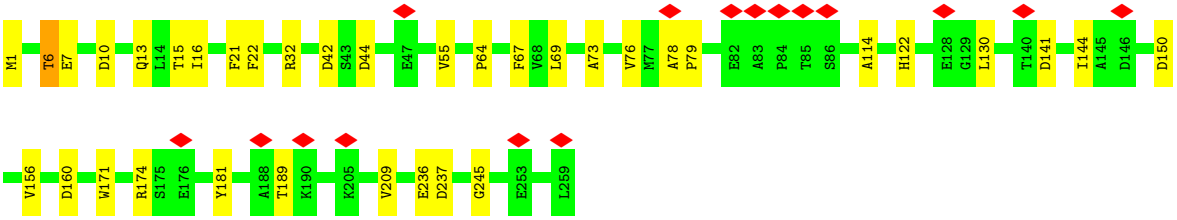


• Molecule 3: Photosynthetic reaction center M subunit

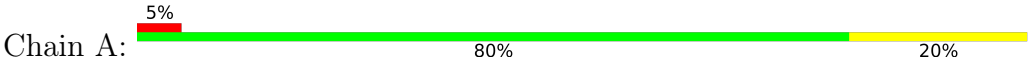
Chain M:

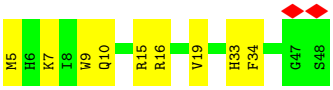
• Molecule 4: Photosynthetic reaction center H subunit

Chain H:

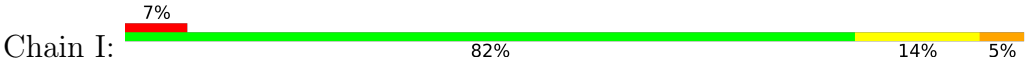


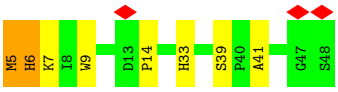
• Molecule 5: Light-harvesting protein LH1 alpha2



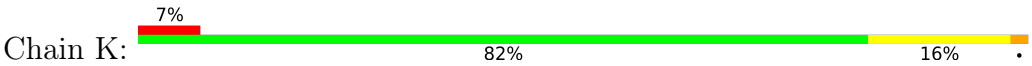


• Molecule 5: Light-harvesting protein LH1 alpha2

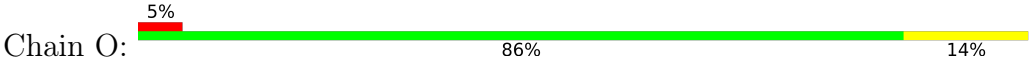


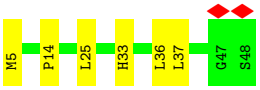


• Molecule 5: Light-harvesting protein LH1 alpha2

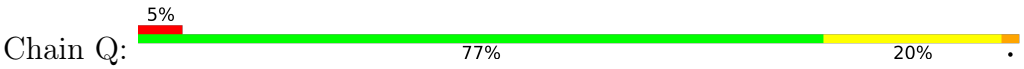


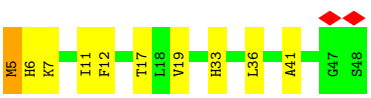
• Molecule 5: Light-harvesting protein LH1 alpha2



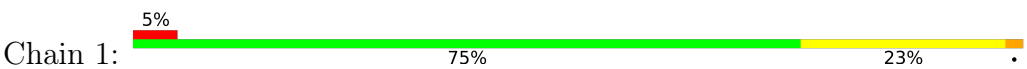


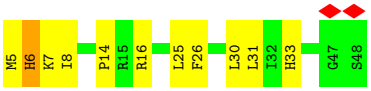
• Molecule 5: Light-harvesting protein LH1 alpha2



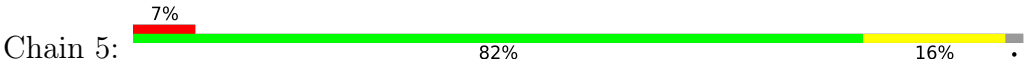


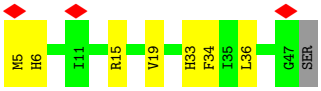
• Molecule 5: Light-harvesting protein LH1 alpha2



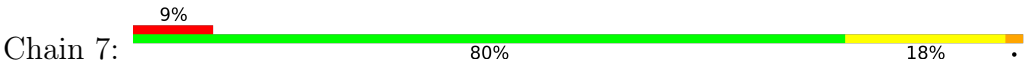


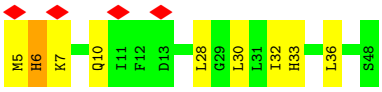
• Molecule 5: Light-harvesting protein LH1 alpha2



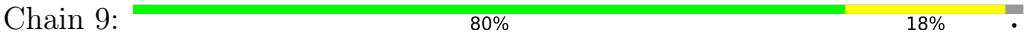


• Molecule 5: Light-harvesting protein LH1 alpha2

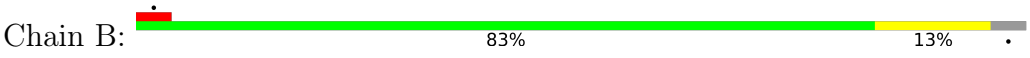


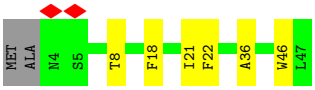


• Molecule 5: Light-harvesting protein LH1 alpha2

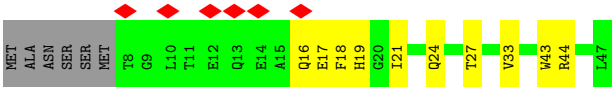


• Molecule 6: Light-harvesting protein LH1 beta1

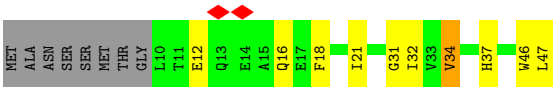




• Molecule 6: Light-harvesting protein LH1 beta1

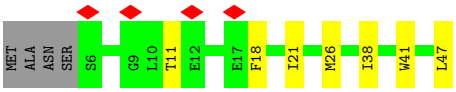


• Molecule 6: Light-harvesting protein LH1 beta1



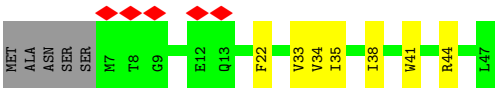
• Molecule 6: Light-harvesting protein LH1 beta1

Chain P:



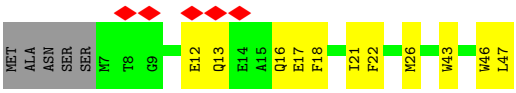
• Molecule 6: Light-harvesting protein LH1 beta1

Chain R:



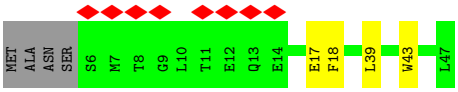
• Molecule 6: Light-harvesting protein LH1 beta1

Chain 2:



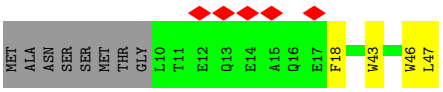
• Molecule 6: Light-harvesting protein LH1 beta1

Chain 4:



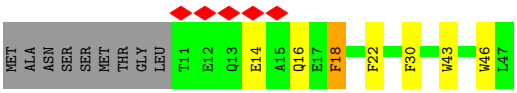
• Molecule 6: Light-harvesting protein LH1 beta1

Chain 6:



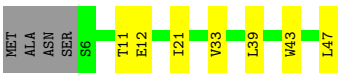
• Molecule 6: Light-harvesting protein LH1 beta1

Chain 8:



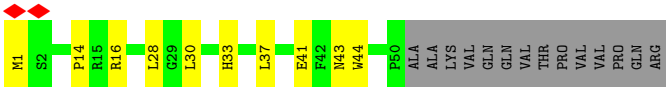
• Molecule 6: Light-harvesting protein LH1 beta1

Chain 0:



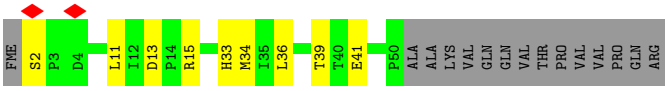
• Molecule 7: Light-harvesting protein LH1 alpha1

Chain D:



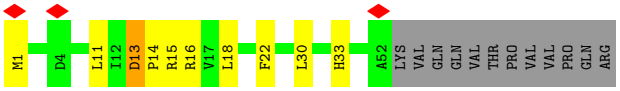
• Molecule 7: Light-harvesting protein LH1 alpha1

Chain F:



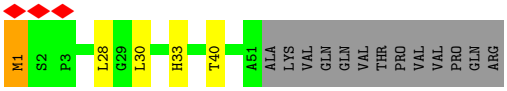
• Molecule 7: Light-harvesting protein LH1 alpha1

Chain S:



• Molecule 7: Light-harvesting protein LH1 alpha1

Chain U:

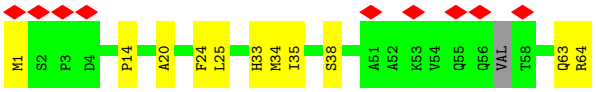


• Molecule 7: Light-harvesting protein LH1 alpha1

Chain W:

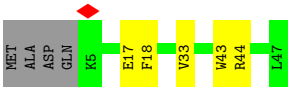
• Molecule 7: Light-harvesting protein LH1 alpha1

Chain Y:



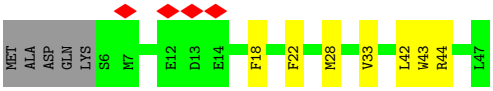
• Molecule 8: Light-harvesting protein LH1 beta3

Chain E:



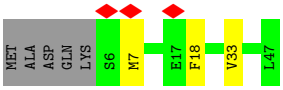
• Molecule 8: Light-harvesting protein LH1 beta3

Chain G:



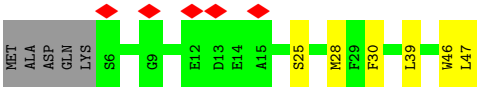
• Molecule 8: Light-harvesting protein LH1 beta3

Chain T:



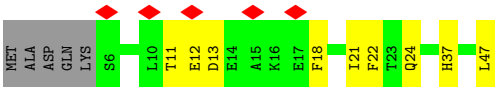
• Molecule 8: Light-harvesting protein LH1 beta3

Chain V:



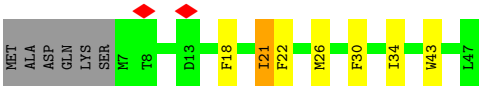
• Molecule 8: Light-harvesting protein LH1 beta3

Chain X:



• Molecule 8: Light-harvesting protein LH1 beta3

Chain Z:



• Molecule 9: Light-harvesting protein LH1 alpha3

Chain 3:

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	156992	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	JEOL CRYO ARM 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.101	Depositor
Minimum map value	-0.051	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.0134	Depositor
Map size (Å)	325.6, 325.6, 325.6	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.814, 0.814, 0.814	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BPH, PLM, DGA, PGV, FME, FE, CRT, HEC, CA, BCL, LMT, LDA, MQ8, UQ8, CDL, MG

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	C	0.28	0/2524	0.48	0/3453
2	L	0.29	0/2297	0.47	0/3139
3	M	0.29	0/2639	0.46	0/3611
4	H	0.28	0/2045	0.50	0/2782
5	1	0.26	0/369	0.43	0/500
5	5	0.27	0/358	0.43	0/488
5	7	0.27	0/365	0.44	0/496
5	9	0.26	0/362	0.44	0/492
5	A	0.27	0/369	0.43	0/500
5	I	0.27	0/369	0.42	0/500
5	K	0.26	0/369	0.42	0/500
5	O	0.26	0/369	0.43	0/500
5	Q	0.27	0/369	0.43	0/500
6	0	0.26	0/357	0.39	0/485
6	2	0.25	0/351	0.40	0/477
6	4	0.26	0/357	0.39	0/485
6	6	0.25	0/332	0.40	0/452
6	8	0.27	0/324	0.38	0/441
6	B	0.28	0/371	0.45	0/504
6	J	0.26	0/343	0.38	0/467
6	N	0.26	0/332	0.40	0/452
6	P	0.25	0/357	0.40	0/485
6	R	0.26	0/351	0.41	0/477
7	D	0.25	0/413	0.45	0/566
7	F	0.24	0/413	0.47	0/566
7	S	0.25	0/421	0.45	0/577
7	U	0.24	0/418	0.49	0/573
7	W	0.24	0/457	0.46	0/625
7	Y	0.27	0/513	0.47	0/702
8	E	0.25	0/365	0.42	0/494
8	G	0.26	0/360	0.41	0/487
8	T	0.26	0/360	0.41	0/487

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
8	V	0.26	0/360	0.41	0/487
8	X	0.25	0/360	0.41	0/487
8	Z	0.25	0/354	0.40	0/479
9	3	0.26	0/517	0.42	0/704
All	All	0.27	0/21590	0.45	0/29420

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	C	2450	0	2362	32	0
2	L	2212	0	2173	25	0
3	M	2539	0	2498	23	0
4	H	1989	0	1993	25	0
5	1	366	0	376	13	0
5	5	355	0	360	5	0
5	7	362	0	365	8	0
5	9	359	0	371	7	0
5	A	366	0	376	6	0
5	I	366	0	376	8	0
5	K	366	0	376	6	0
5	O	366	0	376	6	0
5	Q	366	0	376	10	0
6	0	345	0	334	6	0
6	2	339	0	329	11	0
6	4	345	0	334	4	0
6	6	320	0	310	4	0
6	8	312	0	299	9	0
6	B	359	0	345	6	0
6	J	331	0	320	11	0
6	N	320	0	310	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	P	345	0	334	5	0
6	R	339	0	329	6	0
7	D	411	0	430	8	0
7	F	401	0	419	9	0
7	S	419	0	433	11	0
7	U	416	0	435	6	0
7	W	455	0	478	10	0
7	Y	510	0	537	11	0
8	E	353	0	341	5	0
8	G	348	0	339	7	0
8	T	348	0	339	5	0
8	V	348	0	339	4	0
8	X	348	0	339	6	0
8	Z	342	0	334	7	0
9	3	499	0	506	6	0
10	C	172	0	126	24	0
11	C	1	0	0	0	0
12	C	17	0	15	0	0
13	C	12	0	18	1	0
14	1	27	0	25	2	0
14	5	44	0	56	4	0
14	C	31	0	32	3	0
14	D	35	0	40	0	0
14	H	36	0	42	3	0
14	L	118	0	122	4	0
14	M	104	0	124	3	0
15	0	66	0	74	7	0
15	1	66	0	74	5	0
15	2	66	0	74	6	0
15	3	66	0	74	4	0
15	4	66	0	74	5	0
15	5	66	0	74	4	0
15	6	66	0	74	5	0
15	7	61	0	61	1	0
15	8	66	0	74	9	0
15	9	66	0	74	5	0
15	A	66	0	74	1	0
15	B	66	0	74	7	0
15	D	66	0	74	4	0
15	E	66	0	74	5	0
15	F	66	0	74	6	0
15	G	66	0	74	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	I	66	0	74	3	0
15	J	66	0	74	5	0
15	K	66	0	74	8	0
15	L	198	0	222	9	0
15	M	66	0	74	3	0
15	N	66	0	74	7	0
15	O	66	0	74	4	0
15	P	66	0	74	10	0
15	Q	66	0	74	5	0
15	R	66	0	74	10	0
15	S	66	0	74	3	0
15	T	66	0	74	8	0
15	U	66	0	74	3	0
15	V	66	0	74	7	0
15	W	66	0	74	6	0
15	X	66	0	74	4	0
15	Y	66	0	74	7	0
15	Z	66	0	74	5	0
16	L	65	0	76	4	0
16	M	65	0	76	10	0
17	L	119	0	152	20	0
18	D	58	0	60	4	0
18	H	114	0	126	4	0
18	I	51	0	46	1	0
18	L	84	0	121	1	0
18	M	134	0	168	2	0
18	S	65	0	74	5	0
19	M	1	0	0	0	0
20	M	106	0	144	9	0
21	1	44	0	60	8	0
21	2	44	0	60	6	0
21	4	44	0	60	8	0
21	6	44	0	60	5	0
21	7	44	0	60	4	0
21	8	44	0	60	6	0
21	B	44	0	60	8	0
21	E	44	0	60	5	0
21	G	44	0	60	6	0
21	J	44	0	60	5	0
21	M	44	0	60	3	0
21	N	44	0	60	2	0
21	P	44	0	60	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	Q	44	0	60	6	0
21	R	44	0	60	5	0
21	S	44	0	60	2	0
21	X	44	0	60	5	0
22	0	35	0	46	2	0
22	2	35	0	46	2	0
22	4	70	0	92	4	0
22	8	35	0	46	1	0
22	B	35	0	46	1	0
22	E	35	0	46	1	0
22	G	35	0	46	3	0
22	H	35	0	46	1	0
22	J	70	0	92	1	0
22	K	35	0	46	1	0
22	N	35	0	46	0	0
22	P	35	0	46	1	0
22	T	35	0	46	0	0
22	V	35	0	46	3	0
22	X	35	0	46	0	0
22	Z	35	0	46	2	0
23	D	1	0	0	0	0
23	F	1	0	0	0	0
23	S	1	0	0	0	0
23	U	1	0	0	0	0
23	W	1	0	0	0	0
23	Y	1	0	0	0	0
24	K	16	0	31	1	0
24	O	16	0	31	2	0
25	3	1	0	0	0	0
25	C	18	0	0	0	0
25	L	13	0	0	0	0
25	M	15	0	0	1	0
25	Y	1	0	0	1	0
All	All	26309	0	27095	498	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (498) 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)
1:C:309:CYS:SG	10:C:504:HEC:HAB	1.53	1.48
1:C:252:CYS:SG	10:C:503:HEC:HAC	1.59	1.41
1:C:309:CYS:SG	10:C:504:HEC:CAB	2.07	1.40
1:C:110:CYS:SG	10:C:501:HEC:HAC	1.62	1.40
1:C:157:CYS:SG	10:C:502:HEC:HAC	1.64	1.38
1:C:252:CYS:SG	10:C:503:HEC:CAC	2.22	1.28
1:C:312:CYS:SG	10:C:504:HEC:HAC	1.74	1.25
1:C:157:CYS:SG	10:C:502:HEC:CAC	2.23	1.25
1:C:312:CYS:SG	10:C:504:HEC:CAC	2.25	1.23
1:C:110:CYS:SG	10:C:501:HEC:CAC	2.37	1.11
1:C:110:CYS:HG	10:C:501:HEC:HAC	1.23	1.04
1:C:252:CYS:HG	10:C:503:HEC:HAC	1.18	1.00
1:C:157:CYS:HG	10:C:502:HEC:HAC	0.94	0.88
1:C:309:CYS:SG	10:C:504:HEC:CBB	2.61	0.88
6:N:21:ILE:HD11	21:N:102:CRT:H6	1.60	0.84
1:C:25:ARG:HD3	14:C:508:PGV:H31	1.62	0.82
1:C:107:CYS:HB3	10:C:501:HEC:HAB	1.63	0.79
15:T:102:BCL:H122	15:T:102:BCL:HBB2	1.64	0.79
1:C:309:CYS:CB	10:C:504:HEC:HAB	2.19	0.73
8:X:11:THR:O	8:X:13:ASP:N	2.22	0.73
6:8:43:TRP:HB2	22:8:101:LMT:H42	1.72	0.71
4:H:32:ARG:NH2	18:H:302:CDL:OA3	2.25	0.70
5:Q:11:ILE:HD12	21:Q:102:CRT:H82	1.73	0.69
14:L:506:PGV:H201	7:Y:38:SER:HB2	1.75	0.68
21:B:103:CRT:H82	5:9:11:ILE:HD12	1.74	0.68
6:J:18:PHE:HD1	21:J:103:CRT:H6	1.56	0.68
6:4:43:TRP:HB2	22:4:101:LMT:H31	1.75	0.68
7:S:13:ASP:OD1	7:S:13:ASP:N	2.20	0.67
6:0:33:VAL:HG11	15:0:102:BCL:HBA2	1.77	0.67
18:I:101:CDL:H311	18:I:101:CDL:H551	1.77	0.67
16:M:403:BPH:HBB3	16:M:403:BPH:HHC	1.77	0.66
8:G:42:LEU:O	22:G:101:LMT:O3'	2.13	0.66
4:H:6:THR:HG21	7:F:39:THR:HG22	1.76	0.66
1:C:171:ASP:OD2	7:Y:64:ARG:NH2	2.29	0.66
18:L:510:CDL:H651	18:L:510:CDL:H851	1.76	0.65
5:1:8:ILE:HG12	21:4:103:CRT:H83	1.77	0.65
5:K:36:LEU:HD11	15:N:101:BCL:HHD	1.79	0.65
15:G:102:BCL:H43	15:G:102:BCL:H3A	1.79	0.64
5:O:36:LEU:HD11	15:P:101:BCL:HHD	1.78	0.64
2:L:139:VAL:HG22	14:5:101:PGV:H311	1.80	0.64
7:W:11:LEU:HD21	21:1:402:CRT:H1M1	1.79	0.64
2:L:67:TRP:HE1	14:M:411:PGV:H062	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:S:15:ARG:HH22	18:S:101:CDL:HA21	1.63	0.63
2:L:47:LEU:HD13	5:9:31:LEU:HD22	1.79	0.63
15:G:102:BCL:HBB2	15:G:102:BCL:H101	1.80	0.63
3:M:63:GLY:HA3	16:M:403:BPH:H5C2	1.81	0.63
2:L:224:ILE:HG22	2:L:225:VAL:HG13	1.81	0.62
7:W:1:FME:SD	7:W:1:FME:N	2.70	0.62
5:1:7:LYS:NZ	6:4:17:GLU:OE2	2.27	0.62
8:Z:34:ILE:HD13	15:Z:102:BCL:H93	1.80	0.62
5:K:10:GLN:NE2	6:N:12:GLU:OE1	2.32	0.62
21:G:103:CRT:H393	5:I:33:HIS:HB3	1.82	0.62
1:C:157:CYS:SG	10:C:502:HEC:C3C	2.87	0.61
16:M:403:BPH:HBC3	16:M:403:BPH:HHD	1.81	0.61
3:M:33:PRO:HG3	3:M:49:PRO:HD3	1.81	0.61
4:H:67:PHE:HB2	4:H:76:VAL:HG13	1.82	0.61
7:U:40:THR:HG21	7:W:56:GLN:HB2	1.84	0.60
1:C:185:GLN:NE2	3:M:95:GLU:OE1	2.34	0.60
5:1:33:HIS:CE1	15:2:102:BCL:HMD1	2.37	0.59
5:7:28:LEU:HD23	15:8:102:BCL:HED3	1.83	0.59
2:L:269:ASN:ND2	14:L:506:PGV:O06	2.35	0.59
2:L:33:PHE:HE2	17:L:505:UQ8:H25A	1.67	0.59
3:M:60:ILE:HD12	16:M:403:BPH:H9C2	1.85	0.59
3:M:242:THR:OG1	4:H:237:ASP:OD1	2.22	0.57
4:H:114:ALA:HB2	4:H:245:GLY:HA3	1.86	0.57
3:M:97:PRO:HB3	3:M:106:PRO:HG3	1.86	0.57
1:C:309:CYS:SG	10:C:504:HEC:HBB1	2.45	0.57
4:H:55:VAL:HG13	18:D:102:CDL:HA21	1.86	0.57
15:L:502:BCL:H152	16:L:503:BPH:H3A	1.87	0.56
21:J:103:CRT:H392	15:K:103:BCL:HBB2	1.87	0.56
4:H:78:ALA:HB3	4:H:79:PRO:HD3	1.87	0.56
5:1:26:PHE:CZ	21:1:402:CRT:H343	2.41	0.56
5:9:33:HIS:CE1	15:0:102:BCL:HMD1	2.40	0.56
16:L:503:BPH:HHC	16:L:503:BPH:HBB3	1.87	0.56
5:I:9:TRP:HE1	6:J:19:HIS:HB2	1.71	0.56
5:Q:33:HIS:CE1	15:R:101:BCL:HMD1	2.41	0.56
8:Z:43:TRP:HB2	22:Z:101:LMT:H42	1.87	0.55
6:B:18:PHE:HB2	21:B:103:CRT:H23	1.88	0.55
21:B:103:CRT:H342	15:D:103:BCL:HBA2	1.89	0.55
15:E:102:BCL:H111	15:E:102:BCL:HBB2	1.88	0.55
13:C:507:PLM:H61	14:L:506:PGV:H42	1.88	0.55
4:H:6:THR:HG22	4:H:7:GLU:H	1.72	0.55
6:P:18:PHE:HB2	21:P:102:CRT:H1M1	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Q:5:FME:O	5:Q:7:LYS:N	2.34	0.55
16:L:503:BPH:H101	15:L:508:BCL:H203	1.89	0.55
5:7:33:HIS:CE1	15:8:102:BCL:HMD1	2.42	0.54
8:V:39:LEU:HB3	22:V:101:LMT:H52	1.88	0.54
6:4:39:LEU:HB3	22:4:101:LMT:H42	1.87	0.54
1:C:107:CYS:CB	10:C:501:HEC:HAB	2.37	0.54
7:Y:33:HIS:CE1	15:Z:102:BCL:HMD1	2.43	0.54
5:K:6:HIS:ND1	6:N:16:GLN:OE1	2.41	0.54
4:H:64:PRO:HA	4:H:79:PRO:HD2	1.90	0.54
7:S:33:HIS:CE1	15:T:102:BCL:HMD1	2.42	0.54
7:D:33:HIS:CE1	15:E:102:BCL:HMD1	2.43	0.54
6:P:47:LEU:O	22:P:103:LMT:O3'	2.25	0.54
3:M:160:GLY:HA3	21:M:405:CRT:H292	1.90	0.53
5:I:33:HIS:CE1	15:J:102:BCL:HMD1	2.43	0.53
8:X:47:LEU:HD13	22:Z:101:LMT:H32	1.90	0.53
5:7:6:HIS:CG	6:8:16:GLN:HE22	2.26	0.53
21:7:102:CRT:H42	6:0:21:ILE:HD12	1.90	0.53
7:Y:63:GLN:O	25:Y:201:HOH:O	2.19	0.53
8:G:18:PHE:CD1	21:G:103:CRT:H6	2.44	0.53
18:H:301:CDL:H332	18:D:102:CDL:H142	1.91	0.52
5:O:33:HIS:CE1	15:P:101:BCL:HMD1	2.44	0.52
5:Q:12:PHE:HB3	5:Q:17:THR:HG21	1.89	0.52
15:0:102:BCL:H3A	15:0:102:BCL:H43	1.90	0.52
22:4:104:LMT:H42	6:6:43:TRP:HB2	1.90	0.52
7:S:11:LEU:HD21	21:S:104:CRT:H1M1	1.92	0.52
2:L:202:VAL:HG13	2:L:212:LYS:HB2	1.91	0.52
16:M:403:BPH:H18	16:M:403:BPH:H13	1.91	0.52
5:1:6:HIS:ND1	6:2:16:GLN:OE1	2.42	0.52
7:W:33:HIS:CE1	15:X:102:BCL:HMD1	2.45	0.52
8:X:22:PHE:HA	21:X:103:CRT:H14	1.91	0.52
7:F:33:HIS:CE1	15:G:102:BCL:HMD1	2.46	0.51
7:D:14:PRO:HB3	8:E:18:PHE:CZ	2.46	0.51
1:C:248:ASN:HA	2:L:170:LEU:HD21	1.93	0.51
6:0:39:LEU:HB3	22:0:101:LMT:H42	1.93	0.51
21:Q:102:CRT:H35	15:U:101:BCL:HHB	1.93	0.51
6:2:13:GLN:HE21	6:2:17:GLU:HG2	1.76	0.51
5:7:36:LEU:HD11	15:8:102:BCL:HHD	1.93	0.51
6:8:46:TRP:HZ2	15:8:102:BCL:H141	1.75	0.50
6:8:18:PHE:CD2	21:8:103:CRT:H6	2.47	0.50
7:F:11:LEU:HD23	21:J:103:CRT:H22A	1.92	0.50
6:J:43:TRP:HB2	22:J:101:LMT:H31	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:8:18:PHE:HD2	21:8:103:CRT:H6	1.76	0.50
21:E:103:CRT:H292	15:F:101:BCL:H151	1.92	0.50
8:T:33:VAL:HG11	15:T:102:BCL:HBA2	1.92	0.50
18:M:410:CDL:H792	4:H:22:PHE:HA	1.94	0.50
4:H:171:TRP:HB2	4:H:181:TYR:HB2	1.92	0.50
8:V:46:TRP:CD1	8:V:47:LEU:HG	2.46	0.50
1:C:312:CYS:SG	10:C:504:HEC:C3C	2.98	0.50
5:1:7:LYS:HB2	21:4:103:CRT:H41	1.93	0.50
5:5:33:HIS:CE1	15:6:101:BCL:HMD1	2.47	0.50
2:L:198:LEU:HD22	2:L:221:PHE:CE2	2.47	0.50
5:1:16:ARG:HH22	9:3:15:ARG:NH2	2.08	0.50
14:C:508:PGV:H71	5:1:31:LEU:HD21	1.94	0.50
4:H:141:ASP:OD1	4:H:141:ASP:N	2.44	0.49
5:A:7:LYS:NZ	8:E:17:GLU:OE2	2.40	0.49
8:Z:18:PHE:HB2	21:1:402:CRT:H23	1.93	0.49
6:B:21:ILE:HD12	21:B:103:CRT:H6	1.93	0.49
7:F:41:GLU:O	8:G:44:ARG:NH1	2.45	0.49
4:H:69:LEU:HB2	4:H:73:ALA:HB3	1.95	0.49
7:S:14:PRO:HB3	8:T:18:PHE:CZ	2.48	0.49
7:D:28:LEU:HD23	15:E:102:BCL:HED3	1.94	0.49
5:1:30:LEU:HD23	21:1:402:CRT:H36	1.93	0.49
6:B:46:TRP:HZ2	15:B:102:BCL:H143	1.77	0.49
7:U:1:FME:O1	8:X:24:GLN:NE2	2.45	0.49
16:M:403:BPH:H101	16:M:403:BPH:H142	1.95	0.48
15:6:101:BCL:HMB1	15:6:101:BCL:HBB2	1.95	0.48
3:M:156:TYR:CZ	21:M:405:CRT:H293	2.49	0.48
21:E:103:CRT:H371	15:F:101:BCL:HMB2	1.94	0.48
2:L:198:LEU:HD22	2:L:221:PHE:HE2	1.78	0.48
5:I:5:FME:C	5:I:7:LYS:H	2.27	0.48
18:S:101:CDL:H392	18:S:101:CDL:H331	1.94	0.48
17:L:505:UQ8:H15	17:L:505:UQ8:H12	1.58	0.48
7:D:37:LEU:O	7:D:43:ASN:ND2	2.46	0.48
4:H:21:PHE:HE2	14:H:303:PGV:H291	1.77	0.48
7:D:41:GLU:O	8:E:44:ARG:NH1	2.47	0.48
21:Q:102:CRT:H372	7:U:33:HIS:CG	2.48	0.48
7:W:11:LEU:HD12	21:1:402:CRT:H82	1.95	0.48
15:L:509:BCL:HBB2	15:L:509:BCL:HMB1	1.96	0.48
20:M:404:MQ8:H241	20:M:404:MQ8:H261	1.66	0.48
6:B:36:ALA:HB1	22:B:101:LMT:H111	1.95	0.48
21:X:103:CRT:H371	15:Y:101:BCL:HMB2	1.96	0.48
6:2:12:GLU:O	6:2:16:GLN:HG2	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:252:CYS:SG	10:C:503:HEC:C3C	2.99	0.48
5:K:14:PRO:HB3	6:N:18:PHE:CE2	2.49	0.48
15:W:101:BCL:H62	15:W:101:BCL:H41	1.48	0.48
7:Y:25:LEU:HB2	15:Y:101:BCL:H52	1.95	0.48
6:0:43:TRP:HD1	22:0:101:LMT:H3O2	1.58	0.48
8:Z:30:PHE:CE1	15:Z:102:BCL:H11	2.49	0.47
15:5:102:BCL:H62	15:5:102:BCL:H41	1.66	0.47
15:M:402:BCL:H61	15:M:402:BCL:H41	1.56	0.47
15:J:102:BCL:H62	15:J:102:BCL:H41	1.41	0.47
6:2:43:TRP:HB2	22:2:101:LMT:H31	1.95	0.47
21:8:103:CRT:H36	5:9:30:LEU:HD23	1.96	0.47
4:H:13:GLN:O	4:H:16:ILE:HG22	2.14	0.47
5:K:28:LEU:HD23	15:N:101:BCL:HED3	1.96	0.47
5:1:25:LEU:HB2	15:1:403:BCL:H43	1.96	0.47
6:2:26:MET:HE3	21:2:103:CRT:H19	1.96	0.47
15:8:102:BCL:H161	15:8:102:BCL:H121	1.61	0.47
5:A:33:HIS:CE1	15:B:102:BCL:HMD1	2.50	0.47
6:R:22:PHE:CD1	21:R:102:CRT:H14	2.50	0.47
14:C:508:PGV:H21	14:C:508:PGV:H52	1.70	0.47
2:L:42:ALA:HB1	20:M:404:MQ8:H393	1.96	0.47
17:L:505:UQ8:H17	17:L:505:UQ8:H20	1.62	0.47
17:L:505:UQ8:H32A	17:L:505:UQ8:H28	1.50	0.47
21:P:102:CRT:H10	21:P:102:CRT:H81	1.73	0.47
15:R:101:BCL:H3A	15:R:101:BCL:H51	1.96	0.47
7:Y:35:ILE:HG12	14:1:401:PGV:H42	1.97	0.47
5:O:37:LEU:HD13	24:O:501:LDA:H81	1.96	0.47
15:6:101:BCL:H143	15:6:101:BCL:H112	1.70	0.47
4:H:1:MET:N	5:I:39:SER:OG	2.46	0.47
20:M:406:MQ8:H2M1	20:M:406:MQ8:H112	1.70	0.47
8:T:7:MET:SD	8:T:7:MET:N	2.87	0.47
6:J:33:VAL:HG11	15:J:102:BCL:HAA1	1.97	0.46
6:6:18:PHE:CD1	21:6:102:CRT:H6	2.50	0.46
6:8:14:GLU:O	6:8:18:PHE:HB3	2.15	0.46
4:H:44:ASP:OD2	5:A:15:ARG:NH2	2.49	0.46
6:B:22:PHE:HA	21:B:103:CRT:H14	1.97	0.46
5:9:25:LEU:HB3	15:9:101:BCL:H12	1.96	0.46
1:C:189:SER:OG	7:Y:64:ARG:NH1	2.49	0.46
16:L:503:BPH:HHC	16:L:503:BPH:CBB	2.46	0.46
8:G:33:VAL:HG11	15:G:102:BCL:HAA1	1.97	0.46
2:L:173:HIS:HB3	3:M:182:LEU:HD13	1.98	0.46
3:M:54:PHE:CD1	5:Q:19:VAL:HG21	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:E:103:CRT:H393	7:F:33:HIS:HB3	1.98	0.46
15:I:102:BCL:H41	15:I:102:BCL:H62	1.68	0.46
6:N:46:TRP:CD1	6:N:47:LEU:HG	2.50	0.46
15:P:101:BCL:H72	15:P:101:BCL:H111	1.39	0.46
7:D:16:ARG:NH1	18:D:102:CDL:HA31	2.29	0.46
15:P:101:BCL:HBB2	15:P:101:BCL:HMB1	1.98	0.46
5:Q:36:LEU:HD11	15:R:101:BCL:HHD	1.97	0.46
8:V:25:SER:O	8:V:28:MET:HG3	2.16	0.46
6:2:22:PHE:HA	21:2:103:CRT:H14	1.98	0.46
17:L:512:UQ8:H25	17:L:512:UQ8:H22	1.65	0.46
14:H:303:PGV:H31	7:F:34:MET:HE1	1.97	0.46
3:M:201:HIS:CE1	3:M:205:ILE:HD11	2.51	0.46
8:G:22:PHE:CD1	21:G:103:CRT:H14	2.50	0.46
15:N:101:BCL:H121	15:N:101:BCL:H161	1.83	0.46
21:6:102:CRT:H372	5:7:33:HIS:CG	2.50	0.46
7:F:36:LEU:HD11	15:G:102:BCL:HHD	1.98	0.46
15:R:101:BCL:H11	21:R:102:CRT:H27	1.97	0.46
4:H:67:PHE:HE2	4:H:78:ALA:HB2	1.80	0.46
6:J:18:PHE:CD1	21:J:103:CRT:H6	2.45	0.46
7:U:33:HIS:CE1	15:V:102:BCL:HMD1	2.51	0.46
7:W:14:PRO:HB3	8:X:18:PHE:CZ	2.51	0.46
15:3:101:BCL:HMB1	15:3:101:BCL:HBB3	1.98	0.46
6:0:11:THR:OG1	6:0:12:GLU:N	2.49	0.46
21:E:103:CRT:H241	15:F:101:BCL:H143	1.98	0.46
15:B:102:BCL:H93	15:B:102:BCL:H111	1.81	0.45
6:R:34:VAL:O	6:R:38:ILE:HG12	2.16	0.45
22:V:101:LMT:H3'	22:V:101:LMT:H1B	1.67	0.45
15:2:102:BCL:H203	15:2:102:BCL:H13	1.98	0.45
21:6:102:CRT:H36	5:7:30:LEU:HD23	1.99	0.45
5:A:10:GLN:HB2	21:E:103:CRT:H1M1	1.97	0.45
15:3:101:BCL:HED1	15:3:101:BCL:H93	1.98	0.45
21:4:103:CRT:H342	15:5:102:BCL:HBA2	1.98	0.45
15:7:101:BCL:HBB3	15:7:101:BCL:HMB1	1.98	0.45
6:8:22:PHE:CD1	21:8:103:CRT:H14	2.52	0.45
6:0:47:LEU:HD12	15:0:102:BCL:H193	1.99	0.45
17:L:512:UQ8:H12	17:L:512:UQ8:H15	1.61	0.45
4:H:13:GLN:NE2	14:H:303:PGV:H212	2.32	0.45
15:B:102:BCL:H141	15:B:102:BCL:H162	1.78	0.45
15:R:101:BCL:H111	15:R:101:BCL:H152	1.76	0.45
21:R:102:CRT:H36	7:S:30:LEU:HD23	1.99	0.45
5:1:33:HIS:CG	21:1:402:CRT:H372	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:186:PHE:HB3	16:M:403:BPH:HBB2	1.99	0.45
5:K:33:HIS:CE1	15:N:101:BCL:HMD1	2.51	0.45
18:S:101:CDL:H132	18:S:101:CDL:H161	1.75	0.45
7:W:36:LEU:HD11	15:X:102:BCL:HHD	1.99	0.45
5:5:36:LEU:HD11	15:6:101:BCL:HHD	1.99	0.45
17:L:505:UQ8:H7	17:L:505:UQ8:H10	1.75	0.45
3:M:64:PHE:HD1	16:M:403:BPH:H111	1.82	0.45
15:K:103:BCL:HBC3	15:K:103:BCL:H2C	1.78	0.45
15:K:103:BCL:HMB1	15:K:103:BCL:HBB3	1.99	0.45
21:P:102:CRT:H35	15:Q:101:BCL:HMB2	1.98	0.45
15:W:101:BCL:HMB1	15:W:101:BCL:HBB3	1.99	0.45
9:3:55:LEU:HB3	9:3:59:MET:HG3	1.98	0.45
17:L:505:UQ8:H27	17:L:505:UQ8:H30	1.68	0.45
15:J:102:BCL:HMB3	15:K:103:BCL:CHB	2.47	0.45
21:S:104:CRT:H35	15:W:101:BCL:HHB	1.99	0.45
17:L:505:UQ8:H35	17:L:505:UQ8:H32	1.70	0.45
17:L:505:UQ8:H46	17:L:505:UQ8:H42	1.71	0.45
15:L:508:BCL:H192	15:L:508:BCL:H161	1.73	0.45
15:L:508:BCL:H62	15:L:508:BCL:H92	1.71	0.45
15:F:101:BCL:H41	15:F:101:BCL:H61	1.62	0.45
5:I:6:HIS:CE1	6:J:16:GLN:HE22	2.35	0.45
5:I:41:ALA:O	6:J:44:ARG:NH1	2.50	0.45
15:R:101:BCL:CHB	15:R:101:BCL:H71	2.46	0.45
15:R:101:BCL:HMB1	15:R:101:BCL:HBB2	1.98	0.45
15:V:102:BCL:H18	15:V:102:BCL:H151	1.61	0.45
9:3:44:TRP:CZ2	15:3:101:BCL:HHC	2.52	0.45
5:5:34:PHE:CE1	14:5:101:PGV:H22	2.52	0.45
1:C:181:LYS:H	3:M:109:SER:HB2	1.82	0.45
2:L:40:PHE:CZ	5:9:23:GLY:HA3	2.52	0.45
3:M:3:TYR:CZ	3:M:5:ASN:HA	2.51	0.45
21:B:103:CRT:H36	7:D:30:LEU:HD23	1.99	0.45
15:X:102:BCL:H151	15:X:102:BCL:H18	1.73	0.45
8:Z:21:ILE:H	8:Z:21:ILE:HG12	1.46	0.45
15:4:102:BCL:H143	15:4:102:BCL:H111	1.73	0.45
15:4:102:BCL:H192	15:4:102:BCL:H161	1.79	0.45
5:O:25:LEU:HD13	15:O:502:BCL:H42	1.97	0.45
21:X:103:CRT:H20	21:X:103:CRT:H181	1.81	0.45
2:L:41:PHE:HA	17:L:512:UQ8:H4M	1.99	0.44
4:H:156:VAL:HG22	4:H:209:VAL:HB	1.98	0.44
15:O:502:BCL:HMB1	15:O:502:BCL:HBB3	1.99	0.44
7:Y:25:LEU:HD12	15:Y:101:BCL:H52	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:7:102:CRT:H15	21:7:102:CRT:H131	1.89	0.44
1:C:56:ASN:HD22	1:C:321:TYR:HE2	1.65	0.44
15:J:102:BCL:HBB2	15:J:102:BCL:HMB1	1.99	0.44
15:Y:101:BCL:HBB3	15:Y:101:BCL:HMB1	1.99	0.44
6:6:46:TRP:CD1	6:6:47:LEU:HG	2.52	0.44
15:P:101:BCL:H43	15:P:101:BCL:H3A	1.99	0.44
7:W:7:LYS:HA	7:W:10:LEU:HD13	2.00	0.44
15:9:101:BCL:HBB3	15:9:101:BCL:HMB1	1.99	0.44
15:P:101:BCL:H3A	15:P:101:BCL:O2A	2.17	0.44
15:R:101:BCL:H3A	15:R:101:BCL:H12	1.98	0.44
8:E:43:TRP:HD1	22:E:101:LMT:H3O2	1.65	0.44
6:2:22:PHE:HA	21:2:103:CRT:H11	1.99	0.44
21:8:103:CRT:H20	21:8:103:CRT:H181	1.83	0.44
15:I:102:BCL:HBB3	15:I:102:BCL:HMB1	1.99	0.44
5:O:25:LEU:HB3	15:O:502:BCL:H12	1.99	0.44
5:1:14:PRO:HB3	6:2:18:PHE:CZ	2.53	0.44
6:J:17:GLU:O	6:J:21:ILE:HG12	2.18	0.44
15:1:403:BCL:HMB1	15:1:403:BCL:HBB3	1.99	0.44
21:B:103:CRT:H10	21:B:103:CRT:H81	1.81	0.44
21:G:103:CRT:H35	15:I:102:BCL:HMB2	2.00	0.44
15:1:403:BCL:HBC3	15:1:403:BCL:H2C	1.80	0.44
15:0:102:BCL:HMB1	15:0:102:BCL:HBB2	1.99	0.44
1:C:101:VAL:HG21	10:C:502:HEC:HMB3	2.00	0.44
6:R:33:VAL:HG21	15:R:101:BCL:HBA1	2.00	0.44
16:M:403:BPH:H6C1	16:M:403:BPH:H4C1	1.60	0.43
7:F:13:ASP:OD1	7:F:13:ASP:N	2.50	0.43
15:2:102:BCL:H141	15:2:102:BCL:H161	1.75	0.43
15:2:102:BCL:H93	15:2:102:BCL:H61	1.83	0.43
15:2:102:BCL:HMB1	15:2:102:BCL:HBB2	2.00	0.43
16:M:403:BPH:HBA2	16:M:403:BPH:H3A	1.85	0.43
4:H:181:TYR:OH	4:H:236:GLU:HG3	2.17	0.43
15:X:102:BCL:HBB3	15:X:102:BCL:HMB1	1.99	0.43
21:X:103:CRT:H10	21:X:103:CRT:H81	1.84	0.43
15:4:102:BCL:H61	15:4:102:BCL:H41	1.77	0.43
15:L:509:BCL:H61	15:L:509:BCL:H2	1.66	0.43
20:M:406:MQ8:H391	20:M:406:MQ8:H412	1.52	0.43
15:T:102:BCL:HMB1	15:T:102:BCL:HBB3	2.00	0.43
15:Z:102:BCL:HMB1	15:Z:102:BCL:HBB2	1.99	0.43
6:8:30:PHE:HE2	15:9:101:BCL:H171	1.82	0.43
2:L:31:VAL:HG23	2:L:32:GLY:H	1.83	0.43
18:M:408:CDL:H1	18:M:408:CDL:H311	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:B:102:BCL:H161	15:B:102:BCL:H192	1.76	0.43
15:B:102:BCL:HMB1	15:B:102:BCL:HBB2	1.99	0.43
15:G:102:BCL:HBB3	15:G:102:BCL:HMB1	2.00	0.43
8:X:21:ILE:HD12	21:X:103:CRT:H6	2.00	0.43
17:L:505:UQ8:H22	17:L:505:UQ8:H25	1.86	0.43
15:V:102:BCL:H142	15:V:102:BCL:HBB2	1.99	0.43
6:4:18:PHE:HB2	21:4:103:CRT:H32A	2.00	0.43
15:6:101:BCL:H141	15:6:101:BCL:H162	1.80	0.43
21:8:103:CRT:H10	21:8:103:CRT:H81	1.85	0.43
2:L:273:GLU:HB3	14:L:506:PGV:H212	2.00	0.43
3:M:2:GLU:O	3:M:4:GLN:NE2	2.51	0.43
21:P:102:CRT:H22A	21:P:102:CRT:H5	1.29	0.43
5:Q:41:ALA:O	6:R:44:ARG:NH1	2.51	0.43
15:T:102:BCL:H202	22:V:101:LMT:H22	2.00	0.43
15:V:102:BCL:HMB1	15:V:102:BCL:HBB3	2.00	0.43
7:W:25:LEU:HB3	15:W:101:BCL:H42	2.01	0.43
15:Y:101:BCL:H141	15:Y:101:BCL:H161	1.76	0.43
6:2:21:ILE:HB	21:2:103:CRT:H9	2.00	0.43
5:5:15:ARG:O	5:5:19:VAL:HG23	2.18	0.43
7:D:44:TRP:CZ2	15:D:103:BCL:HHC	2.53	0.43
5:Q:5:FME:C	5:Q:7:LYS:H	2.25	0.43
15:F:101:BCL:HMB1	15:F:101:BCL:HBB3	2.01	0.43
14:M:409:PGV:H272	14:M:409:PGV:H242	1.60	0.43
21:B:103:CRT:H20	21:B:103:CRT:H181	1.83	0.43
15:N:101:BCL:H3A	15:N:101:BCL:O2A	2.19	0.43
15:S:102:BCL:HBB3	15:S:102:BCL:HMB1	2.01	0.43
15:3:101:BCL:H161	15:3:101:BCL:H192	1.76	0.43
24:K:101:LDA:H21	24:K:101:LDA:HM23	1.77	0.43
15:Q:101:BCL:HMB1	15:Q:101:BCL:HBB3	2.01	0.43
21:1:402:CRT:H10	21:1:402:CRT:H81	1.83	0.43
6:2:46:TRP:CE2	15:2:102:BCL:H2C	2.53	0.43
2:L:29:PHE:CE1	18:H:301:CDL:H131	2.54	0.42
17:L:512:UQ8:H17	17:L:512:UQ8:H20	1.77	0.42
4:H:144:ILE:HG13	4:H:150:ASP:OD1	2.19	0.42
15:U:101:BCL:HBA1	15:U:101:BCL:H3A	1.82	0.42
17:L:504:UQ8:H22	17:L:504:UQ8:H25	1.73	0.42
21:7:102:CRT:H10	21:7:102:CRT:H81	1.87	0.42
3:M:58:LEU:HD12	3:M:62:PHE:HE1	1.84	0.42
7:S:15:ARG:HH12	18:S:101:CDL:H1	1.85	0.42
8:V:30:PHE:CE1	15:V:102:BCL:H11	2.54	0.42
15:D:103:BCL:HMB1	15:D:103:BCL:HBB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:E:33:VAL:HG11	15:E:102:BCL:HAA1	2.01	0.42
5:Q:5:FME:C	5:Q:7:LYS:N	2.83	0.42
21:Q:102:CRT:H36	7:U:30:LEU:HD23	2.02	0.42
6:2:47:LEU:HD13	22:4:101:LMT:H32	2.01	0.42
1:C:228:LEU:HD11	3:M:188:PHE:HA	2.02	0.42
9:3:28:LEU:HD23	15:4:102:BCL:HED3	2.01	0.42
5:5:34:PHE:CD1	14:5:101:PGV:H52	2.54	0.42
17:L:505:UQ8:H27	17:L:505:UQ8:H23	1.79	0.42
3:M:174:VAL:HA	3:M:175:PRO:HD3	1.94	0.42
20:M:406:MQ8:H61	25:M:508:HOH:O	2.20	0.42
21:G:103:CRT:H20	21:G:103:CRT:H181	1.91	0.42
6:J:24:GLN:O	6:J:27:THR:HG22	2.20	0.42
15:P:101:BCL:H121	15:P:101:BCL:H162	1.72	0.42
15:Q:101:BCL:H41	15:Q:101:BCL:H61	1.47	0.42
8:Z:22:PHE:O	8:Z:26:MET:HG3	2.20	0.42
20:M:404:MQ8:H312	20:M:404:MQ8:H351	1.76	0.42
14:M:411:PGV:H62	14:M:411:PGV:H91	1.82	0.42
8:T:33:VAL:HG11	15:T:102:BCL:CBA	2.50	0.42
15:Z:102:BCL:H142	15:Z:102:BCL:H112	1.85	0.42
17:L:512:UQ8:H22	17:L:512:UQ8:H18	1.55	0.42
15:D:103:BCL:H62	15:D:103:BCL:H41	1.43	0.42
21:R:102:CRT:H372	7:S:33:HIS:CG	2.55	0.42
7:S:18:LEU:HD23	7:S:18:LEU:HA	1.87	0.42
7:S:22:PHE:CD2	18:S:101:CDL:H131	2.55	0.42
9:3:31:PHE:HE2	21:4:103:CRT:H401	1.85	0.42
2:L:29:PHE:HE1	18:H:301:CDL:H131	1.84	0.42
22:H:304:LMT:H22	22:K:102:LMT:H21	2.01	0.42
15:F:101:BCL:H51	15:F:101:BCL:H12	1.77	0.42
21:J:103:CRT:H15	21:J:103:CRT:H131	1.95	0.42
21:4:103:CRT:H10	21:4:103:CRT:H81	1.94	0.42
2:L:7:ARG:NH2	4:H:42:ASP:OD2	2.50	0.41
17:L:512:UQ8:H7	17:L:512:UQ8:H11A	1.80	0.41
21:2:103:CRT:H31	21:2:103:CRT:H291	1.94	0.41
15:L:508:BCL:H192	15:L:508:BCL:H141	2.02	0.41
20:M:406:MQ8:H201	20:M:406:MQ8:H161	1.73	0.41
5:A:9:TRP:O	6:B:8:THR:HG21	2.20	0.41
21:N:102:CRT:H10	21:N:102:CRT:H81	1.77	0.41
1:C:309:CYS:CA	10:C:504:HEC:HAB	2.50	0.41
3:M:196:TYR:CZ	15:M:402:BCL:HMC2	2.56	0.41
20:M:404:MQ8:H412	20:M:404:MQ8:H391	1.93	0.41
15:A:101:BCL:HMB1	15:A:101:BCL:HBB3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:N:31:GLY:O	6:N:34:VAL:HG12	2.20	0.41
21:P:102:CRT:H371	15:Q:101:BCL:HMB2	2.02	0.41
15:Q:101:BCL:H161	15:Q:101:BCL:H141	1.79	0.41
3:M:58:LEU:HB3	3:M:127:LEU:HD13	2.00	0.41
3:M:295:LEU:HD23	3:M:295:LEU:HA	1.88	0.41
18:D:102:CDL:H572	18:D:102:CDL:H541	1.77	0.41
6:P:41:TRP:CD2	15:P:101:BCL:H193	2.56	0.41
15:W:101:BCL:H8	15:W:101:BCL:H121	1.79	0.41
21:4:103:CRT:H26	21:4:103:CRT:H241	1.90	0.41
15:0:102:BCL:H3A	15:0:102:BCL:HBA1	1.55	0.41
1:C:66:ALA:HA	1:C:67:PRO:HD3	1.97	0.41
17:L:504:UQ8:H7	17:L:504:UQ8:H10	1.75	0.41
7:Y:14:PRO:HB3	8:Z:18:PHE:CZ	2.56	0.41
15:4:102:BCL:H161	15:4:102:BCL:H141	1.83	0.41
15:9:101:BCL:H151	15:9:101:BCL:H112	1.82	0.41
2:L:137:VAL:HG23	2:L:138:VAL:HG23	2.03	0.41
15:Y:101:BCL:HBC3	15:Y:101:BCL:H2C	1.91	0.41
21:7:102:CRT:H131	5:9:22:PHE:HZ	1.86	0.41
15:K:103:BCL:H201	6:N:32:ILE:HD11	2.02	0.41
6:R:35:ILE:HD12	6:R:35:ILE:HA	1.89	0.41
8:T:33:VAL:HG21	15:T:102:BCL:HBA2	2.02	0.41
15:0:102:BCL:H62	15:0:102:BCL:H41	1.79	0.41
3:M:1:PRO:HB2	3:M:2:GLU:H	1.60	0.41
20:M:406:MQ8:H451	20:M:406:MQ8:H462	1.87	0.41
15:K:103:BCL:HHD	15:K:103:BCL:HAC2	1.82	0.41
6:P:21:ILE:HD12	21:P:102:CRT:H6	2.02	0.41
15:P:101:BCL:H62	15:P:101:BCL:H41	1.70	0.41
15:P:101:BCL:H62	15:P:101:BCL:HHB	2.01	0.41
15:S:102:BCL:H192	15:S:102:BCL:H161	1.70	0.41
22:2:101:LMT:H5B	22:2:101:LMT:H6E	2.02	0.41
15:5:102:BCL:HMB1	15:5:102:BCL:HBB3	2.03	0.41
21:6:102:CRT:H26	21:6:102:CRT:H241	1.94	0.41
5:7:7:LYS:HA	5:7:10:GLN:HE22	1.85	0.41
15:8:102:BCL:H112	15:8:102:BCL:H142	1.78	0.41
15:9:101:BCL:H152	15:9:101:BCL:H18	1.71	0.41
10:C:503:HEC:HBB1	2:L:170:LEU:HD22	2.03	0.41
2:L:40:PHE:CD2	17:L:512:UQ8:H10B	2.56	0.41
2:L:147:TRP:NE1	17:L:505:UQ8:H3MA	2.36	0.41
2:L:158:HIS:O	2:L:162:VAL:HG23	2.21	0.41
4:H:130:LEU:HB3	4:H:174:ARG:NH1	2.36	0.41
8:G:43:TRP:CD1	22:G:101:LMT:H2'	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:K:103:BCL:HMD1	6:N:37:HIS:CE1	2.56	0.41
24:O:501:LDA:H21	24:O:501:LDA:HM13	1.84	0.41
15:W:101:BCL:H13	15:W:101:BCL:H171	1.83	0.41
7:Y:34:MET:HB3	14:1:401:PGV:H72	2.03	0.41
21:1:402:CRT:H15	21:1:402:CRT:H131	1.91	0.41
15:1:403:BCL:H72	15:1:403:BCL:H111	1.35	0.41
15:5:102:BCL:HHD	15:5:102:BCL:HAC2	1.86	0.41
5:7:32:ILE:HD12	15:8:102:BCL:O1D	2.20	0.41
6:8:46:TRP:CZ2	15:8:102:BCL:H2C	2.56	0.41
15:B:102:BCL:H93	15:B:102:BCL:H61	1.67	0.41
15:E:102:BCL:HMB1	15:E:102:BCL:HBB3	2.03	0.41
21:G:103:CRT:H26	21:G:103:CRT:H241	1.87	0.41
15:O:502:BCL:H91	15:O:502:BCL:H111	1.75	0.41
21:R:102:CRT:H31	21:R:102:CRT:H291	1.95	0.41
7:S:13:ASP:OD2	7:S:16:ARG:HD3	2.21	0.41
15:T:102:BCL:H111	15:T:102:BCL:H152	1.96	0.41
15:V:102:BCL:H71	15:V:102:BCL:H111	1.36	0.41
15:Y:101:BCL:HHD	15:Y:101:BCL:HAC2	1.87	0.41
21:2:103:CRT:H20	21:2:103:CRT:H181	1.86	0.41
3:M:200:PHE:HZ	4:H:15:THR:HG22	1.87	0.40
7:F:2:SER:OG	6:J:21:ILE:HD12	2.21	0.40
15:K:103:BCL:H102	15:K:103:BCL:H13	1.93	0.40
5:O:14:PRO:HB3	6:P:18:PHE:CZ	2.56	0.40
5:Q:5:FME:O	5:Q:7:LYS:HG2	2.21	0.40
5:1:7:LYS:HB3	21:4:103:CRT:H23	2.03	0.40
15:N:101:BCL:HMB1	15:N:101:BCL:HBB2	2.03	0.40
21:Q:102:CRT:H20	21:Q:102:CRT:H181	1.82	0.40
7:U:28:LEU:HD23	15:V:102:BCL:HED3	2.03	0.40
7:Y:20:ALA:O	7:Y:24:PHE:HB2	2.21	0.40
15:L:508:BCL:HMB1	15:L:508:BCL:HBB2	2.03	0.40
21:Q:102:CRT:H342	15:U:101:BCL:HBA2	2.02	0.40
6:6:18:PHE:HD1	21:6:102:CRT:H6	1.84	0.40
5:A:16:ARG:HA	5:A:19:VAL:HG12	2.03	0.40
8:G:43:TRP:HD1	22:G:101:LMT:H2'	1.86	0.40
6:R:41:TRP:CD1	15:R:101:BCL:H202	2.56	0.40
14:5:101:PGV:H302	14:5:101:PGV:H91	2.03	0.40
15:8:102:BCL:HMB1	15:8:102:BCL:HBB2	2.03	0.40
15:L:502:BCL:H61	15:L:502:BCL:H41	1.84	0.40
15:M:402:BCL:H143	15:M:402:BCL:H161	1.91	0.40
21:M:405:CRT:H181	21:M:405:CRT:H20	1.85	0.40
5:I:14:PRO:HB3	6:J:18:PHE:CZ	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:N:101:BCL:H122	15:N:101:BCL:H8	1.91	0.40
15:S:102:BCL:H51	15:S:102:BCL:H12	1.69	0.40
7:W:49:ILE:HA	7:W:50:PRO:HA	1.90	0.40
15:1:403:BCL:H121	15:1:403:BCL:H161	1.91	0.40
9:3:4:GLN:HB3	9:3:7:LYS:HE3	2.03	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	C	311/405 (77%)	297 (96%)	14 (4%)	0	100	100
2	L	275/277 (99%)	268 (98%)	7 (2%)	0	100	100
3	M	316/324 (98%)	309 (98%)	7 (2%)	0	100	100
4	H	258/259 (100%)	245 (95%)	13 (5%)	0	100	100
5	1	42/44 (96%)	40 (95%)	1 (2%)	1 (2%)	6	19
5	5	41/44 (93%)	40 (98%)	0	1 (2%)	6	19
5	7	42/44 (96%)	37 (88%)	4 (10%)	1 (2%)	6	19
5	9	41/44 (93%)	39 (95%)	2 (5%)	0	100	100
5	A	42/44 (96%)	42 (100%)	0	0	100	100
5	I	42/44 (96%)	40 (95%)	1 (2%)	1 (2%)	6	19
5	K	42/44 (96%)	41 (98%)	1 (2%)	0	100	100
5	O	42/44 (96%)	41 (98%)	1 (2%)	0	100	100
5	Q	42/44 (96%)	40 (95%)	1 (2%)	1 (2%)	6	19
6	0	40/46 (87%)	40 (100%)	0	0	100	100
6	2	39/46 (85%)	39 (100%)	0	0	100	100
6	4	40/46 (87%)	38 (95%)	2 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	6	36/46 (78%)	34 (94%)	2 (6%)	0	100	100
6	8	35/46 (76%)	34 (97%)	1 (3%)	0	100	100
6	B	42/46 (91%)	41 (98%)	1 (2%)	0	100	100
6	J	38/46 (83%)	37 (97%)	1 (3%)	0	100	100
6	N	36/46 (78%)	35 (97%)	1 (3%)	0	100	100
6	P	40/46 (87%)	40 (100%)	0	0	100	100
6	R	39/46 (85%)	39 (100%)	0	0	100	100
7	D	48/64 (75%)	46 (96%)	2 (4%)	0	100	100
7	F	47/64 (73%)	47 (100%)	0	0	100	100
7	S	50/64 (78%)	49 (98%)	1 (2%)	0	100	100
7	U	49/64 (77%)	48 (98%)	1 (2%)	0	100	100
7	W	54/64 (84%)	53 (98%)	1 (2%)	0	100	100
7	Y	59/64 (92%)	56 (95%)	3 (5%)	0	100	100
8	E	41/47 (87%)	40 (98%)	1 (2%)	0	100	100
8	G	40/47 (85%)	40 (100%)	0	0	100	100
8	T	40/47 (85%)	40 (100%)	0	0	100	100
8	V	40/47 (85%)	39 (98%)	1 (2%)	0	100	100
8	X	40/47 (85%)	39 (98%)	0	1 (2%)	5	18
8	Z	39/47 (83%)	39 (100%)	0	0	100	100
9	3	63/67 (94%)	59 (94%)	4 (6%)	0	100	100
All	All	2531/2854 (89%)	2451 (97%)	74 (3%)	6 (0%)	50	76

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	X	12	GLU
5	7	6	HIS
5	Q	6	HIS
5	5	6	HIS
5	1	6	HIS
5	I	6	HIS

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	C	265/322 (82%)	264 (100%)	1 (0%)	91 97
2	L	224/224 (100%)	222 (99%)	2 (1%)	78 93
3	M	252/256 (98%)	248 (98%)	4 (2%)	62 87
4	H	208/208 (100%)	203 (98%)	5 (2%)	49 80
5	1	38/38 (100%)	38 (100%)	0	100 100
5	5	36/38 (95%)	36 (100%)	0	100 100
5	7	37/38 (97%)	37 (100%)	0	100 100
5	9	37/38 (97%)	37 (100%)	0	100 100
5	A	38/38 (100%)	37 (97%)	1 (3%)	46 78
5	I	38/38 (100%)	38 (100%)	0	100 100
5	K	38/38 (100%)	36 (95%)	2 (5%)	22 52
5	O	38/38 (100%)	38 (100%)	0	100 100
5	Q	38/38 (100%)	38 (100%)	0	100 100
6	0	35/38 (92%)	35 (100%)	0	100 100
6	2	34/38 (90%)	34 (100%)	0	100 100
6	4	35/38 (92%)	35 (100%)	0	100 100
6	6	32/38 (84%)	32 (100%)	0	100 100
6	8	31/38 (82%)	30 (97%)	1 (3%)	39 71
6	B	37/38 (97%)	37 (100%)	0	100 100
6	J	33/38 (87%)	33 (100%)	0	100 100
6	N	32/38 (84%)	31 (97%)	1 (3%)	40 72
6	P	35/38 (92%)	32 (91%)	3 (9%)	10 29
6	R	34/38 (90%)	34 (100%)	0	100 100
7	D	44/56 (79%)	44 (100%)	0	100 100
7	F	44/56 (79%)	43 (98%)	1 (2%)	50 80
7	S	43/56 (77%)	42 (98%)	1 (2%)	50 80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	U	44/56 (79%)	44 (100%)	0	100	100
7	W	48/56 (86%)	47 (98%)	1 (2%)	53	82
7	Y	55/56 (98%)	55 (100%)	0	100	100
8	E	36/40 (90%)	36 (100%)	0	100	100
8	G	36/40 (90%)	35 (97%)	1 (3%)	43	76
8	T	36/40 (90%)	36 (100%)	0	100	100
8	V	36/40 (90%)	36 (100%)	0	100	100
8	X	36/40 (90%)	35 (97%)	1 (3%)	43	76
8	Z	35/40 (88%)	34 (97%)	1 (3%)	42	74
9	3	49/51 (96%)	48 (98%)	1 (2%)	55	83
All	All	2167/2359 (92%)	2140 (99%)	27 (1%)	72	91

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	235	TYR
2	L	252	CYS
2	L	277	TRP
3	M	55	THR
3	M	174	VAL
3	M	215	PHE
3	M	242	THR
4	H	6	THR
4	H	10	ASP
4	H	122	HIS
4	H	160	ASP
4	H	189	THR
5	A	34	PHE
7	F	15	ARG
8	G	28	MET
5	K	6	HIS
5	K	34	PHE
6	N	34	VAL
6	P	11	THR
6	P	26	MET
6	P	38	ILE
7	S	13	ASP
7	W	30	LEU

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Mol	Chain	Res	Type
8	X	37	HIS
8	Z	21	ILE
9	3	16	MET
6	8	18	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	56	ASN
1	C	186	ASN
1	C	283	GLN
2	L	269	ASN
3	M	4	GLN
3	M	258	ASN
5	A	6	HIS
6	B	16	GLN
6	J	16	GLN
6	P	13	GLN
6	P	16	GLN
6	2	13	GLN
6	2	16	GLN
5	5	10	GLN
5	7	6	HIS
5	7	10	GLN
6	8	16	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

14 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	$\#\|Z\|>2$
7	FME	D	1	7	8,9,10	0.53	0	7,9,11	1.01	1 (14%)
7	FME	S	1	7	8,9,10	0.51	0	7,9,11	0.97	1 (14%)
5	FME	A	5	5	8,9,10	0.50	0	7,9,11	0.98	1 (14%)
7	FME	Y	1	7	8,9,10	0.52	0	7,9,11	1.00	1 (14%)
5	FME	I	5	5	8,9,10	0.51	0	7,9,11	1.09	1 (14%)
5	FME	K	5	5	8,9,10	0.51	0	7,9,11	1.28	1 (14%)
5	FME	O	5	5	8,9,10	0.53	0	7,9,11	0.98	1 (14%)
5	FME	7	5	5	8,9,10	0.52	0	7,9,11	1.01	1 (14%)
7	FME	U	1	7	8,9,10	0.52	0	7,9,11	1.00	1 (14%)
5	FME	5	5	5	8,9,10	0.54	0	7,9,11	1.03	1 (14%)
5	FME	Q	5	5	8,9,10	0.51	0	7,9,11	0.99	1 (14%)
7	FME	W	1	7	8,9,10	0.52	0	7,9,11	0.97	1 (14%)
5	FME	9	5	5	8,9,10	0.48	0	7,9,11	1.07	1 (14%)
5	FME	1	5	5	8,9,10	0.50	0	7,9,11	1.04	1 (14%)

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
7	FME	D	1	7	-	1/7/9/11	-
7	FME	S	1	7	-	2/7/9/11	-
5	FME	A	5	5	-	2/7/9/11	-
7	FME	Y	1	7	-	0/7/9/11	-
5	FME	I	5	5	-	1/7/9/11	-
5	FME	K	5	5	-	1/7/9/11	-
5	FME	O	5	5	-	0/7/9/11	-
5	FME	7	5	5	-	0/7/9/11	-
7	FME	U	1	7	-	0/7/9/11	-
5	FME	5	5	5	-	3/7/9/11	-
5	FME	Q	5	5	-	1/7/9/11	-
7	FME	W	1	7	-	0/7/9/11	-
5	FME	9	5	5	-	1/7/9/11	-
5	FME	1	5	5	-	0/7/9/11	-

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	K	5	FME	O-C-CA	-2.64	117.87	124.78
5	I	5	FME	O-C-CA	-2.62	117.91	124.78
5	Q	5	FME	O-C-CA	-2.54	118.11	124.78
5	7	5	FME	O-C-CA	-2.54	118.11	124.78
5	9	5	FME	O-C-CA	-2.53	118.16	124.78
7	Y	1	FME	O-C-CA	-2.50	118.23	124.78
5	1	5	FME	O-C-CA	-2.49	118.25	124.78
7	U	1	FME	O-C-CA	-2.48	118.28	124.78
7	W	1	FME	O-C-CA	-2.47	118.30	124.78
5	O	5	FME	O-C-CA	-2.42	118.43	124.78
7	D	1	FME	O-C-CA	-2.41	118.46	124.78
5	5	5	FME	O-C-CA	-2.38	118.55	124.78
5	A	5	FME	O-C-CA	-2.37	118.56	124.78
7	S	1	FME	O-C-CA	-2.29	118.77	124.78

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	5	FME	N-CA-CB-CG
5	K	5	FME	CB-CA-N-CN
5	Q	5	FME	O-C-CA-CB
5	5	5	FME	O1-CN-N-CA
5	5	5	FME	CB-CA-N-CN
7	D	1	FME	O1-CN-N-CA
7	S	1	FME	O1-CN-N-CA
5	5	5	FME	CA-CB-CG-SD
5	9	5	FME	C-CA-CB-CG
7	S	1	FME	N-CA-CB-CG
5	A	5	FME	C-CA-CB-CG
5	I	5	FME	CB-CA-N-CN

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	I	5	FME	1	0
7	U	1	FME	1	0
5	Q	5	FME	4	0
7	W	1	FME	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 114 ligands modelled in this entry, 8 are monoatomic - leaving 106 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	$\#\|Z\| > 2$
22	LMT	J	101	-	36,36,36	0.39	0	47,47,47	0.73	0
15	BCL	6	101	-	58,74,74	1.63	10 (17%)	69,115,115	1.61	14 (20%)
24	LDA	O	501	-	12,15,15	2.08	1 (8%)	14,17,17	0.48	0
22	LMT	N	103	-	36,36,36	0.39	0	47,47,47	0.64	0
22	LMT	P	103	-	36,36,36	0.38	0	47,47,47	0.74	1 (2%)
14	PGV	C	508	-	30,30,50	1.15	2 (6%)	33,36,56	1.28	4 (12%)
21	CRT	1	402	-	41,43,43	0.72	0	50,54,54	1.77	10 (20%)
22	LMT	0	101	-	36,36,36	0.44	0	47,47,47	0.89	1 (2%)
15	BCL	Q	101	-	58,74,74	1.65	10 (17%)	69,115,115	1.64	12 (17%)
14	PGV	M	411	-	35,35,50	1.08	2 (5%)	38,41,56	1.27	4 (10%)
10	HEC	C	503	1	32,50,50	1.56	4 (12%)	24,82,82	1.39	3 (12%)
22	LMT	4	104	-	36,36,36	0.40	0	47,47,47	0.70	1 (2%)
18	CDL	H	302	-	34,34,99	1.21	3 (8%)	39,44,111	1.12	3 (7%)
21	CRT	6	102	-	41,43,43	0.72	0	50,54,54	1.74	14 (28%)
14	PGV	M	407	-	36,36,50	1.05	2 (5%)	39,42,56	1.14	3 (7%)
15	BCL	N	101	-	58,74,74	1.66	11 (18%)	69,115,115	1.63	15 (21%)
10	HEC	C	502	1	32,50,50	1.57	5 (15%)	24,82,82	1.30	1 (4%)
15	BCL	G	102	-	58,74,74	1.63	9 (15%)	69,115,115	1.64	16 (23%)
17	UQ8	L	505	-	53,53,53	1.21	2 (3%)	64,67,67	1.79	20 (31%)
21	CRT	Q	102	-	41,43,43	0.72	0	50,54,54	1.82	11 (22%)
21	CRT	G	103	-	41,43,43	0.69	0	50,54,54	1.52	11 (22%)
15	BCL	F	101	-	58,74,74	1.64	10 (17%)	69,115,115	1.73	14 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
15	BCL	L	509	-	58,74,74	1.64	11 (18%)	69,115,115	1.67	13 (18%)
22	LMT	2	101	-	36,36,36	0.42	0	47,47,47	0.68	0
16	BPH	L	503	-	51,70,70	0.53	0	52,101,101	0.62	0
14	PGV	L	501	-	16,16,50	1.40	2 (12%)	20,21,56	1.41	3 (15%)
21	CRT	N	102	-	41,43,43	0.71	0	50,54,54	1.71	9 (18%)
22	LMT	Z	101	-	36,36,36	0.39	0	47,47,47	0.79	1 (2%)
15	BCL	I	102	-	58,74,74	1.65	11 (18%)	69,115,115	1.56	13 (18%)
15	BCL	K	103	-	58,74,74	1.68	10 (17%)	69,115,115	1.66	15 (21%)
13	PLM	C	507	1	11,11,17	0.39	0	10,10,17	0.44	0
22	LMT	H	304	-	36,36,36	0.41	0	47,47,47	0.70	1 (2%)
15	BCL	P	101	-	58,74,74	1.65	11 (18%)	69,115,115	1.64	17 (24%)
15	BCL	3	101	-	58,74,74	1.68	11 (18%)	69,115,115	1.58	12 (17%)
14	PGV	1	401	-	26,26,50	1.29	2 (7%)	29,31,56	1.18	2 (6%)
15	BCL	9	101	-	58,74,74	1.63	10 (17%)	69,115,115	1.65	15 (21%)
15	BCL	Z	102	-	58,74,74	1.63	10 (17%)	69,115,115	1.66	15 (21%)
17	UQ8	L	512	-	33,33,53	1.55	2 (6%)	40,43,67	1.51	8 (20%)
14	PGV	D	101	-	34,34,50	1.09	2 (5%)	37,40,56	1.05	2 (5%)
15	BCL	D	103	-	58,74,74	1.63	10 (17%)	69,115,115	1.61	13 (18%)
22	LMT	G	101	-	36,36,36	0.42	0	47,47,47	0.74	1 (2%)
15	BCL	7	101	-	53,69,74	1.69	8 (15%)	63,109,115	1.77	16 (25%)
20	MQ8	M	404	-	54,54,54	1.29	2 (3%)	66,69,69	1.47	14 (21%)
14	PGV	H	303	-	35,35,50	1.11	2 (5%)	38,41,56	1.09	2 (5%)
21	CRT	E	103	-	41,43,43	0.68	0	50,54,54	1.65	12 (24%)
21	CRT	2	103	-	41,43,43	0.72	0	50,54,54	2.27	15 (30%)
21	CRT	R	102	-	41,43,43	0.70	0	50,54,54	1.59	12 (24%)
21	CRT	X	103	-	41,43,43	0.72	0	50,54,54	1.75	10 (20%)
15	BCL	W	101	-	58,74,74	1.62	8 (13%)	69,115,115	1.76	17 (24%)
21	CRT	J	103	-	41,43,43	0.71	0	50,54,54	3.36	14 (28%)
22	LMT	J	104	-	36,36,36	0.41	0	47,47,47	0.65	0
22	LMT	K	102	-	36,36,36	0.40	0	47,47,47	0.75	0
15	BCL	V	102	-	58,74,74	1.64	9 (15%)	69,115,115	1.64	15 (21%)
21	CRT	M	405	-	41,43,43	0.71	0	50,54,54	1.63	10 (20%)
15	BCL	T	102	-	58,74,74	1.61	9 (15%)	69,115,115	1.61	15 (21%)
10	HEC	C	504	1	32,50,50	1.58	4 (12%)	24,82,82	1.38	3 (12%)
17	UQ8	L	504	-	33,33,53	1.51	2 (6%)	40,43,67	1.51	7 (17%)
15	BCL	0	102	-	58,74,74	1.63	9 (15%)	69,115,115	1.65	14 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	LMT	E	101	-	36,36,36	0.42	0	47,47,47	0.92	3 (6%)
16	BPH	M	403	-	51,70,70	0.54	1 (1%)	52,101,101	0.60	0
21	CRT	8	103	-	41,43,43	0.69	0	50,54,54	1.69	10 (20%)
15	BCL	M	402	-	58,74,74	1.65	10 (17%)	69,115,115	1.76	13 (18%)
22	LMT	X	101	-	36,36,36	0.44	0	47,47,47	0.86	3 (6%)
14	PGV	L	511	-	32,32,50	1.12	2 (6%)	35,38,56	1.26	4 (11%)
14	PGV	L	507	-	38,38,50	1.01	2 (5%)	41,44,56	1.14	3 (7%)
15	BCL	U	101	-	58,74,74	1.66	10 (17%)	69,115,115	1.65	13 (18%)
21	CRT	7	102	-	41,43,43	0.70	0	50,54,54	1.59	10 (20%)
12	DGA	C	506	1	16,16,43	1.75	3 (18%)	18,18,45	1.83	4 (22%)
15	BCL	2	102	-	58,74,74	1.65	10 (17%)	69,115,115	1.64	16 (23%)
18	CDL	M	408	-	38,38,99	1.29	3 (7%)	43,49,111	1.24	4 (9%)
15	BCL	B	102	-	58,74,74	1.66	10 (17%)	69,115,115	1.61	18 (26%)
15	BCL	R	101	-	58,74,74	1.62	9 (15%)	69,115,115	1.61	15 (21%)
22	LMT	V	101	-	36,36,36	0.44	0	47,47,47	0.68	0
18	CDL	L	510	-	83,83,99	1.04	4 (4%)	89,95,111	1.21	8 (8%)
15	BCL	1	403	-	58,74,74	1.64	11 (18%)	69,115,115	1.60	13 (18%)
21	CRT	4	103	-	41,43,43	0.67	0	50,54,54	1.60	8 (16%)
18	CDL	H	301	-	78,78,99	1.03	4 (5%)	84,90,111	1.08	5 (5%)
18	CDL	D	102	-	57,57,99	1.11	4 (7%)	63,69,111	1.15	4 (6%)
14	PGV	5	101	-	43,43,50	0.97	2 (4%)	46,49,56	1.03	2 (4%)
20	MQ8	M	406	-	54,54,54	1.33	2 (3%)	66,69,69	1.69	17 (25%)
15	BCL	L	508	-	58,74,74	1.61	9 (15%)	69,115,115	1.75	14 (20%)
10	HEC	C	501	1	32,50,50	1.63	4 (12%)	24,82,82	1.35	1 (4%)
22	LMT	8	101	-	36,36,36	0.41	0	47,47,47	0.75	1 (2%)
15	BCL	O	502	-	58,74,74	1.65	10 (17%)	69,115,115	1.62	14 (20%)
21	CRT	S	104	-	41,43,43	0.73	0	50,54,54	2.28	16 (32%)
18	CDL	I	101	-	50,50,99	1.28	4 (8%)	56,62,111	1.34	8 (14%)
22	LMT	B	101	-	36,36,36	0.40	0	47,47,47	0.66	0
22	LMT	4	101	-	36,36,36	0.46	0	47,47,47	0.95	1 (2%)
24	LDA	K	101	-	12,15,15	2.08	1 (8%)	14,17,17	0.53	0
15	BCL	5	102	-	58,74,74	1.67	11 (18%)	69,115,115	1.65	16 (23%)
15	BCL	8	102	-	58,74,74	1.64	9 (15%)	69,115,115	1.63	17 (24%)
15	BCL	J	102	-	58,74,74	1.63	10 (17%)	69,115,115	1.65	15 (21%)
14	PGV	L	506	-	28,28,50	1.21	2 (7%)	31,34,56	1.20	4 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
21	CRT	B	103	-	41,43,43	0.72	0	50,54,54	1.71	11 (22%)
15	BCL	A	101	-	58,74,74	1.64	9 (15%)	69,115,115	1.68	15 (21%)
18	CDL	M	410	-	94,94,99	0.95	4 (4%)	100,106,111	1.08	6 (6%)
15	BCL	4	102	-	58,74,74	1.64	10 (17%)	69,115,115	1.69	15 (21%)
15	BCL	E	102	-	58,74,74	1.63	9 (15%)	69,115,115	1.64	16 (23%)
15	BCL	S	102	-	58,74,74	1.63	10 (17%)	69,115,115	1.60	13 (18%)
22	LMT	T	101	-	36,36,36	0.41	0	47,47,47	0.64	1 (2%)
18	CDL	S	101	-	64,64,99	1.15	4 (6%)	70,76,111	1.15	6 (8%)
15	BCL	X	102	-	58,74,74	1.63	10 (17%)	69,115,115	1.67	16 (23%)
21	CRT	P	102	-	41,43,43	0.71	0	50,54,54	3.54	13 (26%)
15	BCL	Y	101	-	58,74,74	1.66	11 (18%)	69,115,115	1.64	12 (17%)
14	PGV	M	409	-	30,30,50	1.22	2 (6%)	34,35,56	1.28	3 (8%)
15	BCL	L	502	-	58,74,74	1.64	10 (17%)	69,115,115	1.60	14 (20%)

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
22	LMT	J	101	-	-	5/21/61/61	0/2/2/2
15	BCL	6	101	-	-	17/37/137/137	-
24	LDA	O	501	-	-	1/13/13/13	-
22	LMT	N	103	-	-	4/21/61/61	0/2/2/2
22	LMT	P	103	-	-	4/21/61/61	0/2/2/2
14	PGV	C	508	-	-	11/35/35/55	-
21	CRT	1	402	-	-	14/51/51/51	-
22	LMT	0	101	-	-	4/21/61/61	0/2/2/2
15	BCL	Q	101	-	-	16/37/137/137	-
14	PGV	M	411	-	-	12/40/40/55	-
10	HEC	C	503	1	-	0/10/54/54	-
22	LMT	4	104	-	-	1/21/61/61	0/2/2/2
18	CDL	H	302	-	-	14/41/41/110	-
21	CRT	6	102	-	-	7/51/51/51	-
14	PGV	M	407	-	-	5/41/41/55	-
15	BCL	N	101	-	-	13/37/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	HEC	C	502	1	-	5/10/54/54	-
15	BCL	G	102	-	-	14/37/137/137	-
17	UQ8	L	505	-	-	15/51/75/75	0/1/1/1
21	CRT	Q	102	-	-	5/51/51/51	-
21	CRT	G	103	-	-	7/51/51/51	-
15	BCL	F	101	-	-	15/37/137/137	-
15	BCL	L	509	-	-	18/37/137/137	-
22	LMT	2	101	-	-	1/21/61/61	0/2/2/2
16	BPH	L	503	-	-	6/37/105/105	0/5/6/6
14	PGV	L	501	-	-	2/17/17/55	-
21	CRT	N	102	-	-	4/51/51/51	-
22	LMT	Z	101	-	-	8/21/61/61	0/2/2/2
15	BCL	I	102	-	-	16/37/137/137	-
15	BCL	K	103	-	-	16/37/137/137	-
13	PLM	C	507	1	-	0/8/9/15	-
22	LMT	H	304	-	-	1/21/61/61	0/2/2/2
15	BCL	P	101	-	-	25/37/137/137	-
15	BCL	3	101	-	-	12/37/137/137	-
14	PGV	1	401	-	-	12/30/30/55	-
15	BCL	9	101	-	-	13/37/137/137	-
15	BCL	Z	102	-	-	18/37/137/137	-
17	UQ8	L	512	-	-	5/27/51/75	0/1/1/1
14	PGV	D	101	-	-	15/39/39/55	-
15	BCL	D	103	-	-	14/37/137/137	-
22	LMT	G	101	-	-	5/21/61/61	0/2/2/2
15	BCL	7	101	-	-	9/31/131/137	-
20	MQ8	M	404	-	-	6/47/67/67	0/2/2/2
14	PGV	H	303	-	-	10/40/40/55	-
21	CRT	E	103	-	-	4/51/51/51	-
21	CRT	2	103	-	-	5/51/51/51	-
21	CRT	R	102	-	-	2/51/51/51	-
21	CRT	X	103	-	-	6/51/51/51	-
15	BCL	W	101	-	-	17/37/137/137	-
21	CRT	J	103	-	-	3/51/51/51	-
22	LMT	J	104	-	-	1/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	LMT	K	102	-	-	4/21/61/61	0/2/2/2
15	BCL	V	102	-	-	19/37/137/137	-
21	CRT	M	405	-	-	8/51/51/51	-
15	BCL	T	102	-	-	12/37/137/137	-
10	HEC	C	504	1	-	2/10/54/54	-
17	UQ8	L	504	-	-	5/27/51/75	0/1/1/1
15	BCL	0	102	-	-	11/37/137/137	-
22	LMT	E	101	-	-	6/21/61/61	0/2/2/2
16	BPH	M	403	-	-	8/37/105/105	0/5/6/6
21	CRT	8	103	-	-	3/51/51/51	-
15	BCL	M	402	-	-	22/37/137/137	-
22	LMT	X	101	-	-	1/21/61/61	0/2/2/2
14	PGV	L	511	-	-	10/37/37/55	-
14	PGV	L	507	-	-	18/43/43/55	-
15	BCL	U	101	-	-	16/37/137/137	-
21	CRT	7	102	-	-	4/51/51/51	-
12	DGA	C	506	1	-	8/16/16/45	-
15	BCL	2	102	-	-	12/37/137/137	-
18	CDL	M	408	-	-	16/48/48/110	-
15	BCL	B	102	-	-	15/37/137/137	-
15	BCL	R	101	-	-	12/37/137/137	-
22	LMT	V	101	-	-	6/21/61/61	0/2/2/2
18	CDL	L	510	-	-	31/93/93/110	-
15	BCL	1	403	-	-	13/37/137/137	-
21	CRT	4	103	-	-	5/51/51/51	-
18	CDL	H	301	-	-	30/89/89/110	-
18	CDL	D	102	-	-	27/67/67/110	-
14	PGV	5	101	-	-	15/48/48/55	-
20	MQ8	M	406	-	-	7/47/67/67	0/2/2/2
15	BCL	L	508	-	-	11/37/137/137	-
10	HEC	C	501	1	-	2/10/54/54	-
22	LMT	8	101	-	-	2/21/61/61	0/2/2/2
15	BCL	O	502	-	-	15/37/137/137	-
21	CRT	S	104	-	-	9/51/51/51	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CDL	I	101	-	-	14/61/61/110	-
22	LMT	B	101	-	-	6/21/61/61	0/2/2/2
22	LMT	4	101	-	-	3/21/61/61	0/2/2/2
24	LDA	K	101	-	-	5/13/13/13	-
15	BCL	5	102	-	-	18/37/137/137	-
15	BCL	8	102	-	-	18/37/137/137	-
15	BCL	J	102	-	-	13/37/137/137	-
14	PGV	L	506	-	-	11/33/33/55	-
21	CRT	B	103	-	-	9/51/51/51	-
15	BCL	A	101	-	-	16/37/137/137	-
18	CDL	M	410	-	-	35/105/105/110	-
15	BCL	4	102	-	-	20/37/137/137	-
15	BCL	E	102	-	-	16/37/137/137	-
15	BCL	S	102	-	-	14/37/137/137	-
22	LMT	T	101	-	-	5/21/61/61	0/2/2/2
18	CDL	S	101	-	-	20/75/75/110	-
15	BCL	X	102	-	-	18/37/137/137	-
21	CRT	P	102	-	-	8/51/51/51	-
15	BCL	Y	101	-	-	17/37/137/137	-
14	PGV	M	409	-	-	6/32/32/55	-
15	BCL	L	502	-	-	13/37/137/137	-

All (442) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	L	512	UQ8	C6-C1	7.84	1.49	1.35
20	M	406	MQ8	C3-C2	7.82	1.49	1.35
20	M	404	MQ8	C3-C2	7.78	1.49	1.35
17	L	504	UQ8	C6-C1	7.63	1.49	1.35
17	L	505	UQ8	C6-C1	7.56	1.49	1.35
24	K	101	LDA	O1-N1	-7.16	1.25	1.42
24	O	501	LDA	O1-N1	-7.16	1.25	1.42
15	L	502	BCL	O2D-CGD	5.20	1.45	1.33
15	X	102	BCL	O2D-CGD	5.13	1.45	1.33
15	5	102	BCL	O2D-CGD	5.11	1.45	1.33
15	2	102	BCL	O2D-CGD	5.10	1.45	1.33
15	T	102	BCL	O2D-CGD	5.09	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	J	102	BCL	O2D-CGD	5.09	1.45	1.33
15	B	102	BCL	O2D-CGD	5.09	1.45	1.33
15	0	102	BCL	O2D-CGD	5.08	1.45	1.33
15	Z	102	BCL	O2D-CGD	5.08	1.45	1.33
15	9	101	BCL	O2D-CGD	5.07	1.45	1.33
15	O	502	BCL	O2D-CGD	5.06	1.45	1.33
15	E	102	BCL	O2D-CGD	5.06	1.45	1.33
15	G	102	BCL	O2D-CGD	5.06	1.45	1.33
15	4	102	BCL	O2D-CGD	5.05	1.45	1.33
15	P	101	BCL	O2D-CGD	5.04	1.45	1.33
15	D	103	BCL	O2D-CGD	5.04	1.45	1.33
15	Q	101	BCL	O2D-CGD	5.04	1.45	1.33
15	R	101	BCL	O2D-CGD	5.04	1.45	1.33
15	V	102	BCL	O2D-CGD	5.04	1.45	1.33
15	1	403	BCL	O2D-CGD	5.03	1.45	1.33
15	K	103	BCL	O2D-CGD	5.03	1.45	1.33
15	Y	101	BCL	O2D-CGD	5.02	1.45	1.33
15	N	101	BCL	O2D-CGD	5.02	1.45	1.33
15	8	102	BCL	O2D-CGD	5.02	1.45	1.33
15	S	102	BCL	O2D-CGD	5.01	1.45	1.33
15	M	402	BCL	C3B-C2B	5.00	1.48	1.39
15	3	101	BCL	O2D-CGD	4.99	1.45	1.33
15	6	101	BCL	O2D-CGD	4.98	1.45	1.33
15	M	402	BCL	O2D-CGD	4.98	1.45	1.33
15	F	101	BCL	O2D-CGD	4.98	1.45	1.33
15	U	101	BCL	O2D-CGD	4.97	1.45	1.33
15	W	101	BCL	O2D-CGD	4.96	1.45	1.33
15	I	102	BCL	O2D-CGD	4.96	1.45	1.33
15	L	509	BCL	O2D-CGD	4.92	1.45	1.33
20	M	406	MQ8	C10-C5	4.90	1.48	1.40
15	N	101	BCL	C3B-C2B	4.89	1.48	1.39
15	L	508	BCL	O2D-CGD	4.88	1.45	1.33
15	B	102	BCL	C3B-C2B	4.88	1.48	1.39
15	A	101	BCL	O2D-CGD	4.86	1.45	1.33
15	7	101	BCL	O2D-CGD	4.84	1.45	1.33
15	L	502	BCL	C3B-C2B	4.84	1.48	1.39
15	5	102	BCL	C3B-C2B	4.81	1.48	1.39
15	4	102	BCL	C3B-C2B	4.80	1.48	1.39
15	Z	102	BCL	C3B-C2B	4.77	1.48	1.39
15	3	101	BCL	C3B-C2B	4.77	1.48	1.39
18	L	510	CDL	OA6-CA5	4.76	1.46	1.35
15	U	101	BCL	C3B-C2B	4.76	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	2	102	BCL	C3B-C2B	4.76	1.48	1.39
12	C	506	DGA	OG2-CB1	4.74	1.45	1.35
15	Y	101	BCL	C3B-C2B	4.74	1.47	1.39
15	F	101	BCL	C3B-C2B	4.72	1.47	1.39
15	T	102	BCL	C3B-C2B	4.72	1.47	1.39
15	Q	101	BCL	C3B-C2B	4.71	1.47	1.39
15	6	101	BCL	C3B-C2B	4.69	1.47	1.39
15	P	101	BCL	C3B-C2B	4.69	1.47	1.39
15	L	509	BCL	C3B-C2B	4.68	1.47	1.39
15	K	103	BCL	C3B-C2B	4.67	1.47	1.39
15	I	102	BCL	C3B-C2B	4.67	1.47	1.39
15	X	102	BCL	C3B-C2B	4.65	1.47	1.39
15	V	102	BCL	C3B-C2B	4.63	1.47	1.39
15	E	102	BCL	OBD-CAD	4.63	1.28	1.22
15	O	502	BCL	C3B-C2B	4.63	1.47	1.39
15	0	102	BCL	C3B-C2B	4.62	1.47	1.39
15	L	508	BCL	C3B-C2B	4.61	1.47	1.39
15	1	403	BCL	C3B-C2B	4.61	1.47	1.39
15	G	102	BCL	C3B-C2B	4.61	1.47	1.39
15	8	102	BCL	C3B-C2B	4.60	1.47	1.39
15	I	102	BCL	OBD-CAD	4.59	1.28	1.22
15	A	101	BCL	C3B-C2B	4.59	1.47	1.39
15	J	102	BCL	C3B-C2B	4.59	1.47	1.39
15	8	102	BCL	OBD-CAD	4.58	1.28	1.22
20	M	404	MQ8	C10-C5	4.58	1.48	1.40
15	2	102	BCL	OBD-CAD	4.58	1.28	1.22
15	E	102	BCL	C3B-C2B	4.57	1.47	1.39
15	W	101	BCL	C3B-C2B	4.57	1.47	1.39
15	R	101	BCL	C3B-C2B	4.57	1.47	1.39
15	7	101	BCL	C3B-C2B	4.56	1.47	1.39
15	V	102	BCL	OBD-CAD	4.56	1.28	1.22
15	J	102	BCL	OBD-CAD	4.54	1.28	1.22
15	9	101	BCL	C3B-C2B	4.54	1.47	1.39
15	K	103	BCL	OBD-CAD	4.54	1.28	1.22
15	U	101	BCL	OBD-CAD	4.53	1.28	1.22
15	D	103	BCL	OBD-CAD	4.52	1.28	1.22
15	0	102	BCL	OBD-CAD	4.52	1.28	1.22
10	C	501	HEC	C2B-C3B	-4.52	1.36	1.40
15	6	101	BCL	OBD-CAD	4.52	1.28	1.22
15	D	103	BCL	C3B-C2B	4.51	1.47	1.39
15	1	403	BCL	OBD-CAD	4.50	1.28	1.22
15	3	101	BCL	OBD-CAD	4.50	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	4	102	BCL	OBD-CAD	4.50	1.28	1.22
15	N	101	BCL	OBD-CAD	4.50	1.28	1.22
15	A	101	BCL	OBD-CAD	4.50	1.28	1.22
15	F	101	BCL	OBD-CAD	4.49	1.28	1.22
15	T	102	BCL	OBD-CAD	4.48	1.28	1.22
15	5	102	BCL	OBD-CAD	4.48	1.28	1.22
15	P	101	BCL	OBD-CAD	4.47	1.28	1.22
15	G	102	BCL	OBD-CAD	4.47	1.28	1.22
15	Q	101	BCL	OBD-CAD	4.47	1.28	1.22
15	2	102	BCL	C3D-C2D	4.47	1.47	1.39
15	M	402	BCL	OBD-CAD	4.47	1.28	1.22
14	1	401	PGV	O01-C1	4.46	1.46	1.34
15	R	101	BCL	OBD-CAD	4.46	1.28	1.22
15	3	101	BCL	C3D-C2D	4.45	1.47	1.39
15	B	102	BCL	OBD-CAD	4.44	1.28	1.22
15	L	502	BCL	OBD-CAD	4.44	1.28	1.22
15	S	102	BCL	OBD-CAD	4.43	1.28	1.22
15	Y	101	BCL	OBD-CAD	4.43	1.28	1.22
15	S	102	BCL	C3B-C2B	4.43	1.47	1.39
15	K	103	BCL	C3D-C2D	4.42	1.47	1.39
15	O	502	BCL	OBD-CAD	4.42	1.28	1.22
15	7	101	BCL	OBD-CAD	4.42	1.28	1.22
15	W	101	BCL	OBD-CAD	4.41	1.28	1.22
15	L	509	BCL	C3D-C2D	4.40	1.47	1.39
15	L	509	BCL	OBD-CAD	4.40	1.28	1.22
15	X	102	BCL	OBD-CAD	4.39	1.28	1.22
15	5	102	BCL	C3D-C2D	4.38	1.47	1.39
15	9	101	BCL	OBD-CAD	4.38	1.28	1.22
10	C	504	HEC	CBC-CAC	-4.38	1.33	1.49
10	C	503	HEC	CBC-CAC	-4.37	1.33	1.49
18	S	101	CDL	OB8-CB7	4.36	1.46	1.33
15	J	102	BCL	C3D-C2D	4.36	1.47	1.39
18	M	408	CDL	OA8-CA7	4.36	1.46	1.33
15	A	101	BCL	O2A-CGA	4.35	1.46	1.33
15	P	101	BCL	C3D-C2D	4.35	1.47	1.39
10	C	501	HEC	CBC-CAC	-4.34	1.33	1.49
15	I	102	BCL	O2A-CGA	4.34	1.46	1.33
15	L	509	BCL	O2A-CGA	4.34	1.46	1.33
15	S	102	BCL	O2A-CGA	4.33	1.46	1.33
15	L	502	BCL	O2A-CGA	4.33	1.46	1.33
18	H	301	CDL	OA8-CA7	4.33	1.46	1.33
15	1	403	BCL	O2A-CGA	4.32	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	L	508	BCL	C3D-C2D	4.32	1.47	1.39
15	Z	102	BCL	OBD-CAD	4.32	1.28	1.22
15	O	502	BCL	O2A-CGA	4.31	1.45	1.33
10	C	504	HEC	CBB-CAB	-4.31	1.33	1.49
10	C	502	HEC	CBB-CAB	-4.31	1.33	1.49
15	A	101	BCL	C3D-C2D	4.31	1.47	1.39
10	C	502	HEC	CBC-CAC	-4.31	1.33	1.49
15	Y	101	BCL	O2A-CGA	4.30	1.45	1.33
15	N	101	BCL	C3D-C2D	4.30	1.47	1.39
15	0	102	BCL	C3D-C2D	4.29	1.47	1.39
18	I	101	CDL	OB8-CB7	4.29	1.45	1.33
15	5	102	BCL	O2A-CGA	4.29	1.45	1.33
18	M	410	CDL	OA8-CA7	4.29	1.45	1.33
14	H	303	PGV	O01-C1	4.29	1.46	1.34
15	Q	101	BCL	C3D-C2D	4.28	1.47	1.39
14	L	506	PGV	O03-C19	4.28	1.45	1.33
15	U	101	BCL	C3D-C2D	4.28	1.47	1.39
15	E	102	BCL	C3D-C2D	4.28	1.47	1.39
15	M	402	BCL	O2A-CGA	4.28	1.45	1.33
15	L	508	BCL	OBD-CAD	4.28	1.28	1.22
15	R	101	BCL	O2A-CGA	4.27	1.45	1.33
14	1	401	PGV	O03-C19	4.27	1.45	1.33
18	H	301	CDL	OA6-CA5	4.27	1.46	1.34
15	N	101	BCL	O2A-CGA	4.27	1.45	1.33
14	H	303	PGV	O03-C19	4.27	1.45	1.33
10	C	503	HEC	CBB-CAB	-4.27	1.33	1.49
10	C	501	HEC	CBB-CAB	-4.27	1.33	1.49
15	S	102	BCL	C3D-C2D	4.27	1.47	1.39
15	B	102	BCL	C3D-C2D	4.27	1.47	1.39
15	7	101	BCL	O2A-CGA	4.27	1.45	1.33
15	G	102	BCL	O2A-CGA	4.26	1.45	1.33
14	M	409	PGV	O03-C19	4.25	1.45	1.33
15	O	502	BCL	C3D-C2D	4.25	1.47	1.39
18	I	101	CDL	OA8-CA7	4.25	1.45	1.33
18	H	302	CDL	OB8-CB7	4.25	1.45	1.33
18	S	101	CDL	OA8-CA7	4.25	1.45	1.33
15	4	102	BCL	C3D-C2D	4.25	1.47	1.39
18	M	410	CDL	OB8-CB7	4.24	1.45	1.33
15	Z	102	BCL	C3D-C2D	4.24	1.47	1.39
15	8	102	BCL	C3D-C2D	4.24	1.47	1.39
15	9	101	BCL	C3D-C2D	4.24	1.47	1.39
15	V	102	BCL	C3D-C2D	4.24	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	Y	101	BCL	C3D-C2D	4.24	1.47	1.39
14	C	508	PGV	O03-C19	4.24	1.45	1.33
12	C	506	DGA	OG1-CA1	4.23	1.45	1.33
15	W	101	BCL	C3D-C2D	4.23	1.47	1.39
18	S	101	CDL	OA6-CA5	4.22	1.46	1.34
15	B	102	BCL	O2A-CGA	4.22	1.45	1.33
15	1	403	BCL	C3D-C2D	4.22	1.47	1.39
15	6	101	BCL	O2A-CGA	4.22	1.45	1.33
15	F	101	BCL	C3D-C2D	4.22	1.47	1.39
15	T	102	BCL	O2A-CGA	4.22	1.45	1.33
18	L	510	CDL	OA8-CA7	4.22	1.45	1.33
15	4	102	BCL	O2A-CGA	4.21	1.45	1.33
15	D	103	BCL	C3D-C2D	4.21	1.47	1.39
15	G	102	BCL	C3D-C2D	4.21	1.47	1.39
15	E	102	BCL	O2A-CGA	4.21	1.45	1.33
14	M	411	PGV	O03-C19	4.20	1.45	1.33
18	M	408	CDL	OA6-CA5	4.20	1.46	1.34
15	8	102	BCL	O2A-CGA	4.20	1.45	1.33
15	6	101	BCL	C3D-C2D	4.19	1.46	1.39
15	L	502	BCL	C3D-C2D	4.19	1.46	1.39
15	P	101	BCL	O2A-CGA	4.19	1.45	1.33
15	2	102	BCL	O2A-CGA	4.19	1.45	1.33
15	3	101	BCL	O2A-CGA	4.19	1.45	1.33
14	D	101	PGV	O03-C19	4.18	1.45	1.33
15	9	101	BCL	O2A-CGA	4.18	1.45	1.33
14	M	409	PGV	O01-C1	4.18	1.46	1.34
18	D	102	CDL	OB8-CB7	4.18	1.45	1.33
15	V	102	BCL	O2A-CGA	4.17	1.45	1.33
15	7	101	BCL	C3D-C2D	4.17	1.46	1.39
14	L	511	PGV	O03-C19	4.16	1.45	1.33
15	J	102	BCL	O2A-CGA	4.15	1.45	1.33
15	F	101	BCL	O2A-CGA	4.15	1.45	1.33
15	W	101	BCL	O2A-CGA	4.15	1.45	1.33
15	Z	102	BCL	O2A-CGA	4.15	1.45	1.33
10	C	504	HEC	C2B-C3B	-4.14	1.36	1.40
15	L	508	BCL	O2A-CGA	4.14	1.45	1.33
14	5	101	PGV	O03-C19	4.14	1.45	1.33
15	I	102	BCL	C3D-C2D	4.14	1.46	1.39
15	D	103	BCL	O2A-CGA	4.14	1.45	1.33
15	R	101	BCL	C3D-C2D	4.14	1.46	1.39
15	Q	101	BCL	O2A-CGA	4.14	1.45	1.33
18	L	510	CDL	OB6-CB5	4.14	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	M	407	PGV	O03-C19	4.13	1.45	1.33
15	X	102	BCL	O2A-CGA	4.13	1.45	1.33
15	0	102	BCL	O2A-CGA	4.13	1.45	1.33
18	L	510	CDL	OB8-CB7	4.13	1.45	1.33
18	I	101	CDL	OA6-CA5	4.13	1.45	1.34
15	T	102	BCL	C3D-C2D	4.12	1.46	1.39
18	D	102	CDL	OA6-CA5	4.12	1.45	1.34
15	K	103	BCL	O2A-CGA	4.12	1.45	1.33
10	C	502	HEC	C2B-C3B	-4.11	1.36	1.40
15	X	102	BCL	C3D-C2D	4.11	1.46	1.39
15	U	101	BCL	O2A-CGA	4.10	1.45	1.33
14	5	101	PGV	O01-C1	4.10	1.45	1.34
18	H	301	CDL	OB6-CB5	4.09	1.45	1.34
18	M	410	CDL	OA6-CA5	4.09	1.45	1.34
18	S	101	CDL	OB6-CB5	4.08	1.45	1.34
10	C	503	HEC	C2B-C3B	-4.07	1.36	1.40
14	L	501	PGV	O01-C1	4.07	1.45	1.34
18	I	101	CDL	OB6-CB5	4.05	1.45	1.34
14	L	506	PGV	O01-C1	4.05	1.45	1.34
18	H	301	CDL	OB8-CB7	4.04	1.45	1.33
18	D	102	CDL	OB6-CB5	4.04	1.45	1.34
18	H	302	CDL	OB6-CB5	4.03	1.45	1.34
14	D	101	PGV	O01-C1	4.01	1.45	1.34
14	L	507	PGV	O03-C19	4.01	1.45	1.33
14	M	407	PGV	O01-C1	3.98	1.45	1.34
14	L	507	PGV	O01-C1	3.98	1.45	1.34
18	M	410	CDL	OB6-CB5	3.98	1.45	1.34
14	L	511	PGV	O01-C1	3.97	1.45	1.34
15	M	402	BCL	C3D-C2D	3.96	1.46	1.39
18	M	408	CDL	OB6-CB5	3.95	1.45	1.34
14	M	411	PGV	O01-C1	3.90	1.45	1.34
14	C	508	PGV	O01-C1	3.89	1.45	1.34
15	K	103	BCL	C2D-C1D	3.72	1.51	1.42
15	1	403	BCL	C2D-C1D	3.70	1.50	1.42
15	U	101	BCL	C2D-C1D	3.67	1.50	1.42
15	Q	101	BCL	C2D-C1D	3.65	1.50	1.42
15	S	102	BCL	C2D-C1D	3.61	1.50	1.42
15	O	502	BCL	C2D-C1D	3.61	1.50	1.42
15	9	101	BCL	C2D-C1D	3.61	1.50	1.42
15	3	101	BCL	C2D-C1D	3.60	1.50	1.42
15	D	103	BCL	C2D-C1D	3.60	1.50	1.42
15	Y	101	BCL	C2D-C1D	3.59	1.50	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	7	101	BCL	C2D-C1D	3.57	1.50	1.42
15	I	102	BCL	C2D-C1D	3.56	1.50	1.42
15	5	102	BCL	C2D-C1D	3.55	1.50	1.42
15	8	102	BCL	C2D-C1D	3.54	1.50	1.42
15	4	102	BCL	C2D-C1D	3.52	1.50	1.42
15	W	101	BCL	C2D-C1D	3.51	1.50	1.42
15	F	101	BCL	C2D-C1D	3.50	1.50	1.42
15	L	509	BCL	C2D-C1D	3.48	1.50	1.42
15	V	102	BCL	C2D-C1D	3.47	1.50	1.42
15	L	508	BCL	C2D-C1D	3.46	1.50	1.42
15	P	101	BCL	C2D-C1D	3.46	1.50	1.42
15	N	101	BCL	C2D-C1D	3.45	1.50	1.42
15	A	101	BCL	C2D-C1D	3.45	1.50	1.42
15	X	102	BCL	C2D-C1D	3.44	1.50	1.42
15	M	402	BCL	C2D-C1D	3.43	1.50	1.42
15	L	502	BCL	C2D-C1D	3.40	1.50	1.42
15	B	102	BCL	C2D-C1D	3.39	1.50	1.42
15	6	101	BCL	C2D-C1D	3.38	1.50	1.42
15	0	102	BCL	C2D-C1D	3.35	1.50	1.42
15	J	102	BCL	C2D-C1D	3.28	1.50	1.42
15	E	102	BCL	C2D-C1D	3.25	1.49	1.42
15	2	102	BCL	C2D-C1D	3.24	1.49	1.42
15	Z	102	BCL	C2D-C1D	3.24	1.49	1.42
15	T	102	BCL	C2D-C1D	3.22	1.49	1.42
15	G	102	BCL	C2D-C1D	3.22	1.49	1.42
17	L	505	UQ8	C4-C3	3.20	1.49	1.36
15	R	101	BCL	C2D-C1D	3.19	1.49	1.42
10	C	501	HEC	C4B-C3B	3.10	1.48	1.43
17	L	512	UQ8	C4-C3	3.08	1.48	1.36
17	L	504	UQ8	C4-C3	3.05	1.48	1.36
10	C	503	HEC	C4B-C3B	2.83	1.48	1.43
10	C	504	HEC	C4B-C3B	2.72	1.48	1.43
15	K	103	BCL	MG-NA	-2.69	1.99	2.06
10	C	502	HEC	C4B-C3B	2.62	1.47	1.43
15	3	101	BCL	MG-NA	-2.54	2.00	2.06
14	L	501	PGV	O03-C19	2.53	1.45	1.33
18	D	102	CDL	OA8-CA7	2.49	1.45	1.33
18	H	302	CDL	OA8-CA7	2.49	1.45	1.33
15	Y	101	BCL	MG-NA	-2.46	2.00	2.06
15	3	101	BCL	MG-NC	-2.46	2.00	2.06
15	F	101	BCL	MG-NA	-2.44	2.00	2.06
15	U	101	BCL	MG-NA	-2.43	2.00	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	P	101	BCL	MG-NC	-2.41	2.00	2.06
15	L	509	BCL	MG-NA	-2.39	2.00	2.06
15	B	102	BCL	MG-NC	-2.39	2.00	2.06
15	I	102	BCL	MG-NA	-2.38	2.00	2.06
12	C	506	DGA	OG2-CG2	-2.38	1.43	1.47
15	W	101	BCL	MG-NA	-2.36	2.00	2.06
15	I	102	BCL	C1B-CHB	2.36	1.47	1.41
15	8	102	BCL	C1B-CHB	2.35	1.47	1.41
15	Q	101	BCL	MG-NA	-2.34	2.00	2.06
15	N	101	BCL	MG-NA	-2.34	2.00	2.06
15	R	101	BCL	C1B-CHB	2.33	1.47	1.41
15	F	101	BCL	C1B-CHB	2.32	1.47	1.41
15	P	101	BCL	MG-NA	-2.32	2.00	2.06
15	5	102	BCL	MG-NA	-2.30	2.00	2.06
15	B	102	BCL	MG-NA	-2.29	2.00	2.06
15	G	102	BCL	C1B-CHB	2.29	1.47	1.41
15	5	102	BCL	C1B-CHB	2.29	1.47	1.41
15	K	103	BCL	C1B-CHB	2.29	1.47	1.41
15	Y	101	BCL	C1B-CHB	2.28	1.47	1.41
15	O	502	BCL	MG-NA	-2.28	2.00	2.06
15	W	101	BCL	C1B-CHB	2.28	1.47	1.41
15	2	102	BCL	MG-NA	-2.28	2.00	2.06
15	D	103	BCL	MG-NA	-2.27	2.00	2.06
15	3	101	BCL	C1B-CHB	2.27	1.47	1.41
15	M	402	BCL	MG-NC	-2.27	2.00	2.06
15	6	101	BCL	MG-NC	-2.27	2.00	2.06
15	U	101	BCL	C1B-CHB	2.26	1.47	1.41
15	B	102	BCL	C1B-CHB	2.25	1.47	1.41
15	8	102	BCL	MG-NA	-2.25	2.00	2.06
15	A	101	BCL	MG-NA	-2.25	2.00	2.06
15	E	102	BCL	C1B-CHB	2.24	1.47	1.41
15	M	402	BCL	MG-NA	-2.23	2.01	2.06
15	J	102	BCL	MG-NA	-2.23	2.01	2.06
15	X	102	BCL	MG-NC	-2.23	2.01	2.06
15	O	502	BCL	MG-NC	-2.22	2.01	2.06
15	N	101	BCL	MG-NC	-2.22	2.01	2.06
15	9	101	BCL	MG-NA	-2.22	2.01	2.06
15	K	103	BCL	MG-NC	-2.22	2.01	2.06
15	7	101	BCL	MG-NA	-2.22	2.01	2.06
15	1	403	BCL	MG-NA	-2.21	2.01	2.06
15	2	102	BCL	C1B-CHB	2.21	1.47	1.41
15	S	102	BCL	MG-NA	-2.21	2.01	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	L	508	BCL	MG-NA	-2.21	2.01	2.06
15	S	102	BCL	C1B-CHB	2.20	1.47	1.41
15	V	102	BCL	MG-NA	-2.20	2.01	2.06
15	J	102	BCL	C1B-CHB	2.20	1.47	1.41
15	N	101	BCL	C1B-CHB	2.19	1.47	1.41
15	I	102	BCL	MG-NC	-2.19	2.01	2.06
15	O	502	BCL	C1B-CHB	2.19	1.47	1.41
15	Q	101	BCL	C1B-CHB	2.19	1.47	1.41
15	Y	101	BCL	MG-NC	-2.18	2.01	2.06
15	X	102	BCL	MG-NA	-2.18	2.01	2.06
15	Z	102	BCL	MG-NC	-2.18	2.01	2.06
15	9	101	BCL	C1B-CHB	2.18	1.47	1.41
15	G	102	BCL	MG-NA	-2.18	2.01	2.06
15	5	102	BCL	MG-NC	-2.18	2.01	2.06
15	L	509	BCL	MG-NC	-2.17	2.01	2.06
15	L	502	BCL	C1B-CHB	2.17	1.47	1.41
15	7	101	BCL	C1B-CHB	2.17	1.47	1.41
15	1	403	BCL	C1B-CHB	2.17	1.47	1.41
15	Z	102	BCL	MG-NA	-2.16	2.01	2.06
15	2	102	BCL	MG-NC	-2.16	2.01	2.06
16	M	403	BPH	C3A-C2A	-2.16	1.52	1.54
15	3	101	BCL	CHD-C4C	2.16	1.47	1.41
15	F	101	BCL	MG-NC	-2.16	2.01	2.06
15	Z	102	BCL	C1B-CHB	2.15	1.47	1.41
15	9	101	BCL	MG-NC	-2.15	2.01	2.06
15	M	402	BCL	C4B-CHC	2.15	1.47	1.41
15	U	101	BCL	MG-NC	-2.15	2.01	2.06
15	L	509	BCL	C4B-CHC	2.14	1.46	1.41
15	0	102	BCL	MG-NC	-2.14	2.01	2.06
15	L	508	BCL	MG-NC	-2.14	2.01	2.06
15	0	102	BCL	MG-NA	-2.13	2.01	2.06
15	6	101	BCL	MG-NA	-2.13	2.01	2.06
15	L	502	BCL	C4B-CHC	2.13	1.46	1.41
15	R	101	BCL	MG-NA	-2.12	2.01	2.06
15	3	101	BCL	C4B-CHC	2.12	1.46	1.41
15	R	101	BCL	MG-NC	-2.12	2.01	2.06
15	1	403	BCL	CHD-C4C	2.12	1.47	1.41
15	I	102	BCL	C4B-CHC	2.12	1.46	1.41
15	A	101	BCL	C1B-CHB	2.12	1.46	1.41
15	E	102	BCL	MG-NA	-2.11	2.01	2.06
15	V	102	BCL	C1B-CHB	2.11	1.46	1.41
15	V	102	BCL	MG-NC	-2.11	2.01	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	4	102	BCL	MG-NC	-2.10	2.01	2.06
15	A	101	BCL	MG-NC	-2.10	2.01	2.06
15	N	101	BCL	C4B-CHC	2.10	1.46	1.41
15	G	102	BCL	MG-NC	-2.09	2.01	2.06
15	S	102	BCL	MG-NC	-2.09	2.01	2.06
15	K	103	BCL	CHD-C4C	2.09	1.47	1.41
15	D	103	BCL	C1B-CHB	2.09	1.46	1.41
15	M	402	BCL	C1B-CHB	2.09	1.46	1.41
15	N	101	BCL	CHD-C4C	2.09	1.47	1.41
15	6	101	BCL	C1B-CHB	2.08	1.46	1.41
10	C	502	HEC	C3C-C2C	-2.08	1.38	1.40
15	5	102	BCL	CHD-C4C	2.08	1.47	1.41
15	P	101	BCL	C1B-CHB	2.08	1.46	1.41
15	1	403	BCL	C4B-CHC	2.08	1.46	1.41
15	Q	101	BCL	CHD-C4C	2.08	1.47	1.41
15	D	103	BCL	MG-NC	-2.07	2.01	2.06
15	4	102	BCL	MG-NA	-2.07	2.01	2.06
15	U	101	BCL	CHD-C4C	2.07	1.47	1.41
15	L	508	BCL	C1B-CHB	2.07	1.46	1.41
15	P	101	BCL	C4B-CHC	2.07	1.46	1.41
15	B	102	BCL	C4B-CHC	2.07	1.46	1.41
15	0	102	BCL	C1B-CHB	2.07	1.46	1.41
15	8	102	BCL	MG-NC	-2.07	2.01	2.06
15	Y	101	BCL	C4B-CHC	2.07	1.46	1.41
15	T	102	BCL	C1B-CHB	2.07	1.46	1.41
15	O	502	BCL	CHD-C4C	2.07	1.47	1.41
15	6	101	BCL	C4B-CHC	2.07	1.46	1.41
15	L	509	BCL	C1B-CHB	2.06	1.46	1.41
15	X	102	BCL	C4B-CHC	2.06	1.46	1.41
15	Q	101	BCL	MG-NC	-2.06	2.01	2.06
15	4	102	BCL	C1B-CHB	2.06	1.46	1.41
15	I	102	BCL	CHD-C4C	2.05	1.47	1.41
15	5	102	BCL	C4B-CHC	2.05	1.46	1.41
15	S	102	BCL	CHD-C4C	2.05	1.47	1.41
15	1	403	BCL	MG-NC	-2.05	2.01	2.06
15	Y	101	BCL	CHD-C4C	2.04	1.47	1.41
15	X	102	BCL	C1B-CHB	2.04	1.46	1.41
15	F	101	BCL	C4B-CHC	2.04	1.46	1.41
15	T	102	BCL	MG-NC	-2.03	2.01	2.06
15	D	103	BCL	CHD-C4C	2.03	1.47	1.41
15	T	102	BCL	C4B-CHC	2.03	1.46	1.41
15	9	101	BCL	CHD-C4C	2.03	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	2	102	BCL	C4B-CHC	2.03	1.46	1.41
15	E	102	BCL	MG-NC	-2.02	2.01	2.06
15	4	102	BCL	C4B-CHC	2.02	1.46	1.41
15	Z	102	BCL	C4B-CHC	2.02	1.46	1.41
15	L	502	BCL	MG-NC	-2.02	2.01	2.06
15	L	509	BCL	CHD-C4C	2.01	1.47	1.41
15	P	101	BCL	CHD-C4C	2.01	1.47	1.41
15	J	102	BCL	C4B-CHC	2.01	1.46	1.41
15	L	502	BCL	MG-NA	-2.00	2.01	2.06
15	J	102	BCL	MG-NC	-2.00	2.01	2.06

All (895) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	P	102	CRT	C3-C1-C4	-16.52	85.50	110.86
21	J	103	CRT	C3-C1-C4	-14.49	88.61	110.86
21	J	103	CRT	C2-C1-C4	-13.85	89.59	110.86
21	P	102	CRT	C2-C1-C4	-13.10	90.74	110.86
21	S	104	CRT	C39-C38-C37	6.04	120.13	110.86
15	L	508	BCL	O2D-CGD-CBD	5.91	121.77	111.27
21	2	103	CRT	C40-C38-C37	5.90	119.92	110.86
21	M	405	CRT	C21-C22-C23	-5.75	119.10	127.31
15	W	101	BCL	O2D-CGD-CBD	5.57	121.16	111.27
20	M	406	MQ8	C11-C12-C13	-5.53	117.59	126.79
21	J	103	CRT	C3-C1-C2	5.49	120.70	110.37
15	M	402	BCL	O2D-CGD-CBD	5.46	120.97	111.27
15	L	509	BCL	O2D-CGD-CBD	5.41	120.89	111.27
21	S	104	CRT	C40-C38-C39	5.38	120.49	110.37
18	L	510	CDL	OA6-CA5-C11	5.32	120.88	111.09
21	6	102	CRT	C21-C22-C23	-5.32	119.72	127.31
15	K	103	BCL	O2D-CGD-CBD	5.30	120.69	111.27
21	2	103	CRT	C40-C38-C39	5.29	120.33	110.37
21	2	103	CRT	C39-C38-C37	5.15	118.77	110.86
15	F	101	BCL	O2D-CGD-CBD	5.10	120.34	111.27
15	M	402	BCL	CHD-C4C-NC	5.07	130.71	125.08
21	J	103	CRT	C21-C22-C23	-5.02	120.14	127.31
15	A	101	BCL	O2D-CGD-CBD	5.00	120.15	111.27
21	P	102	CRT	C3-C1-C2	4.97	119.73	110.37
15	Y	101	BCL	O2D-CGD-CBD	4.95	120.06	111.27
21	1	402	CRT	C21-C22-C23	-4.93	120.28	127.31
12	C	506	DGA	OG2-CB1-CB2	4.90	120.11	111.09
21	Q	102	CRT	C10-C9-C7	-4.90	120.31	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	S	104	CRT	C40-C38-C37	4.89	118.37	110.86
15	7	101	BCL	O2D-CGD-CBD	4.86	119.91	111.27
15	T	102	BCL	CHD-C4C-NC	4.83	130.44	125.08
15	5	102	BCL	O2D-CGD-CBD	4.78	119.76	111.27
21	P	102	CRT	C5-C6-C7	-4.78	118.67	125.89
21	G	103	CRT	C21-C22-C23	-4.77	120.50	127.31
21	S	104	CRT	C10-C9-C7	-4.76	120.52	127.31
15	T	102	BCL	C3C-C4C-CHD	-4.72	113.30	123.39
15	O	502	BCL	O2D-CGD-CBD	4.72	119.65	111.27
21	X	103	CRT	C21-C22-C23	-4.71	120.59	127.31
15	Q	101	BCL	O2D-CGD-CBD	4.70	119.62	111.27
15	9	101	BCL	O2D-CGD-CBD	4.69	119.61	111.27
15	3	101	BCL	O2D-CGD-CBD	4.69	119.59	111.27
15	4	102	BCL	CHD-C4C-NC	4.68	130.27	125.08
15	M	402	BCL	CMB-C2B-C3B	4.67	133.42	124.68
21	E	103	CRT	C21-C22-C23	-4.67	120.65	127.31
21	P	102	CRT	C10-C9-C7	-4.65	120.67	127.31
15	1	403	BCL	O2D-CGD-CBD	4.65	119.52	111.27
15	S	102	BCL	O2D-CGD-CBD	4.64	119.51	111.27
15	U	101	BCL	O2D-CGD-CBD	4.63	119.50	111.27
15	N	101	BCL	O2D-CGD-CBD	4.62	119.48	111.27
21	B	103	CRT	C21-C22-C23	-4.60	120.75	127.31
21	S	104	CRT	C21-C22-C23	-4.57	120.79	127.31
21	Q	102	CRT	C21-C22-C23	-4.56	120.80	127.31
21	2	103	CRT	C21-C22-C23	-4.56	120.81	127.31
15	M	402	BCL	C3C-C4C-CHD	-4.55	113.68	123.39
15	G	102	BCL	CHD-C4C-NC	4.53	130.10	125.08
17	L	505	UQ8	C35-C34-C36	4.51	122.86	115.27
15	9	101	BCL	CHD-C4C-NC	4.49	130.06	125.08
15	X	102	BCL	CHD-C4C-NC	4.48	130.05	125.08
14	M	411	PGV	O01-C1-C2	4.47	121.14	111.50
15	7	101	BCL	CHD-C4C-NC	4.47	130.04	125.08
15	A	101	BCL	CHD-C4C-NC	4.47	130.04	125.08
15	F	101	BCL	CHD-C4C-NC	4.47	130.04	125.08
15	0	102	BCL	CHD-C4C-NC	4.45	130.02	125.08
18	M	410	CDL	OA6-CA5-C11	4.43	121.04	111.50
15	L	508	BCL	CHD-C4C-NC	4.42	129.99	125.08
15	V	102	BCL	CHD-C4C-NC	4.42	129.98	125.08
15	L	502	BCL	CHD-C4C-NC	4.41	129.97	125.08
15	W	101	BCL	CHD-C4C-NC	4.41	129.97	125.08
18	L	510	CDL	OB6-CB5-C51	4.41	121.00	111.50
15	4	102	BCL	C3C-C4C-CHD	-4.38	114.03	123.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	O	502	BCL	CHD-C4C-NC	4.36	129.92	125.08
15	J	102	BCL	CHD-C4C-NC	4.36	129.92	125.08
15	0	102	BCL	C3C-C4C-CHD	-4.35	114.10	123.39
15	L	502	BCL	CMB-C2B-C3B	4.35	132.82	124.68
15	L	502	BCL	C3C-C4C-CHD	-4.34	114.11	123.39
15	5	102	BCL	CHD-C4C-NC	4.33	129.89	125.08
21	P	102	CRT	C21-C22-C23	-4.32	121.14	127.31
21	8	103	CRT	C21-C22-C23	-4.32	121.14	127.31
15	P	101	BCL	O2D-CGD-CBD	4.32	118.94	111.27
15	G	102	BCL	C3C-C4C-CHD	-4.31	114.17	123.39
15	E	102	BCL	CHD-C4C-NC	4.31	129.87	125.08
14	C	508	PGV	O01-C1-C2	4.31	120.79	111.50
15	2	102	BCL	O2D-CGD-CBD	4.30	118.91	111.27
15	E	102	BCL	C3C-C4C-CHD	-4.29	114.22	123.39
15	4	102	BCL	CMB-C2B-C3B	4.29	132.70	124.68
15	R	101	BCL	CHD-C4C-NC	4.26	129.81	125.08
15	Q	101	BCL	CHD-C4C-NC	4.26	129.81	125.08
15	Y	101	BCL	CHD-C4C-NC	4.26	129.81	125.08
15	Z	102	BCL	CHD-C4C-NC	4.25	129.80	125.08
15	U	101	BCL	CHD-C4C-NC	4.25	129.80	125.08
15	N	101	BCL	CMB-C2B-C3B	4.25	132.62	124.68
15	6	101	BCL	O2D-CGD-CBD	4.24	118.80	111.27
15	I	102	BCL	O2D-CGD-CBD	4.24	118.80	111.27
18	I	101	CDL	OA6-CA5-C11	4.24	120.63	111.50
15	X	102	BCL	C3C-C4C-CHD	-4.23	114.35	123.39
18	H	301	CDL	OA6-CA5-C11	4.23	120.61	111.50
15	L	509	BCL	CMB-C2B-C3B	4.22	132.57	124.68
15	L	508	BCL	C1-C2-C3	-4.21	118.75	126.04
15	8	102	BCL	O2D-CGD-CBD	4.21	118.75	111.27
21	4	103	CRT	C21-C22-C23	-4.21	121.30	127.31
15	S	102	BCL	CHD-C4C-NC	4.20	129.74	125.08
15	W	101	BCL	C3C-C4C-CHD	-4.18	114.46	123.39
15	D	103	BCL	O2D-CGD-CBD	4.17	118.68	111.27
15	Q	101	BCL	CMB-C2B-C3B	4.17	132.48	124.68
15	0	102	BCL	CMB-C2B-C3B	4.17	132.47	124.68
14	L	511	PGV	O01-C1-C2	4.16	120.47	111.50
21	2	103	CRT	C10-C9-C7	-4.15	121.39	127.31
21	N	102	CRT	C10-C9-C7	-4.14	121.40	127.31
21	4	103	CRT	C20-C19-C17	-4.14	121.40	127.31
21	8	103	CRT	C20-C19-C17	-4.14	121.40	127.31
15	R	101	BCL	C3C-C4C-CHD	-4.13	114.56	123.39
15	6	101	BCL	CHD-C4C-NC	4.13	129.66	125.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	Z	102	BCL	C3C-C4C-CHD	-4.12	114.58	123.39
15	L	509	BCL	CHD-C4C-NC	4.12	129.65	125.08
15	7	101	BCL	C3C-C4C-CHD	-4.11	114.60	123.39
15	1	403	BCL	CHD-C4C-NC	4.10	129.63	125.08
15	J	102	BCL	C3C-C4C-CHD	-4.10	114.64	123.39
15	Z	102	BCL	O2D-CGD-CBD	4.10	118.55	111.27
15	F	101	BCL	CMB-C2B-C3B	4.09	132.32	124.68
15	A	101	BCL	C3C-C4C-CHD	-4.07	114.70	123.39
15	5	102	BCL	CMB-C2B-C3B	4.06	132.28	124.68
18	I	101	CDL	OB6-CB5-C51	4.06	120.26	111.50
15	D	103	BCL	CHD-C4C-NC	4.06	129.58	125.08
15	E	102	BCL	O2D-CGD-CBD	4.06	118.48	111.27
14	L	507	PGV	O01-C1-C2	4.06	120.24	111.50
15	X	102	BCL	C1-C2-C3	-4.05	119.03	126.04
15	B	102	BCL	CMB-C2B-C3B	4.05	132.25	124.68
15	V	102	BCL	C3C-C4C-CHD	-4.05	114.74	123.39
21	N	102	CRT	C5-C6-C7	-4.05	119.77	125.89
15	L	508	BCL	C3C-C4C-CHD	-4.04	114.77	123.39
15	2	102	BCL	CMB-C2B-C3B	4.03	132.23	124.68
14	1	401	PGV	O01-C1-C2	4.03	120.18	111.50
15	6	101	BCL	CMB-C2B-C3B	4.03	132.21	124.68
14	H	303	PGV	O01-C1-C2	4.03	120.18	111.50
15	8	102	BCL	CHD-C4C-NC	4.03	129.55	125.08
14	M	409	PGV	O01-C1-C2	4.01	120.14	111.50
18	H	301	CDL	OB6-CB5-C51	4.00	120.12	111.50
15	J	102	BCL	O2D-CGD-CBD	3.99	118.36	111.27
15	A	101	BCL	CMB-C2B-C3B	3.98	132.13	124.68
14	M	407	PGV	O01-C1-C2	3.98	120.07	111.50
15	9	101	BCL	C3C-C4C-CHD	-3.97	114.91	123.39
15	K	103	BCL	CMB-C2B-C3B	3.96	132.09	124.68
15	Z	102	BCL	CMB-C2B-C3B	3.95	132.08	124.68
15	Q	101	BCL	C3C-C4C-CHD	-3.95	114.95	123.39
15	L	508	BCL	CMB-C2B-C3B	3.95	132.06	124.68
15	F	101	BCL	C3C-C4C-CHD	-3.95	114.96	123.39
15	S	102	BCL	C3C-C4C-CHD	-3.94	114.96	123.39
21	X	103	CRT	C20-C19-C17	-3.94	121.69	127.31
15	3	101	BCL	CHD-C4C-NC	3.94	129.45	125.08
14	L	506	PGV	O01-C1-C2	3.93	119.98	111.50
15	V	102	BCL	CMB-C2B-C3B	3.93	132.03	124.68
15	O	502	BCL	C3C-C4C-CHD	-3.92	115.01	123.39
15	J	102	BCL	C1-C2-C3	-3.92	119.27	126.04
15	P	101	BCL	C1-C2-C3	-3.91	119.27	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	0	102	BCL	O2D-CGD-CBD	3.90	118.20	111.27
15	2	102	BCL	CHD-C4C-NC	3.90	129.41	125.08
14	5	101	PGV	O01-C1-C2	3.89	119.89	111.50
15	I	102	BCL	CMB-C2B-C3B	3.89	131.95	124.68
15	U	101	BCL	CMB-C2B-C3B	3.89	131.95	124.68
15	4	102	BCL	C4-C3-C5	3.87	121.79	115.27
15	T	102	BCL	CMB-C2B-C3B	3.87	131.92	124.68
21	7	102	CRT	C20-C19-C17	-3.86	121.80	127.31
21	1	402	CRT	C20-C19-C17	-3.86	121.81	127.31
15	2	102	BCL	C3C-C4C-CHD	-3.86	115.15	123.39
15	I	102	BCL	CHD-C4C-NC	3.85	129.35	125.08
21	R	102	CRT	C21-C22-C23	-3.84	121.83	127.31
15	W	101	BCL	CMB-C2B-C3B	3.83	131.85	124.68
15	U	101	BCL	C3C-C4C-CHD	-3.83	115.20	123.39
15	P	101	BCL	CMB-C2B-C3B	3.83	131.84	124.68
15	Y	101	BCL	CMB-C2B-C3B	3.83	131.84	124.68
21	Q	102	CRT	C5-C6-C7	-3.82	120.11	125.89
21	N	102	CRT	C21-C22-C23	-3.82	121.86	127.31
18	S	101	CDL	OB6-CB5-C51	3.82	119.73	111.50
15	8	102	BCL	C3C-C4C-CHD	-3.81	115.24	123.39
18	D	102	CDL	OB6-CB5-C51	3.81	119.72	111.50
15	4	102	BCL	O2D-CGD-CBD	3.81	118.04	111.27
15	6	101	BCL	C3C-C4C-CHD	-3.81	115.26	123.39
18	M	408	CDL	OB6-CB5-C51	3.81	119.70	111.50
15	X	102	BCL	O2D-CGD-CBD	3.80	118.02	111.27
21	Q	102	CRT	C20-C19-C17	-3.79	121.90	127.31
15	Z	102	BCL	C1-C2-C3	-3.79	119.49	126.04
15	D	103	BCL	C3C-C4C-CHD	-3.78	115.33	123.39
15	K	103	BCL	CHD-C4C-NC	3.77	129.26	125.08
21	N	102	CRT	C20-C19-C17	-3.77	121.93	127.31
15	5	102	BCL	C3C-C4C-CHD	-3.77	115.35	123.39
15	B	102	BCL	O2D-CGD-CBD	3.76	117.95	111.27
15	X	102	BCL	CMB-C2B-C3B	3.76	131.71	124.68
14	D	101	PGV	O01-C1-C2	3.75	119.59	111.50
15	D	103	BCL	C1-C2-C3	-3.75	119.55	126.04
21	M	405	CRT	C20-C19-C17	-3.75	121.96	127.31
18	D	102	CDL	OA6-CA5-C11	3.75	119.57	111.50
15	O	502	BCL	CMB-C2B-C3B	3.73	131.66	124.68
15	7	101	BCL	CMB-C2B-C3B	3.73	131.66	124.68
15	U	101	BCL	C1-C2-C3	-3.73	119.60	126.04
15	D	103	BCL	CMB-C2B-C3B	3.73	131.65	124.68
21	R	102	CRT	C20-C19-C17	-3.72	122.00	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	S	101	CDL	OA6-CA5-C11	3.71	119.50	111.50
21	7	102	CRT	C21-C22-C23	-3.70	122.02	127.31
15	R	101	BCL	O2D-CGD-CBD	3.68	117.80	111.27
15	1	403	BCL	CMB-C2B-C3B	3.67	131.54	124.68
17	L	504	UQ8	C7-C8-C9	-3.66	120.70	126.79
15	T	102	BCL	O2D-CGD-CBD	3.66	117.77	111.27
15	V	102	BCL	O2D-CGD-CBD	3.64	117.75	111.27
15	N	101	BCL	CHD-C4C-NC	3.64	129.12	125.08
18	M	410	CDL	OB6-CB5-C51	3.63	119.31	111.50
15	B	102	BCL	CHD-C4C-NC	3.62	129.10	125.08
21	B	103	CRT	C20-C19-C17	-3.62	122.15	127.31
15	Y	101	BCL	C3C-C4C-CHD	-3.61	115.67	123.39
21	X	103	CRT	C10-C9-C7	-3.61	122.16	127.31
21	1	402	CRT	C10-C9-C7	-3.60	122.17	127.31
15	Y	101	BCL	C1-C2-C3	-3.60	119.81	126.04
15	J	102	BCL	CMB-C2B-C3B	3.60	131.41	124.68
15	1	403	BCL	C3C-C4C-CHD	-3.60	115.70	123.39
18	L	510	CDL	CA4-OA6-CA5	-3.60	111.19	117.90
17	L	505	UQ8	C40-C39-C41	3.59	121.31	115.27
15	B	102	BCL	C4C-CHD-C1D	-3.57	120.61	125.88
15	R	101	BCL	CMB-C2B-C3B	3.57	131.35	124.68
15	W	101	BCL	C1-C2-C3	-3.56	119.89	126.04
15	3	101	BCL	CMB-C2B-C3B	3.54	131.31	124.68
15	Y	101	BCL	C4C-CHD-C1D	-3.54	120.66	125.88
15	I	102	BCL	C4C-CHD-C1D	-3.54	120.66	125.88
15	L	509	BCL	C3C-C4C-CHD	-3.53	115.84	123.39
17	L	512	UQ8	C10-C9-C11	3.53	121.21	115.27
15	K	103	BCL	C4C-CHD-C1D	-3.52	120.68	125.88
15	P	101	BCL	CHD-C4C-NC	3.52	128.99	125.08
15	N	101	BCL	C4C-CHD-C1D	-3.51	120.69	125.88
21	B	103	CRT	C10-C9-C7	-3.51	122.30	127.31
15	G	102	BCL	C1-C2-C3	-3.51	119.97	126.04
15	G	102	BCL	CMB-C2B-C3B	3.51	131.24	124.68
15	7	101	BCL	C1-C2-C3	-3.50	120.00	126.04
15	V	102	BCL	C1-C2-C3	-3.49	120.01	126.04
15	3	101	BCL	C4B-CHC-C1C	-3.49	123.21	130.12
15	F	101	BCL	C1-C2-C3	-3.49	120.01	126.04
15	2	102	BCL	C1-C2-C3	-3.48	120.02	126.04
21	2	103	CRT	C20-C19-C17	-3.47	122.36	127.31
21	2	103	CRT	C5-C6-C7	-3.47	120.65	125.89
15	L	502	BCL	O2D-CGD-CBD	3.46	117.42	111.27
15	6	101	BCL	C4C-CHD-C1D	-3.46	120.78	125.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	1	402	CRT	C26-C27-C28	-3.45	122.38	127.31
15	9	101	BCL	CMB-C2B-C3B	3.45	131.14	124.68
10	C	503	HEC	CBA-CAA-C2A	-3.45	106.79	112.60
15	P	101	BCL	C4C-CHD-C1D	-3.44	120.80	125.88
15	2	102	BCL	C4C-CHD-C1D	-3.44	120.80	125.88
21	S	104	CRT	C20-C19-C17	-3.44	122.40	127.31
15	0	102	BCL	C4-C3-C5	3.44	121.05	115.27
15	1	403	BCL	C4C-CHD-C1D	-3.43	120.83	125.88
14	L	501	PGV	O01-C1-C2	3.41	120.32	110.80
15	6	101	BCL	C1-C2-C3	-3.40	120.17	126.04
20	M	406	MQ8	C21-C22-C23	-3.38	119.51	127.66
15	N	101	BCL	C3C-C4C-CHD	-3.37	116.19	123.39
15	F	101	BCL	C4C-CHD-C1D	-3.37	120.91	125.88
15	E	102	BCL	CMB-C2B-C3B	3.37	130.98	124.68
18	H	302	CDL	OB6-CB5-C51	3.37	120.19	110.80
21	J	103	CRT	C21-C20-C19	-3.36	116.59	123.47
15	B	102	BCL	C3C-C4C-CHD	-3.36	116.22	123.39
15	I	102	BCL	C3C-C4C-CHD	-3.34	116.26	123.39
17	L	505	UQ8	C10-C9-C11	3.34	120.89	115.27
15	G	102	BCL	O2D-CGD-CBD	3.34	117.20	111.27
21	N	102	CRT	C15-C14-C12	-3.33	122.56	127.31
15	R	101	BCL	C4C-CHD-C1D	-3.31	121.00	125.88
15	8	102	BCL	CMB-C2B-C3B	3.30	130.86	124.68
15	G	102	BCL	C4C-CHD-C1D	-3.30	121.01	125.88
15	L	502	BCL	O2A-CGA-CBA	3.30	122.27	111.91
21	6	102	CRT	C20-C19-C17	-3.30	122.60	127.31
21	S	104	CRT	O2-C38-C39	-3.29	86.34	108.97
21	R	102	CRT	C26-C27-C28	-3.28	122.63	127.31
21	8	103	CRT	C10-C9-C7	-3.28	122.63	127.31
15	8	102	BCL	C4C-CHD-C1D	-3.27	121.06	125.88
15	S	102	BCL	CMB-C2B-C3B	3.25	130.76	124.68
15	A	101	BCL	C4C-CHD-C1D	-3.25	121.09	125.88
15	P	101	BCL	C3C-C4C-CHD	-3.24	116.47	123.39
15	Z	102	BCL	C4C-CHD-C1D	-3.24	121.10	125.88
15	B	102	BCL	C4-C3-C5	3.24	120.72	115.27
15	M	402	BCL	C4C-CHD-C1D	-3.24	121.10	125.88
15	3	101	BCL	C3C-C4C-CHD	-3.24	116.48	123.39
22	4	101	LMT	C1B-O1B-C4'	-3.23	109.97	117.96
17	L	505	UQ8	C12-C13-C14	-3.22	119.91	127.66
15	K	103	BCL	C3C-C4C-CHD	-3.22	116.52	123.39
18	M	408	CDL	OA8-CA7-C31	3.22	119.81	111.38
15	5	102	BCL	C4C-CHD-C1D	-3.21	121.15	125.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	X	103	CRT	C15-C14-C12	-3.20	122.74	127.31
21	S	104	CRT	C5-C6-C7	-3.20	121.06	125.89
21	E	103	CRT	C20-C19-C17	-3.20	122.75	127.31
20	M	406	MQ8	C14-C13-C15	3.20	120.65	115.27
15	L	509	BCL	C4C-CHD-C1D	-3.19	121.17	125.88
15	T	102	BCL	C4C-CHD-C1D	-3.19	121.17	125.88
15	Q	101	BCL	C4-C3-C5	3.18	120.62	115.27
15	V	102	BCL	C4C-CHD-C1D	-3.18	121.19	125.88
15	I	102	BCL	C4-C3-C5	3.17	120.61	115.27
15	S	102	BCL	C1-C2-C3	-3.17	120.56	126.04
14	L	511	PGV	C02-O01-C1	-3.17	109.99	117.79
15	L	508	BCL	C4-C3-C5	3.17	120.60	115.27
15	B	102	BCL	C4B-CHC-C1C	-3.16	123.86	130.12
15	V	102	BCL	O2A-CGA-CBA	3.16	121.81	111.91
15	N	101	BCL	O2A-CGA-CBA	3.13	121.73	111.91
15	J	102	BCL	C4C-CHD-C1D	-3.13	121.27	125.88
20	M	406	MQ8	C11-C3-C4	3.12	121.84	118.50
15	E	102	BCL	C4C-CHD-C1D	-3.12	121.28	125.88
15	U	101	BCL	C4-C3-C5	3.11	120.51	115.27
20	M	404	MQ8	C26-C27-C28	-3.11	120.16	127.66
15	F	101	BCL	C4-C3-C5	3.11	120.50	115.27
15	5	102	BCL	C4-C3-C5	3.11	120.50	115.27
15	4	102	BCL	O2A-CGA-CBA	3.10	121.62	111.91
15	L	508	BCL	C4C-CHD-C1D	-3.09	121.32	125.88
21	2	103	CRT	O2-C38-C39	-3.09	87.71	108.97
15	E	102	BCL	C1-C2-C3	-3.09	120.69	126.04
15	L	509	BCL	O2A-CGA-CBA	3.09	121.59	111.91
21	P	102	CRT	C32-C31-C30	-3.09	113.59	123.22
15	7	101	BCL	C4C-CHD-C1D	-3.08	121.34	125.88
15	G	102	BCL	C4-C3-C5	3.07	120.43	115.27
21	2	103	CRT	O2-C38-C40	-3.07	87.87	108.97
21	1	402	CRT	C5-C6-C7	-3.06	121.27	125.89
15	3	101	BCL	C1-C2-C3	-3.06	120.75	126.04
15	B	102	BCL	O2A-CGA-CBA	3.05	121.49	111.91
15	3	101	BCL	C4C-CHD-C1D	-3.05	121.37	125.88
17	L	512	UQ8	C12-C13-C14	-3.05	120.31	127.66
21	B	103	CRT	C15-C14-C12	-3.05	122.96	127.31
21	B	103	CRT	C32-C31-C30	-3.04	113.72	123.22
17	L	505	UQ8	C22-C23-C24	-3.04	120.34	127.66
15	V	102	BCL	CHB-C4A-NA	3.04	128.71	124.51
15	L	502	BCL	C4C-CHD-C1D	-3.03	121.42	125.88
21	M	405	CRT	C14-C15-C16	-3.03	113.77	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	S	104	CRT	C15-C14-C12	-3.03	122.99	127.31
22	G	101	LMT	C1B-O1B-C4'	-3.02	110.49	117.96
15	M	402	BCL	O2A-CGA-CBA	3.02	121.37	111.91
20	M	406	MQ8	C39-C38-C40	3.02	120.34	115.27
15	L	508	BCL	O2D-CGD-O1D	-3.01	117.95	123.84
21	M	405	CRT	C32-C31-C30	-3.01	113.82	123.22
21	4	103	CRT	C15-C14-C12	-3.01	123.02	127.31
12	C	506	DGA	CG2-OG2-CB1	-3.00	113.13	118.31
15	0	102	BCL	C4C-CHD-C1D	-3.00	121.45	125.88
15	W	101	BCL	CHC-C1C-NC	2.99	128.65	124.51
15	E	102	BCL	O2A-CGA-CBA	2.99	121.28	111.91
15	2	102	BCL	C4-C3-C5	2.98	120.29	115.27
15	4	102	BCL	C4C-CHD-C1D	-2.98	121.48	125.88
17	L	505	UQ8	C17-C18-C19	-2.98	120.49	127.66
15	X	102	BCL	C4C-CHD-C1D	-2.98	121.49	125.88
15	W	101	BCL	C4C-CHD-C1D	-2.97	121.50	125.88
15	T	102	BCL	CHB-C4A-NA	2.97	128.62	124.51
15	O	502	BCL	C1-C2-C3	-2.96	120.93	126.04
15	R	101	BCL	C1-C2-C3	-2.96	120.93	126.04
14	L	507	PGV	C02-O01-C1	-2.96	110.51	117.79
15	Q	101	BCL	C1-C2-C3	-2.96	120.93	126.04
15	8	102	BCL	C4-C3-C5	2.95	120.23	115.27
21	X	103	CRT	C32-C31-C30	-2.94	114.03	123.22
15	5	102	BCL	C1-C2-C3	-2.94	120.95	126.04
15	0	102	BCL	C1-C2-C3	-2.93	120.97	126.04
15	S	102	BCL	C4C-CHD-C1D	-2.93	121.56	125.88
15	Z	102	BCL	C4-C3-C5	2.93	120.19	115.27
17	L	505	UQ8	C20-C19-C21	2.93	120.19	115.27
15	A	101	BCL	C1-C2-C3	-2.93	120.98	126.04
18	M	410	CDL	CA4-OA6-CA5	-2.92	110.59	117.79
15	E	102	BCL	CHB-C4A-NA	2.92	128.56	124.51
15	K	103	BCL	C1-C2-C3	-2.92	120.99	126.04
14	C	508	PGV	C02-O01-C1	-2.92	110.60	117.79
21	7	102	CRT	C10-C9-C7	-2.92	123.14	127.31
15	8	102	BCL	O2A-CGA-CBA	2.92	121.07	111.91
15	L	509	BCL	C4B-CHC-C1C	-2.92	124.34	130.12
15	E	102	BCL	C4-C3-C5	2.92	120.18	115.27
15	K	103	BCL	O2D-CGD-O1D	-2.92	118.14	123.84
12	C	506	DGA	OG1-CA1-CA2	2.91	121.04	111.91
20	M	404	MQ8	C39-C38-C40	2.91	120.16	115.27
15	0	102	BCL	C2A-C1A-CHA	-2.91	118.77	123.86
15	S	102	BCL	CHC-C1C-NC	2.91	128.53	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	M	408	CDL	OA6-CA5-C11	2.91	118.91	110.80
15	6	101	BCL	C4-C3-C5	2.91	120.16	115.27
21	B	103	CRT	C5-C6-C7	-2.90	121.50	125.89
15	4	102	BCL	CHB-C4A-NA	2.90	128.53	124.51
21	8	103	CRT	C32-C31-C30	-2.89	114.19	123.22
20	M	406	MQ8	C24-C23-C25	2.89	120.13	115.27
21	E	103	CRT	C32-C31-C30	-2.89	114.21	123.22
21	2	103	CRT	C31-C32-C33	-2.88	123.19	127.31
15	Q	101	BCL	C4C-CHD-C1D	-2.88	121.63	125.88
15	M	402	BCL	CAA-C2A-C3A	-2.88	104.88	112.78
21	E	103	CRT	C5-C6-C7	-2.88	121.54	125.89
17	L	505	UQ8	C27-C28-C29	-2.88	120.72	127.66
18	I	101	CDL	CA4-OA6-CA5	-2.88	110.70	117.79
18	L	510	CDL	CB4-OB6-CB5	-2.88	110.70	117.79
14	L	506	PGV	O03-C19-C20	2.88	120.94	111.91
15	Q	101	BCL	CHC-C1C-NC	2.88	128.49	124.51
21	4	103	CRT	C32-C31-C30	-2.88	114.24	123.22
15	K	103	BCL	C4-C3-C5	2.88	120.11	115.27
18	M	410	CDL	OA8-CA7-C31	2.87	120.93	111.91
17	L	504	UQ8	C1M-C1-C6	-2.87	119.72	124.40
21	G	103	CRT	C9-C10-C11	-2.87	114.28	123.22
21	4	103	CRT	C5-C6-C7	-2.86	121.56	125.89
10	C	501	HEC	CBA-CAA-C2A	-2.86	107.78	112.60
21	S	104	CRT	O2-C38-C40	-2.86	89.28	108.97
17	L	504	UQ8	C20-C19-C21	2.86	120.08	115.27
15	Y	101	BCL	O2A-CGA-CBA	2.86	120.88	111.91
15	V	102	BCL	CHC-C1C-NC	2.86	128.47	124.51
14	M	407	PGV	C02-O01-C1	-2.86	110.76	117.79
15	L	508	BCL	CHC-C1C-NC	2.86	128.46	124.51
21	X	103	CRT	C5-C6-C7	-2.86	121.58	125.89
18	H	301	CDL	OA8-CA7-C31	2.85	120.87	111.91
15	L	509	BCL	O2D-CGD-O1D	-2.85	118.26	123.84
15	0	102	BCL	CHB-C4A-NA	2.85	128.46	124.51
15	4	102	BCL	CHC-C1C-NC	2.85	128.45	124.51
15	7	101	BCL	CHB-C4A-NA	2.85	128.45	124.51
15	W	101	BCL	C4-C3-C5	2.85	120.06	115.27
15	U	101	BCL	C4C-CHD-C1D	-2.84	121.68	125.88
21	8	103	CRT	C5-C6-C7	-2.84	121.60	125.89
21	1	402	CRT	C31-C32-C33	-2.83	123.27	127.31
21	6	102	CRT	C21-C20-C19	-2.83	117.67	123.47
15	4	102	BCL	C1-C2-C3	-2.83	121.16	126.04
15	X	102	BCL	C4-C3-C5	2.82	120.02	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	Y	101	BCL	O2D-CGD-O1D	-2.82	118.32	123.84
15	W	101	BCL	O2D-CGD-O1D	-2.81	118.34	123.84
20	M	406	MQ8	C19-C18-C20	2.81	120.00	115.27
14	M	409	PGV	O03-C19-C20	2.81	120.73	111.91
22	4	104	LMT	C1B-O1B-C4'	-2.81	111.01	117.96
15	R	101	BCL	C4-C3-C5	2.81	120.00	115.27
15	9	101	BCL	C4C-CHD-C1D	-2.81	121.74	125.88
15	G	102	BCL	CHB-C4A-NA	2.81	128.39	124.51
21	7	102	CRT	C15-C14-C12	-2.80	123.31	127.31
21	Q	102	CRT	C8-C7-C9	-2.80	119.00	122.92
15	3	101	BCL	C4-C3-C5	2.80	119.97	115.27
15	A	101	BCL	CHC-C1C-NC	2.79	128.38	124.51
17	L	505	UQ8	C30-C29-C31	2.79	119.97	115.27
14	L	511	PGV	O03-C19-C20	2.79	120.67	111.91
15	0	102	BCL	CHC-C1C-NC	2.79	128.37	124.51
15	U	101	BCL	CHC-C1C-NC	2.79	128.37	124.51
15	O	502	BCL	C4C-CHD-C1D	-2.79	121.77	125.88
14	M	411	PGV	C02-O01-C1	-2.78	110.94	117.79
15	9	101	BCL	O2A-CGA-CBA	2.78	120.63	111.91
15	R	101	BCL	CHB-C4A-NA	2.78	128.35	124.51
18	M	410	CDL	OB8-CB7-C71	2.78	120.62	111.91
18	D	102	CDL	OB8-CB7-C71	2.78	120.62	111.91
18	H	301	CDL	OB8-CB7-C71	2.77	120.61	111.91
15	9	101	BCL	C1-C2-C3	-2.77	121.25	126.04
10	C	502	HEC	CBA-CAA-C2A	-2.77	107.94	112.60
21	J	103	CRT	C20-C19-C17	-2.77	123.36	127.31
15	D	103	BCL	C4-C3-C5	2.76	119.92	115.27
15	J	102	BCL	CHB-C4A-NA	2.76	128.33	124.51
15	B	102	BCL	C4A-NA-C1A	2.76	107.94	106.71
22	0	101	LMT	C1B-O1B-C4'	-2.76	111.14	117.96
15	D	103	BCL	O2A-CGA-CBA	2.75	120.55	111.91
14	1	401	PGV	O03-C19-C20	2.75	120.55	111.91
15	L	509	BCL	C4-C3-C5	2.75	119.90	115.27
15	Y	101	BCL	CHC-C1C-NC	2.75	128.32	124.51
15	S	102	BCL	O2A-CGA-CBA	2.75	120.53	111.91
15	F	101	BCL	CHC-C1C-NC	2.74	128.30	124.51
15	P	101	BCL	CHB-C4A-NA	2.74	128.30	124.51
14	C	508	PGV	O03-C19-C20	2.74	120.50	111.91
21	6	102	CRT	C32-C31-C30	-2.73	114.70	123.22
15	N	101	BCL	C1-C2-C3	-2.73	121.33	126.04
15	Z	102	BCL	O2A-CGA-CBA	2.72	120.45	111.91
21	E	103	CRT	C10-C9-C7	-2.72	123.42	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	T	102	BCL	CAD-C3D-C4D	2.72	109.99	108.47
15	X	102	BCL	CHB-C4A-NA	2.72	128.27	124.51
14	M	411	PGV	O03-C19-C20	2.71	120.42	111.91
15	L	502	BCL	CHC-C1C-NC	2.71	128.26	124.51
15	T	102	BCL	C4-C3-C5	2.71	119.83	115.27
15	D	103	BCL	CHB-C4A-NA	2.71	128.26	124.51
15	4	102	BCL	C2A-C1A-CHA	-2.71	119.13	123.86
15	L	502	BCL	CED-O2D-CGD	2.70	122.05	115.94
15	P	101	BCL	C4B-CHC-C1C	-2.70	124.76	130.12
15	9	101	BCL	C4-C3-C5	2.70	119.82	115.27
15	1	403	BCL	C4B-CHC-C1C	-2.70	124.77	130.12
21	7	102	CRT	C32-C31-C30	-2.70	114.80	123.22
15	R	101	BCL	C2A-C1A-CHA	-2.70	119.14	123.86
20	M	404	MQ8	C45-C43-C44	2.70	119.81	115.27
14	H	303	PGV	O03-C19-C20	2.69	120.36	111.91
15	N	101	BCL	C4-C3-C5	2.69	119.80	115.27
15	T	102	BCL	CHC-C1C-NC	2.69	128.24	124.51
15	U	101	BCL	O2A-CGA-CBA	2.69	120.36	111.91
15	F	101	BCL	O2A-CGA-CBA	2.69	120.35	111.91
15	1	403	BCL	CHB-C4A-NA	2.69	128.23	124.51
18	M	408	CDL	CB4-OB6-CB5	-2.69	111.17	117.79
15	N	101	BCL	C4B-CHC-C1C	-2.69	124.79	130.12
21	N	102	CRT	C32-C31-C30	-2.69	114.84	123.22
20	M	404	MQ8	C41-C42-C43	-2.68	121.20	127.66
15	8	102	BCL	CAD-C3D-C4D	2.68	109.97	108.47
15	M	402	BCL	O2D-CGD-O1D	-2.68	118.60	123.84
21	M	405	CRT	C9-C10-C11	-2.68	114.86	123.22
20	M	404	MQ8	C14-C13-C15	2.68	119.77	115.27
18	I	101	CDL	OB8-CB7-C71	2.67	120.30	111.91
15	J	102	BCL	C4-C3-C5	2.67	119.76	115.27
15	A	101	BCL	CHB-C4A-NA	2.67	128.20	124.51
15	J	102	BCL	CHC-C1C-NC	2.67	128.20	124.51
15	R	101	BCL	CHC-C1C-NC	2.66	128.20	124.51
21	6	102	CRT	C34-C33-C35	2.66	122.28	118.08
15	G	102	BCL	CAD-C3D-C4D	2.66	109.95	108.47
15	7	101	BCL	C4B-CHC-C1C	-2.66	124.85	130.12
15	S	102	BCL	CHB-C4A-NA	2.66	128.19	124.51
21	P	102	CRT	C21-C20-C19	-2.66	118.03	123.47
21	E	103	CRT	C21-C20-C19	-2.66	118.03	123.47
18	S	101	CDL	OB8-CB7-C71	2.65	120.22	111.91
17	L	512	UQ8	C20-C19-C21	2.65	119.73	115.27
21	G	103	CRT	C20-C19-C17	-2.65	123.53	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	X	102	BCL	CAD-C3D-C4D	2.65	109.95	108.47
21	7	102	CRT	C34-C33-C35	2.64	122.24	118.08
20	M	406	MQ8	C41-C42-C43	-2.64	121.31	127.66
21	P	102	CRT	C15-C14-C12	-2.64	123.55	127.31
15	9	101	BCL	CHB-C4A-NA	2.64	128.16	124.51
15	W	101	BCL	CHB-C4A-NA	2.64	128.16	124.51
15	U	101	BCL	O2D-CGD-O1D	-2.63	118.69	123.84
17	L	512	UQ8	C15-C14-C16	2.63	119.70	115.27
14	5	101	PGV	O03-C19-C20	2.63	120.17	111.91
21	2	103	CRT	C15-C14-C12	-2.63	123.56	127.31
20	M	406	MQ8	C2M-C2-C3	-2.63	120.12	124.40
15	5	102	BCL	CHC-C1C-NC	2.63	128.14	124.51
20	M	406	MQ8	C36-C37-C38	-2.62	121.36	127.66
15	L	502	BCL	CAD-C3D-C4D	2.62	109.93	108.47
15	F	101	BCL	O2D-CGD-O1D	-2.62	118.72	123.84
15	X	102	BCL	CHC-C1C-NC	2.62	128.13	124.51
21	J	103	CRT	C9-C10-C11	-2.61	115.06	123.22
18	H	302	CDL	CB4-OB6-CB5	-2.61	111.36	117.79
15	D	103	BCL	C4C-CHD-C1D	-2.60	122.04	125.88
15	8	102	BCL	C2A-C1A-CHA	-2.60	119.31	123.86
15	Z	102	BCL	C2A-C1A-CHA	-2.60	119.31	123.86
15	R	101	BCL	C1C-NC-C4C	-2.59	105.54	106.71
21	J	103	CRT	C26-C27-C28	-2.59	123.61	127.31
21	B	103	CRT	C26-C27-C28	-2.59	123.61	127.31
15	V	102	BCL	C4-C3-C5	2.59	119.62	115.27
21	6	102	CRT	C14-C15-C16	-2.59	115.14	123.22
14	M	407	PGV	O03-C19-C20	2.59	120.03	111.91
18	I	101	CDL	OA8-CA7-C31	2.58	120.01	111.91
15	L	508	BCL	CHB-C4A-NA	2.58	128.08	124.51
17	L	512	UQ8	C7-C8-C9	-2.58	122.50	126.79
21	1	402	CRT	C15-C14-C12	-2.58	123.63	127.31
15	E	102	BCL	CHC-C1C-NC	2.58	128.07	124.51
20	M	406	MQ8	C45-C43-C44	2.58	119.60	115.27
21	Q	102	CRT	C32-C31-C30	-2.58	115.18	123.22
15	R	101	BCL	O2A-CGA-CBA	2.57	119.98	111.91
15	O	502	BCL	CHB-C4A-NA	2.57	128.06	124.51
15	W	101	BCL	O2A-CGA-CBA	2.57	119.96	111.91
21	Q	102	CRT	C26-C27-C28	-2.56	123.65	127.31
15	E	102	BCL	C1C-NC-C4C	-2.56	105.56	106.71
15	A	101	BCL	O2D-CGD-O1D	-2.56	118.84	123.84
20	M	404	MQ8	C29-C28-C30	2.56	119.57	115.27
15	J	102	BCL	C1-O2A-CGA	2.56	123.15	116.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	8	102	BCL	C4B-CHC-C1C	-2.55	125.06	130.12
15	9	101	BCL	C4B-CHC-C1C	-2.55	125.06	130.12
15	4	102	BCL	CAD-C3D-C4D	2.55	109.89	108.47
15	1	403	BCL	C4-C3-C5	2.54	119.55	115.27
17	L	504	UQ8	C17-C18-C19	-2.54	121.54	127.66
15	Q	101	BCL	O2A-CGA-CBA	2.54	119.89	111.91
14	L	507	PGV	O03-C19-C20	2.54	119.88	111.91
15	7	101	BCL	O2A-CGA-CBA	2.54	119.88	111.91
15	K	103	BCL	CHC-C1C-NC	2.54	128.02	124.51
15	W	101	BCL	C1C-NC-C4C	-2.54	105.57	106.71
20	M	404	MQ8	C34-C33-C35	2.52	119.51	115.27
17	L	505	UQ8	C25-C24-C26	2.52	119.51	115.27
15	6	101	BCL	CHB-C4A-NA	2.52	128.00	124.51
15	L	502	BCL	C4-C3-C5	2.52	119.51	115.27
15	7	101	BCL	O2D-CGD-O1D	-2.52	118.91	123.84
22	E	101	LMT	C2'-C3'-C4'	2.52	115.43	109.68
15	5	102	BCL	CHB-C4A-NA	2.52	127.99	124.51
22	X	101	LMT	C1B-O1B-C4'	-2.52	111.74	117.96
15	K	103	BCL	O2A-CGA-CBA	2.51	119.79	111.91
17	L	512	UQ8	C1M-C1-C6	-2.51	120.30	124.40
21	6	102	CRT	C26-C27-C28	-2.51	123.73	127.31
17	L	512	UQ8	C17-C18-C19	-2.51	121.62	127.66
15	8	102	BCL	C1-C2-C3	-2.51	121.70	126.04
15	P	101	BCL	O2A-CGA-CBA	2.50	119.77	111.91
15	8	102	BCL	CHC-C1C-NC	2.50	127.97	124.51
15	3	101	BCL	O2D-CGD-O1D	-2.50	118.95	123.84
15	T	102	BCL	C1C-NC-C4C	-2.50	105.58	106.71
15	S	102	BCL	O2D-CGD-O1D	-2.50	118.95	123.84
15	3	101	BCL	O2A-CGA-CBA	2.50	119.75	111.91
15	9	101	BCL	O2D-CGD-O1D	-2.50	118.95	123.84
15	7	101	BCL	CHC-C1C-NC	2.50	127.96	124.51
21	X	103	CRT	C26-C27-C28	-2.49	123.75	127.31
21	E	103	CRT	C14-C15-C16	-2.49	115.44	123.22
20	M	404	MQ8	C19-C18-C20	2.49	119.46	115.27
15	5	102	BCL	O2D-CGD-O1D	-2.49	118.97	123.84
15	O	502	BCL	C4-C3-C5	2.49	119.45	115.27
18	S	101	CDL	OA8-CA7-C31	2.49	119.71	111.91
15	O	502	BCL	O2D-CGD-O1D	-2.48	118.99	123.84
21	G	103	CRT	C21-C20-C19	-2.48	118.39	123.47
15	1	403	BCL	O2A-CGA-CBA	2.48	119.68	111.91
15	Y	101	BCL	C4-C3-C5	2.48	119.44	115.27
15	1	403	BCL	O2D-CGD-O1D	-2.47	119.00	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	L	505	UQ8	C32-C33-C34	-2.47	121.71	127.66
15	Q	101	BCL	O2D-CGD-O1D	-2.47	119.01	123.84
15	3	101	BCL	C1B-CHB-C4A	-2.47	125.22	130.12
15	F	101	BCL	CHB-C4A-NA	2.47	127.92	124.51
17	L	504	UQ8	C15-C14-C16	2.47	119.42	115.27
15	R	101	BCL	CAD-C3D-C4D	2.47	109.84	108.47
22	E	101	LMT	C1'-C2'-C3'	2.46	115.11	110.00
15	Z	102	BCL	CHC-C1C-NC	2.45	127.91	124.51
20	M	404	MQ8	C16-C17-C18	-2.45	121.75	127.66
21	S	104	CRT	C31-C32-C33	-2.45	123.81	127.31
15	D	103	BCL	O2D-CGD-O1D	-2.45	119.05	123.84
15	P	101	BCL	C6-C5-C3	-2.45	107.03	113.45
15	D	103	BCL	C4B-CHC-C1C	-2.45	125.27	130.12
15	O	502	BCL	C4B-CHC-C1C	-2.45	125.27	130.12
15	O	502	BCL	O2A-CGA-CBA	2.45	119.59	111.91
21	G	103	CRT	C31-C32-C33	-2.45	123.82	127.31
14	L	501	PGV	O14-P-O13	2.44	120.25	110.68
15	1	403	BCL	CHC-C1C-NC	2.44	127.89	124.51
21	6	102	CRT	C15-C14-C12	-2.44	123.83	127.31
15	P	101	BCL	C4A-NA-C1A	2.44	107.80	106.71
15	G	102	BCL	CHC-C1C-NC	2.44	127.89	124.51
15	E	102	BCL	C2A-C1A-CHA	-2.44	119.59	123.86
15	X	102	BCL	C1-O2A-CGA	2.44	122.84	116.44
18	S	101	CDL	CA6-CA4-CA3	-2.43	106.03	111.79
20	M	406	MQ8	C31-C32-C33	-2.43	121.80	127.66
15	W	101	BCL	C4A-NA-C1A	2.43	107.80	106.71
22	8	101	LMT	C1B-O1B-C4'	-2.43	111.95	117.96
20	M	404	MQ8	C36-C37-C38	-2.43	121.81	127.66
21	7	102	CRT	C27-C26-C25	-2.43	115.64	123.22
17	L	505	UQ8	C37-C38-C39	-2.43	121.82	127.66
21	R	102	CRT	C32-C31-C30	-2.43	115.65	123.22
15	G	102	BCL	C4B-CHC-C1C	-2.42	125.31	130.12
15	2	102	BCL	C1C-NC-C4C	-2.42	105.62	106.71
15	T	102	BCL	C2A-C1A-CHA	-2.42	119.62	123.86
15	8	102	BCL	CHB-C4A-NA	2.42	127.86	124.51
21	8	103	CRT	C14-C15-C16	-2.42	115.65	123.22
15	5	102	BCL	O2A-CGA-CBA	2.42	119.50	111.91
15	G	102	BCL	C2A-C1A-CHA	-2.42	119.63	123.86
21	P	102	CRT	C20-C19-C17	-2.42	123.86	127.31
15	K	103	BCL	CHB-C4A-NA	2.42	127.85	124.51
21	8	103	CRT	C34-C33-C35	2.42	121.88	118.08
17	L	505	UQ8	O5-C5-C6	-2.42	117.31	121.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	X	103	CRT	C34-C33-C35	2.41	121.88	118.08
15	1	403	BCL	C2A-C1A-CHA	-2.41	119.64	123.86
15	A	101	BCL	CBA-CAA-C2A	-2.41	106.74	113.86
21	N	102	CRT	C34-C33-C35	2.41	121.88	118.08
21	E	103	CRT	C26-C27-C28	-2.41	123.87	127.31
15	K	103	BCL	C4A-NA-C1A	2.41	107.79	106.71
15	9	101	BCL	CHC-C1C-NC	2.41	127.84	124.51
15	I	102	BCL	C4B-CHC-C1C	-2.41	125.35	130.12
15	Z	102	BCL	CAD-C3D-C4D	2.41	109.81	108.47
17	L	505	UQ8	C1M-C1-C6	-2.41	120.47	124.40
21	R	102	CRT	C14-C15-C16	-2.40	115.71	123.22
21	X	103	CRT	C29-C28-C30	2.40	121.86	118.08
21	E	103	CRT	C9-C10-C11	-2.40	115.72	123.22
10	C	504	HEC	CBA-CAA-C2A	-2.39	108.57	112.60
17	L	504	UQ8	C25-C24-C26	2.39	119.89	114.60
21	J	103	CRT	C31-C32-C33	-2.39	123.90	127.31
22	T	101	LMT	C1B-O1B-C4'	-2.39	112.04	117.96
15	7	101	BCL	C4-C3-C5	2.39	119.29	115.27
15	I	102	BCL	O2A-CGA-CBA	2.39	119.41	111.91
15	M	402	BCL	C4-C3-C5	2.39	119.29	115.27
15	P	101	BCL	C2A-C1A-CHA	-2.39	119.68	123.86
15	L	509	BCL	C4A-NA-C1A	2.39	107.78	106.71
18	H	302	CDL	OB8-CB7-C71	2.38	119.39	111.91
15	N	101	BCL	O2D-CGD-O1D	-2.38	119.18	123.84
15	L	502	BCL	C1-C2-C3	-2.38	121.92	126.04
15	K	103	BCL	C2A-C1A-CHA	-2.38	119.70	123.86
21	S	104	CRT	C32-C31-C30	-2.38	115.79	123.22
15	S	102	BCL	C4-C3-C5	2.38	119.27	115.27
15	Q	101	BCL	CHB-C4A-NA	2.38	127.80	124.51
17	L	505	UQ8	C15-C14-C16	2.38	119.27	115.27
15	I	102	BCL	CHB-C4A-NA	2.38	127.80	124.51
15	P	101	BCL	O2D-CGD-O1D	-2.38	119.19	123.84
15	0	102	BCL	CAD-C3D-C4D	2.37	109.79	108.47
15	F	101	BCL	C4A-NA-C1A	2.37	107.77	106.71
15	7	101	BCL	CAD-C3D-C4D	2.37	109.79	108.47
15	K	103	BCL	C4B-CHC-C1C	-2.37	125.42	130.12
15	A	101	BCL	C4-C3-C5	2.37	119.26	115.27
15	L	509	BCL	CHB-C4A-NA	2.37	127.79	124.51
21	Q	102	CRT	C15-C14-C12	-2.37	123.93	127.31
21	R	102	CRT	C34-C33-C35	2.37	121.81	118.08
15	G	102	BCL	O2A-CGA-CBA	2.37	119.34	111.91
15	L	502	BCL	CHB-C4A-NA	2.37	127.78	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	L	510	CDL	OB8-CB7-C71	2.37	119.33	111.91
15	2	102	BCL	CHB-C4A-NA	2.36	127.78	124.51
21	6	102	CRT	C9-C10-C11	-2.36	115.85	123.22
15	2	102	BCL	O2D-CGD-O1D	-2.36	119.23	123.84
18	I	101	CDL	CB4-OB6-CB5	-2.36	111.98	117.79
15	6	101	BCL	C4B-CHC-C1C	-2.36	125.45	130.12
15	L	508	BCL	O2A-CGA-CBA	2.36	119.31	111.91
15	M	402	BCL	CHC-C1C-NC	2.36	127.77	124.51
15	A	101	BCL	C1C-NC-C4C	-2.36	105.65	106.71
15	I	102	BCL	CHC-C1C-NC	2.36	127.77	124.51
20	M	404	MQ8	C31-C32-C33	-2.35	122.00	127.66
15	8	102	BCL	C4A-NA-C1A	2.35	107.76	106.71
15	6	101	BCL	O2D-CGD-O1D	-2.35	119.25	123.84
15	D	103	BCL	CHC-C1C-NC	2.35	127.76	124.51
15	8	102	BCL	O2D-CGD-O1D	-2.35	119.25	123.84
17	L	504	UQ8	C12-C13-C14	-2.34	122.02	127.66
15	A	101	BCL	O2A-CGA-CBA	2.34	119.26	111.91
21	G	103	CRT	C32-C31-C30	-2.34	115.91	123.22
15	2	102	BCL	C2A-C1A-CHA	-2.34	119.77	123.86
15	L	502	BCL	O2A-CGA-O1A	-2.34	117.69	123.59
15	P	101	BCL	CAD-C3D-C4D	2.34	109.77	108.47
15	2	102	BCL	CHC-C1C-NC	2.34	127.74	124.51
21	B	103	CRT	C34-C33-C35	2.34	121.76	118.08
15	5	102	BCL	C1-O2A-CGA	2.34	122.57	116.44
15	X	102	BCL	C4B-CHC-C1C	-2.34	125.49	130.12
20	M	406	MQ8	C50-C48-C49	2.34	119.76	114.60
15	6	101	BCL	C2A-C1A-CHA	-2.34	119.78	123.86
15	2	102	BCL	O2A-CGA-CBA	2.33	119.23	111.91
15	B	102	BCL	C1-C2-C3	-2.33	122.01	126.04
15	E	102	BCL	O2D-CGD-O1D	-2.33	119.28	123.84
21	2	103	CRT	C36-C35-C33	-2.33	122.37	125.89
20	M	404	MQ8	C50-C48-C49	2.33	119.74	114.60
15	Z	102	BCL	O2D-CGD-O1D	-2.32	119.30	123.84
15	M	402	BCL	CAD-C3D-C4D	2.32	109.76	108.47
15	P	101	BCL	C1-O2A-CGA	2.32	122.53	116.44
21	E	103	CRT	C29-C28-C30	2.32	121.73	118.08
20	M	406	MQ8	C34-C33-C35	2.32	119.17	115.27
21	G	103	CRT	C13-C12-C11	2.32	121.73	118.08
15	5	102	BCL	C4B-CHC-C1C	-2.31	125.53	130.12
15	G	102	BCL	C1C-NC-C4C	-2.31	105.67	106.71
15	6	101	BCL	CHC-C1C-NC	2.31	127.71	124.51
15	6	101	BCL	O2A-CGA-CBA	2.31	119.16	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	E	103	CRT	C13-C12-C11	2.31	121.71	118.08
21	R	102	CRT	C9-C10-C11	-2.30	116.02	123.22
15	E	102	BCL	CAD-C3D-C4D	2.30	109.75	108.47
15	2	102	BCL	C4B-CHC-C1C	-2.30	125.56	130.12
17	L	512	UQ8	C25-C24-C26	2.30	119.69	114.60
15	Z	102	BCL	C1C-NC-C4C	-2.30	105.67	106.71
15	Z	102	BCL	C4B-CHC-C1C	-2.30	125.57	130.12
15	1	403	BCL	C1-C2-C3	-2.30	122.07	126.04
21	P	102	CRT	C8-C7-C9	-2.30	119.71	122.92
15	X	102	BCL	O2A-CGA-CBA	2.29	119.10	111.91
15	Z	102	BCL	CHB-C4A-NA	2.29	127.67	124.51
15	6	101	BCL	CAD-C3D-C4D	2.29	109.75	108.47
21	1	402	CRT	C36-C35-C33	-2.29	122.44	125.89
15	O	502	BCL	CHC-C1C-NC	2.28	127.67	124.51
20	M	406	MQ8	C29-C28-C30	2.28	119.11	115.27
15	V	102	BCL	C2A-C1A-CHA	-2.28	119.87	123.86
21	S	104	CRT	C21-C20-C19	-2.28	118.80	123.47
21	S	104	CRT	C8-C7-C9	-2.28	119.73	122.92
21	X	103	CRT	C21-C20-C19	-2.28	118.81	123.47
21	2	103	CRT	C21-C20-C19	-2.28	118.81	123.47
22	P	103	LMT	C1B-O1B-C4'	-2.28	112.33	117.96
22	E	101	LMT	C1B-O1B-C4'	-2.27	112.34	117.96
21	Q	102	CRT	C34-C33-C35	2.27	121.66	118.08
15	U	101	BCL	C2A-C1A-CHA	-2.27	119.89	123.86
15	X	102	BCL	C2A-C1A-CHA	-2.27	119.89	123.86
15	5	102	BCL	C2A-C1A-CHA	-2.27	119.89	123.86
14	L	501	PGV	C02-O01-C1	-2.27	112.21	117.79
21	P	102	CRT	C29-C28-C30	2.27	121.65	118.08
15	9	101	BCL	C2A-C1A-CHA	-2.27	119.90	123.86
21	7	102	CRT	C5-C6-C7	-2.26	122.47	125.89
21	6	102	CRT	C13-C12-C11	2.26	121.64	118.08
15	N	101	BCL	CHB-C4A-NA	2.26	127.64	124.51
21	M	405	CRT	C13-C12-C11	2.26	121.64	118.08
14	D	101	PGV	O03-C19-C20	2.25	118.98	111.91
15	Y	101	BCL	CHB-C4A-NA	2.25	127.63	124.51
15	L	508	BCL	C2A-C1A-CHA	-2.25	119.92	123.86
15	J	102	BCL	CAD-C3D-C4D	2.25	109.73	108.47
21	S	104	CRT	C27-C26-C25	-2.25	116.19	123.22
15	S	102	BCL	C2A-C1A-CHA	-2.25	119.92	123.86
15	V	102	BCL	O2A-CGA-O1A	-2.25	117.92	123.59
21	1	402	CRT	C29-C28-C30	2.25	121.62	118.08
15	7	101	BCL	C1C-NC-C4C	-2.24	105.70	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	M	405	CRT	C24-C23-C22	-2.24	119.78	122.92
14	M	409	PGV	O14-P-O13	2.24	119.45	110.68
15	I	102	BCL	C4A-NA-C1A	2.24	107.71	106.71
21	6	102	CRT	C31-C32-C33	-2.24	124.12	127.31
21	8	103	CRT	C9-C10-C11	-2.24	116.24	123.22
15	V	102	BCL	CAD-C3D-C4D	2.24	109.72	108.47
15	W	101	BCL	C2A-C1A-CHA	-2.23	119.95	123.86
17	L	505	UQ8	C46-C44-C45	2.23	119.54	114.60
15	0	102	BCL	O2D-CGD-O1D	-2.23	119.48	123.84
14	L	506	PGV	C02-O01-C1	-2.23	112.30	117.79
15	L	502	BCL	C2A-C1A-CHA	-2.23	119.96	123.86
18	L	510	CDL	OA8-CA7-C31	2.23	118.90	111.91
15	U	101	BCL	CAD-C3D-C4D	2.23	109.71	108.47
15	L	509	BCL	CHC-C1C-NC	2.22	127.59	124.51
15	S	102	BCL	C4B-CHC-C1C	-2.22	125.72	130.12
21	7	102	CRT	C29-C28-C30	2.22	121.58	118.08
10	C	504	HEC	CMC-C2C-C1C	-2.22	125.06	128.46
15	X	102	BCL	CED-O2D-CGD	2.22	120.95	115.94
21	2	103	CRT	C32-C31-C30	-2.21	116.31	123.22
22	X	101	LMT	C2'-C3'-C4'	2.21	114.72	109.68
15	J	102	BCL	C4B-CHC-C1C	-2.20	125.75	130.12
21	R	102	CRT	C18-C17-C16	2.20	121.55	118.08
21	R	102	CRT	C13-C12-C11	2.20	121.54	118.08
21	J	103	CRT	C8-C7-C6	2.20	121.54	118.08
21	J	103	CRT	C14-C15-C16	-2.20	116.36	123.22
20	M	404	MQ8	C24-C23-C25	2.20	118.97	115.27
15	3	101	BCL	C4A-NA-C1A	2.20	107.69	106.71
15	9	101	BCL	CAD-C3D-C4D	2.19	109.69	108.47
20	M	406	MQ8	C46-C47-C48	-2.19	120.26	127.75
15	V	102	BCL	CED-O2D-CGD	2.19	120.89	115.94
15	J	102	BCL	O2D-CGD-O1D	-2.19	119.56	123.84
15	7	101	BCL	C2A-C1A-CHA	-2.19	120.03	123.86
15	5	102	BCL	CAD-C3D-C4D	2.19	109.69	108.47
15	2	102	BCL	C1-O2A-CGA	2.18	122.17	116.44
15	X	102	BCL	O2D-CGD-O1D	-2.18	119.57	123.84
15	Q	101	BCL	C2A-C1A-CHA	-2.18	120.05	123.86
18	M	410	CDL	CB4-OB6-CB5	-2.18	112.43	117.79
15	O	502	BCL	C2A-C1A-CHA	-2.18	120.05	123.86
15	N	101	BCL	CHC-C1C-NC	2.18	127.52	124.51
21	2	103	CRT	C8-C7-C9	-2.17	119.88	122.92
15	P	101	BCL	C4-C3-C5	2.17	118.93	115.27
15	I	102	BCL	O2D-CGD-O1D	-2.17	119.59	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	U	101	BCL	CHB-C4A-NA	2.17	127.51	124.51
21	8	103	CRT	C21-C20-C19	-2.17	119.03	123.47
15	T	102	BCL	C4B-CHC-C1C	-2.17	125.82	130.12
15	B	102	BCL	CED-O2D-CGD	2.17	120.84	115.94
15	2	102	BCL	C1B-CHB-C4A	-2.16	125.83	130.12
15	0	102	BCL	CED-O2D-CGD	2.16	120.83	115.94
15	T	102	BCL	O2D-CGD-O1D	-2.16	119.62	123.84
21	6	102	CRT	C10-C9-C7	-2.16	124.23	127.31
18	S	101	CDL	CB4-OB6-CB5	-2.16	112.48	117.79
15	M	402	BCL	C4-C3-C2	-2.15	118.15	123.68
22	X	101	LMT	C1'-C2'-C3'	2.15	114.48	110.00
20	M	406	MQ8	C16-C17-C18	-2.15	122.47	127.66
20	M	404	MQ8	C2M-C2-C3	-2.15	120.89	124.40
21	N	102	CRT	C26-C27-C28	-2.15	124.24	127.31
21	M	405	CRT	C26-C27-C28	-2.15	124.25	127.31
15	W	101	BCL	CBA-CAA-C2A	-2.15	107.53	113.86
21	G	103	CRT	C26-C27-C28	-2.15	124.25	127.31
21	B	103	CRT	C29-C28-C30	2.15	121.46	118.08
15	V	102	BCL	C1C-NC-C4C	-2.14	105.74	106.71
15	4	102	BCL	O2D-CGD-O1D	-2.14	119.65	123.84
21	M	405	CRT	C34-C33-C35	2.14	121.45	118.08
21	4	103	CRT	C34-C33-C35	2.14	121.45	118.08
21	8	103	CRT	C13-C12-C11	2.14	121.45	118.08
21	Q	102	CRT	C14-C15-C16	-2.14	116.53	123.22
14	M	411	PGV	O01-C1-O02	-2.14	118.53	123.70
15	T	102	BCL	C1-C2-C3	-2.14	122.34	126.04
15	G	102	BCL	CED-O2D-CGD	2.13	120.77	115.94
15	J	102	BCL	C2A-C1A-CHA	-2.13	120.13	123.86
15	A	101	BCL	C4B-CHC-C1C	-2.13	125.89	130.12
15	R	101	BCL	O2D-CGD-O1D	-2.13	119.67	123.84
22	Z	101	LMT	C1-O1'-C1'	-2.13	110.31	113.84
15	B	102	BCL	CAD-C3D-C4D	2.13	109.66	108.47
21	G	103	CRT	C8-C7-C6	2.13	121.43	118.08
21	Q	102	CRT	C21-C20-C19	-2.13	119.12	123.47
15	7	101	BCL	CBA-CAA-C2A	-2.13	107.59	113.86
21	P	102	CRT	C27-C26-C25	-2.13	116.58	123.22
15	E	102	BCL	C4B-CHC-C1C	-2.12	125.91	130.12
15	O	502	BCL	CAD-C3D-C4D	2.12	109.65	108.47
21	G	103	CRT	C14-C15-C16	-2.12	116.60	123.22
15	P	101	BCL	CHC-C1C-NC	2.12	127.44	124.51
21	4	103	CRT	C10-C9-C7	-2.11	124.29	127.31
15	F	101	BCL	C1C-NC-C4C	-2.11	105.76	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	0	102	BCL	C1C-NC-C4C	-2.11	105.76	106.71
15	N	101	BCL	C2A-C1A-CHA	-2.11	120.17	123.86
21	J	103	CRT	C32-C31-C30	-2.11	116.63	123.22
15	4	102	BCL	CED-O2D-CGD	2.11	120.70	115.94
15	M	402	BCL	CHB-C4A-NA	2.11	127.42	124.51
15	8	102	BCL	C1C-NC-C4C	-2.10	105.76	106.71
15	B	102	BCL	CHB-C4A-NA	2.10	127.42	124.51
21	J	103	CRT	C13-C12-C11	2.10	121.39	118.08
18	D	102	CDL	CA6-CA4-CA3	-2.10	106.82	111.79
15	B	102	BCL	C2A-C1A-CHA	-2.10	120.19	123.86
15	G	102	BCL	O2D-CGD-O1D	-2.10	119.74	123.84
18	I	101	CDL	CA6-CA4-CA3	-2.09	106.84	111.79
17	L	505	UQ8	C4M-O4-C4	2.09	123.87	116.47
15	F	101	BCL	C2A-C1A-CHA	-2.09	120.21	123.86
15	Y	101	BCL	CAD-C3D-C4D	2.09	109.63	108.47
14	C	508	PGV	O01-C1-O02	-2.08	118.66	123.70
15	J	102	BCL	O2A-CGA-CBA	2.08	118.44	111.91
21	4	103	CRT	C26-C27-C28	-2.08	124.34	127.31
18	L	510	CDL	OB6-CB5-OB7	-2.08	118.68	123.70
21	6	102	CRT	C18-C17-C16	2.08	121.35	118.08
15	K	103	BCL	CAD-C3D-C4D	2.07	109.63	108.47
21	E	103	CRT	C34-C33-C35	2.07	121.34	118.08
15	D	103	BCL	CAD-C3D-C4D	2.07	109.62	108.47
15	N	101	BCL	O2A-CGA-O1A	-2.07	118.37	123.59
21	M	405	CRT	C8-C7-C6	2.07	121.33	118.08
15	B	102	BCL	C1C-NC-C4C	-2.06	105.78	106.71
17	L	505	UQ8	C7-C8-C9	-2.06	123.36	126.79
15	N	101	BCL	CAD-C3D-C4D	2.06	109.62	108.47
18	L	510	CDL	OA6-CA5-OA7	-2.06	118.88	122.96
15	B	102	BCL	O2D-CGD-O1D	-2.06	119.82	123.84
15	L	508	BCL	O1D-CGD-CBD	-2.06	120.28	124.48
17	L	505	UQ8	O4-C4-C5	2.05	123.51	116.56
21	1	402	CRT	C21-C20-C19	-2.05	119.27	123.47
15	5	102	BCL	CED-O2D-CGD	2.05	120.58	115.94
21	S	104	CRT	C34-C33-C35	2.05	121.31	118.08
21	R	102	CRT	C26-C25-C23	-2.05	120.65	126.42
15	R	101	BCL	C4B-CHC-C1C	-2.05	126.06	130.12
15	W	101	BCL	C4B-CHC-C1C	-2.05	126.06	130.12
18	H	301	CDL	OB8-CB7-OB9	-2.04	118.43	123.59
21	B	103	CRT	C8-C7-C9	-2.04	120.06	122.92
10	C	503	HEC	CBD-CAD-C3D	-2.04	109.14	112.62
15	A	101	BCL	C2A-C1A-CHA	-2.04	120.30	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	B	102	BCL	C1B-CHB-C4A	-2.04	126.08	130.12
21	R	102	CRT	C5-C6-C7	-2.04	122.81	125.89
21	6	102	CRT	C27-C26-C25	-2.04	116.86	123.22
15	B	102	BCL	O2A-CGA-O1A	-2.04	118.45	123.59
15	8	102	BCL	CED-O2D-CGD	2.04	120.54	115.94
15	4	102	BCL	O2A-CGA-O1A	-2.03	118.46	123.59
18	I	101	CDL	OA6-CA5-OA7	-2.03	118.79	123.70
15	E	102	BCL	O2A-CGA-O1A	-2.03	118.46	123.59
10	C	503	HEC	CMC-C2C-C1C	-2.03	125.35	128.46
17	L	505	UQ8	C42-C43-C44	-2.03	120.82	127.75
21	G	103	CRT	C34-C33-C35	2.03	121.27	118.08
14	L	506	PGV	O01-C1-O02	-2.03	118.81	123.70
15	L	509	BCL	C1-C2-C3	-2.02	122.55	126.04
21	7	102	CRT	C20-C21-C22	-2.02	119.33	123.47
15	9	101	BCL	O2A-CGA-O1A	-2.02	118.50	123.59
21	B	103	CRT	C21-C20-C19	-2.02	119.34	123.47
12	C	506	DGA	OG2-CG2-CG1	2.02	110.80	106.13
14	L	511	PGV	O03-C19-O04	-2.02	118.50	123.59
15	W	101	BCL	CAD-C3D-C4D	2.02	109.59	108.47
10	C	504	HEC	O2D-CGD-CBD	2.01	120.50	114.03
15	T	102	BCL	CED-O2D-CGD	2.01	120.49	115.94
21	N	102	CRT	C29-C28-C30	2.01	121.25	118.08
21	J	103	CRT	C15-C14-C12	-2.01	124.45	127.31
15	I	102	BCL	C1-C2-C3	-2.01	122.57	126.04
15	L	508	BCL	C4B-CHC-C1C	-2.00	126.15	130.12
22	H	304	LMT	C1B-O1B-C4'	-2.00	113.01	117.96
21	R	102	CRT	C31-C32-C33	-2.00	124.45	127.31

There are no chirality outliers.

All (1113) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	C	506	DGA	OG1-CG1-CG2-OG2
12	C	506	DGA	OG1-CG1-CG2-CG3
14	C	508	PGV	C03-O11-P-O12
14	C	508	PGV	C04-O12-P-O14
14	L	506	PGV	C03-O11-P-O13
14	L	506	PGV	O12-C04-C05-O05
14	L	507	PGV	C03-O11-P-O12
14	L	507	PGV	C03-O11-P-O13
14	L	511	PGV	C04-O12-P-O14
14	M	409	PGV	O02-C1-O01-C02

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Mol	Chain	Res	Type	Atoms
14	M	409	PGV	C2-C1-O01-C02
14	H	303	PGV	C03-O11-P-O12
14	H	303	PGV	C04-O12-P-O13
14	D	101	PGV	C04-O12-P-O13
14	D	101	PGV	C04-O12-P-O14
14	D	101	PGV	O12-C04-C05-C06
14	D	101	PGV	O12-C04-C05-O05
14	1	401	PGV	C03-O11-P-O14
14	1	401	PGV	O01-C02-C03-O11
15	L	502	BCL	C2-C3-C5-C6
15	L	502	BCL	C4-C3-C5-C6
15	M	402	BCL	C2-C3-C5-C6
15	M	402	BCL	C4-C3-C5-C6
15	A	101	BCL	C2C-C3C-CAC-CBC
15	A	101	BCL	C4C-C3C-CAC-CBC
15	B	102	BCL	C1A-C2A-CAA-CBA
15	B	102	BCL	C2C-C3C-CAC-CBC
15	B	102	BCL	C4C-C3C-CAC-CBC
15	B	102	BCL	C6-C7-C8-C9
15	D	103	BCL	C2C-C3C-CAC-CBC
15	D	103	BCL	C4C-C3C-CAC-CBC
15	D	103	BCL	C2-C3-C5-C6
15	D	103	BCL	C4-C3-C5-C6
15	E	102	BCL	C2C-C3C-CAC-CBC
15	E	102	BCL	C4C-C3C-CAC-CBC
15	F	101	BCL	C2-C3-C5-C6
15	F	101	BCL	C4-C3-C5-C6
15	J	102	BCL	C4-C3-C5-C6
15	K	103	BCL	C2C-C3C-CAC-CBC
15	K	103	BCL	CHA-CBD-CGD-O1D
15	N	101	BCL	C2C-C3C-CAC-CBC
15	N	101	BCL	C4C-C3C-CAC-CBC
15	O	502	BCL	C4C-C3C-CAC-CBC
15	O	502	BCL	CHA-CBD-CGD-O1D
15	O	502	BCL	C11-C10-C8-C9
15	P	101	BCL	C4C-C3C-CAC-CBC
15	Q	101	BCL	C2C-C3C-CAC-CBC
15	Q	101	BCL	C4C-C3C-CAC-CBC
15	Q	101	BCL	C4-C3-C5-C6
15	R	101	BCL	C1A-C2A-CAA-CBA
15	R	101	BCL	C4C-C3C-CAC-CBC
15	R	101	BCL	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
15	R	101	BCL	C4-C3-C5-C6
15	S	102	BCL	C2C-C3C-CAC-CBC
15	S	102	BCL	C4C-C3C-CAC-CBC
15	T	102	BCL	C3A-C2A-CAA-CBA
15	U	101	BCL	C2C-C3C-CAC-CBC
15	U	101	BCL	C4C-C3C-CAC-CBC
15	U	101	BCL	C2-C3-C5-C6
15	U	101	BCL	C4-C3-C5-C6
15	V	102	BCL	C4C-C3C-CAC-CBC
15	V	102	BCL	C11-C10-C8-C7
15	W	101	BCL	C2C-C3C-CAC-CBC
15	W	101	BCL	C4C-C3C-CAC-CBC
15	W	101	BCL	CHA-CBD-CGD-O1D
15	W	101	BCL	CHA-CBD-CGD-O2D
15	W	101	BCL	C4-C3-C5-C6
15	X	102	BCL	C1A-C2A-CAA-CBA
15	Z	102	BCL	C1A-C2A-CAA-CBA
15	Z	102	BCL	C2C-C3C-CAC-CBC
15	Z	102	BCL	C4C-C3C-CAC-CBC
15	2	102	BCL	C2C-C3C-CAC-CBC
15	2	102	BCL	C4C-C3C-CAC-CBC
15	3	101	BCL	C3A-C2A-CAA-CBA
15	4	102	BCL	C4-C3-C5-C6
15	5	102	BCL	C2-C3-C5-C6
15	5	102	BCL	C4-C3-C5-C6
15	6	101	BCL	C2C-C3C-CAC-CBC
15	6	101	BCL	C4C-C3C-CAC-CBC
15	7	101	BCL	C2C-C3C-CAC-CBC
15	7	101	BCL	C4C-C3C-CAC-CBC
15	8	102	BCL	C4C-C3C-CAC-CBC
15	9	101	BCL	C4C-C3C-CAC-CBC
15	0	102	BCL	C1A-C2A-CAA-CBA
15	0	102	BCL	C3A-C2A-CAA-CBA
15	0	102	BCL	C2-C3-C5-C6
15	0	102	BCL	C4-C3-C5-C6
17	L	504	UQ8	C19-C21-C22-C23
17	L	504	UQ8	C14-C16-C17-C18
17	L	505	UQ8	C35-C34-C36-C37
17	L	505	UQ8	C33-C34-C36-C37
17	L	512	UQ8	C19-C21-C22-C23
18	L	510	CDL	CA3-OA5-PA1-OA3
18	L	510	CDL	CB2-OB2-PB2-OB3

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Mol	Chain	Res	Type	Atoms
18	L	510	CDL	CB2-OB2-PB2-OB4
18	L	510	CDL	CB2-OB2-PB2-OB5
18	L	510	CDL	C51-CB5-OB6-CB4
18	M	408	CDL	CA2-OA2-PA1-OA3
18	M	408	CDL	CA2-OA2-PA1-OA4
18	M	408	CDL	CA3-OA5-PA1-OA2
18	M	408	CDL	CA3-OA5-PA1-OA3
18	M	408	CDL	CA3-OA5-PA1-OA4
18	M	408	CDL	CB2-OB2-PB2-OB3
18	M	408	CDL	CB2-OB2-PB2-OB5
18	M	410	CDL	CA2-OA2-PA1-OA4
18	M	410	CDL	CB2-OB2-PB2-OB5
18	H	301	CDL	CA2-OA2-PA1-OA4
18	H	301	CDL	C11-CA5-OA6-CA4
18	H	302	CDL	CA2-OA2-PA1-OA3
18	H	302	CDL	CA2-OA2-PA1-OA5
18	D	102	CDL	CA2-C1-CB2-OB2
18	D	102	CDL	CA2-OA2-PA1-OA3
18	D	102	CDL	CA3-OA5-PA1-OA2
18	D	102	CDL	CA3-OA5-PA1-OA3
18	D	102	CDL	CA3-OA5-PA1-OA4
18	D	102	CDL	C11-CA5-OA6-CA4
18	D	102	CDL	CB2-OB2-PB2-OB3
18	D	102	CDL	CB3-OB5-PB2-OB2
18	D	102	CDL	CB3-OB5-PB2-OB3
18	I	101	CDL	CA2-OA2-PA1-OA3
18	I	101	CDL	CA3-OA5-PA1-OA3
18	I	101	CDL	C11-CA5-OA6-CA4
18	S	101	CDL	CA2-OA2-PA1-OA3
18	S	101	CDL	CB3-OB5-PB2-OB2
18	S	101	CDL	CB3-OB5-PB2-OB3
18	S	101	CDL	CB3-OB5-PB2-OB4
20	M	404	MQ8	C37-C38-C40-C41
20	M	404	MQ8	C39-C38-C40-C41
20	M	406	MQ8	C33-C35-C36-C37
20	M	406	MQ8	C39-C38-C40-C41
21	B	103	CRT	O1-C1-C4-C5
21	B	103	CRT	C2-C1-C4-C5
21	B	103	CRT	C3-C1-C4-C5
21	B	103	CRT	C10-C11-C12-C13
21	B	103	CRT	C15-C16-C17-C18
21	B	103	CRT	C15-C16-C17-C19

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Mol	Chain	Res	Type	Atoms
21	G	103	CRT	C2-C1-C4-C5
21	G	103	CRT	C3-C1-C4-C5
21	J	103	CRT	C3-C1-O1-C1M
21	N	102	CRT	C15-C16-C17-C18
21	N	102	CRT	C15-C16-C17-C19
21	P	102	CRT	C15-C16-C17-C18
21	Q	102	CRT	C10-C11-C12-C13
21	R	102	CRT	C22-C23-C25-C26
21	R	102	CRT	C24-C23-C25-C26
21	S	104	CRT	O1-C1-C4-C5
21	S	104	CRT	C2-C1-C4-C5
21	S	104	CRT	C3-C1-C4-C5
21	S	104	CRT	C15-C16-C17-C18
21	S	104	CRT	C15-C16-C17-C19
21	S	104	CRT	C36-C37-C38-C39
21	S	104	CRT	C36-C37-C38-C40
21	X	103	CRT	C15-C16-C17-C18
21	X	103	CRT	C15-C16-C17-C19
21	1	402	CRT	O1-C1-C4-C5
21	1	402	CRT	C2-C1-C4-C5
21	1	402	CRT	C3-C1-C4-C5
21	1	402	CRT	C32-C33-C35-C36
21	1	402	CRT	C34-C33-C35-C36
21	1	402	CRT	C36-C37-C38-C39
21	1	402	CRT	C36-C37-C38-C40
21	2	103	CRT	C10-C11-C12-C13
21	2	103	CRT	C36-C37-C38-C39
21	2	103	CRT	C36-C37-C38-C40
21	6	102	CRT	C2-C1-C4-C5
21	6	102	CRT	C34-C33-C35-C36
21	7	102	CRT	C10-C11-C12-C13
21	7	102	CRT	C10-C11-C12-C14
21	7	102	CRT	C15-C16-C17-C18
21	7	102	CRT	C15-C16-C17-C19
21	8	103	CRT	C1-C4-C5-C6
21	8	103	CRT	C5-C6-C7-C8
22	P	103	LMT	O5'-C1'-O1'-C1
15	M	402	BCL	CBD-CGD-O2D-CED
15	0	102	BCL	O1A-CGA-O2A-C1
15	T	102	BCL	O1A-CGA-O2A-C1
12	C	506	DGA	CB2-CB1-OG2-CG2
14	5	101	PGV	O02-C1-O01-C02

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Mol	Chain	Res	Type	Atoms
18	L	510	CDL	OB7-CB5-OB6-CB4
18	H	301	CDL	OA7-CA5-OA6-CA4
18	D	102	CDL	OA7-CA5-OA6-CA4
15	M	402	BCL	C3-C5-C6-C7
15	D	103	BCL	C3-C5-C6-C7
15	Q	101	BCL	C3-C5-C6-C7
14	1	401	PGV	C20-C19-O03-C01
15	K	103	BCL	CBA-CGA-O2A-C1
15	0	102	BCL	CBA-CGA-O2A-C1
14	5	101	PGV	C2-C1-O01-C02
15	P	101	BCL	C4-C3-C5-C6
15	J	102	BCL	C2-C3-C5-C6
15	W	101	BCL	C2-C3-C5-C6
20	M	406	MQ8	C37-C38-C40-C41
15	P	101	BCL	CBD-CGD-O2D-CED
15	J	102	BCL	C3-C5-C6-C7
15	P	101	BCL	C3-C5-C6-C7
15	T	102	BCL	C3-C5-C6-C7
15	L	509	BCL	CBA-CGA-O2A-C1
15	T	102	BCL	CBA-CGA-O2A-C1
18	I	101	CDL	OA7-CA5-OA6-CA4
15	L	509	BCL	O1A-CGA-O2A-C1
15	5	102	BCL	CBD-CGD-O2D-CED
18	H	301	CDL	O1-C1-CA2-OA2
18	H	301	CDL	O1-C1-CB2-OB2
18	D	102	CDL	O1-C1-CB2-OB2
15	G	102	BCL	C3-C5-C6-C7
14	1	401	PGV	O04-C19-O03-C01
15	K	103	BCL	O1A-CGA-O2A-C1
15	M	402	BCL	O1D-CGD-O2D-CED
22	N	103	LMT	O5'-C5'-C6'-O6'
22	Z	101	LMT	O5'-C5'-C6'-O6'
15	Q	101	BCL	C5-C6-C7-C8
15	I	102	BCL	C5-C6-C7-C8
15	I	102	BCL	C4-C3-C5-C6
16	M	403	BPH	C4-C3-C5-C6
17	L	505	UQ8	C40-C39-C41-C42
17	L	505	UQ8	C12-C11-C9-C10
15	I	102	BCL	C2-C3-C5-C6
15	Q	101	BCL	C2-C3-C5-C6
15	4	102	BCL	C2-C3-C5-C6
16	M	403	BPH	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
17	L	505	UQ8	C38-C39-C41-C42
17	L	505	UQ8	C12-C11-C9-C8
15	J	102	BCL	CBD-CGD-O2D-CED
15	N	101	BCL	C2A-CAA-CBA-CGA
15	5	102	BCL	C2A-CAA-CBA-CGA
22	G	101	LMT	O5'-C1'-O1'-C1
17	L	504	UQ8	C9-C11-C12-C13
17	L	505	UQ8	C29-C31-C32-C33
20	M	406	MQ8	C38-C40-C41-C42
15	M	402	BCL	CBA-CGA-O2A-C1
18	S	101	CDL	C31-CA7-OA8-CA6
14	M	411	PGV	C2-C1-O01-C02
14	L	506	PGV	O12-C04-C05-C06
18	S	101	CDL	OA9-CA7-OA8-CA6
15	E	102	BCL	C3-C5-C6-C7
15	8	102	BCL	C3-C5-C6-C7
15	1	403	BCL	CBA-CGA-O2A-C1
15	4	102	BCL	CBA-CGA-O2A-C1
15	B	102	BCL	C8-C10-C11-C12
18	L	510	CDL	OA5-CA3-CA4-OA6
15	F	101	BCL	C8-C10-C11-C12
15	K	103	BCL	C15-C16-C17-C18
18	L	510	CDL	O1-C1-CB2-OB2
18	D	102	CDL	O1-C1-CA2-OA2
15	P	101	BCL	C2-C3-C5-C6
15	L	509	BCL	C11-C10-C8-C9
15	M	402	BCL	C11-C10-C8-C9
15	A	101	BCL	C6-C7-C8-C9
15	D	103	BCL	C11-C10-C8-C9
15	E	102	BCL	C6-C7-C8-C9
15	K	103	BCL	C11-C10-C8-C9
15	N	101	BCL	C6-C7-C8-C9
15	O	502	BCL	C6-C7-C8-C9
15	P	101	BCL	C11-C12-C13-C14
15	R	101	BCL	C6-C7-C8-C9
15	S	102	BCL	C6-C7-C8-C9
15	T	102	BCL	C11-C10-C8-C9
15	U	101	BCL	C6-C7-C8-C9
15	V	102	BCL	C6-C7-C8-C9
15	V	102	BCL	C11-C12-C13-C14
15	W	101	BCL	C6-C7-C8-C9
15	Y	101	BCL	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
15	Z	102	BCL	C6-C7-C8-C9
15	2	102	BCL	C11-C10-C8-C9
15	6	101	BCL	C11-C10-C8-C9
15	6	101	BCL	C11-C12-C13-C14
15	0	102	BCL	C11-C10-C8-C9
12	C	506	DGA	OB1-CB1-OG2-CG2
15	E	102	BCL	C5-C6-C7-C8
15	F	101	BCL	C2A-CAA-CBA-CGA
21	M	405	CRT	C24-C23-C25-C26
21	B	103	CRT	C24-C23-C25-C26
21	N	102	CRT	C5-C6-C7-C8
21	X	103	CRT	C10-C11-C12-C13
21	1	402	CRT	C10-C11-C12-C13
14	M	407	PGV	C19-C20-C21-C22
18	I	101	CDL	CA7-C31-C32-C33
22	V	101	LMT	C5'-C4'-O1B-C1B
22	K	102	LMT	O5'-C5'-C6'-O6'
15	L	509	BCL	C3-C5-C6-C7
15	G	102	BCL	CBD-CGD-O2D-CED
15	G	102	BCL	C8-C10-C11-C12
15	P	101	BCL	C10-C11-C12-C13
15	T	102	BCL	C5-C6-C7-C8
15	1	403	BCL	C10-C11-C12-C13
15	4	102	BCL	C15-C16-C17-C18
15	6	101	BCL	C15-C16-C17-C18
15	8	102	BCL	C10-C11-C12-C13
14	5	101	PGV	C19-C20-C21-C22
18	M	410	CDL	CB7-C71-C72-C73
15	4	102	BCL	C10-C11-C12-C13
15	6	101	BCL	C10-C11-C12-C13
22	V	101	LMT	C3'-C4'-O1B-C1B
15	L	509	BCL	C2-C1-O2A-CGA
15	2	102	BCL	C15-C16-C17-C18
15	B	102	BCL	C6-C7-C8-C10
15	P	101	BCL	C11-C10-C8-C7
15	R	101	BCL	C6-C7-C8-C10
15	1	403	BCL	C11-C10-C8-C7
15	7	101	BCL	C11-C10-C8-C7
15	4	102	BCL	O1A-CGA-O2A-C1
15	M	402	BCL	C2A-CAA-CBA-CGA
15	L	502	BCL	C10-C11-C12-C13
15	L	509	BCL	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
15	2	102	BCL	C5-C6-C7-C8
15	Q	101	BCL	C13-C15-C16-C17
17	L	505	UQ8	C24-C26-C27-C28
17	L	505	UQ8	C14-C16-C17-C18
20	M	406	MQ8	C28-C30-C31-C32
14	M	411	PGV	O02-C1-O01-C02
15	T	102	BCL	C13-C15-C16-C17
15	V	102	BCL	C13-C15-C16-C17
15	8	102	BCL	C5-C6-C7-C8
15	D	103	BCL	CBA-CGA-O2A-C1
15	M	402	BCL	O1A-CGA-O2A-C1
15	1	403	BCL	O1A-CGA-O2A-C1
15	L	508	BCL	C13-C15-C16-C17
15	N	101	BCL	C13-C15-C16-C17
15	S	102	BCL	C15-C16-C17-C18
15	Y	101	BCL	C5-C6-C7-C8
15	8	102	BCL	C13-C15-C16-C17
18	M	408	CDL	C11-CA5-OA6-CA4
15	T	102	BCL	C8-C10-C11-C12
15	Z	102	BCL	C13-C15-C16-C17
14	C	508	PGV	C04-O12-P-O11
14	D	101	PGV	C03-O11-P-O12
14	D	101	PGV	C04-O12-P-O11
14	1	401	PGV	C03-O11-P-O12
18	L	510	CDL	CB3-OB5-PB2-OB2
18	M	408	CDL	CA2-OA2-PA1-OA5
18	M	410	CDL	CA2-OA2-PA1-OA5
18	M	410	CDL	CB3-OB5-PB2-OB2
18	H	301	CDL	CA3-OA5-PA1-OA2
18	H	301	CDL	CB2-OB2-PB2-OB5
18	H	302	CDL	CB2-OB2-PB2-OB5
18	D	102	CDL	C31-CA7-OA8-CA6
15	L	509	BCL	C8-C10-C11-C12
18	H	301	CDL	CA2-C1-CB2-OB2
15	E	102	BCL	C8-C10-C11-C12
15	Q	101	BCL	C15-C16-C17-C18
15	W	101	BCL	C10-C11-C12-C13
15	Z	102	BCL	C2A-CAA-CBA-CGA
15	J	102	BCL	C16-C17-C18-C19
15	P	101	BCL	C16-C17-C18-C19
15	W	101	BCL	C16-C17-C18-C19
15	I	102	BCL	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
15	R	101	BCL	CBA-CGA-O2A-C1
15	X	102	BCL	C8-C10-C11-C12
14	L	511	PGV	C2-C1-O01-C02
14	L	507	PGV	C24-C25-C26-C27
18	L	510	CDL	C62-C63-C64-C65
14	M	411	PGV	C20-C19-O03-C01
18	M	410	CDL	C36-C37-C38-C39
18	S	101	CDL	C35-C36-C37-C38
14	L	511	PGV	O02-C1-O01-C02
18	M	408	CDL	OA7-CA5-OA6-CA4
18	L	510	CDL	C77-C78-C79-C80
18	S	101	CDL	C71-C72-C73-C74
15	A	101	BCL	C5-C6-C7-C8
14	L	507	PGV	C1-C2-C3-C4
14	L	507	PGV	C19-C20-C21-C22
15	P	101	BCL	O1D-CGD-O2D-CED
15	Y	101	BCL	CBA-CGA-O2A-C1
14	L	507	PGV	C25-C26-C27-C28
15	L	502	BCL	C8-C10-C11-C12
15	E	102	BCL	C16-C17-C18-C19
15	5	102	BCL	C16-C17-C18-C19
15	9	101	BCL	C16-C17-C18-C19
17	L	505	UQ8	C25-C24-C26-C27
15	Y	101	BCL	C11-C10-C8-C9
16	M	403	BPH	C6-C7-C8-C9
14	M	411	PGV	C23-C24-C25-C26
15	V	102	BCL	C2A-CAA-CBA-CGA
18	H	301	CDL	C15-C16-C17-C18
14	D	101	PGV	C04-C05-C06-O06
21	6	102	CRT	C32-C33-C35-C36
21	8	103	CRT	C5-C6-C7-C9
14	1	401	PGV	O02-C1-O01-C02
15	L	508	BCL	C15-C16-C17-C18
15	N	101	BCL	C5-C6-C7-C8
14	1	401	PGV	C2-C1-O01-C02
18	M	410	CDL	C11-CA5-OA6-CA4
18	M	410	CDL	C71-C72-C73-C74
18	H	301	CDL	C58-C59-C60-C61
14	H	303	PGV	C22-C23-C24-C25
15	J	102	BCL	C16-C17-C18-C20
15	P	101	BCL	C16-C17-C18-C20
15	W	101	BCL	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
15	L	509	BCL	CBD-CGD-O2D-CED
15	D	103	BCL	O1A-CGA-O2A-C1
18	M	410	CDL	C52-C53-C54-C55
15	6	101	BCL	C3-C5-C6-C7
14	M	409	PGV	C22-C23-C24-C25
15	5	102	BCL	O1D-CGD-O2D-CED
10	C	502	HEC	C3D-CAD-CBD-CGD
15	M	402	BCL	C3A-C2A-CAA-CBA
15	B	102	BCL	C3A-C2A-CAA-CBA
15	I	102	BCL	C3A-C2A-CAA-CBA
15	R	101	BCL	C3A-C2A-CAA-CBA
15	X	102	BCL	C3A-C2A-CAA-CBA
15	Y	101	BCL	C3A-C2A-CAA-CBA
15	Z	102	BCL	C3A-C2A-CAA-CBA
15	4	102	BCL	C3A-C2A-CAA-CBA
22	Z	101	LMT	C2-C1-O1'-C1'
22	8	101	LMT	C2-C1-O1'-C1'
14	5	101	PGV	C28-C29-C30-C31
15	5	102	BCL	C16-C17-C18-C20
18	L	510	CDL	O1-C1-CA2-OA2
18	S	101	CDL	O1-C1-CB2-OB2
15	E	102	BCL	C15-C16-C17-C18
15	3	101	BCL	C8-C10-C11-C12
15	K	103	BCL	C3-C5-C6-C7
15	W	101	BCL	C3-C5-C6-C7
15	R	101	BCL	O1A-CGA-O2A-C1
14	M	407	PGV	C26-C27-C28-C29
18	M	410	CDL	C34-C35-C36-C37
18	M	410	CDL	OA7-CA5-OA6-CA4
15	L	508	BCL	C5-C6-C7-C8
14	M	411	PGV	O04-C19-O03-C01
15	Y	101	BCL	O1A-CGA-O2A-C1
22	N	103	LMT	C4'-C5'-C6'-O6'
22	T	101	LMT	C2-C3-C4-C5
22	4	101	LMT	C5-C6-C7-C8
15	A	101	BCL	C10-C11-C12-C13
15	Y	101	BCL	C15-C16-C17-C18
15	5	102	BCL	C13-C15-C16-C17
22	Z	101	LMT	C1-C2-C3-C4
15	O	502	BCL	C6-C7-C8-C10
15	Q	101	BCL	C11-C12-C13-C15
15	U	101	BCL	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
15	U	101	BCL	C11-C12-C13-C15
15	V	102	BCL	C11-C12-C13-C15
15	Y	101	BCL	C11-C10-C8-C7
15	Z	102	BCL	C6-C7-C8-C10
15	5	102	BCL	C11-C10-C8-C7
15	6	101	BCL	C11-C12-C13-C15
16	M	403	BPH	C6-C7-C8-C10
17	L	505	UQ8	C13-C14-C16-C17
15	3	101	BCL	C15-C16-C17-C18
17	L	505	UQ8	C3-C4-O4-C4M
15	5	102	BCL	CBA-CGA-O2A-C1
15	B	102	BCL	C2A-CAA-CBA-CGA
15	E	102	BCL	C2A-CAA-CBA-CGA
15	6	101	BCL	C2A-CAA-CBA-CGA
15	8	102	BCL	C2A-CAA-CBA-CGA
15	B	102	BCL	C5-C6-C7-C8
15	P	101	BCL	C5-C6-C7-C8
15	J	102	BCL	O1D-CGD-O2D-CED
22	P	103	LMT	C3-C4-C5-C6
15	K	103	BCL	C5-C6-C7-C8
22	H	304	LMT	C2-C3-C4-C5
22	G	101	LMT	O5'-C5'-C6'-O6'
15	2	102	BCL	C16-C17-C18-C19
15	D	103	BCL	C8-C10-C11-C12
15	V	102	BCL	C8-C10-C11-C12
22	N	103	LMT	C2-C3-C4-C5
14	H	303	PGV	C1-C2-C3-C4
22	Z	101	LMT	C4'-C5'-C6'-O6'
15	9	101	BCL	C5-C6-C7-C8
15	K	103	BCL	CBD-CGD-O2D-CED
15	X	102	BCL	CBD-CGD-O2D-CED
18	S	101	CDL	O1-C1-CA2-OA2
15	E	102	BCL	C16-C17-C18-C20
22	0	101	LMT	O5B-C5B-C6B-O6B
15	5	102	BCL	C10-C11-C12-C13
17	L	505	UQ8	C15-C14-C16-C17
15	L	508	BCL	C6-C7-C8-C9
15	U	101	BCL	C11-C12-C13-C14
15	Y	101	BCL	C6-C7-C8-C9
15	5	102	BCL	C11-C10-C8-C9
15	7	101	BCL	C11-C10-C8-C9
18	D	102	CDL	OA9-CA7-OA8-CA6

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Mol	Chain	Res	Type	Atoms
15	J	102	BCL	C2A-CAA-CBA-CGA
15	3	101	BCL	C2A-CAA-CBA-CGA
22	Z	101	LMT	O5B-C5B-C6B-O6B
15	9	101	BCL	CBA-CGA-O2A-C1
21	S	104	CRT	C10-C11-C12-C13
21	4	103	CRT	C15-C16-C17-C18
15	G	102	BCL	O1D-CGD-O2D-CED
15	O	502	BCL	C15-C16-C17-C18
21	P	102	CRT	C15-C16-C17-C19
21	Q	102	CRT	C10-C11-C12-C14
21	2	103	CRT	C10-C11-C12-C14
15	L	508	BCL	C1A-C2A-CAA-CBA
15	M	402	BCL	C1A-C2A-CAA-CBA
15	T	102	BCL	C1A-C2A-CAA-CBA
15	Y	101	BCL	C1A-C2A-CAA-CBA
15	3	101	BCL	C1A-C2A-CAA-CBA
15	4	102	BCL	C1A-C2A-CAA-CBA
15	2	102	BCL	C16-C17-C18-C20
15	9	101	BCL	C16-C17-C18-C20
18	M	410	CDL	C16-C17-C18-C19
15	O	502	BCL	C8-C10-C11-C12
14	1	401	PGV	C3-C4-C5-C6
15	1	403	BCL	C8-C10-C11-C12
14	5	101	PGV	C01-C02-C03-O11
18	L	510	CDL	OA5-CA3-CA4-CA6
18	H	301	CDL	OA5-CA3-CA4-CA6
18	M	410	CDL	CA5-C11-C12-C13
18	M	410	CDL	C12-C13-C14-C15
15	M	402	BCL	C15-C16-C17-C18
15	4	102	BCL	C13-C15-C16-C17
22	2	101	LMT	O5B-C5B-C6B-O6B
21	M	405	CRT	C1-C4-C5-C6
14	5	101	PGV	C20-C19-O03-C01
15	U	101	BCL	CBA-CGA-O2A-C1
15	O	502	BCL	C2C-C3C-CAC-CBC
15	P	101	BCL	C2C-C3C-CAC-CBC
15	R	101	BCL	C2C-C3C-CAC-CBC
15	V	102	BCL	C2C-C3C-CAC-CBC
15	8	102	BCL	C2C-C3C-CAC-CBC
15	9	101	BCL	C2C-C3C-CAC-CBC
17	L	505	UQ8	C23-C24-C26-C27
22	V	101	LMT	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
15	5	102	BCL	O1A-CGA-O2A-C1
22	J	104	LMT	C6-C7-C8-C9
15	B	102	BCL	C10-C11-C12-C13
15	V	102	BCL	C15-C16-C17-C18
15	O	502	BCL	C16-C17-C18-C19
15	Z	102	BCL	C16-C17-C18-C19
14	L	507	PGV	O03-C01-C02-C03
14	H	303	PGV	O03-C01-C02-C03
18	L	510	CDL	CA3-CA4-CA6-OA8
18	H	301	CDL	CA3-CA4-CA6-OA8
18	H	302	CDL	CB3-CB4-CB6-OB8
20	M	406	MQ8	C12-C11-C3-C2
22	E	101	LMT	O1'-C1-C2-C3
22	T	101	LMT	O5B-C5B-C6B-O6B
22	4	101	LMT	O5'-C5'-C6'-O6'
14	L	506	PGV	C2-C1-O01-C02
18	M	410	CDL	C41-C42-C43-C44
22	N	103	LMT	O5B-C5B-C6B-O6B
15	V	102	BCL	C4-C3-C5-C6
17	L	512	UQ8	C20-C19-C21-C22
22	B	101	LMT	O5B-C5B-C6B-O6B
22	X	101	LMT	O5'-C5'-C6'-O6'
18	D	102	CDL	C57-C58-C59-C60
15	P	101	BCL	C8-C10-C11-C12
15	U	101	BCL	C13-C15-C16-C17
15	Z	102	BCL	C15-C16-C17-C18
16	L	503	BPH	C5-C6-C7-C8
20	M	406	MQ8	C12-C11-C3-C4
14	5	101	PGV	C01-C02-O01-C1
22	V	101	LMT	O5'-C5'-C6'-O6'
15	G	102	BCL	C2-C1-O2A-CGA
22	E	101	LMT	O5'-C5'-C6'-O6'
18	M	410	CDL	C37-C38-C39-C40
18	M	408	CDL	C31-CA7-OA8-CA6
15	U	101	BCL	O1A-CGA-O2A-C1
15	9	101	BCL	O1A-CGA-O2A-C1
21	P	102	CRT	C2-C1-O1-C1M
14	L	511	PGV	O03-C01-C02-O01
14	H	303	PGV	O03-C01-C02-O01
14	D	101	PGV	C3-C4-C5-C6
21	M	405	CRT	C36-C37-C38-C39
21	M	405	CRT	C36-C37-C38-C40

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Mol	Chain	Res	Type	Atoms
21	E	103	CRT	C3-C1-C4-C5
21	E	103	CRT	C36-C37-C38-C39
21	E	103	CRT	C36-C37-C38-C40
21	G	103	CRT	C36-C37-C38-C39
21	P	102	CRT	C36-C37-C38-C39
21	P	102	CRT	C36-C37-C38-C40
21	Q	102	CRT	C2-C1-C4-C5
21	Q	102	CRT	C3-C1-C4-C5
21	4	103	CRT	C36-C37-C38-C39
21	6	102	CRT	C3-C1-C4-C5
21	6	102	CRT	C36-C37-C38-C39
18	D	102	CDL	C55-C56-C57-C58
15	X	102	BCL	C4-C3-C5-C6
15	Y	101	BCL	C13-C15-C16-C17
15	L	508	BCL	C11-C10-C8-C7
15	A	101	BCL	C6-C7-C8-C10
15	E	102	BCL	C6-C7-C8-C10
15	E	102	BCL	C11-C10-C8-C7
15	F	101	BCL	C11-C10-C8-C7
15	Q	101	BCL	C11-C10-C8-C7
15	S	102	BCL	C6-C7-C8-C10
15	V	102	BCL	C2-C3-C5-C6
15	W	101	BCL	C6-C7-C8-C10
15	X	102	BCL	C2-C3-C5-C6
15	Y	101	BCL	C6-C7-C8-C10
15	1	403	BCL	C6-C7-C8-C10
15	4	102	BCL	C11-C10-C8-C7
16	L	503	BPH	C12-C13-C15-C16
15	M	402	BCL	C6-C7-C8-C9
15	A	101	BCL	C11-C10-C8-C9
15	B	102	BCL	C11-C10-C8-C9
15	F	101	BCL	C11-C10-C8-C9
15	G	102	BCL	C14-C13-C15-C16
15	I	102	BCL	C11-C10-C8-C9
15	Q	101	BCL	C11-C10-C8-C9
15	R	101	BCL	C11-C10-C8-C9
15	X	102	BCL	C6-C7-C8-C9
15	1	403	BCL	C6-C7-C8-C9
15	4	102	BCL	C11-C10-C8-C9
15	9	101	BCL	C11-C10-C8-C9
16	L	503	BPH	C14-C13-C15-C16
22	8	101	LMT	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
15	I	102	BCL	C15-C16-C17-C18
15	4	102	BCL	C5-C6-C7-C8
15	Y	101	BCL	C2A-CAA-CBA-CGA
21	E	103	CRT	C36-C37-C38-O2
21	G	103	CRT	O1-C1-C4-C5
21	P	102	CRT	C36-C37-C38-O2
21	Q	102	CRT	O1-C1-C4-C5
21	1	402	CRT	C36-C37-C38-O2
21	1	402	CRT	C15-C16-C17-C18
15	Z	102	BCL	C16-C17-C18-C20
21	B	103	CRT	C22-C23-C25-C26
24	K	101	LDA	N1-C1-C2-C3
15	6	101	BCL	C5-C6-C7-C8
12	C	506	DGA	CA2-CA1-OG1-CG1
15	S	102	BCL	CBA-CGA-O2A-C1
18	H	301	CDL	C71-CB7-OB8-CB6
12	C	506	DGA	CG3-CG2-OG2-CB1
15	W	101	BCL	C13-C15-C16-C17
14	1	401	PGV	C01-C02-C03-O11
18	L	510	CDL	C58-C59-C60-C61
14	5	101	PGV	O04-C19-O03-C01
15	G	102	BCL	C5-C6-C7-C8
15	V	102	BCL	C10-C11-C12-C13
18	M	410	CDL	C15-C16-C17-C18
22	V	101	LMT	C2-C1-O1'-C1'
15	Y	101	BCL	C10-C11-C12-C13
18	M	408	CDL	OA9-CA7-OA8-CA6
18	M	410	CDL	C71-CB7-OB8-CB6
14	C	508	PGV	O03-C01-C02-C03
14	L	506	PGV	O03-C01-C02-C03
14	L	506	PGV	O02-C1-O01-C02
18	H	301	CDL	C55-C56-C57-C58
16	M	403	BPH	O2A-C1-C2-C3
14	M	407	PGV	C29-C30-C31-C32
15	8	102	BCL	C4-C3-C5-C6
20	M	404	MQ8	C24-C23-C25-C26
15	O	502	BCL	C16-C17-C18-C20
15	L	509	BCL	O1D-CGD-O2D-CED
15	K	103	BCL	O1D-CGD-O2D-CED
22	4	101	LMT	C6-C7-C8-C9
24	K	101	LDA	C4-C5-C6-C7
15	X	102	BCL	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
15	2	102	BCL	C13-C15-C16-C17
18	D	102	CDL	OB5-CB3-CB4-OB6
14	M	409	PGV	C24-C25-C26-C27
22	K	102	LMT	C4'-C5'-C6'-O6'
14	C	508	PGV	O03-C01-C02-O01
18	L	510	CDL	OA6-CA4-CA6-OA8
18	H	301	CDL	OB6-CB4-CB6-OB8
18	D	102	CDL	OB6-CB4-CB6-OB8
18	H	301	CDL	CB2-C1-CA2-OA2
15	S	102	BCL	C2-C1-O2A-CGA
15	L	502	BCL	C6-C7-C8-C9
15	L	508	BCL	C11-C10-C8-C9
15	E	102	BCL	C11-C10-C8-C9
15	F	101	BCL	C6-C7-C8-C9
15	G	102	BCL	C6-C7-C8-C9
15	P	101	BCL	C6-C7-C8-C9
15	4	102	BCL	C6-C7-C8-C9
15	4	102	BCL	C11-C12-C13-C14
15	G	102	BCL	C2A-CAA-CBA-CGA
21	P	102	CRT	C10-C11-C12-C13
22	0	101	LMT	C3'-C4'-O1B-C1B
21	B	103	CRT	C10-C11-C12-C14
21	X	103	CRT	C10-C11-C12-C14
14	L	511	PGV	C20-C21-C22-C23
15	L	502	BCL	C6-C7-C8-C10
15	M	402	BCL	C6-C7-C8-C10
15	A	101	BCL	C11-C10-C8-C7
15	D	103	BCL	C6-C7-C8-C10
15	F	101	BCL	C6-C7-C8-C10
15	G	102	BCL	C6-C7-C8-C10
15	I	102	BCL	C11-C10-C8-C7
15	J	102	BCL	C12-C13-C15-C16
15	K	103	BCL	C12-C13-C15-C16
15	N	101	BCL	C6-C7-C8-C10
15	S	102	BCL	C11-C12-C13-C15
15	T	102	BCL	C11-C10-C8-C7
15	V	102	BCL	C6-C7-C8-C10
15	Z	102	BCL	C11-C10-C8-C7
15	3	101	BCL	C11-C10-C8-C7
15	6	101	BCL	C11-C10-C8-C7
15	7	101	BCL	C6-C7-C8-C10
15	9	101	BCL	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
15	0	102	BCL	C11-C10-C8-C7
17	L	512	UQ8	C18-C19-C21-C22
15	U	101	BCL	C3-C5-C6-C7
15	X	102	BCL	CBA-CGA-O2A-C1
18	S	101	CDL	C37-C38-C39-C40
15	D	103	BCL	C5-C6-C7-C8
15	U	101	BCL	C2A-CAA-CBA-CGA
18	L	510	CDL	C63-C64-C65-C66
18	H	301	CDL	C57-C58-C59-C60
15	L	509	BCL	CAD-CBD-CGD-O2D
18	M	408	CDL	CA3-CA4-OA6-CA5
22	E	101	LMT	C4B-C5B-C6B-O6B
14	L	507	PGV	C20-C19-O03-C01
15	P	101	BCL	CBA-CGA-O2A-C1
15	L	508	BCL	C16-C17-C18-C19
22	B	101	LMT	O5'-C1'-O1'-C1
14	1	401	PGV	O03-C01-C02-C03
12	C	506	DGA	OA1-CA1-OG1-CG1
18	H	301	CDL	OB9-CB7-OB8-CB6
14	L	507	PGV	C2-C1-O01-C02
18	H	301	CDL	OA5-CA3-CA4-OA6
15	F	101	BCL	C5-C6-C7-C8
15	P	101	BCL	CAA-CBA-CGA-O2A
15	D	103	BCL	C2A-CAA-CBA-CGA
18	M	410	CDL	C82-C83-C84-C85
14	L	507	PGV	O02-C1-O01-C02
15	M	402	BCL	CHA-CBD-CGD-O1D
15	M	402	BCL	CHA-CBD-CGD-O2D
15	K	103	BCL	CHA-CBD-CGD-O2D
15	O	502	BCL	CHA-CBD-CGD-O2D
15	N	101	BCL	C3-C5-C6-C7
15	S	102	BCL	O1A-CGA-O2A-C1
18	M	410	CDL	OB9-CB7-OB8-CB6
15	0	102	BCL	C13-C15-C16-C17
22	T	101	LMT	O1'-C1-C2-C3
14	L	506	PGV	O03-C01-C02-O01
14	L	507	PGV	O03-C01-C02-O01
18	H	301	CDL	OA6-CA4-CA6-OA8
18	H	302	CDL	OB6-CB4-CB6-OB8
14	D	101	PGV	C4-C5-C6-C7
15	P	101	BCL	O1A-CGA-O2A-C1
15	Z	102	BCL	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
17	L	504	UQ8	C12-C11-C9-C10
17	L	512	UQ8	C15-C14-C16-C17
15	X	102	BCL	O1A-CGA-O2A-C1
15	Z	102	BCL	C2-C3-C5-C6
17	L	512	UQ8	C13-C14-C16-C17
15	D	103	BCL	C6-C7-C8-C9
15	V	102	BCL	C11-C10-C8-C9
15	Z	102	BCL	C11-C10-C8-C9
15	3	101	BCL	C11-C10-C8-C9
15	3	101	BCL	C11-C12-C13-C14
15	5	102	BCL	C6-C7-C8-C9
14	5	101	PGV	C1-C2-C3-C4
14	L	507	PGV	C2-C3-C4-C5
18	L	510	CDL	C31-C32-C33-C34
22	B	101	LMT	O1'-C1-C2-C3
14	H	303	PGV	C4-C5-C6-C7
21	1	402	CRT	C24-C23-C25-C26
21	N	102	CRT	C5-C6-C7-C9
21	1	402	CRT	C10-C11-C12-C14
21	4	103	CRT	C15-C16-C17-C19
15	I	102	BCL	C1A-C2A-CAA-CBA
15	V	102	BCL	C1A-C2A-CAA-CBA
15	1	403	BCL	C1A-C2A-CAA-CBA
15	8	102	BCL	C1A-C2A-CAA-CBA
15	6	101	BCL	C16-C17-C18-C19
18	I	101	CDL	C12-C13-C14-C15
18	S	101	CDL	C32-C33-C34-C35
14	L	506	PGV	C03-O11-P-O12
14	L	511	PGV	C04-O12-P-O11
18	L	510	CDL	CA3-OA5-PA1-OA2
18	D	102	CDL	CA2-OA2-PA1-OA5
18	D	102	CDL	CB2-OB2-PB2-OB5
18	S	101	CDL	CA2-OA2-PA1-OA5
18	D	102	CDL	C13-C14-C15-C16
15	N	101	BCL	C4-C3-C5-C6
17	L	504	UQ8	C12-C11-C9-C8
14	C	508	PGV	C03-O11-P-O14
14	H	303	PGV	C03-O11-P-O14
14	D	101	PGV	C03-O11-P-O13
18	L	510	CDL	CB3-OB5-PB2-OB3
18	M	410	CDL	CB2-OB2-PB2-OB4
18	M	410	CDL	CB3-OB5-PB2-OB3

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Mol	Chain	Res	Type	Atoms
18	H	301	CDL	CA3-OA5-PA1-OA3
18	H	301	CDL	CB2-OB2-PB2-OB4
18	H	302	CDL	CB2-OB2-PB2-OB3
15	K	103	BCL	C13-C15-C16-C17
18	M	410	CDL	OA5-CA3-CA4-CA6
18	D	102	CDL	OB5-CB3-CB4-CB6
14	C	508	PGV	C2-C3-C4-C5
14	M	407	PGV	C27-C28-C29-C30
18	H	301	CDL	C16-C17-C18-C19
21	J	103	CRT	C35-C36-C37-C38
22	P	103	LMT	O1'-C1-C2-C3
14	5	101	PGV	C2-C3-C4-C5
14	5	101	PGV	O01-C02-C03-O11
15	L	509	BCL	C11-C10-C8-C7
15	L	509	BCL	C12-C13-C15-C16
15	M	402	BCL	C11-C12-C13-C15
15	I	102	BCL	C6-C7-C8-C10
15	W	101	BCL	C11-C12-C13-C15
15	X	102	BCL	C11-C12-C13-C15
15	2	102	BCL	C11-C10-C8-C7
15	3	101	BCL	C11-C12-C13-C15
15	4	102	BCL	C6-C7-C8-C10
18	M	410	CDL	OA5-CA3-CA4-OA6
14	L	507	PGV	O04-C19-O03-C01
18	L	510	CDL	C80-C81-C82-C83
22	K	102	LMT	C2-C3-C4-C5
24	K	101	LDA	C11-C10-C9-C8
14	L	511	PGV	O03-C01-C02-C03
18	S	101	CDL	OA6-CA4-CA6-OA8
22	J	101	LMT	C3'-C4'-O1B-C1B
15	3	101	BCL	C10-C11-C12-C13
15	K	103	BCL	C14-C13-C15-C16
15	S	102	BCL	C11-C12-C13-C14
15	1	403	BCL	C11-C10-C8-C9
15	7	101	BCL	C6-C7-C8-C9
18	L	510	CDL	C81-C82-C83-C84
15	6	101	BCL	C16-C17-C18-C20
17	L	505	UQ8	C9-C11-C12-C13
20	M	404	MQ8	C23-C25-C26-C27
21	M	405	CRT	C5-C6-C7-C8
21	M	405	CRT	C29-C28-C30-C31
15	X	102	BCL	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
15	A	101	BCL	C8-C10-C11-C12
15	F	101	BCL	C15-C16-C17-C18
18	M	410	CDL	C14-C15-C16-C17
15	B	102	BCL	C15-C16-C17-C18
15	L	508	BCL	C3-C5-C6-C7
15	O	502	BCL	C3-C5-C6-C7
14	1	401	PGV	C01-C02-O01-C1
18	H	302	CDL	C31-CA7-OA8-CA6
18	L	510	CDL	CA2-C1-CB2-OB2
15	Z	102	BCL	C2-C1-O2A-CGA
15	4	102	BCL	C2-C1-O2A-CGA
22	0	101	LMT	C5'-C4'-O1B-C1B
18	M	410	CDL	CA7-C31-C32-C33
14	M	411	PGV	C02-C03-O11-P
15	0	102	BCL	C16-C17-C18-C19
15	T	102	BCL	C4-C3-C5-C6
14	L	506	PGV	C20-C19-O03-C01
22	E	101	LMT	O5B-C1B-O1B-C4'
18	L	510	CDL	C37-C38-C39-C40
14	L	511	PGV	C2-C3-C4-C5
14	L	506	PGV	C04-O12-P-O11
14	L	507	PGV	C04-O12-P-O11
14	M	407	PGV	C03-O11-P-O12
14	M	411	PGV	C04-O12-P-O11
14	H	303	PGV	C04-O12-P-O11
14	5	101	PGV	C03-O11-P-O12
14	5	101	PGV	C04-O12-P-O11
18	L	510	CDL	CA2-OA2-PA1-OA5
18	M	408	CDL	CB3-OB5-PB2-OB2
18	M	410	CDL	CA3-OA5-PA1-OA2
18	H	301	CDL	CA2-OA2-PA1-OA5
18	H	301	CDL	CB3-OB5-PB2-OB2
18	H	302	CDL	CA3-OA5-PA1-OA2
18	H	302	CDL	CB3-OB5-PB2-OB2
18	I	101	CDL	CA2-OA2-PA1-OA5
18	I	101	CDL	CB2-OB2-PB2-OB5
18	I	101	CDL	CB3-OB5-PB2-OB2
18	S	101	CDL	CB2-OB2-PB2-OB5
18	D	102	CDL	CA5-C11-C12-C13
22	G	101	LMT	C3'-C4'-O1B-C1B
21	G	103	CRT	C36-C37-C38-C40
21	X	103	CRT	C36-C37-C38-C39

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Mol	Chain	Res	Type	Atoms
21	2	103	CRT	C3-C1-C4-C5
18	S	101	CDL	CA3-CA4-CA6-OA8
15	1	403	BCL	C4-C3-C5-C6
22	J	101	LMT	C5'-C4'-O1B-C1B
15	M	402	BCL	C11-C10-C8-C7
15	B	102	BCL	C11-C10-C8-C7
15	D	103	BCL	C11-C10-C8-C7
15	N	101	BCL	C2-C3-C5-C6
15	P	101	BCL	C6-C7-C8-C10
15	X	102	BCL	C6-C7-C8-C10
15	X	102	BCL	CAA-CBA-CGA-O2A
15	J	102	BCL	C14-C13-C15-C16
15	P	101	BCL	C11-C10-C8-C9
15	Q	101	BCL	C11-C12-C13-C14
15	X	102	BCL	C11-C12-C13-C14
22	0	101	LMT	C2-C3-C4-C5
18	L	510	CDL	C36-C37-C38-C39
21	G	103	CRT	C36-C37-C38-O2
21	6	102	CRT	C36-C37-C38-O2
18	M	410	CDL	CA4-CA3-OA5-PA1
18	H	302	CDL	C1-CB2-OB2-PB2
18	L	510	CDL	C71-C72-C73-C74
18	S	101	CDL	C73-C74-C75-C76
15	A	101	BCL	C3-C5-C6-C7
15	8	102	BCL	C2-C3-C5-C6
15	S	102	BCL	C16-C17-C18-C19
15	G	102	BCL	CBA-CGA-O2A-C1
18	H	302	CDL	C71-CB7-OB8-CB6
22	Z	101	LMT	C2-C3-C4-C5
14	M	411	PGV	C4-C5-C6-C7
15	G	102	BCL	O1A-CGA-O2A-C1
15	O	502	BCL	CBA-CGA-O2A-C1
18	H	301	CDL	OB5-CB3-CB4-OB6
18	I	101	CDL	OB5-CB3-CB4-OB6
14	L	506	PGV	O04-C19-O03-C01
15	I	102	BCL	C10-C11-C12-C13
18	S	101	CDL	C34-C35-C36-C37
15	O	502	BCL	O1A-CGA-O2A-C1
15	M	402	BCL	C2-C1-O2A-CGA
15	P	101	BCL	C15-C16-C17-C18
15	K	103	BCL	C2A-CAA-CBA-CGA
15	4	102	BCL	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
15	U	101	BCL	C15-C16-C17-C18
15	V	102	BCL	C3A-C2A-CAA-CBA
15	1	403	BCL	C3A-C2A-CAA-CBA
15	8	102	BCL	C3A-C2A-CAA-CBA
10	C	501	HEC	CAA-CBA-CGA-O1A
15	J	102	BCL	CAA-CBA-CGA-O2A
22	T	101	LMT	C3-C4-C5-C6
10	C	502	HEC	CAA-CBA-CGA-O2A
15	3	101	BCL	C4-C3-C5-C6
15	M	402	BCL	C11-C12-C13-C14
15	E	102	BCL	C14-C13-C15-C16
15	G	102	BCL	C11-C12-C13-C14
15	I	102	BCL	C6-C7-C8-C9
15	I	102	BCL	C14-C13-C15-C16
15	1	403	BCL	C15-C16-C17-C18
22	B	101	LMT	C6-C7-C8-C9
14	M	409	PGV	C23-C24-C25-C26
14	1	401	PGV	C04-O12-P-O14
10	C	502	HEC	CAA-CBA-CGA-O1A
22	P	103	LMT	C2-C3-C4-C5
22	4	104	LMT	C7-C8-C9-C10
18	M	410	CDL	CA6-CA4-OA6-CA5
18	H	301	CDL	CA6-CA4-OA6-CA5
18	S	101	CDL	CA6-CA4-OA6-CA5
15	A	101	BCL	C1A-C2A-CAA-CBA
15	P	101	BCL	C1A-C2A-CAA-CBA
14	M	411	PGV	C7-C8-C9-C10
15	B	102	BCL	C11-C12-C13-C15
15	P	101	BCL	C11-C12-C13-C15
15	8	102	BCL	C6-C7-C8-C10
16	L	503	BPH	C11-C12-C13-C15
15	J	102	BCL	C15-C16-C17-C18
15	L	502	BCL	O1A-CGA-O2A-C1
15	S	102	BCL	C10-C11-C12-C13
15	8	102	BCL	C8-C10-C11-C12
15	L	509	BCL	C16-C17-C18-C19
15	L	502	BCL	C2A-CAA-CBA-CGA
15	W	101	BCL	C5-C6-C7-C8
15	5	102	BCL	C15-C16-C17-C18
18	D	102	CDL	C15-C16-C17-C18
14	C	508	PGV	O01-C02-C03-O11
18	D	102	CDL	OA5-CA3-CA4-OA6

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Mol	Chain	Res	Type	Atoms
22	J	101	LMT	O5B-C1B-O1B-C4'
15	L	502	BCL	CBA-CGA-O2A-C1
14	C	508	PGV	C20-C21-C22-C23
18	L	510	CDL	C42-C43-C44-C45
22	G	101	LMT	C5'-C4'-O1B-C1B
18	H	302	CDL	OB9-CB7-OB8-CB6
15	T	102	BCL	C2-C3-C5-C6
15	1	403	BCL	C2-C3-C5-C6
15	3	101	BCL	C2-C3-C5-C6
22	V	101	LMT	O1'-C1-C2-C3
15	M	402	BCL	C16-C17-C18-C19
14	D	101	PGV	C22-C23-C24-C25
14	M	411	PGV	O03-C01-C02-O01
18	I	101	CDL	OA6-CA4-CA6-OA8
21	J	103	CRT	C1-C4-C5-C6
21	X	103	CRT	C1-C4-C5-C6
15	N	101	BCL	C16-C17-C18-C19
15	I	102	BCL	C2-C1-O2A-CGA
15	O	502	BCL	C2-C1-O2A-CGA
15	V	102	BCL	C2-C1-O2A-CGA
15	W	101	BCL	C2-C1-O2A-CGA
15	4	102	BCL	C2C-C3C-CAC-CBC
18	M	410	CDL	C13-C14-C15-C16
15	2	102	BCL	CAA-CBA-CGA-O2A
15	8	102	BCL	C11-C10-C8-C9
10	C	501	HEC	CAA-CBA-CGA-O2A
15	8	102	BCL	C16-C17-C18-C19
15	Q	101	BCL	C10-C11-C12-C13
18	M	408	CDL	CA3-CA4-CA6-OA8
10	C	504	HEC	CAA-CBA-CGA-O1A
14	L	511	PGV	C04-C05-C06-O06
15	Y	101	BCL	C4-C3-C5-C6
22	E	101	LMT	O5B-C5B-C6B-O6B
21	S	104	CRT	C10-C11-C12-C14
18	M	408	CDL	OA5-CA3-CA4-OA6
18	I	101	CDL	C31-C32-C33-C34
15	Z	102	BCL	O1D-CGD-O2D-CED
15	Q	101	BCL	C16-C17-C18-C19
18	M	410	CDL	C60-C61-C62-C63
14	C	508	PGV	C01-C02-C03-O11
15	Y	101	BCL	C11-C12-C13-C15
15	4	102	BCL	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
15	8	102	BCL	C11-C10-C8-C7
15	5	102	BCL	C8-C10-C11-C12
14	D	101	PGV	O05-C05-C06-O06
18	L	510	CDL	C79-C80-C81-C82
15	V	102	BCL	CAA-CBA-CGA-O2A
15	6	101	BCL	O1A-CGA-O2A-C1
16	M	403	BPH	C15-C16-C17-C18
14	H	303	PGV	C23-C24-C25-C26
15	6	101	BCL	CBA-CGA-O2A-C1
15	E	102	BCL	CAA-CBA-CGA-O2A
18	D	102	CDL	C72-C71-CB7-OB8
22	T	101	LMT	C4-C5-C6-C7
15	A	101	BCL	C4-C3-C5-C6
15	6	101	BCL	C4-C3-C5-C6
22	E	101	LMT	C2B-C1B-O1B-C4'
15	L	502	BCL	C11-C10-C8-C9
15	B	102	BCL	C11-C12-C13-C14
15	W	101	BCL	C11-C12-C13-C14
22	K	102	LMT	C6-C7-C8-C9
14	L	507	PGV	O01-C1-C2-C3
18	H	301	CDL	C80-C81-C82-C83
15	L	502	BCL	CAD-CBD-CGD-O2D
15	L	508	BCL	CAD-CBD-CGD-O2D
16	L	503	BPH	CAD-CBD-CGD-O2D
18	M	410	CDL	CA3-CA4-OA6-CA5
14	C	508	PGV	C21-C22-C23-C24
15	L	502	BCL	C5-C6-C7-C8
15	9	101	BCL	C13-C15-C16-C17
14	L	501	PGV	O02-C1-O01-C02
18	H	301	CDL	C77-C78-C79-C80
15	Q	101	BCL	C8-C10-C11-C12
22	J	101	LMT	C2B-C1B-O1B-C4'
14	L	507	PGV	C31-C32-C33-C34
22	Z	101	LMT	C5'-C4'-O1B-C1B
15	K	103	BCL	C4-C3-C5-C6
21	M	405	CRT	C5-C6-C7-C9
21	M	405	CRT	C22-C23-C25-C26
21	P	102	CRT	C10-C11-C12-C14
21	1	402	CRT	C15-C16-C17-C19
21	1	402	CRT	C22-C23-C25-C26
14	M	411	PGV	C6-C7-C8-C9
15	P	101	BCL	O2A-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
15	R	101	BCL	O2A-C1-C2-C3
16	L	503	BPH	O2A-C1-C2-C3
22	B	101	LMT	C2-C3-C4-C5
14	5	101	PGV	C9-C10-C11-C12
15	M	402	BCL	C16-C17-C18-C20
15	A	101	BCL	CHA-CBD-CGD-O1D
15	A	101	BCL	CHA-CBD-CGD-O2D
15	I	102	BCL	CHA-CBD-CGD-O1D
15	N	101	BCL	CHA-CBD-CGD-O1D
15	N	101	BCL	CHA-CBD-CGD-O2D
15	S	102	BCL	CHA-CBD-CGD-O1D
15	S	102	BCL	CHA-CBD-CGD-O2D
15	7	101	BCL	CHA-CBD-CGD-O1D
15	7	101	BCL	CHA-CBD-CGD-O2D
15	8	102	BCL	CHA-CBD-CGD-O1D
15	7	101	BCL	C4-C3-C5-C6
20	M	404	MQ8	C19-C18-C20-C21
22	G	101	LMT	C6-C7-C8-C9
15	L	509	BCL	C2-C3-C5-C6
15	A	101	BCL	C2-C3-C5-C6
15	Y	101	BCL	C2-C3-C5-C6
15	6	101	BCL	C2-C3-C5-C6
15	0	102	BCL	C5-C6-C7-C8
14	L	507	PGV	C21-C22-C23-C24
21	G	103	CRT	C39-C38-O2-C2M
14	M	409	PGV	C21-C22-C23-C24
24	K	101	LDA	C9-C10-C11-C12
10	C	504	HEC	CAA-CBA-CGA-O2A
15	9	101	BCL	CAA-CBA-CGA-O2A
21	4	103	CRT	C36-C37-C38-C40
21	6	102	CRT	C36-C37-C38-C40
24	O	501	LDA	C9-C10-C11-C12
15	F	101	BCL	C11-C12-C13-C15
15	U	101	BCL	C12-C13-C15-C16
20	M	404	MQ8	C22-C23-C25-C26
18	I	101	CDL	C1-CA2-OA2-PA1
15	L	509	BCL	C14-C13-C15-C16
15	F	101	BCL	C11-C12-C13-C14
15	8	102	BCL	C6-C7-C8-C9
15	F	101	BCL	C10-C11-C12-C13
15	X	102	BCL	C15-C16-C17-C18
15	P	101	BCL	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
14	D	101	PGV	C1-C2-C3-C4
18	L	510	CDL	C53-C54-C55-C56
21	4	103	CRT	C36-C37-C38-O2
18	M	410	CDL	C51-C52-C53-C54
15	E	102	BCL	CAA-CBA-CGA-O1A
18	L	510	CDL	C78-C79-C80-C81
15	2	102	BCL	C1A-C2A-CAA-CBA
15	A	101	BCL	C2-C1-O2A-CGA
15	F	101	BCL	C2-C1-O2A-CGA
22	J	101	LMT	C5-C6-C7-C8
15	J	102	BCL	C13-C15-C16-C17
22	Z	101	LMT	C3'-C4'-O1B-C1B
10	C	502	HEC	CAD-CBD-CGD-O1D
18	I	101	CDL	CA3-CA4-CA6-OA8
18	M	410	CDL	C18-C19-C20-C21
14	L	507	PGV	O02-C1-C2-C3
15	9	101	BCL	CAA-CBA-CGA-O1A
18	D	102	CDL	C72-C71-CB7-OB9
22	B	101	LMT	C3'-C4'-O1B-C1B
14	L	511	PGV	C04-O12-P-O13
14	M	411	PGV	C04-O12-P-O13
14	D	101	PGV	C03-O11-P-O14
18	H	301	CDL	CA2-OA2-PA1-OA3
18	H	302	CDL	CB3-OB5-PB2-OB3
18	S	101	CDL	CB2-OB2-PB2-OB3
15	5	102	BCL	C3-C5-C6-C7
15	Q	101	BCL	CAA-CBA-CGA-O2A
15	4	102	BCL	CAA-CBA-CGA-O2A
15	G	102	BCL	C13-C15-C16-C17
15	L	509	BCL	C4-C3-C5-C6
14	L	501	PGV	C2-C1-O01-C02
14	D	101	PGV	C20-C21-C22-C23
15	F	101	BCL	CAD-CBD-CGD-O1D
15	I	102	BCL	CAD-CBD-CGD-O1D
15	L	502	BCL	C15-C16-C17-C18
15	U	101	BCL	C14-C13-C15-C16
12	C	506	DGA	CG1-CG2-OG2-CB1
15	L	508	BCL	C16-C17-C18-C20
24	K	101	LDA	C6-C7-C8-C9
18	H	302	CDL	OA9-CA7-OA8-CA6
15	9	101	BCL	C15-C16-C17-C18
16	M	403	BPH	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
18	M	410	CDL	C53-C54-C55-C56
15	X	102	BCL	C2C-C3C-CAC-CBC
15	X	102	BCL	C11-C10-C8-C7
15	5	102	BCL	C6-C7-C8-C10
16	M	403	BPH	C11-C12-C13-C15
14	5	101	PGV	C3-C4-C5-C6
15	L	509	BCL	C16-C17-C18-C20
15	Z	102	BCL	CAA-CBA-CGA-O2A
10	C	502	HEC	CAD-CBD-CGD-O2D
15	L	509	BCL	C2A-CAA-CBA-CGA
15	2	102	BCL	C4-C3-C5-C6

There are no ring outliers.

96 monomers are involved in 386 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	J	101	LMT	1	0
15	6	101	BCL	5	0
24	O	501	LDA	2	0
22	P	103	LMT	1	0
14	C	508	PGV	3	0
21	1	402	CRT	8	0
22	0	101	LMT	2	0
15	Q	101	BCL	5	0
14	M	411	PGV	2	0
10	C	503	HEC	5	0
22	4	104	LMT	1	0
18	H	302	CDL	1	0
21	6	102	CRT	5	0
15	N	101	BCL	7	0
10	C	502	HEC	5	0
15	G	102	BCL	6	0
17	L	505	UQ8	11	0
21	Q	102	CRT	6	0
21	G	103	CRT	6	0
15	F	101	BCL	6	0
15	L	509	BCL	2	0
22	2	101	LMT	2	0
16	L	503	BPH	4	0
21	N	102	CRT	2	0
22	Z	101	LMT	2	0
15	I	102	BCL	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	K	103	BCL	8	0
13	C	507	PLM	1	0
22	H	304	LMT	1	0
15	P	101	BCL	10	0
15	3	101	BCL	4	0
14	1	401	PGV	2	0
15	9	101	BCL	5	0
15	Z	102	BCL	5	0
17	L	512	UQ8	7	0
15	D	103	BCL	4	0
22	G	101	LMT	3	0
15	7	101	BCL	1	0
20	M	404	MQ8	4	0
14	H	303	PGV	3	0
21	E	103	CRT	5	0
21	2	103	CRT	6	0
21	R	102	CRT	5	0
21	X	103	CRT	5	0
15	W	101	BCL	6	0
21	J	103	CRT	5	0
22	K	102	LMT	1	0
15	V	102	BCL	7	0
21	M	405	CRT	3	0
15	T	102	BCL	8	0
10	C	504	HEC	9	0
17	L	504	UQ8	2	0
15	0	102	BCL	7	0
22	E	101	LMT	1	0
16	M	403	BPH	10	0
21	8	103	CRT	6	0
15	M	402	BCL	3	0
15	U	101	BCL	3	0
21	7	102	CRT	4	0
15	2	102	BCL	6	0
18	M	408	CDL	1	0
15	B	102	BCL	7	0
15	R	101	BCL	10	0
22	V	101	LMT	3	0
18	L	510	CDL	1	0
15	1	403	BCL	5	0
21	4	103	CRT	8	0
18	H	301	CDL	3	0

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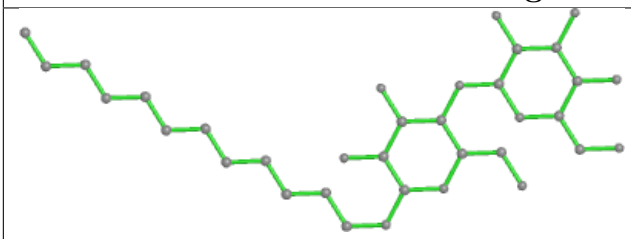
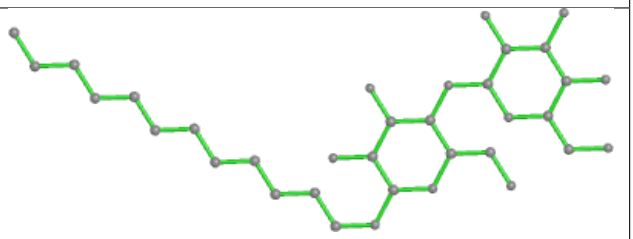
Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	D	102	CDL	4	0
14	5	101	PGV	4	0
20	M	406	MQ8	5	0
15	L	508	BCL	5	0
10	C	501	HEC	5	0
22	8	101	LMT	1	0
15	O	502	BCL	4	0
21	S	104	CRT	2	0
18	I	101	CDL	1	0
22	B	101	LMT	1	0
22	4	101	LMT	3	0
24	K	101	LDA	1	0
15	5	102	BCL	4	0
15	8	102	BCL	9	0
15	J	102	BCL	5	0
14	L	506	PGV	4	0
21	B	103	CRT	8	0
15	A	101	BCL	1	0
18	M	410	CDL	1	0
15	4	102	BCL	5	0
15	E	102	BCL	5	0
15	S	102	BCL	3	0
18	S	101	CDL	5	0
15	X	102	BCL	4	0
21	P	102	CRT	6	0
15	Y	101	BCL	7	0
14	M	409	PGV	1	0
15	L	502	BCL	2	0

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

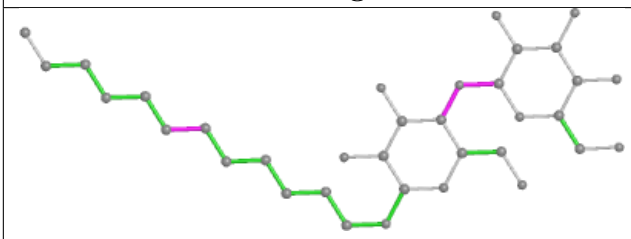
Ligand LMT J 101



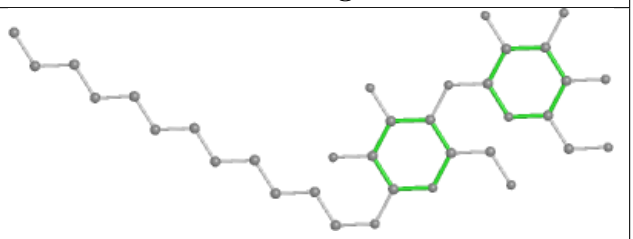
Bond lengths



Bond angles

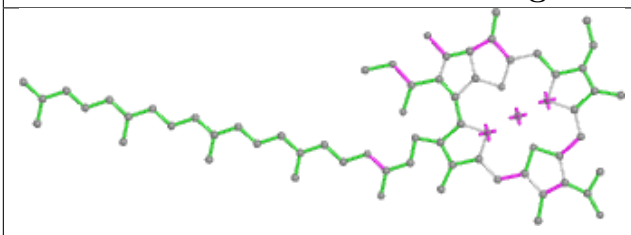


Torsions

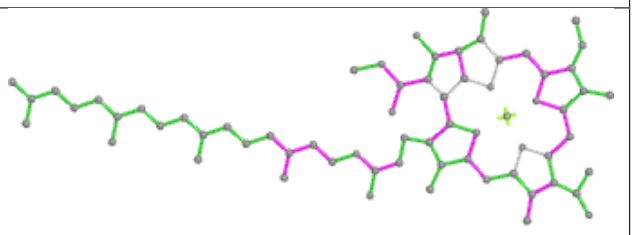


Rings

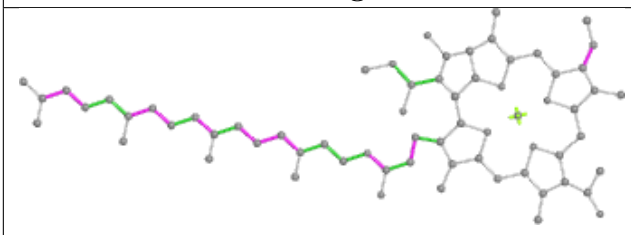
Ligand BCL 6 101



Bond lengths



Bond angles



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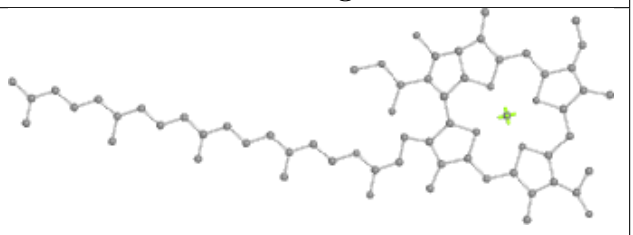
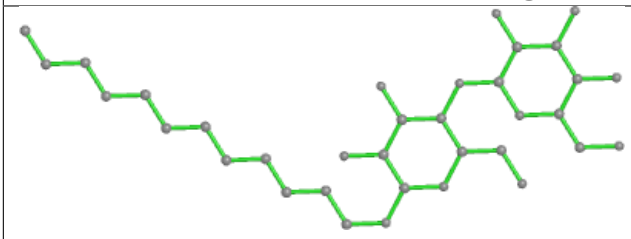
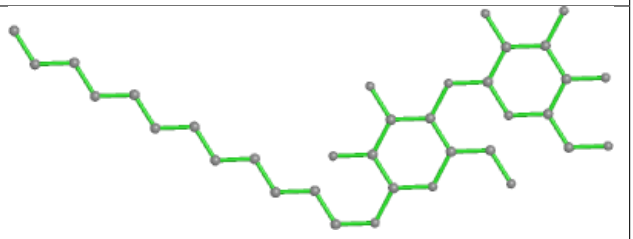


Rings

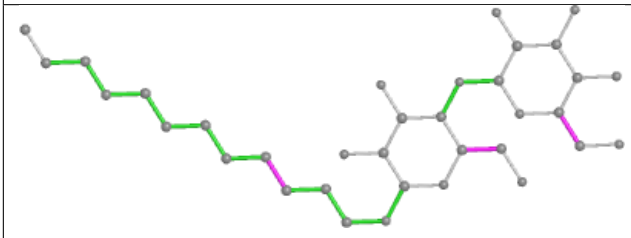
Ligand LMT N 103



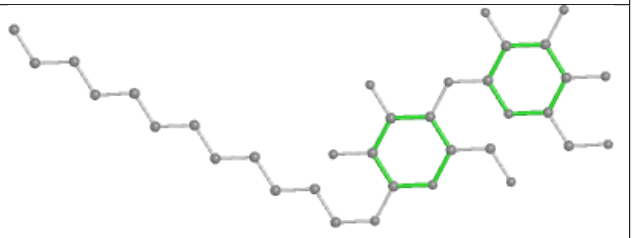
Bond lengths



Bond angles

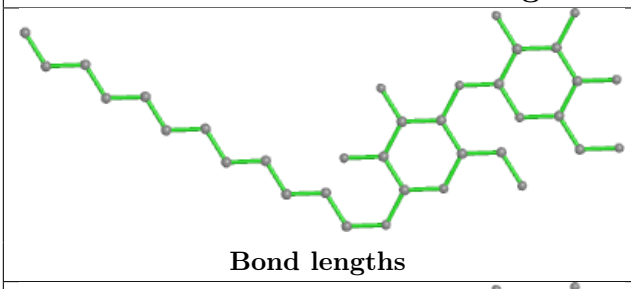


Torsions

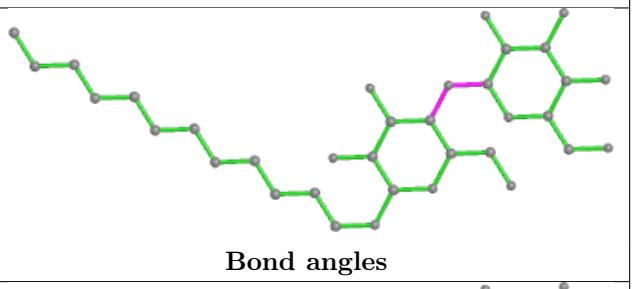


Rings

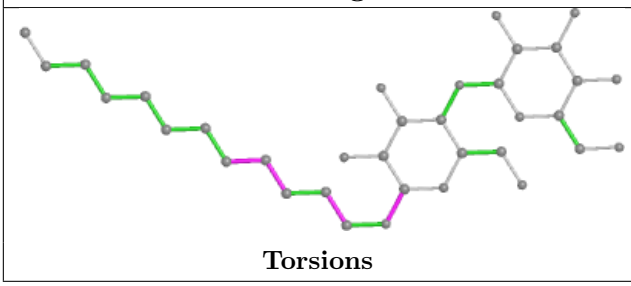
Ligand LMT P 103



Bond lengths



Bond angles



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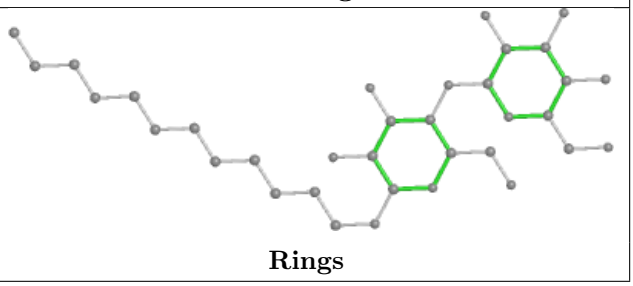
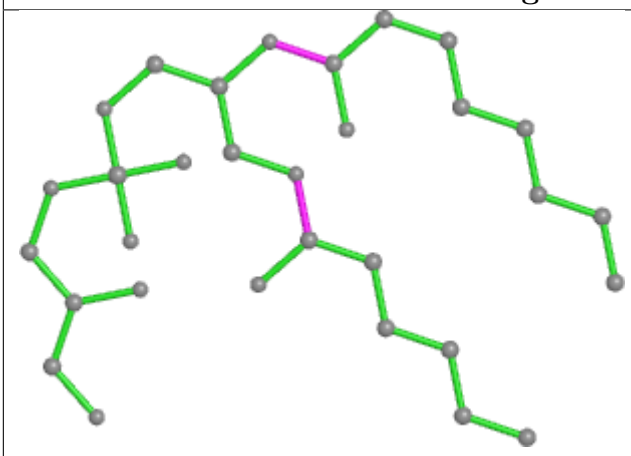
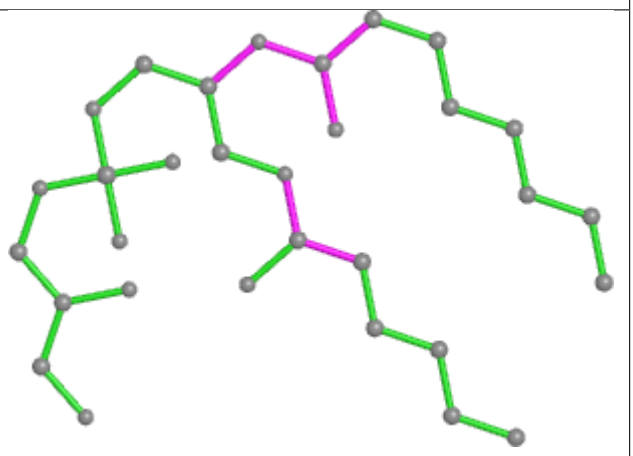


Rings

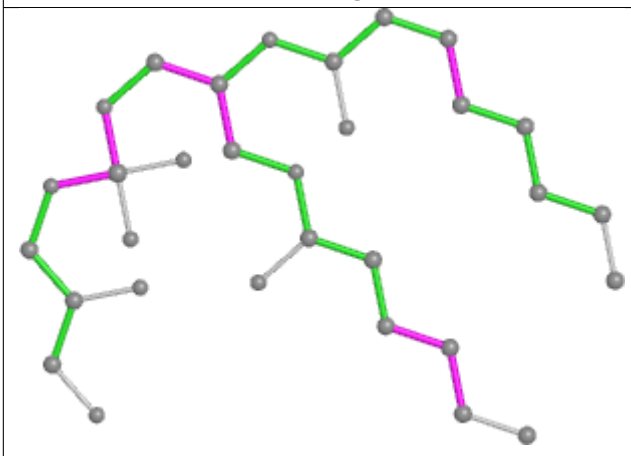
Ligand PGV C 508



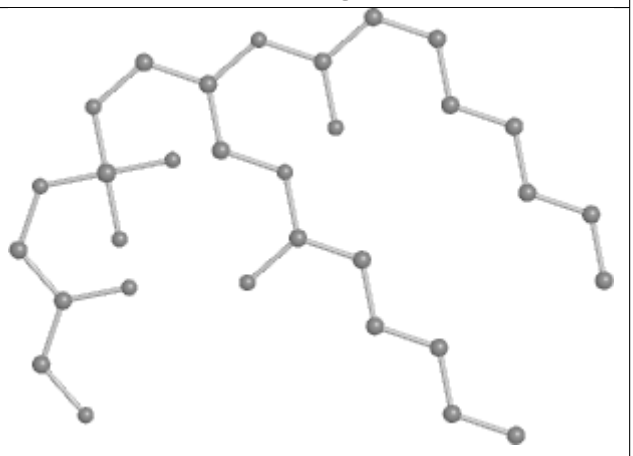
Bond lengths



Bond angles

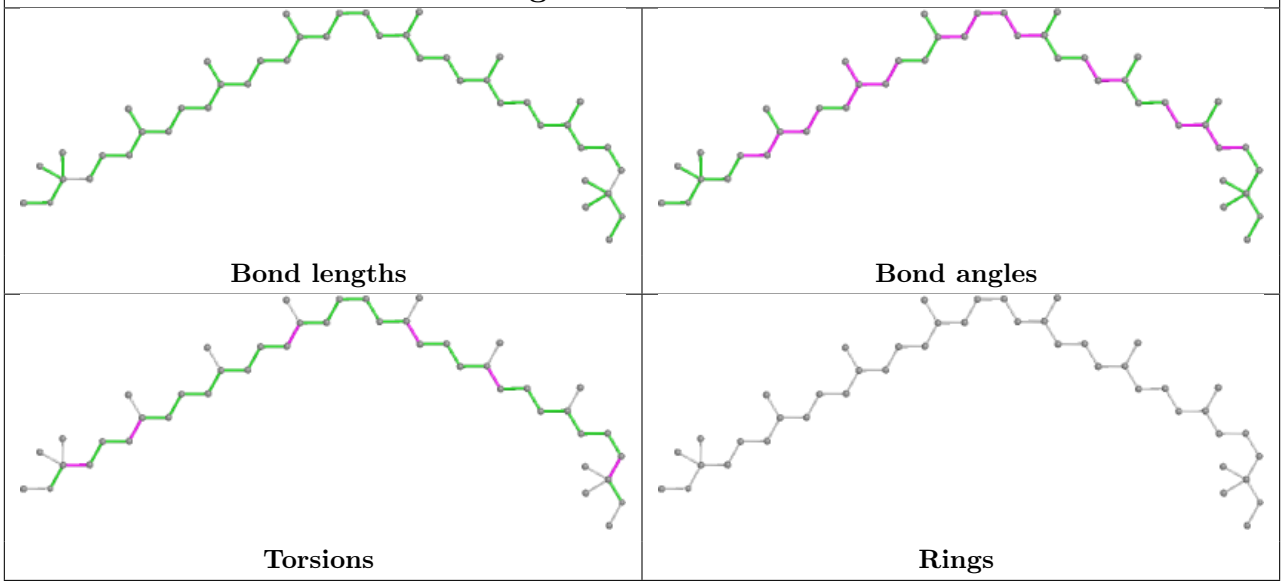


Torsions

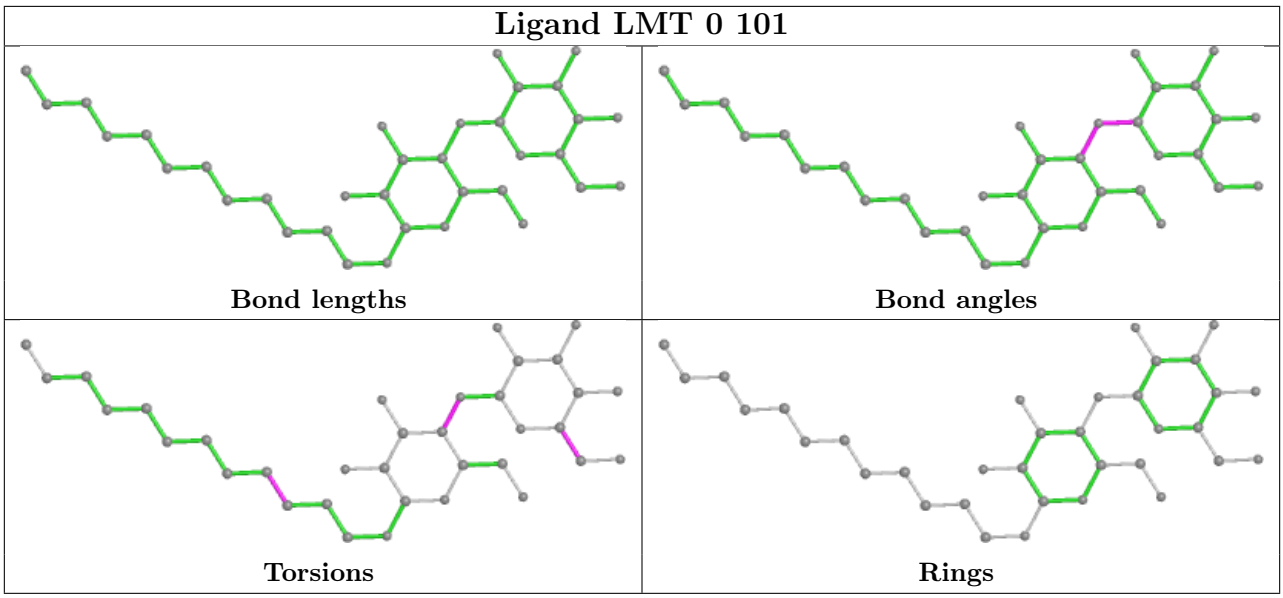


Rings

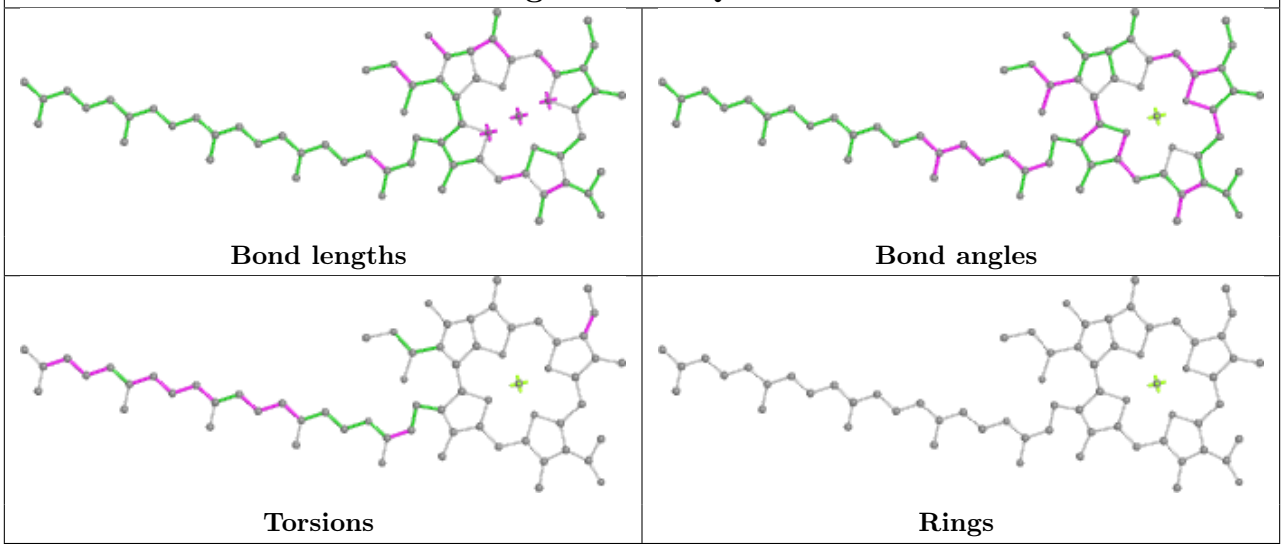
Ligand CRT 1 402



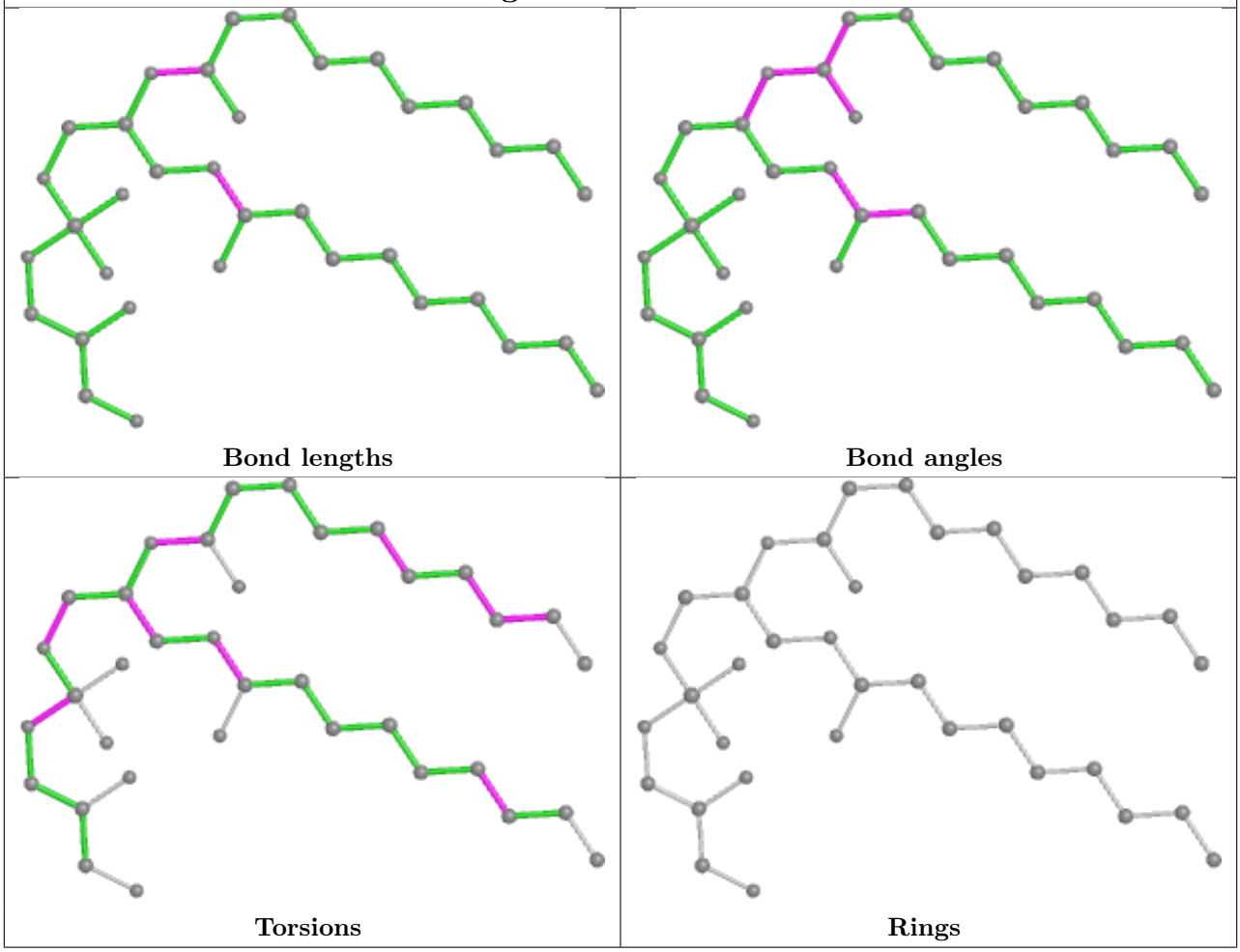
Ligand LMT 0 101



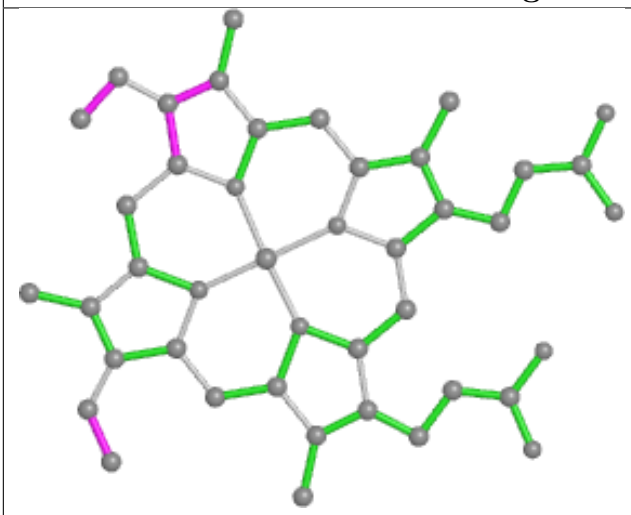
Ligand BCL Q 101



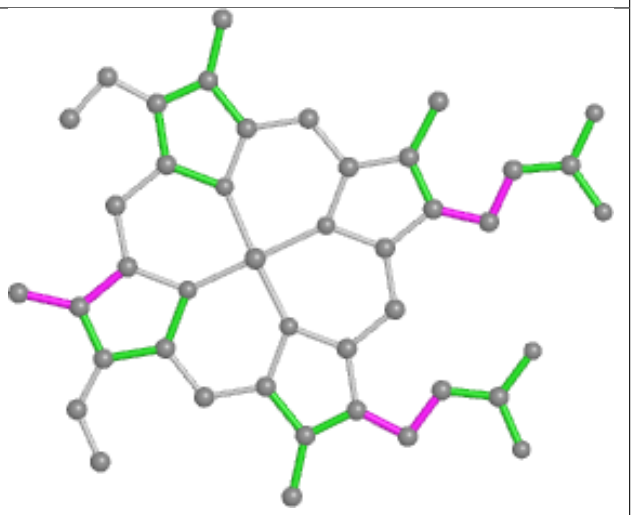
Ligand PGV M 411



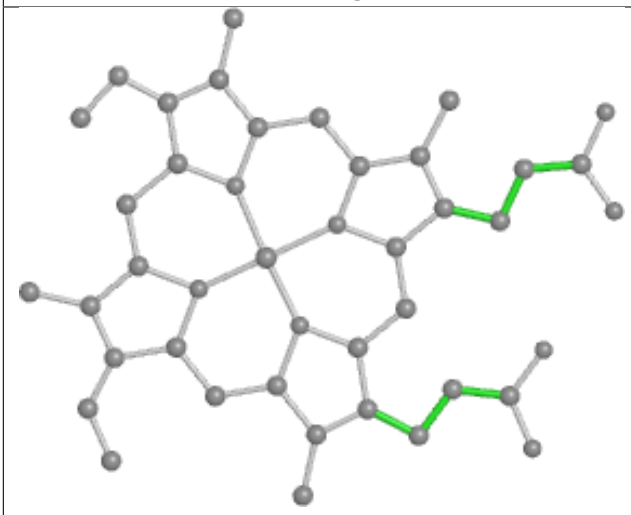
Ligand HEC C 503



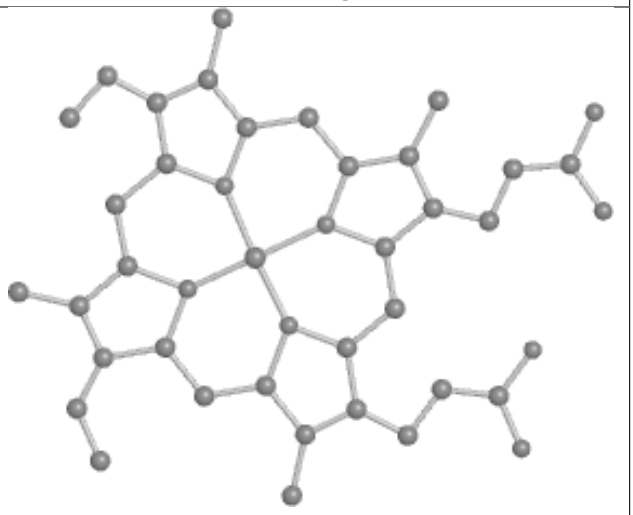
Bond lengths



Bond angles

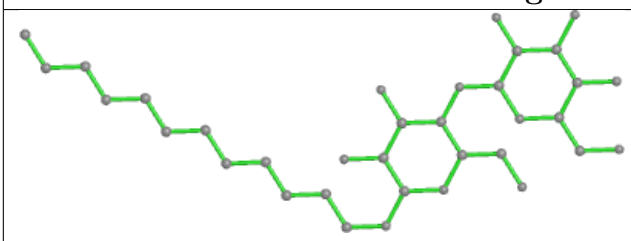


Torsions

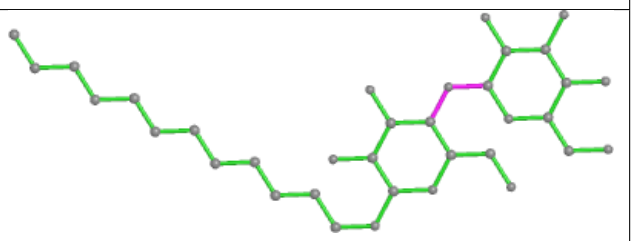


Rings

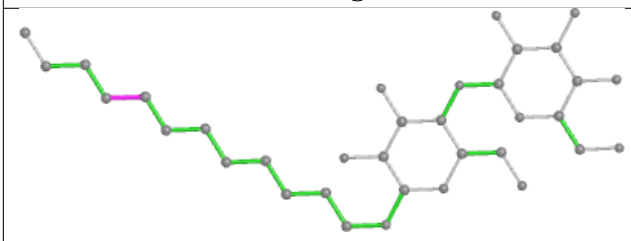
Ligand LMT 4 104



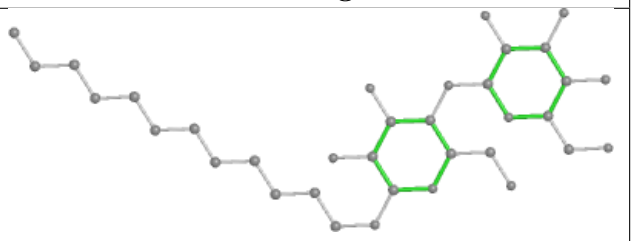
Bond lengths



Bond angles

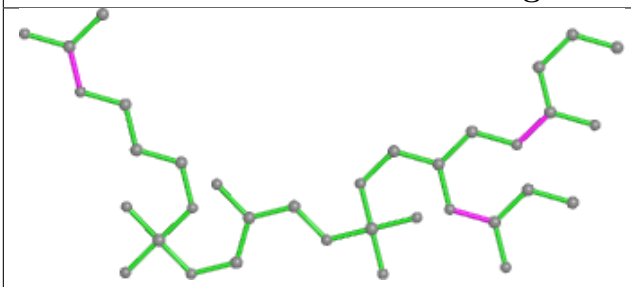


Torsions

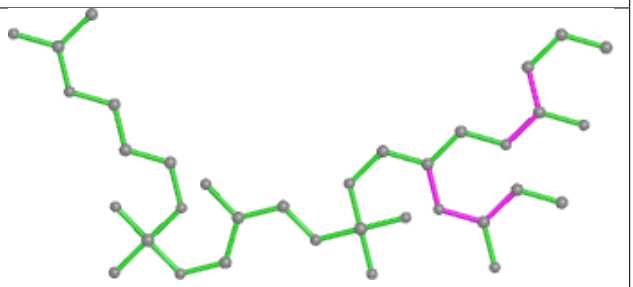


Rings

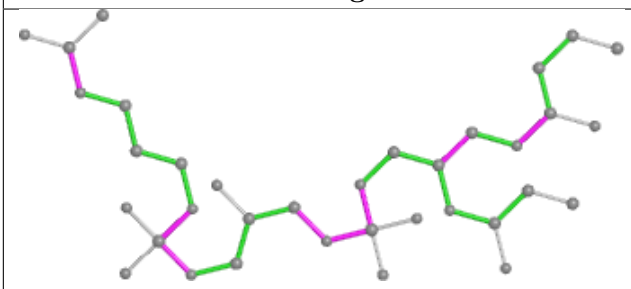
Ligand CDL H 302



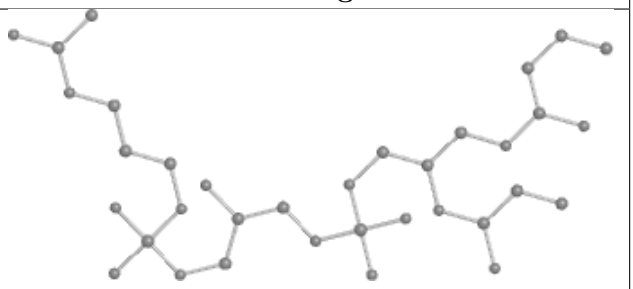
Bond lengths



Bond angles

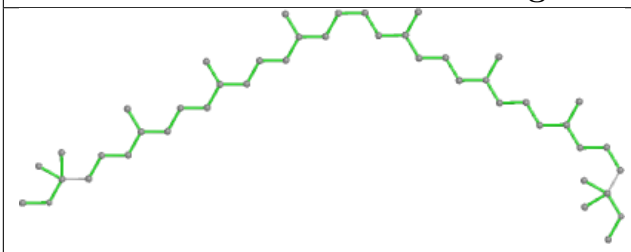


Torsions

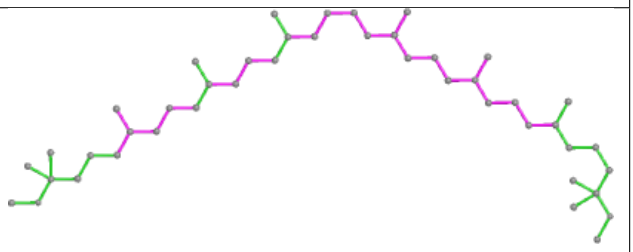


Rings

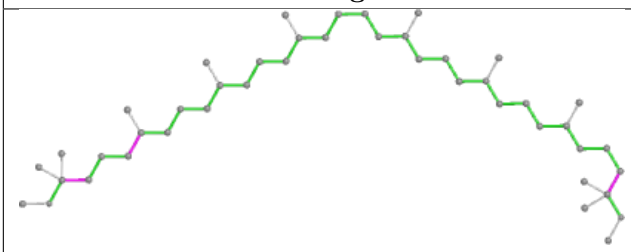
Ligand CRT 6 102



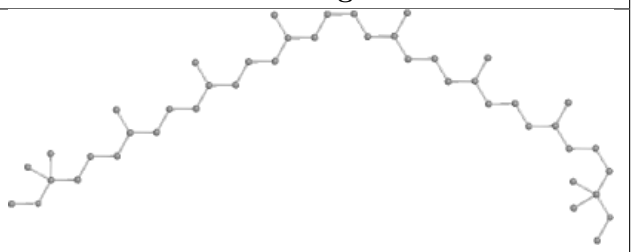
Bond lengths



Bond angles

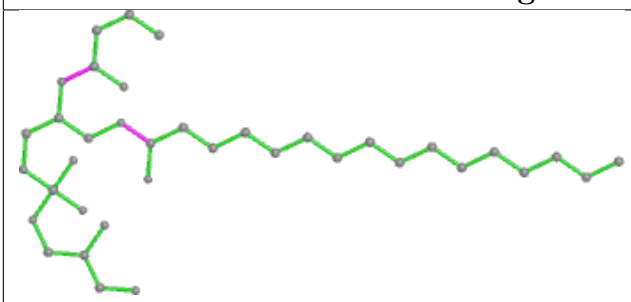


Torsions

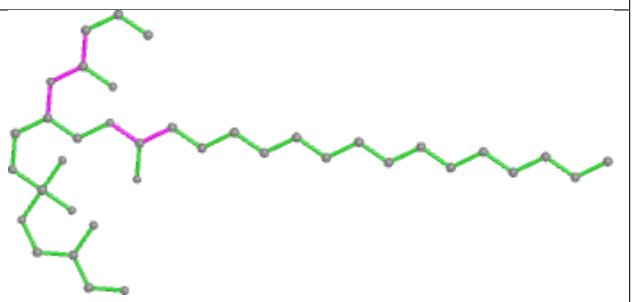


Rings

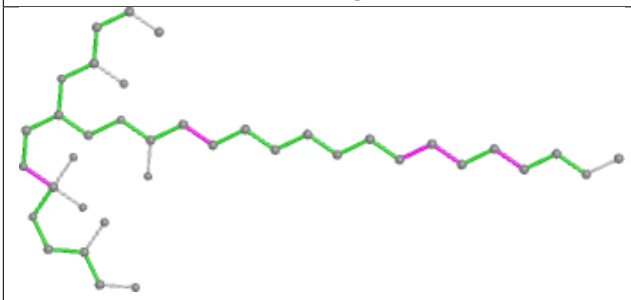
Ligand PGV M 407



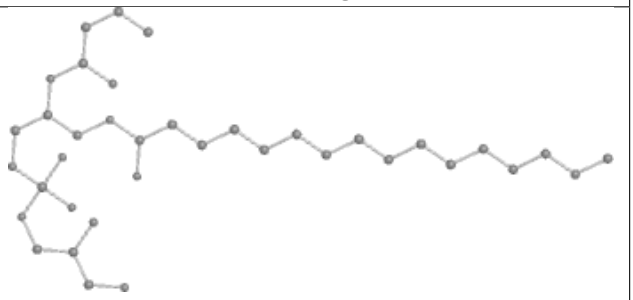
Bond lengths



Bond angles

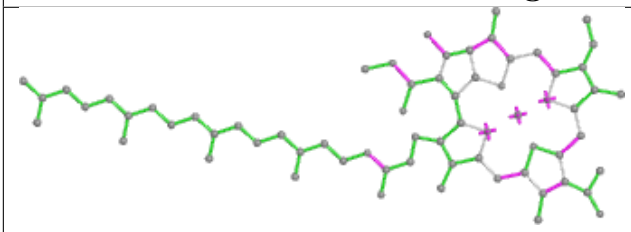


Torsions

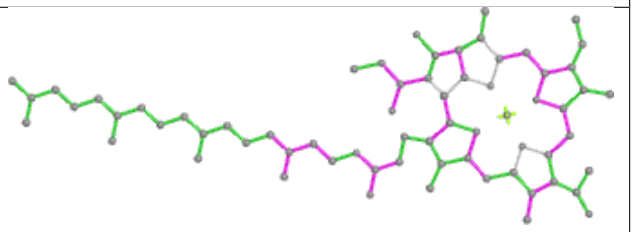


Rings

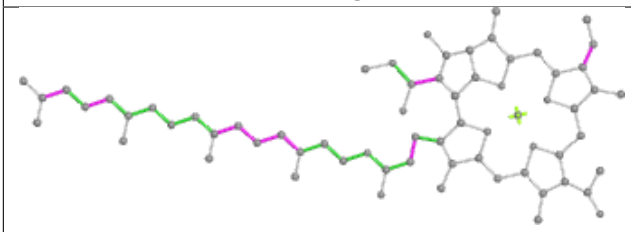
Ligand BCL N 101



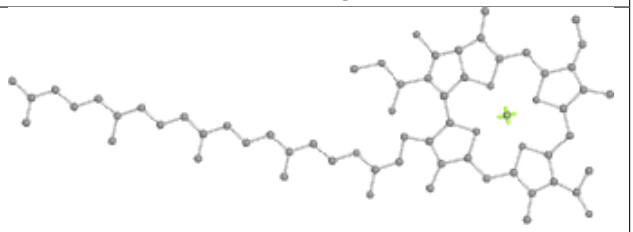
Bond lengths



Bond angles

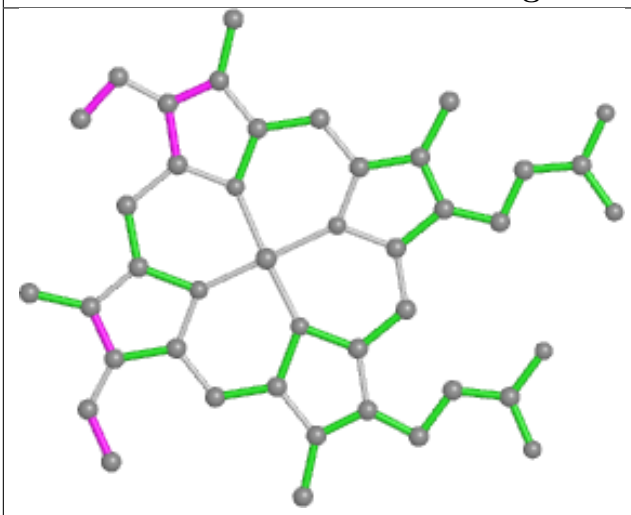


Torsions

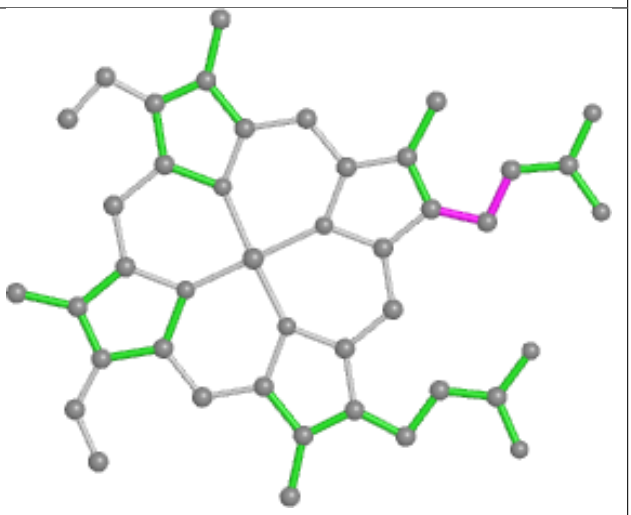


Rings

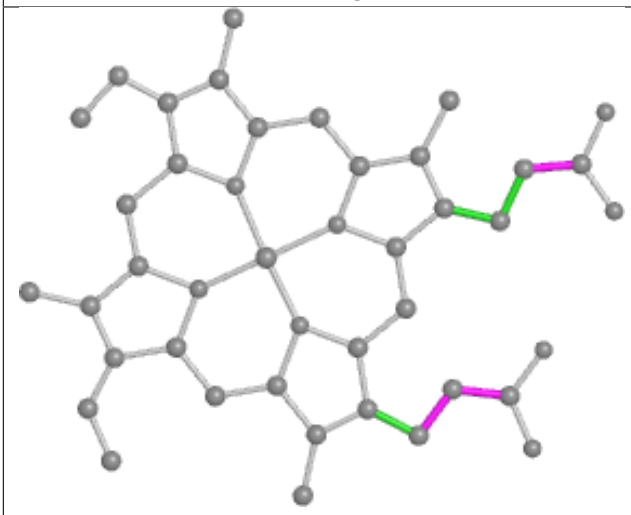
Ligand HEC C 502



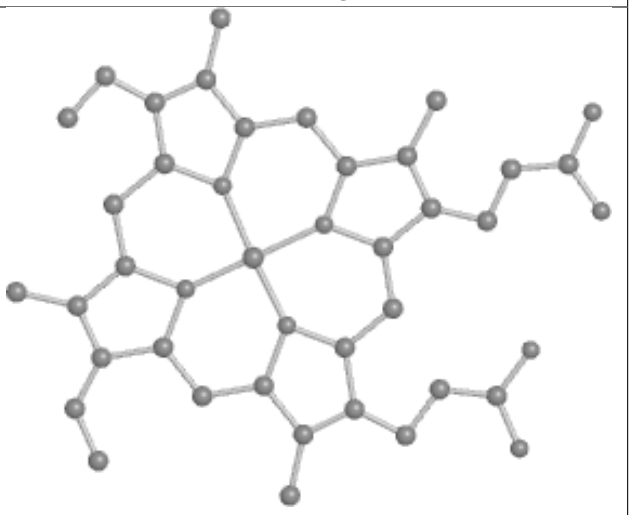
Bond lengths



Bond angles

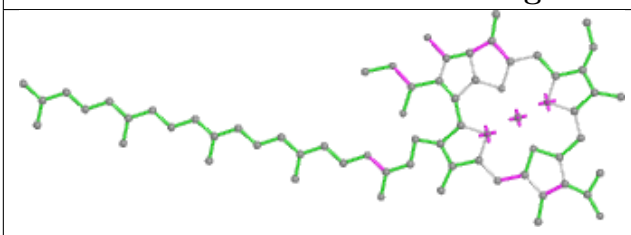


Torsions

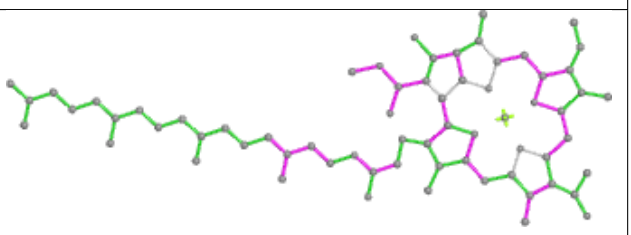


Rings

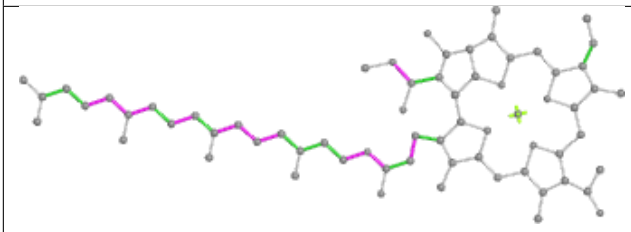
Ligand BCL G 102



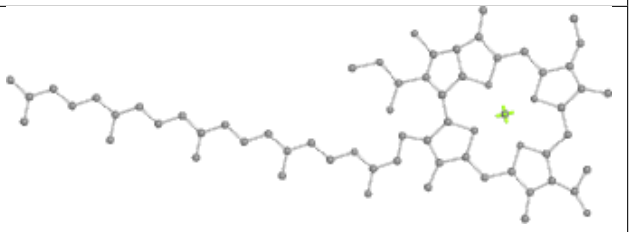
Bond lengths



Bond angles

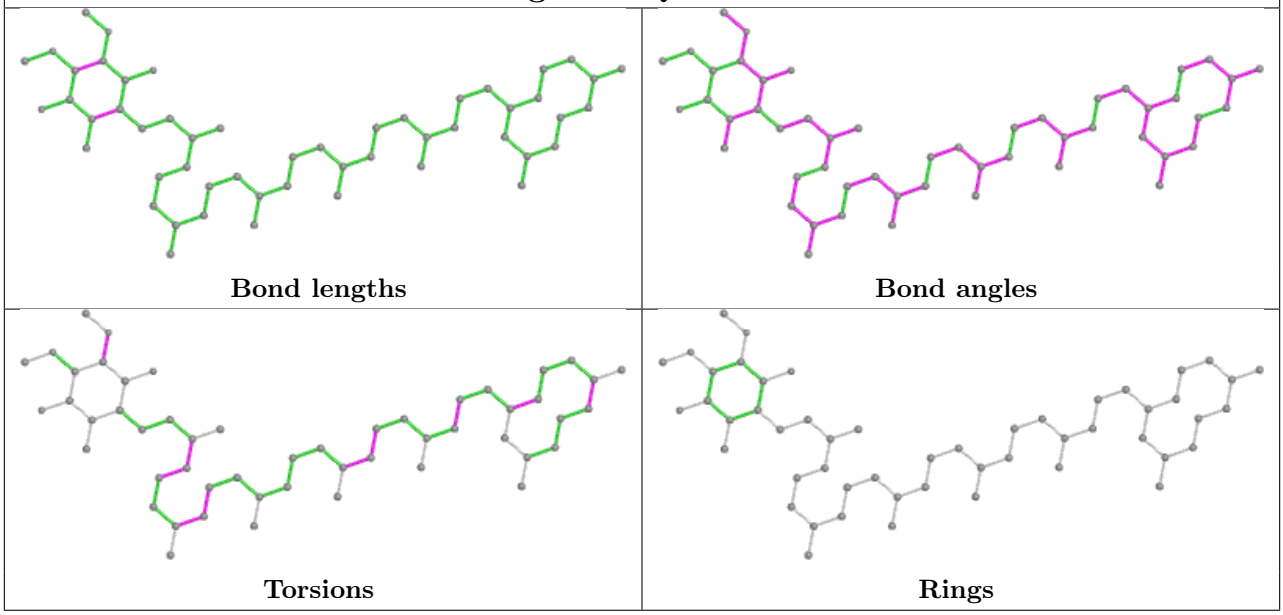


Torsions

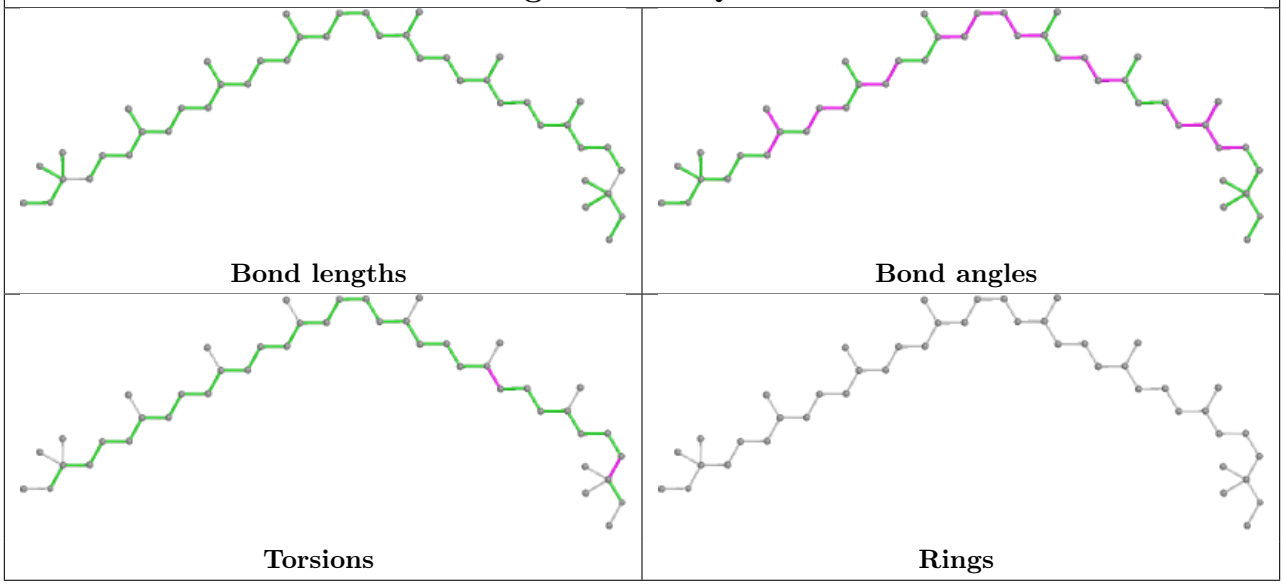


Rings

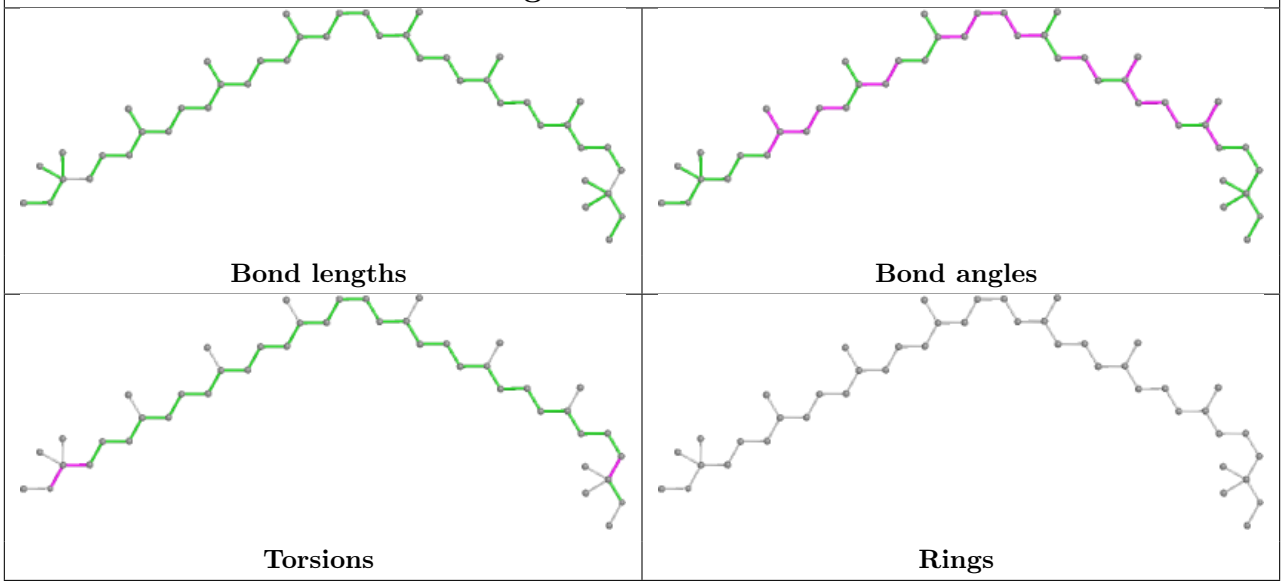
Ligand UQ8 L 505



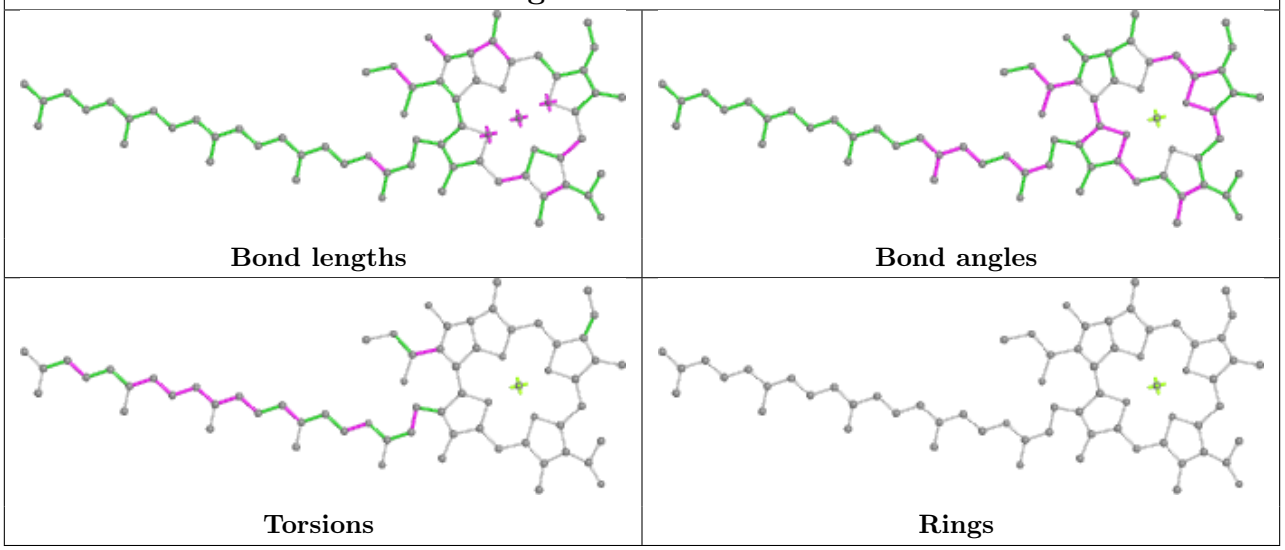
Ligand CRT Q 102



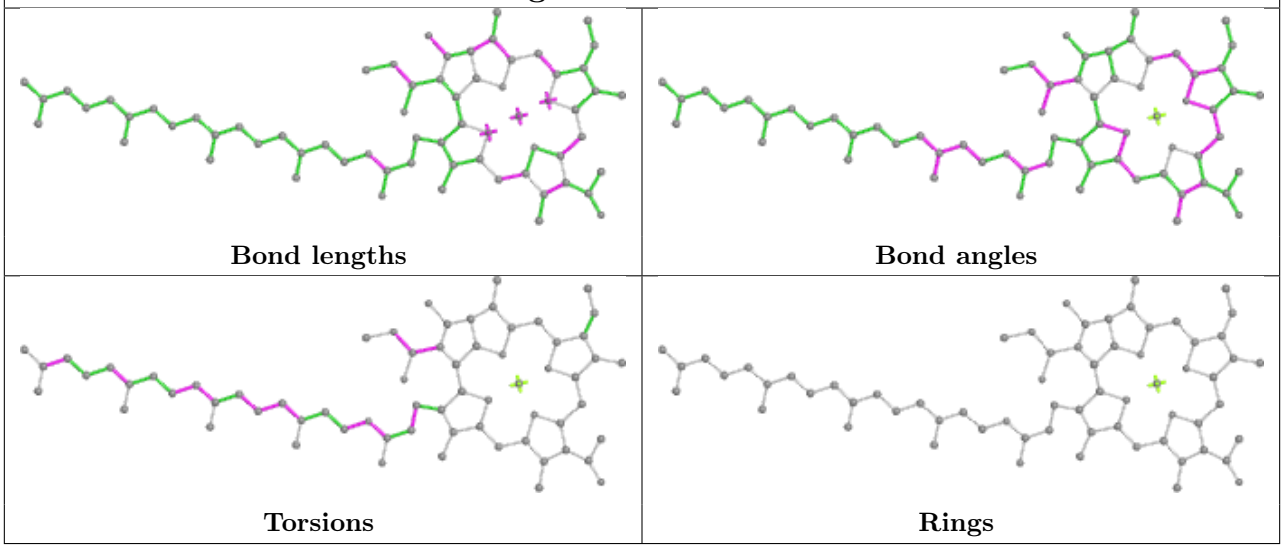
Ligand CRT G 103



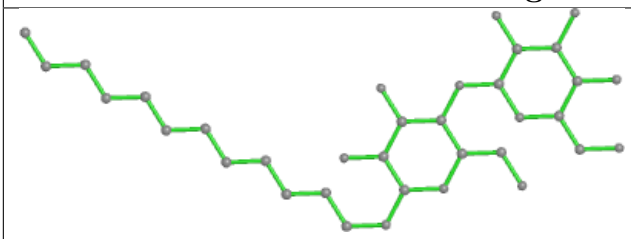
Ligand BCL F 101



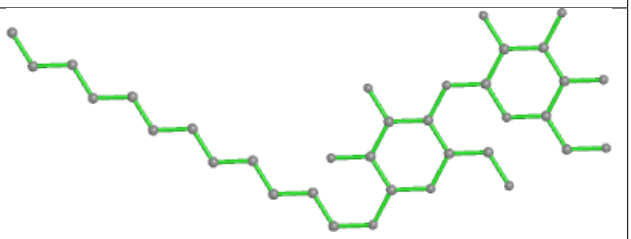
Ligand BCL L 509



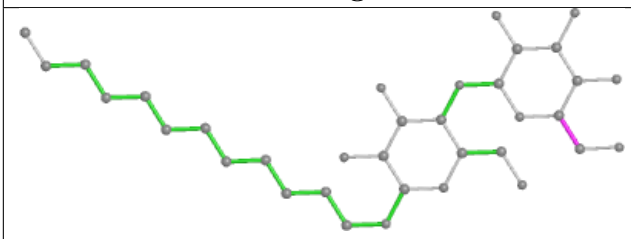
Ligand LMT 2 101



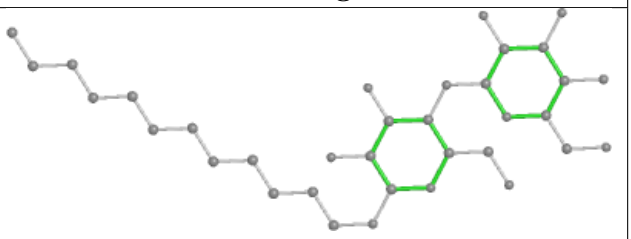
Bond lengths



Bond angles

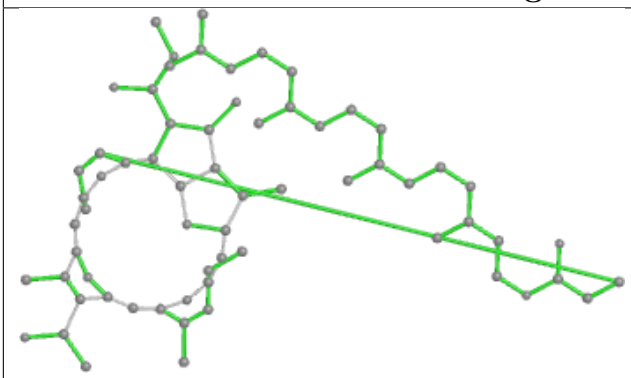


Torsions

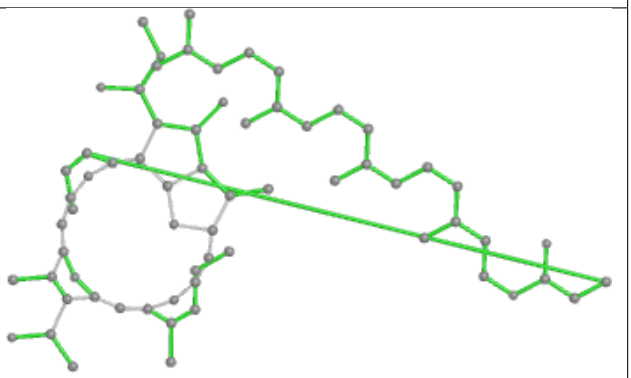


Rings

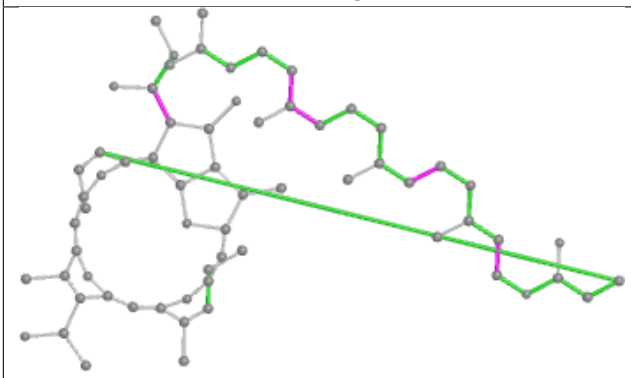
Ligand BPH L 503



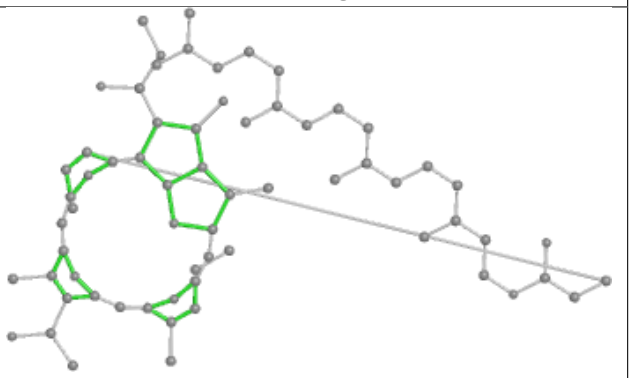
Bond lengths



Bond angles

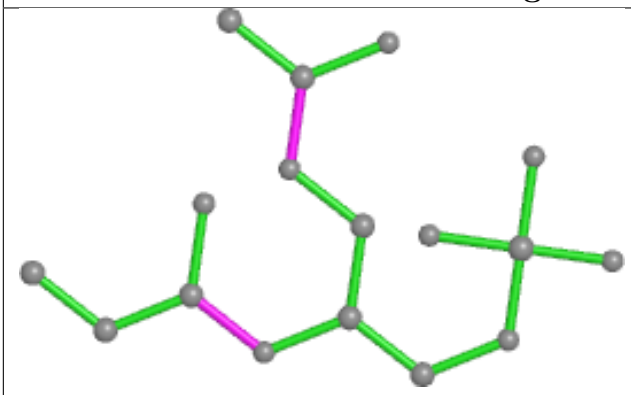


Torsions

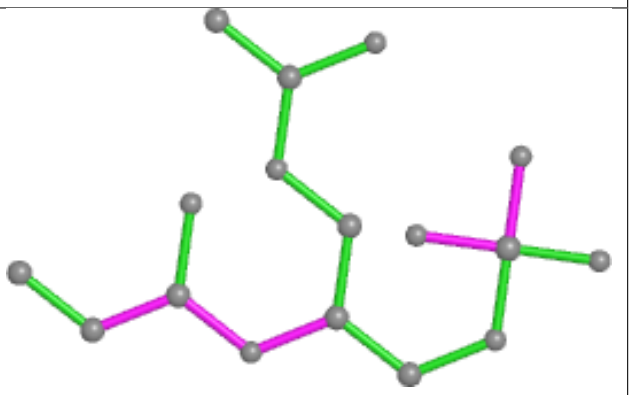


Rings

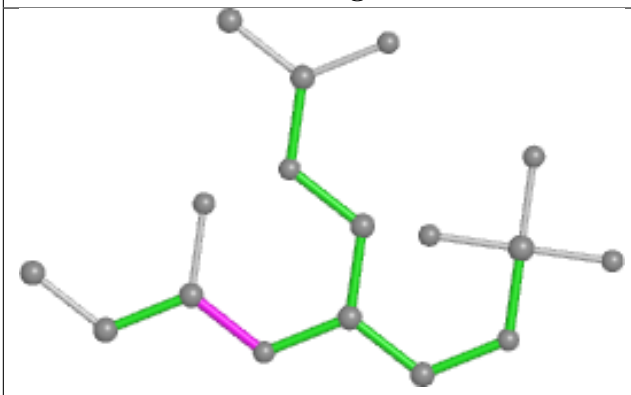
Ligand PGV L 501



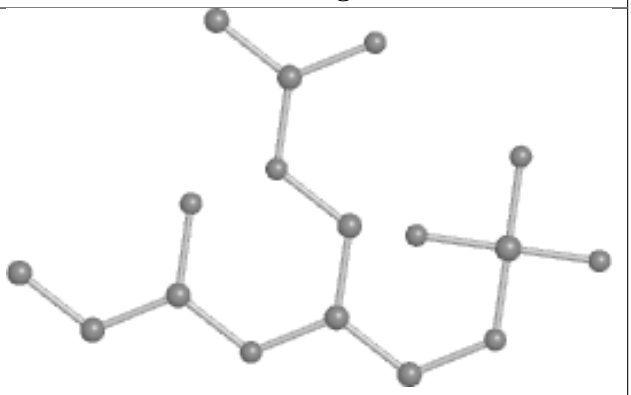
Bond lengths



Bond angles

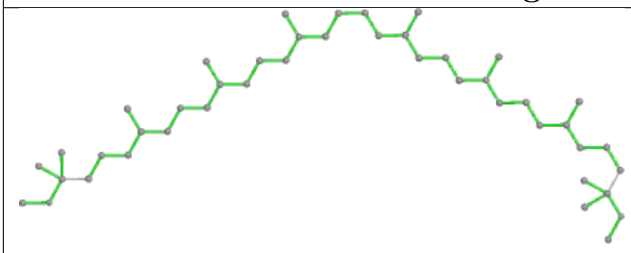


Torsions

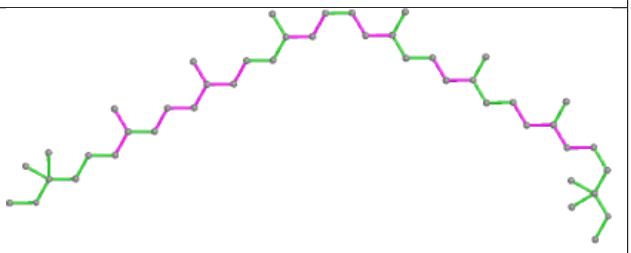


Rings

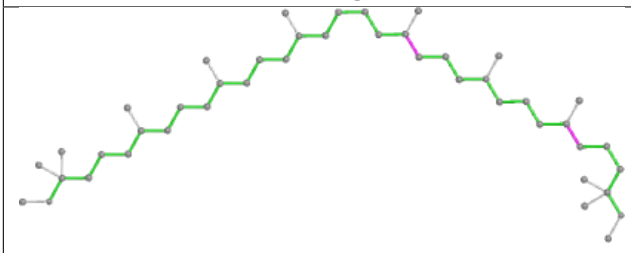
Ligand CRT N 102



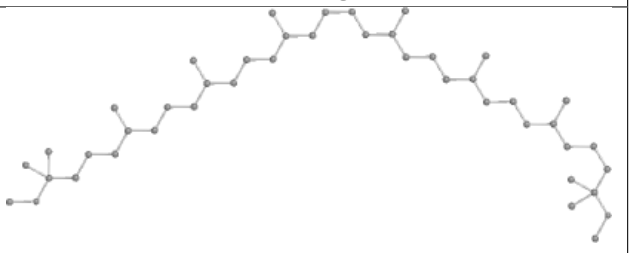
Bond lengths



Bond angles

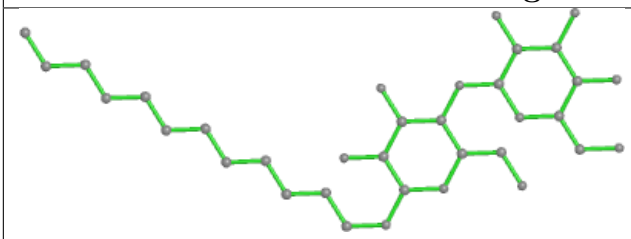


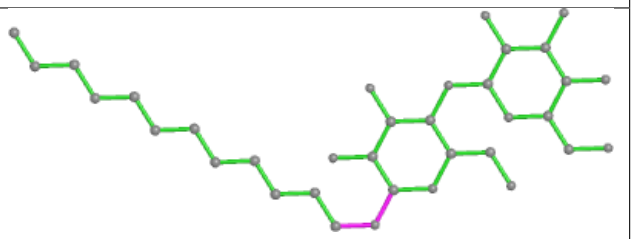
Torsions

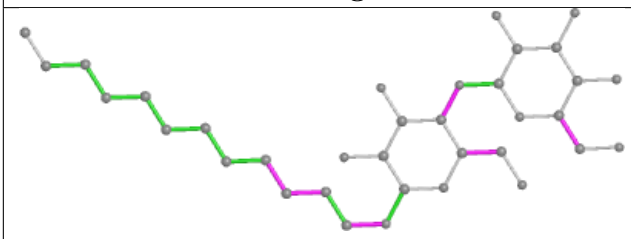


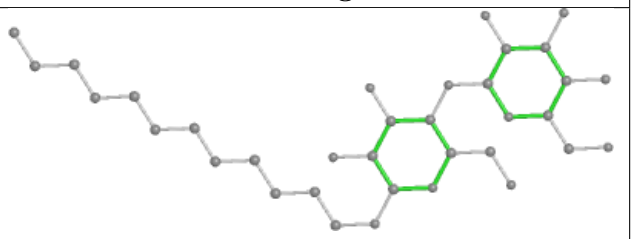
Rings

Ligand LMT Z 101

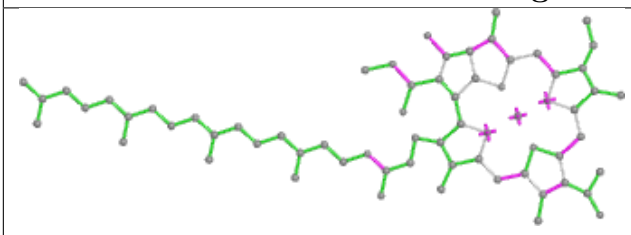

Bond lengths

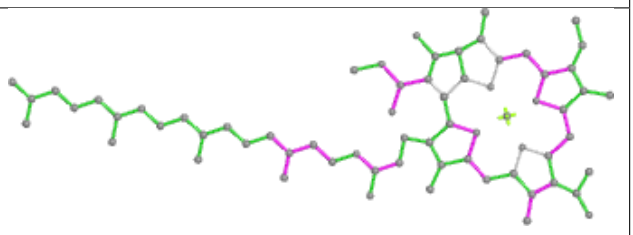

Bond angles

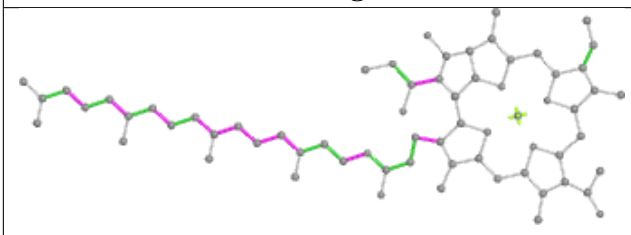

Torsions

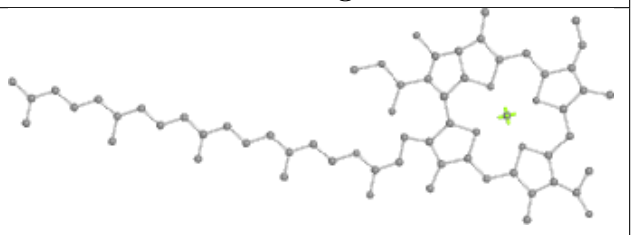

Rings

Ligand BCL I 102

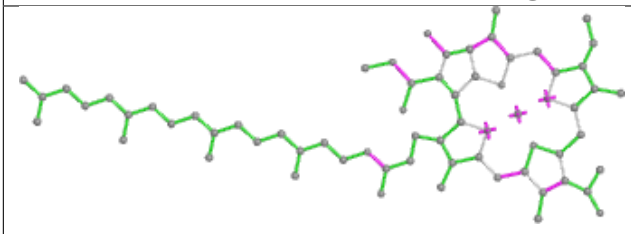

Bond lengths

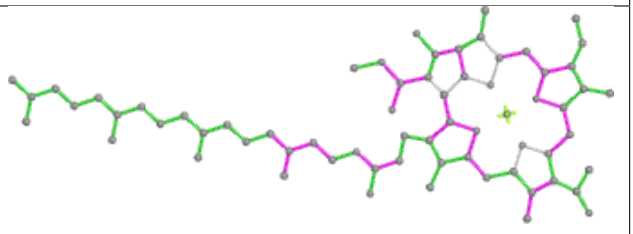

Bond angles

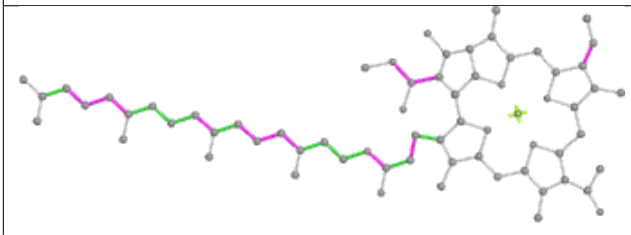

Torsions

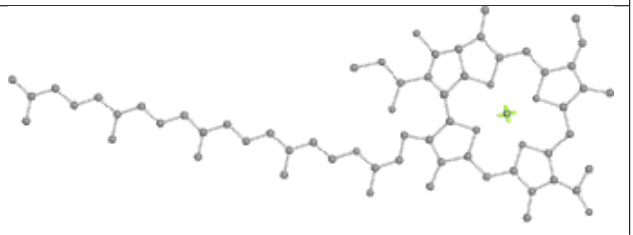

Rings

Ligand BCL K 103

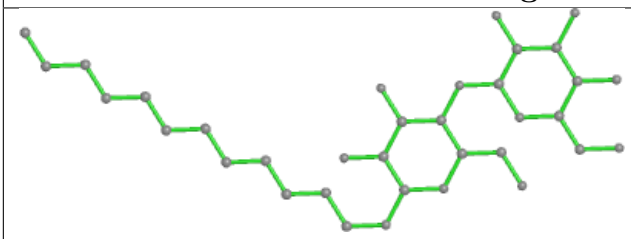

Bond lengths


Bond angles

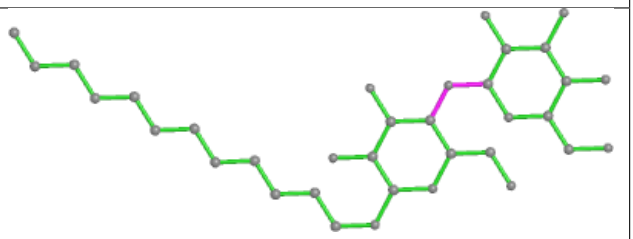

Torsions


Rings

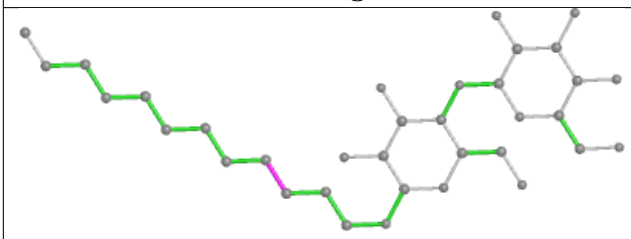
Ligand LMT H 304



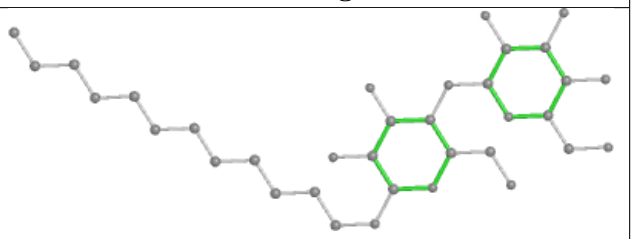
Bond lengths



Bond angles

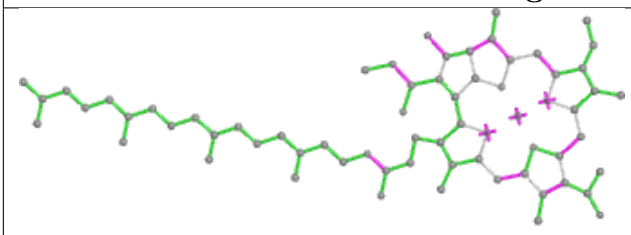


Torsions

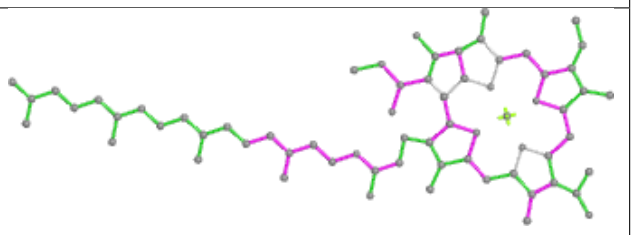


Rings

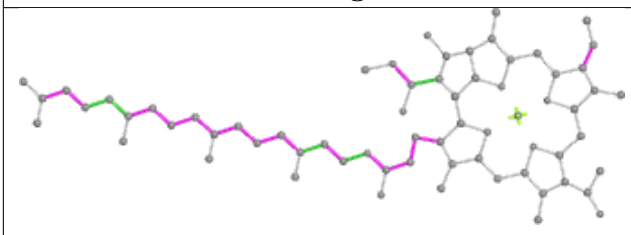
Ligand BCL P 101



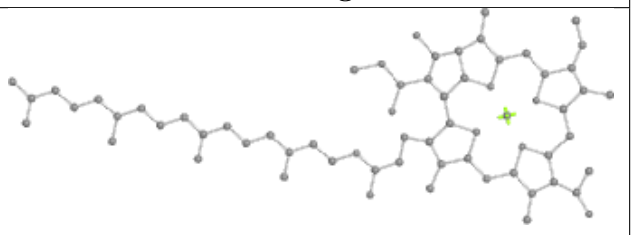
Bond lengths



Bond angles

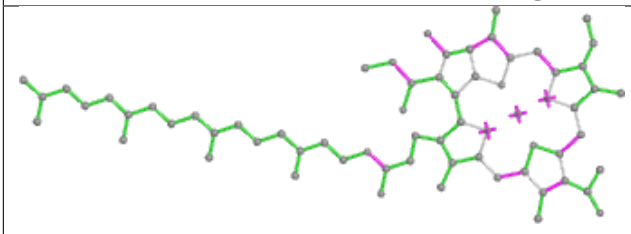


Torsions

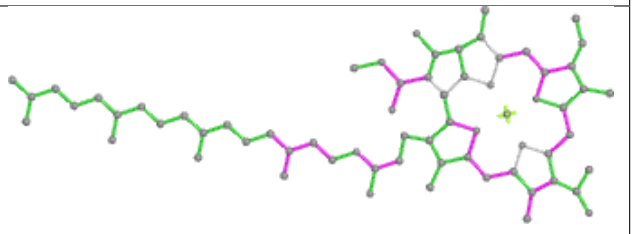


Rings

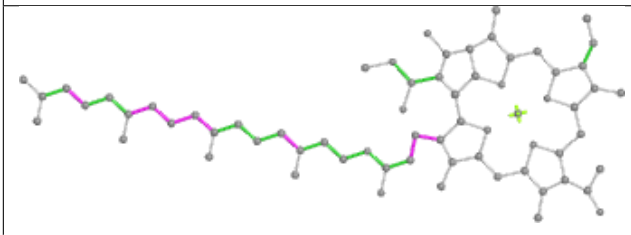
Ligand BCL 3 101



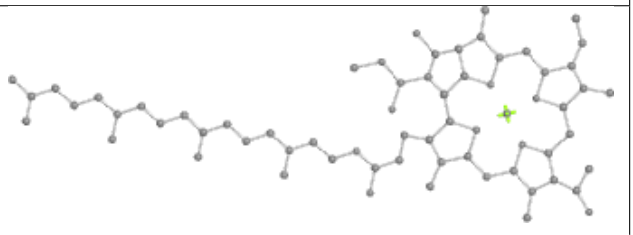
Bond lengths



Bond angles

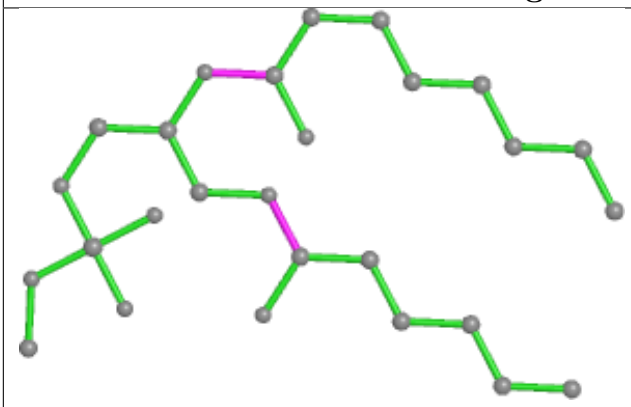


Torsions



Rings

Ligand PGV 1 401



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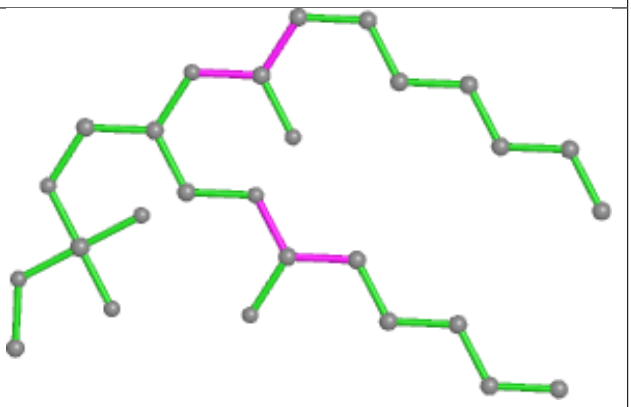
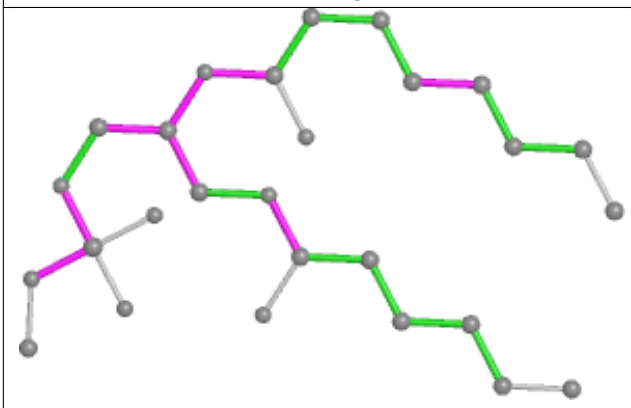


Bond angles



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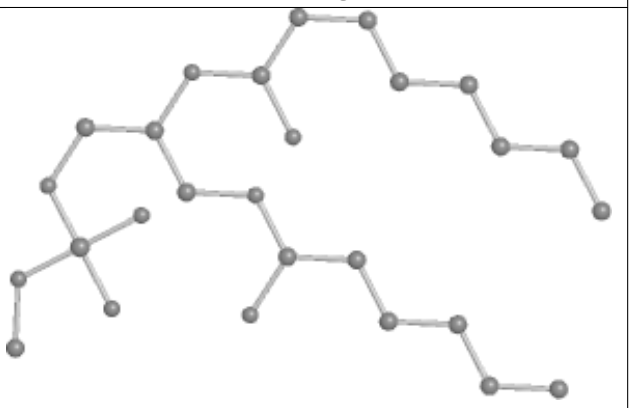
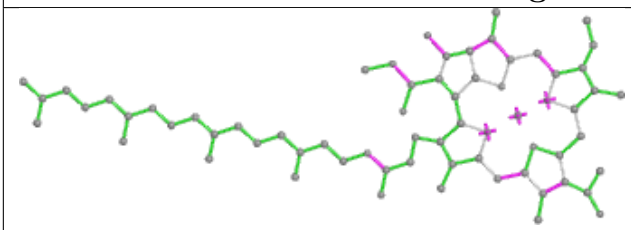
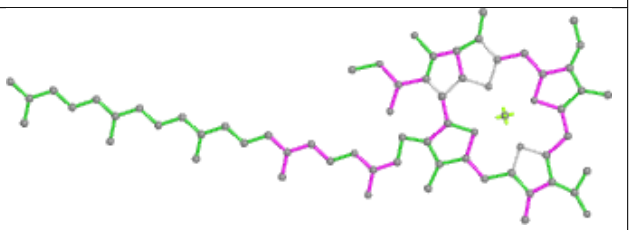


Rings

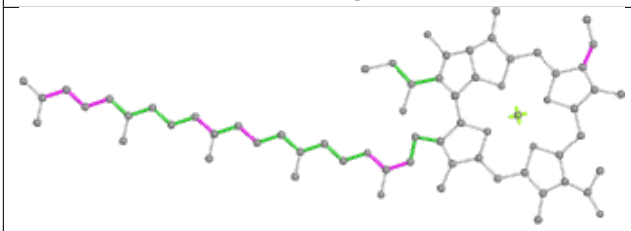
Ligand BCL 9 101



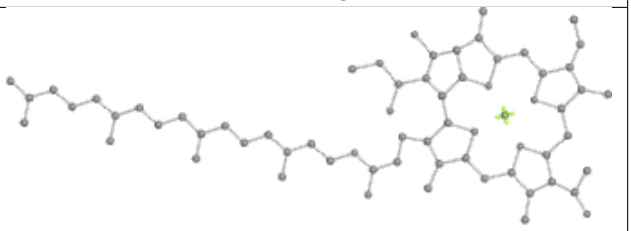
Bond lengths



Bond angles

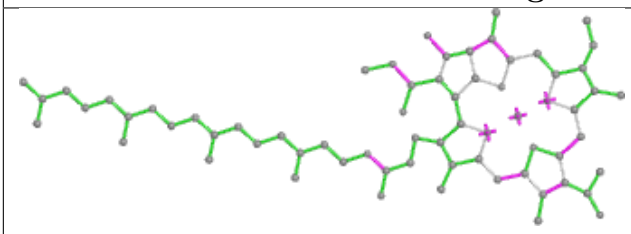


Torsions

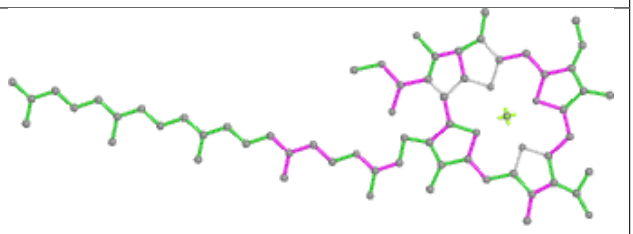


Rings

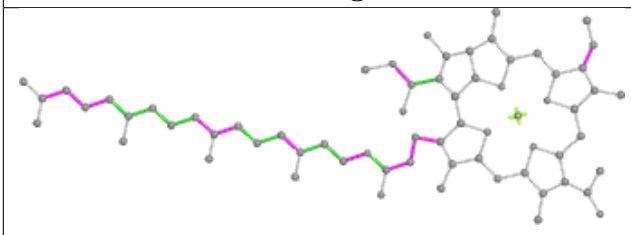
Ligand BCL Z 102



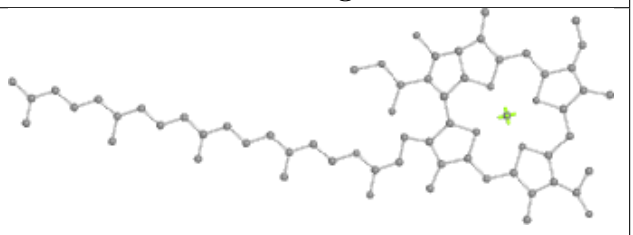
Bond lengths



Bond angles

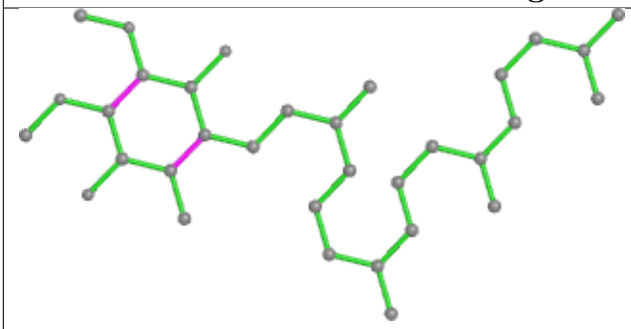


Torsions

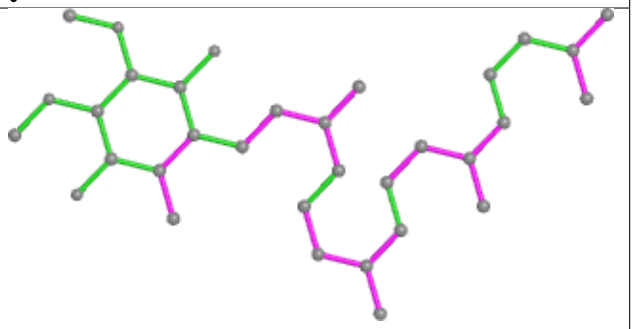


Rings

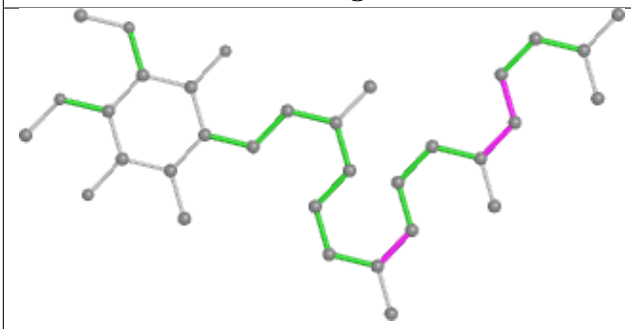
Ligand UQ8 L 512



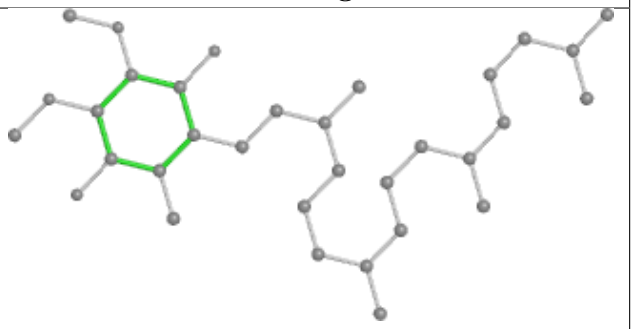
Bond lengths



Bond angles

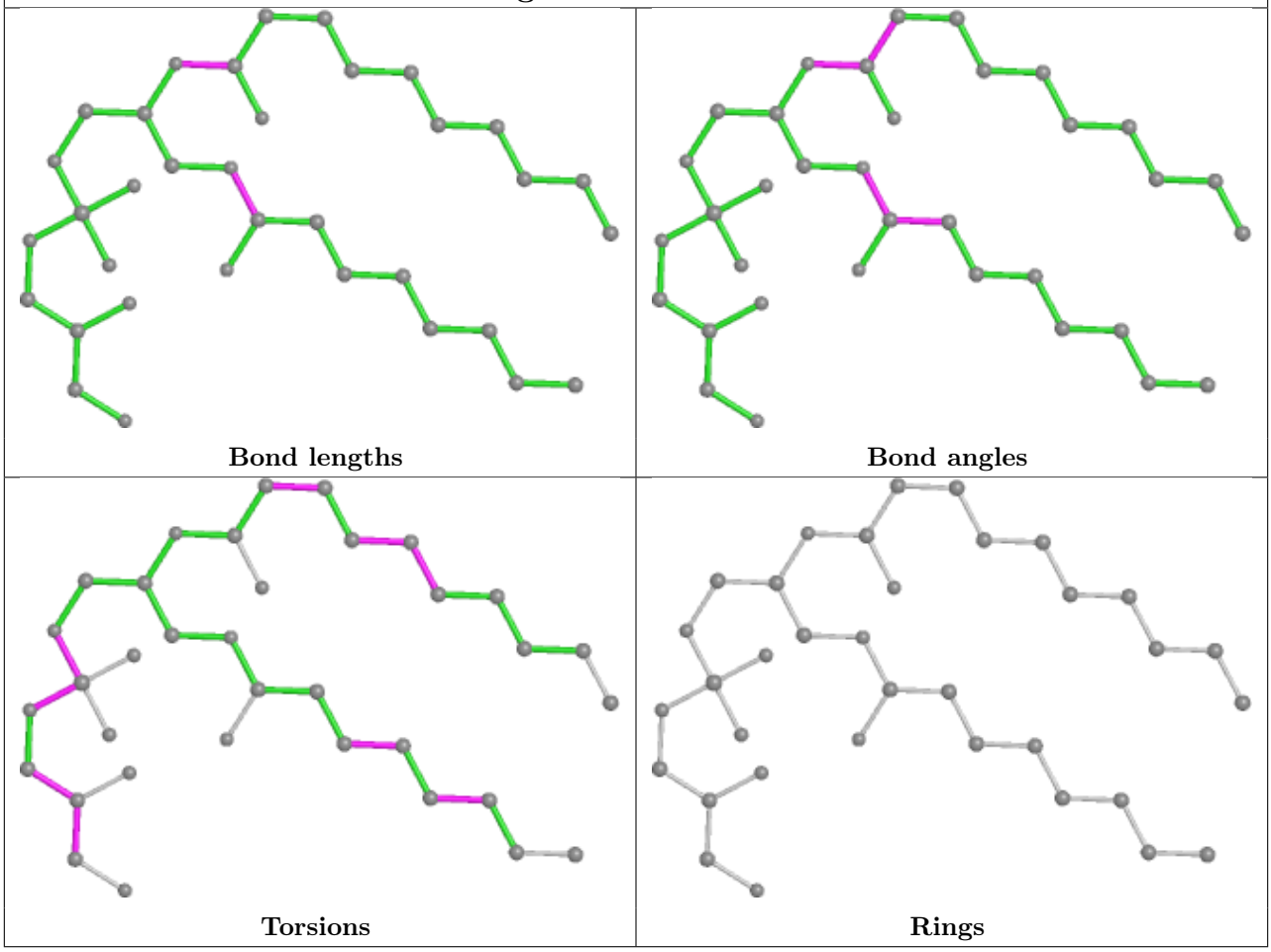


Torsions

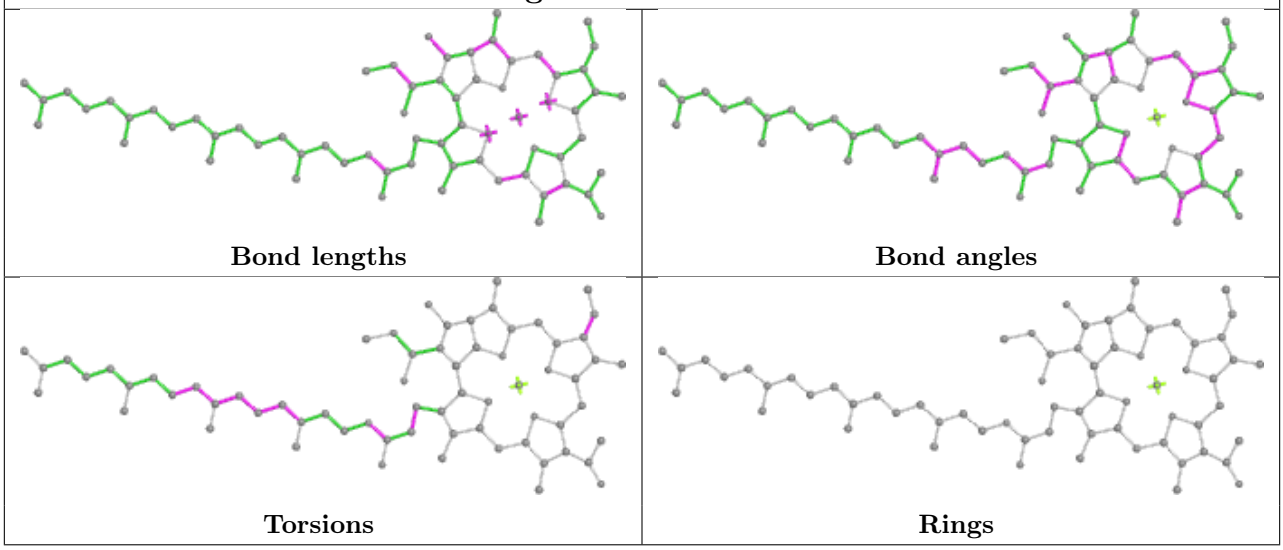


Rings

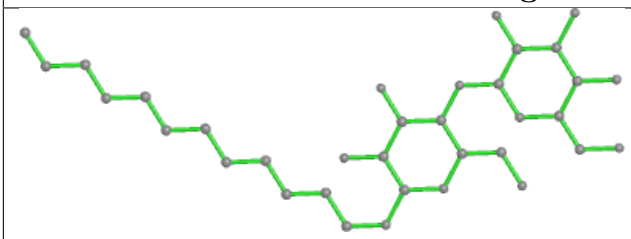
Ligand PGV D 101

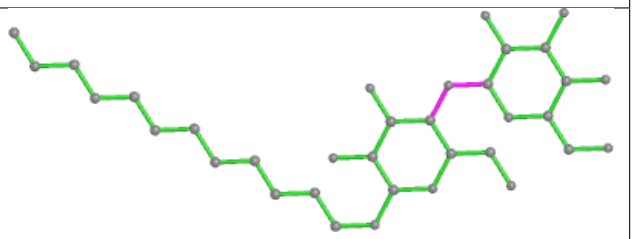


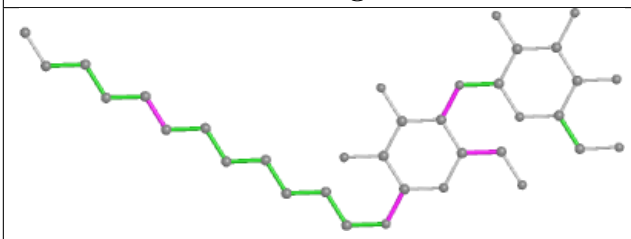
Ligand BCL D 103

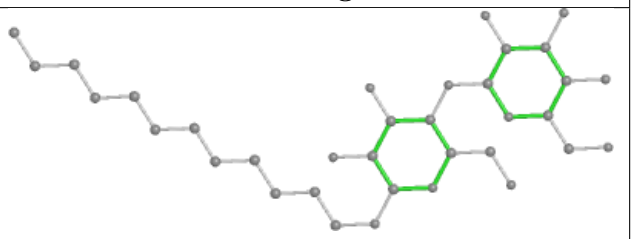


Ligand LMT G 101

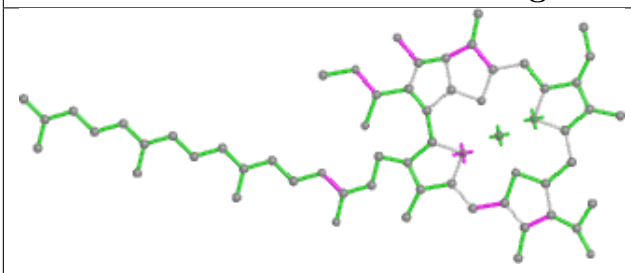

Bond lengths

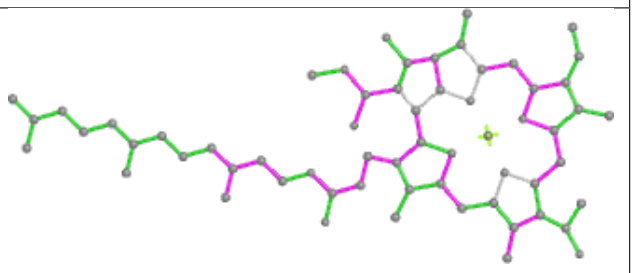

Bond angles

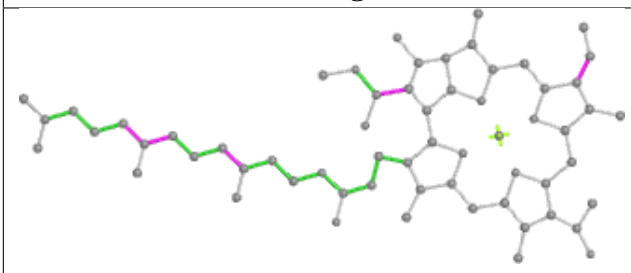

Torsions

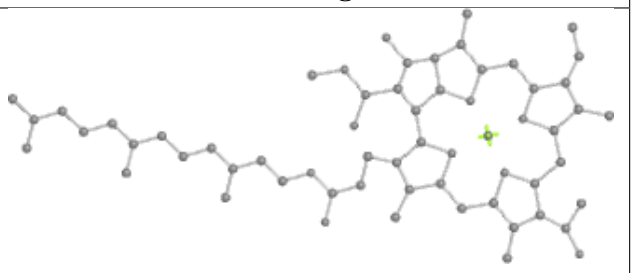

Rings

Ligand BCL 7 101

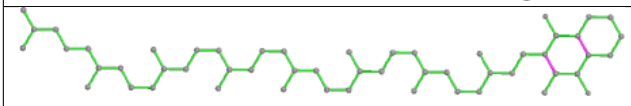

Bond lengths

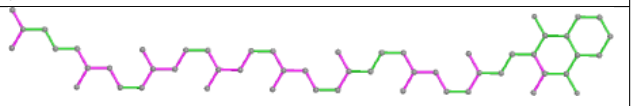

Bond angles

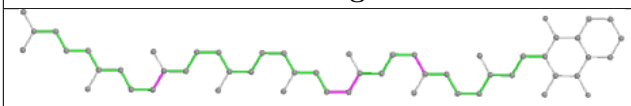

Torsions

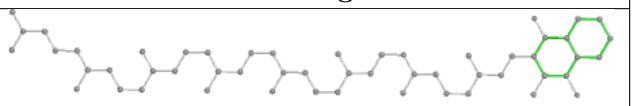

Rings

Ligand MQ8 M 404

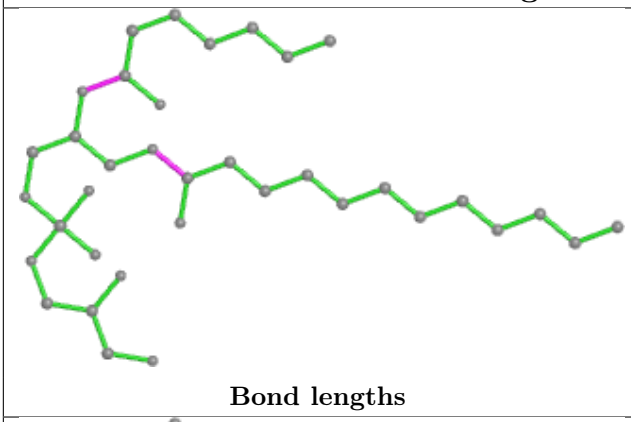

Bond lengths


Bond angles

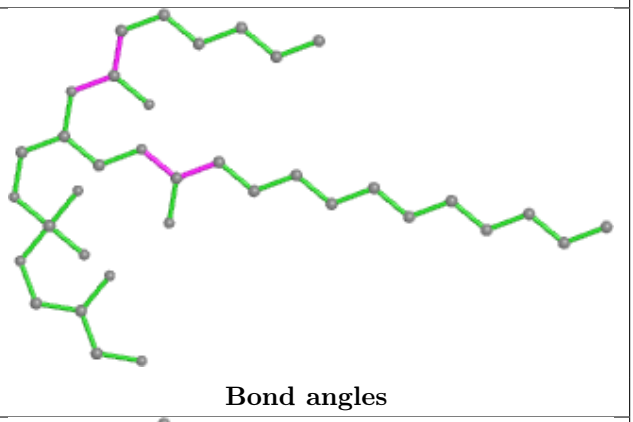

Torsions


Rings

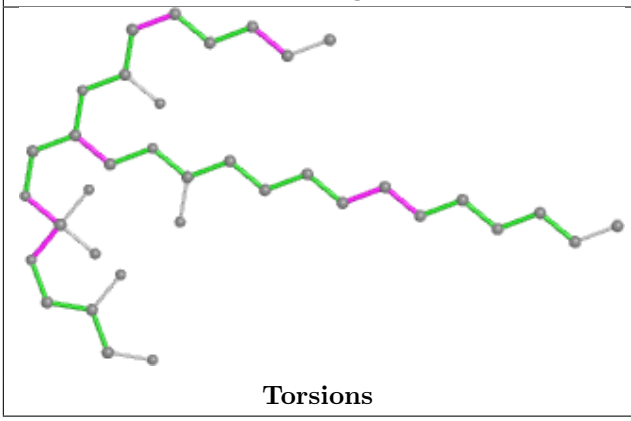
Ligand PGV H 303



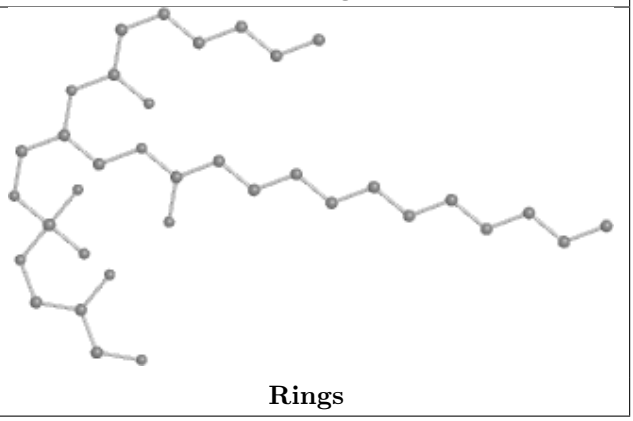
Bond lengths



Bond angles

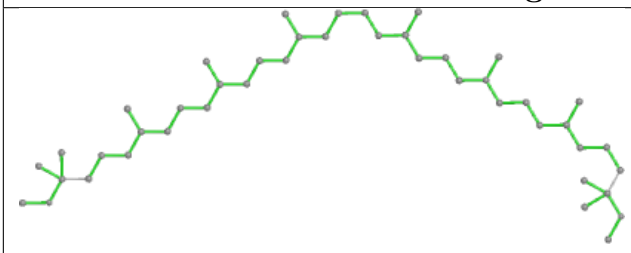


Torsions

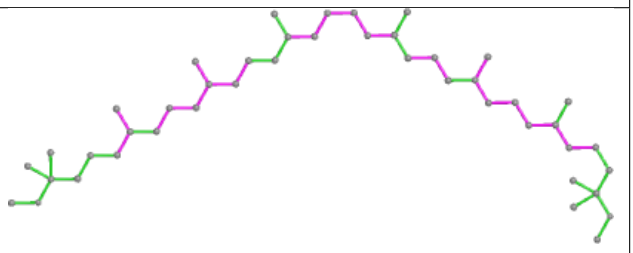


Rings

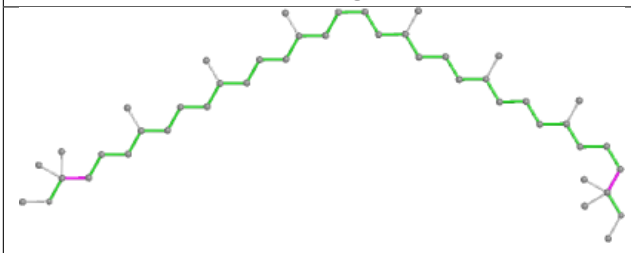
Ligand CRT E 103



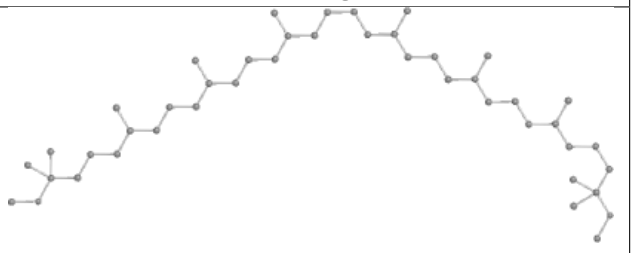
Bond lengths



Bond angles

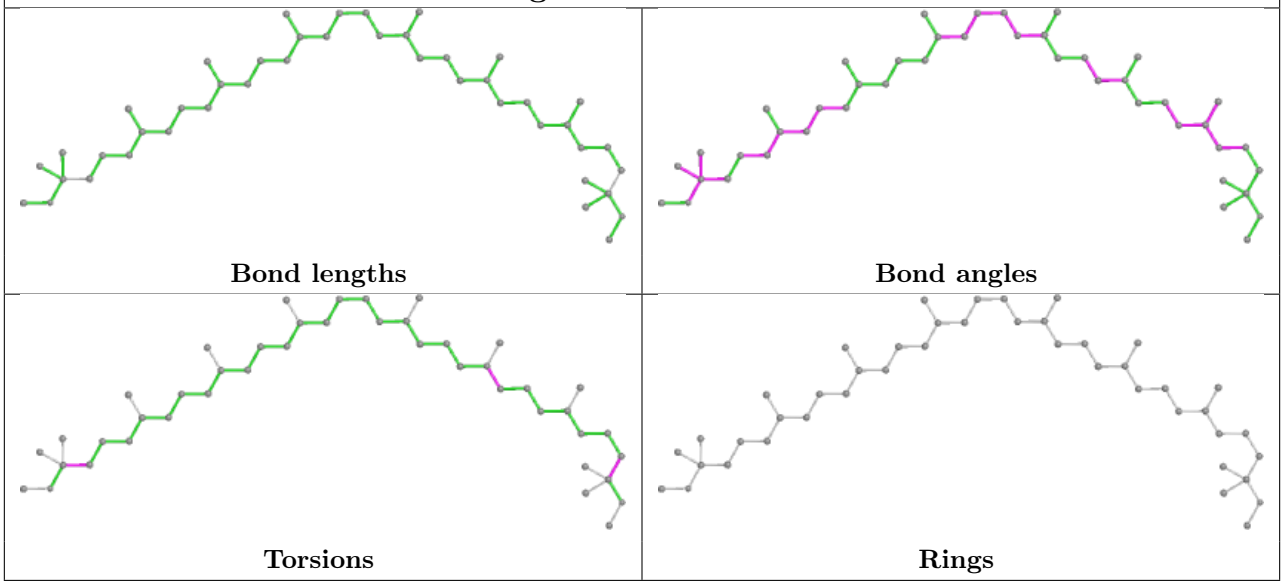


Torsions

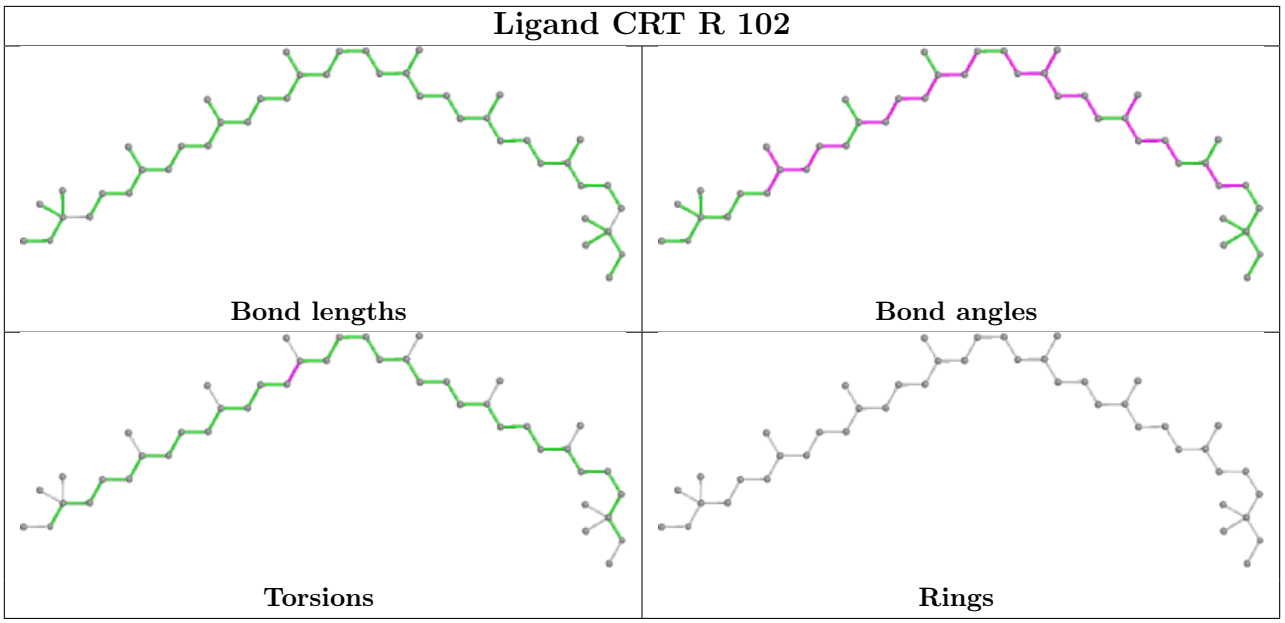


Rings

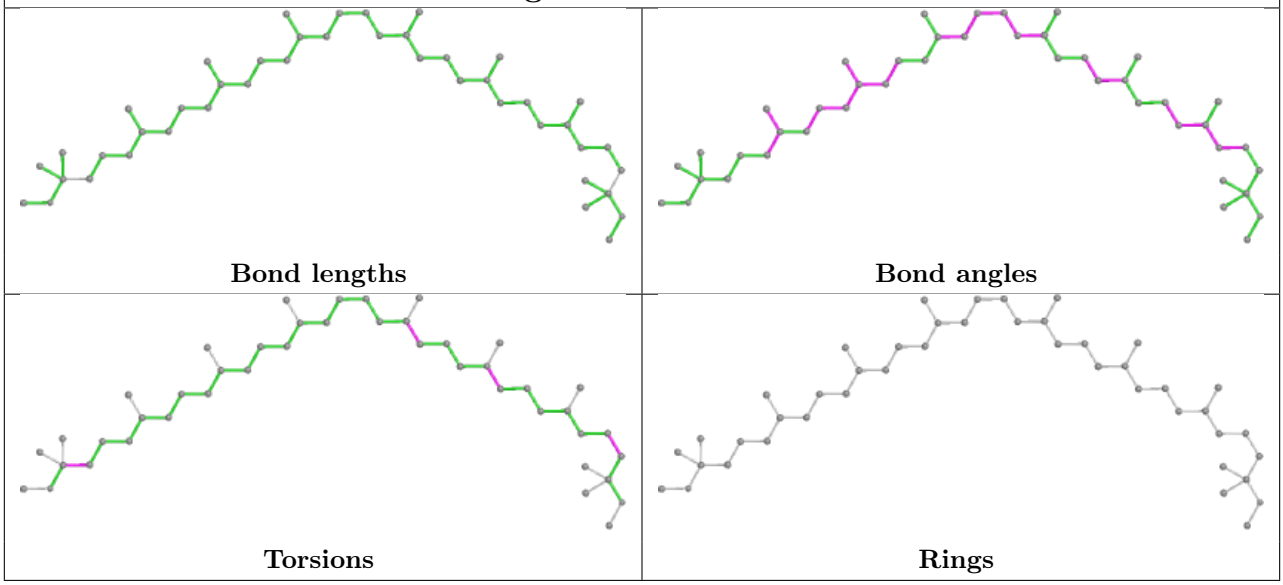
Ligand CRT 2 103



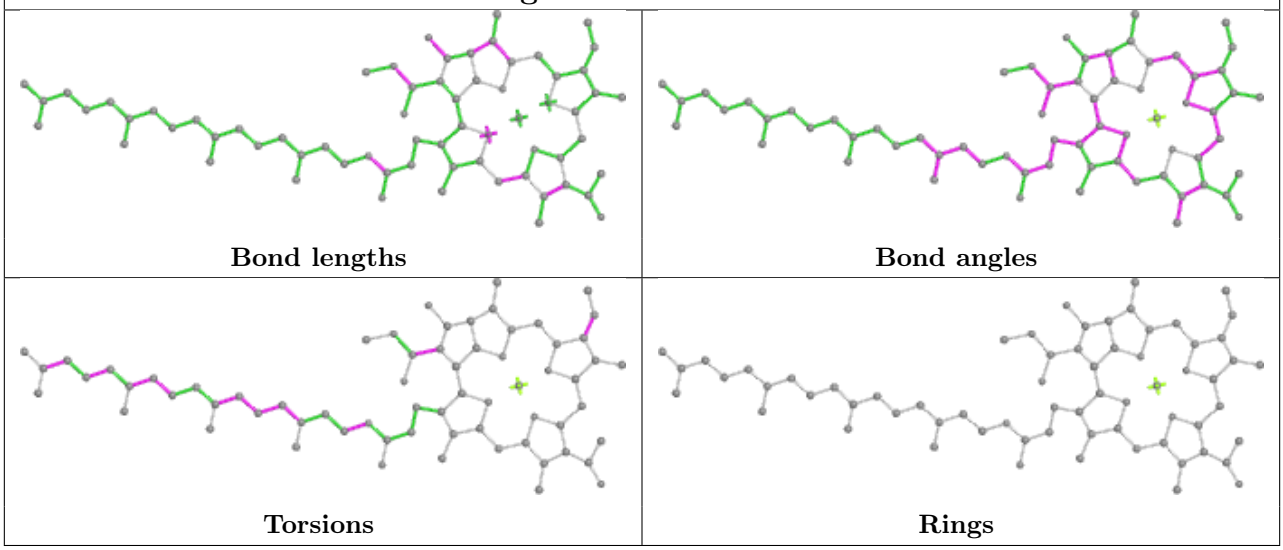
Ligand CRT R 102



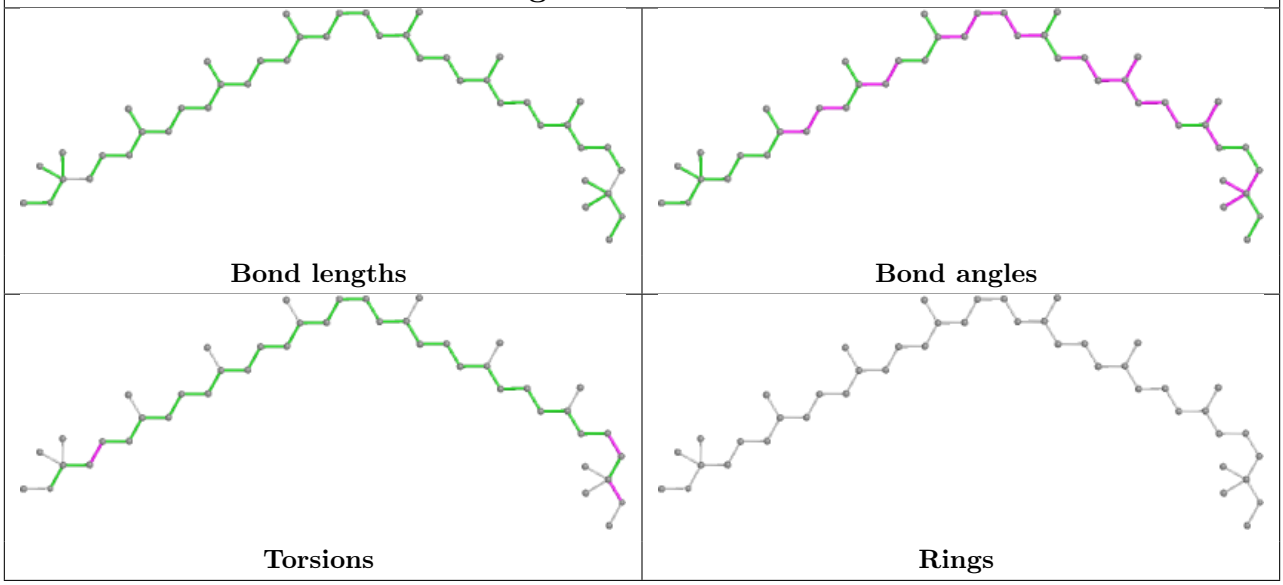
Ligand CRT X 103



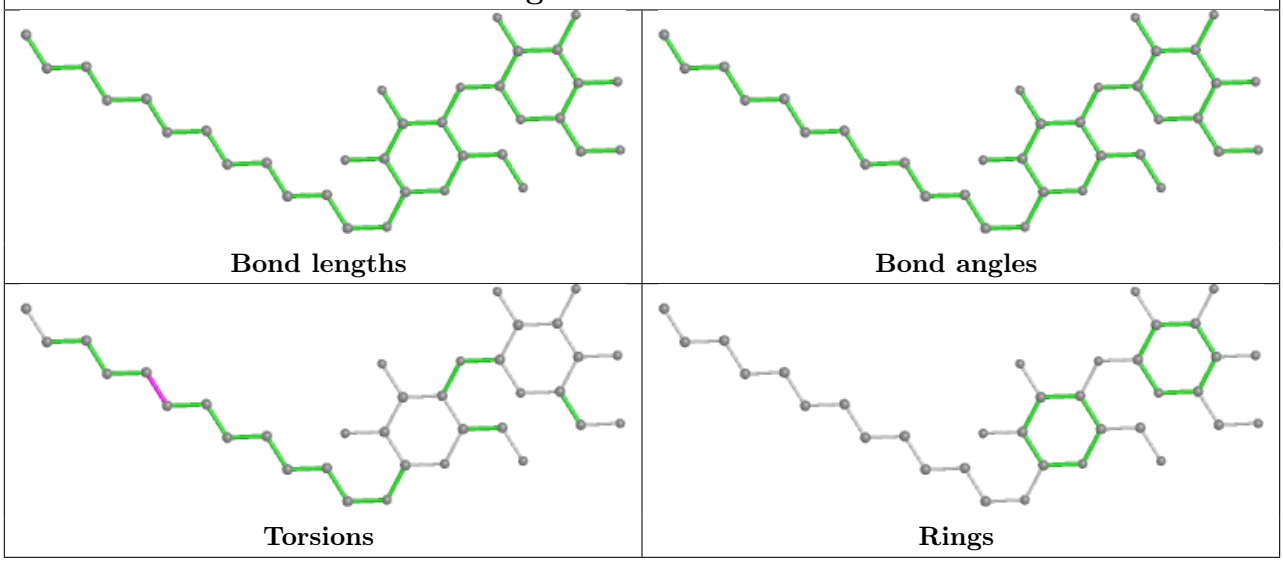
Ligand BCL W 101



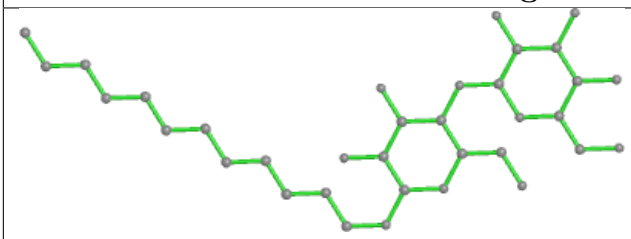
Ligand CRT J 103



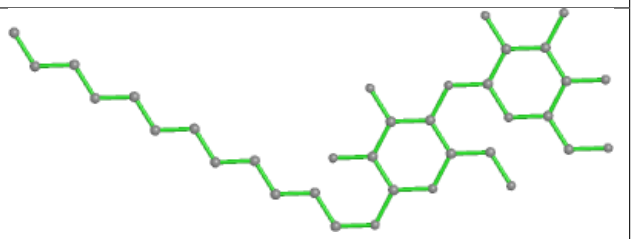
Ligand LMT J 104



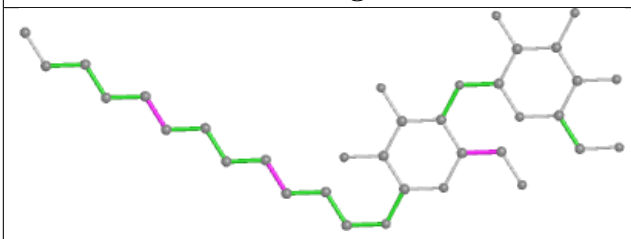
Ligand LMT K 102



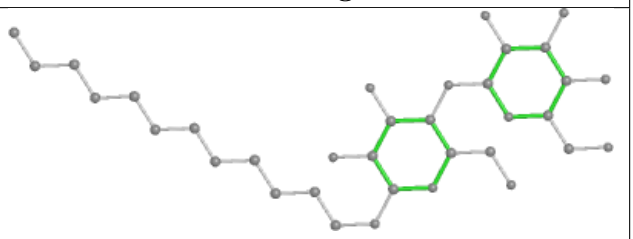
Bond lengths



Bond angles

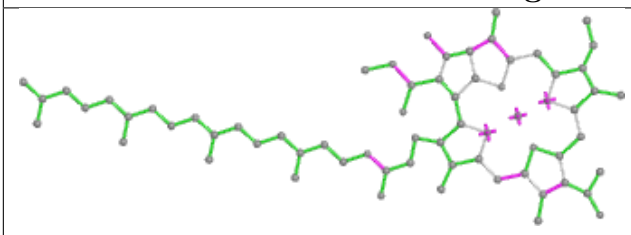


Torsions

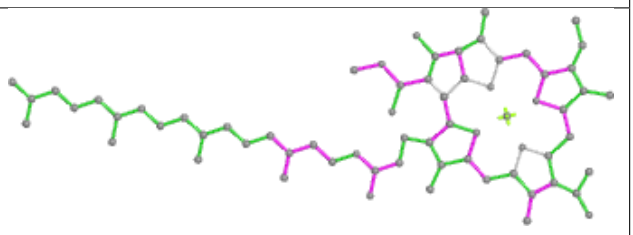


Rings

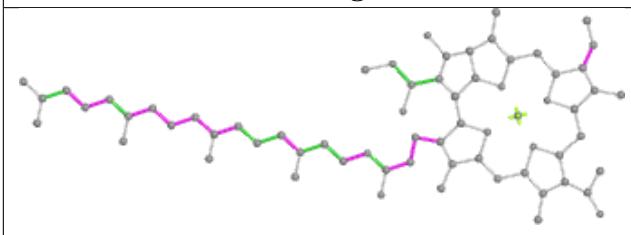
Ligand BCL V 102



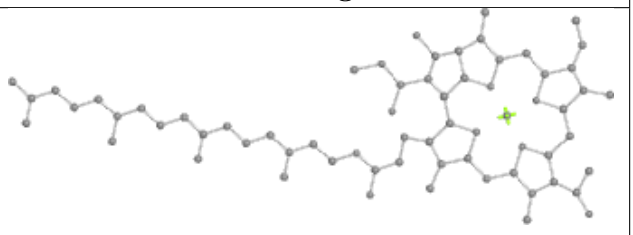
Bond lengths



Bond angles

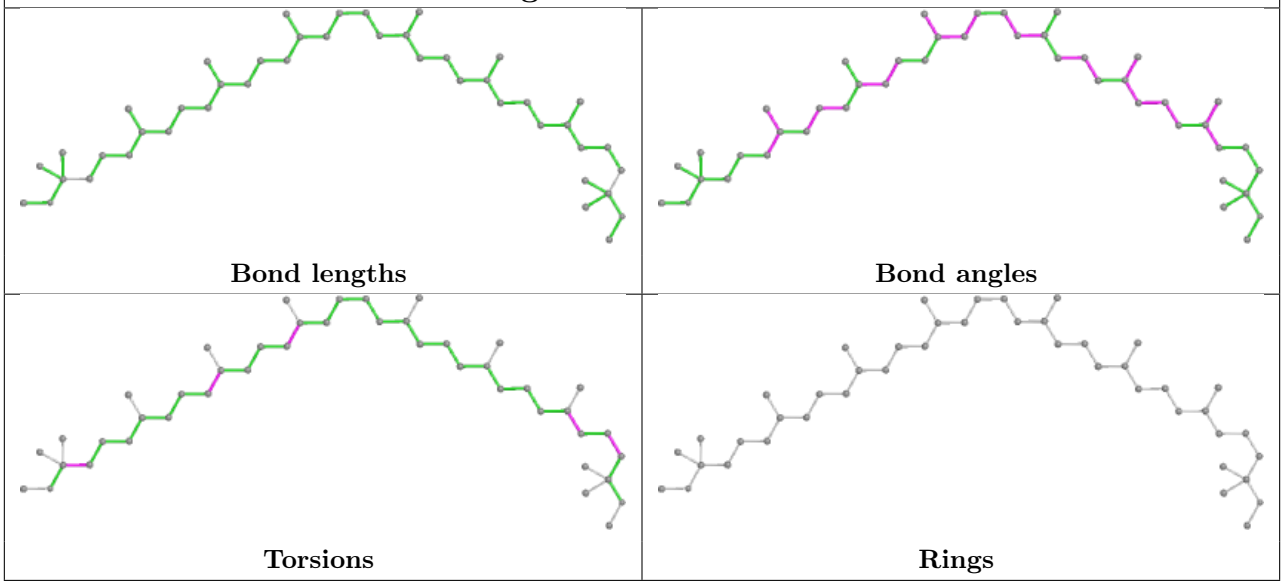


Torsions

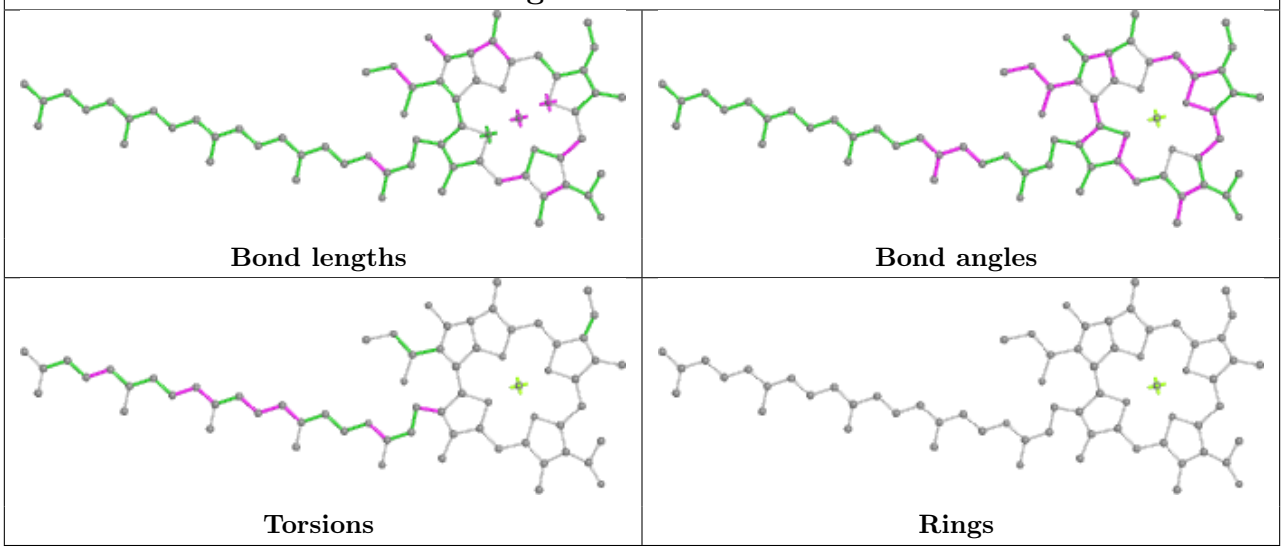


Rings

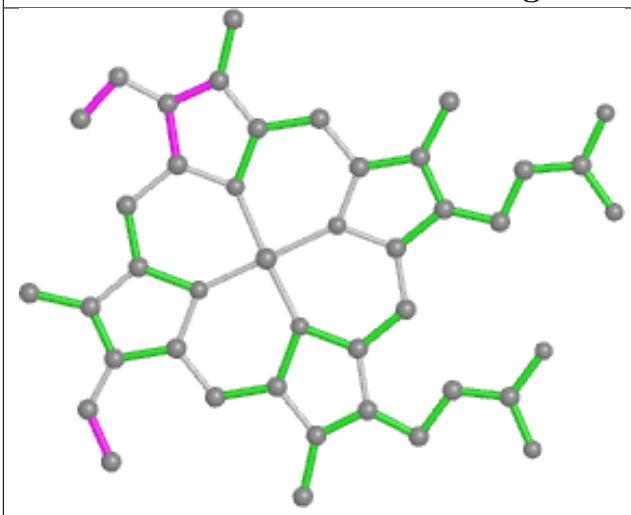
Ligand CRT M 405



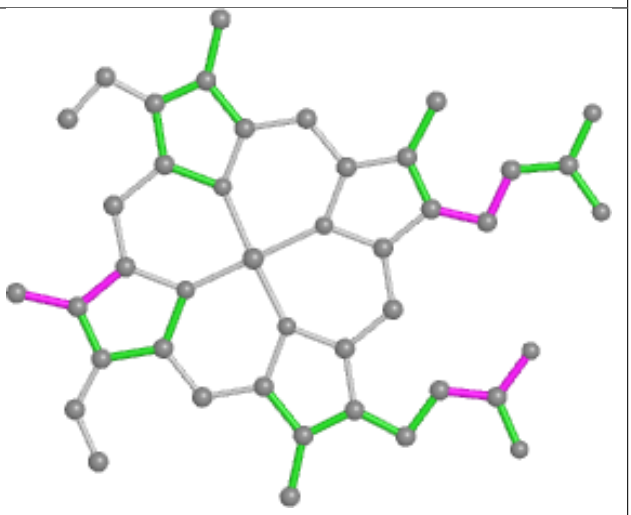
Ligand BCL T 102



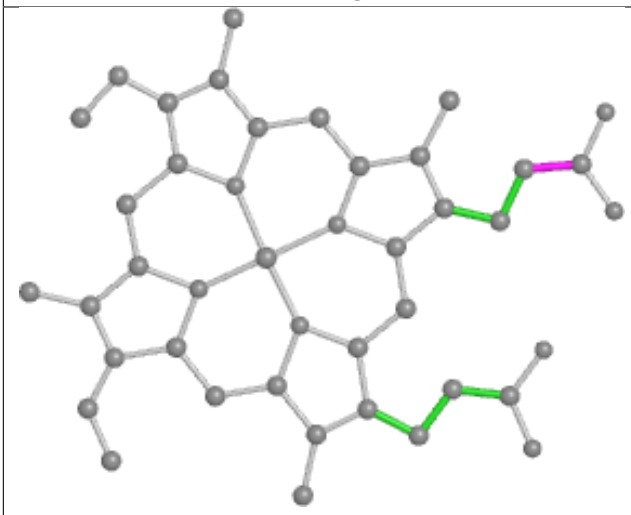
Ligand HEC C 504



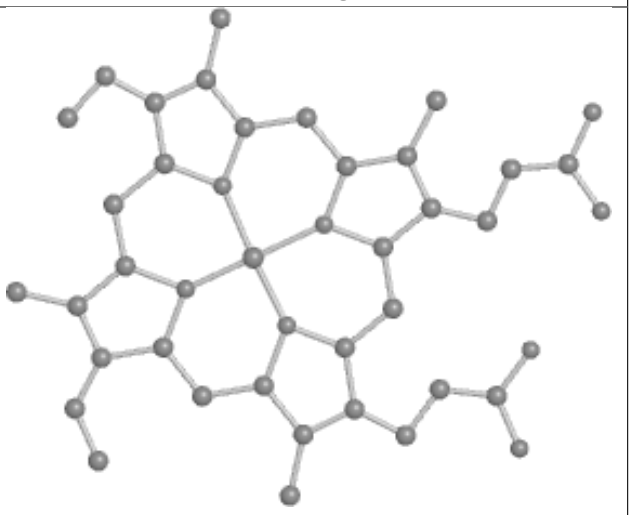
Bond lengths



Bond angles

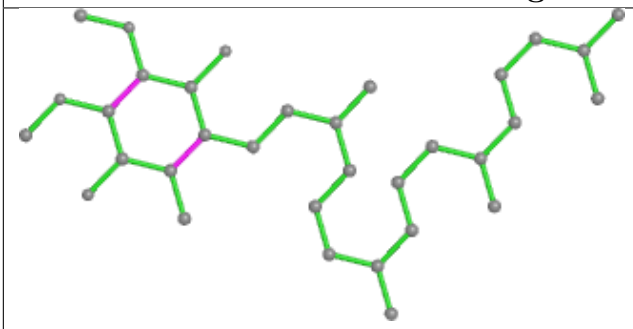


Torsions

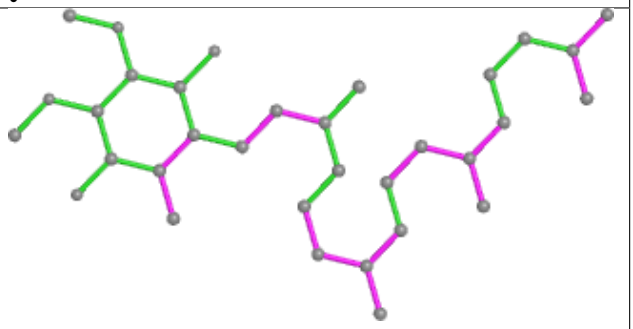


Rings

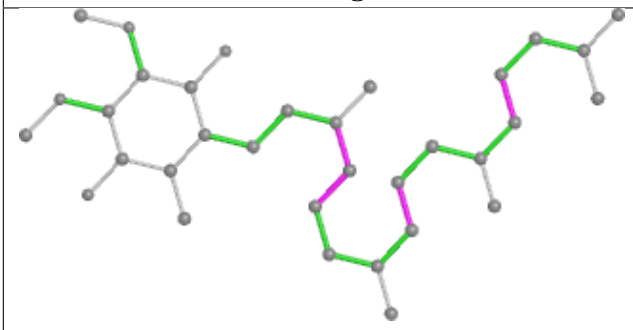
Ligand UQ8 L 504



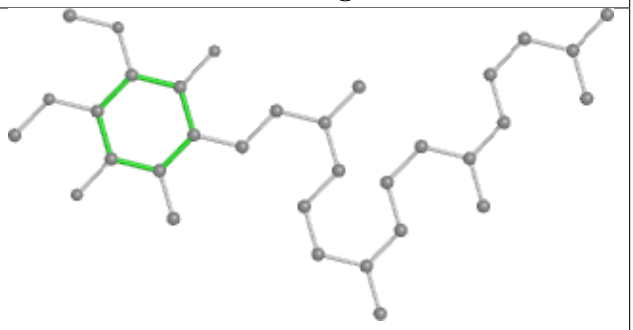
Bond lengths



Bond angles

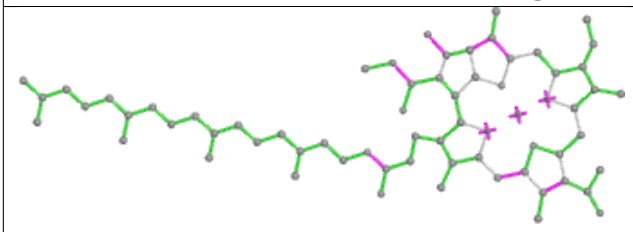


Torsions

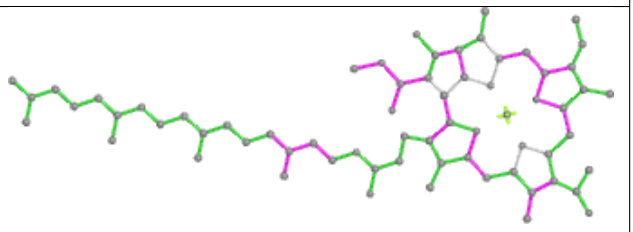


Rings

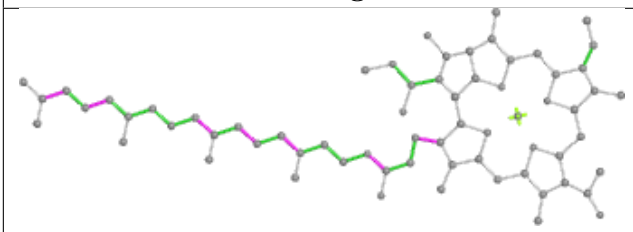
Ligand BCL 0 102



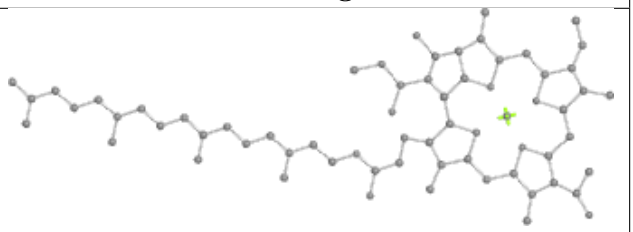
Bond lengths



Bond angles

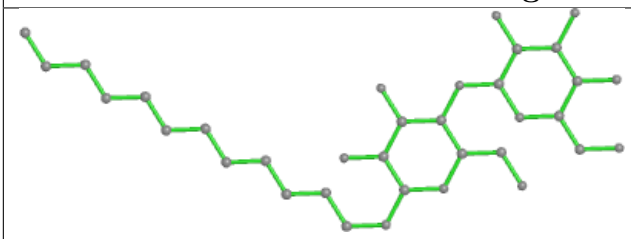


Torsions

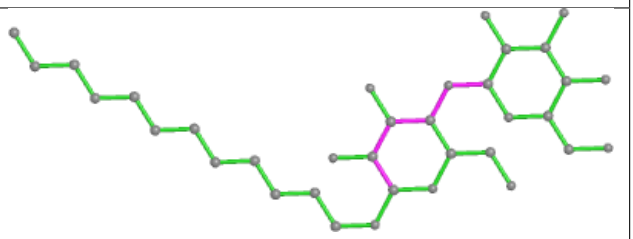


Rings

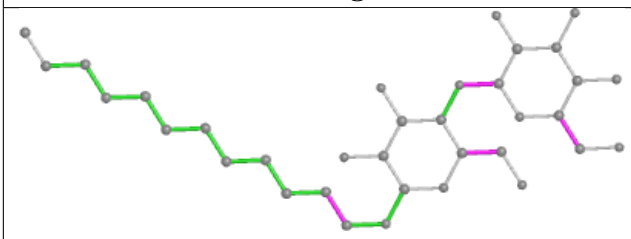
Ligand LMT E 101



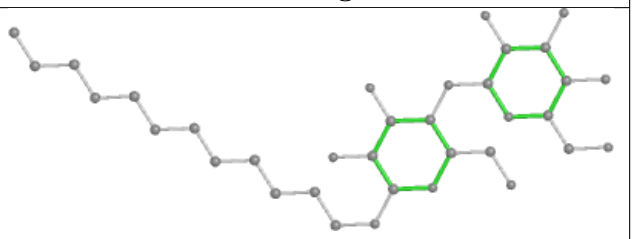
Bond lengths



Bond angles

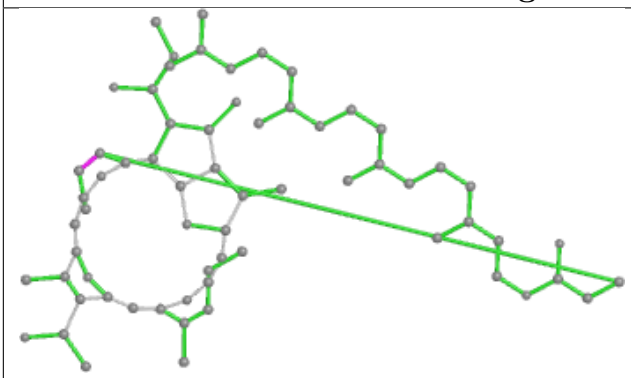


Torsions

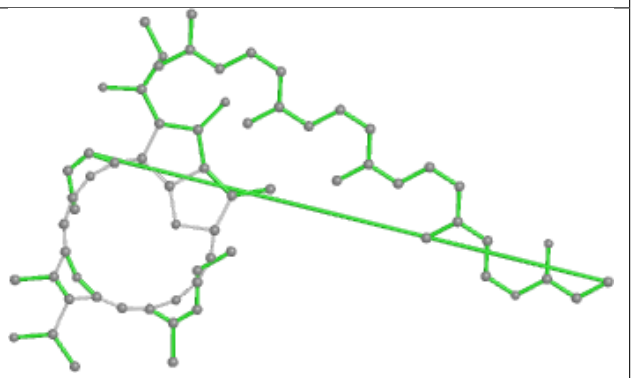


Rings

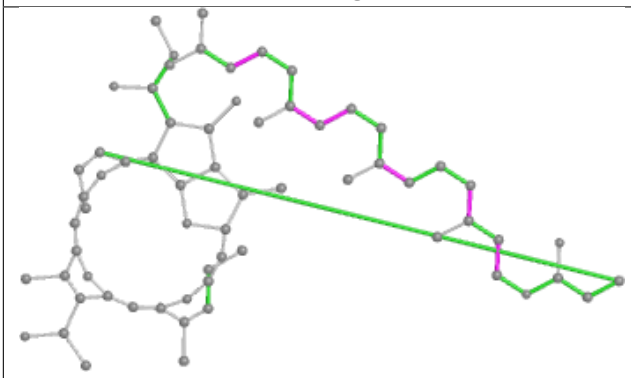
Ligand BPH M 403



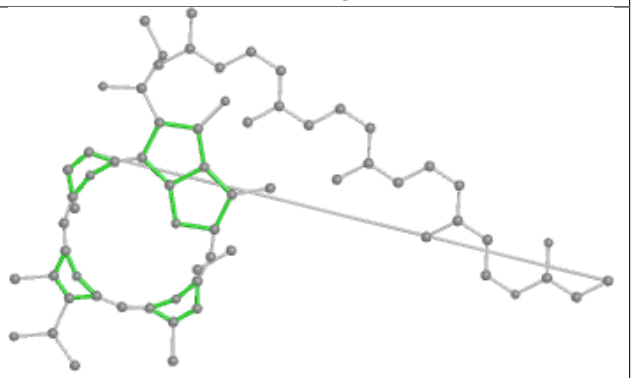
Bond lengths



Bond angles

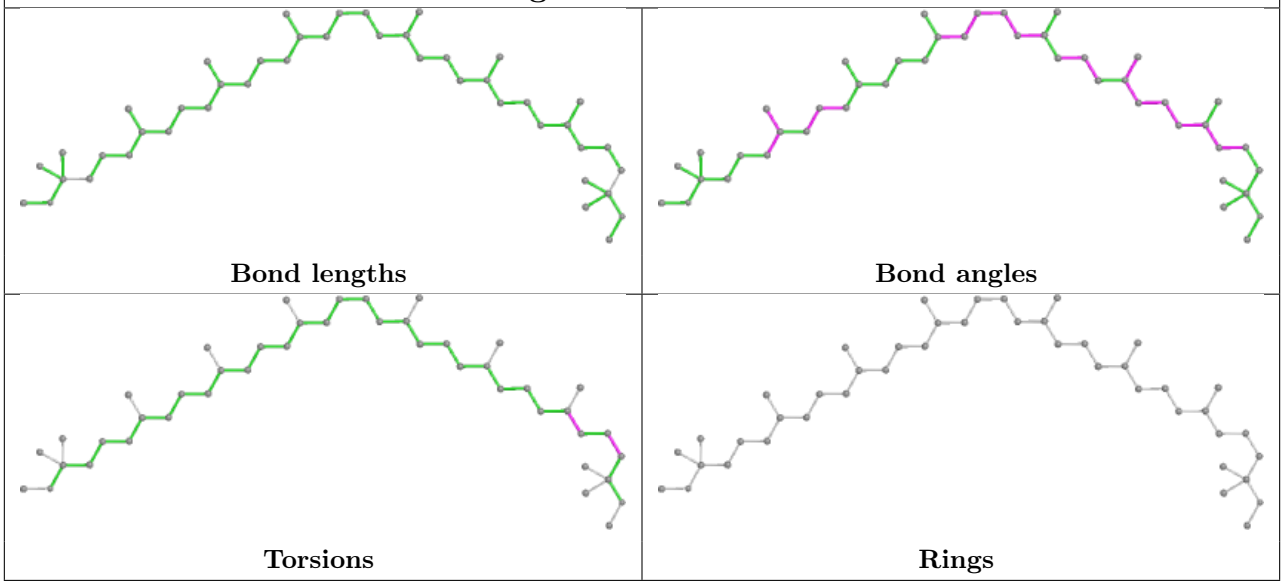


Torsions

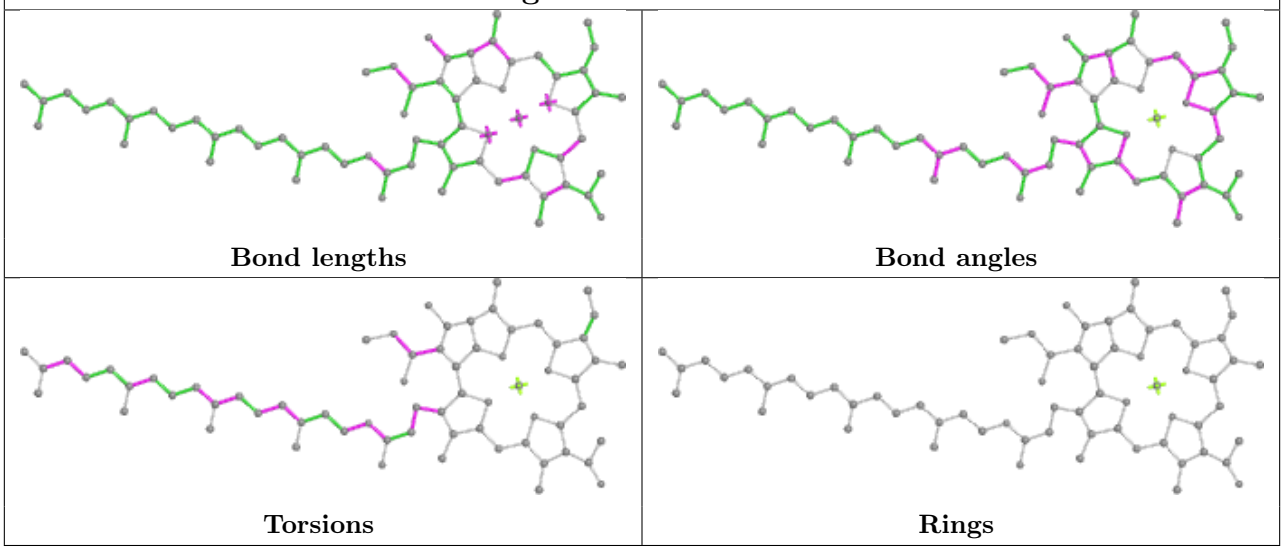


Rings

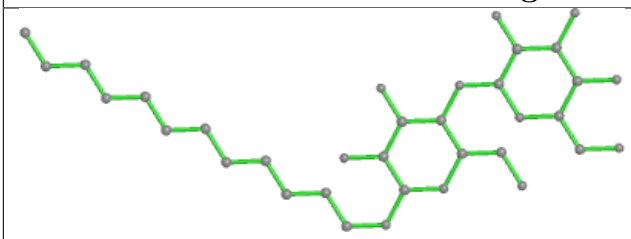
Ligand CRT 8 103



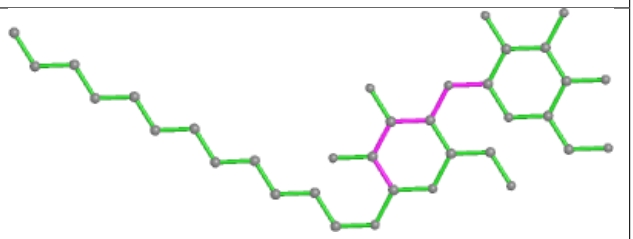
Ligand BCL M 402



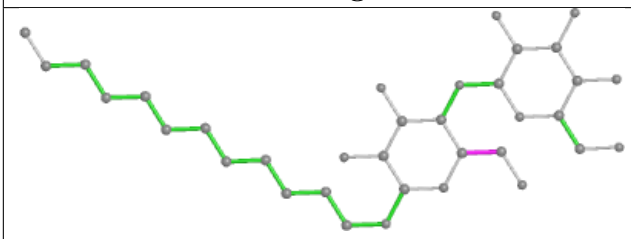
Ligand LMT X 101



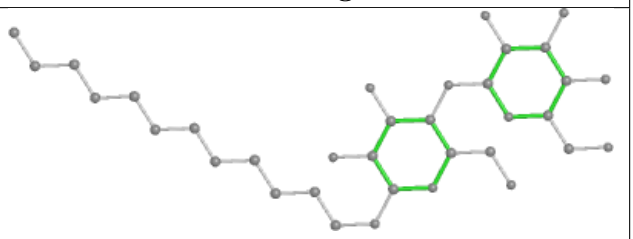
Bond lengths



Bond angles

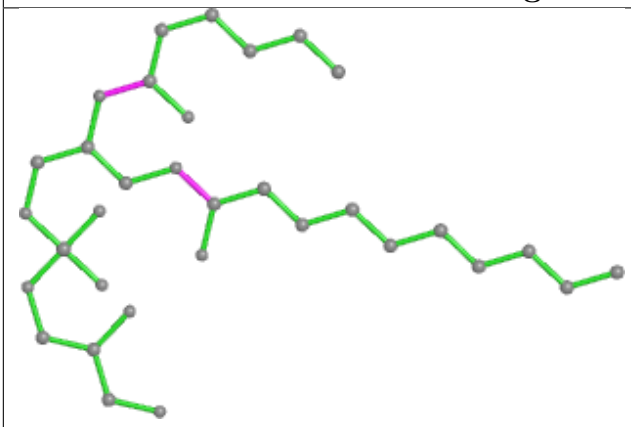


Torsions

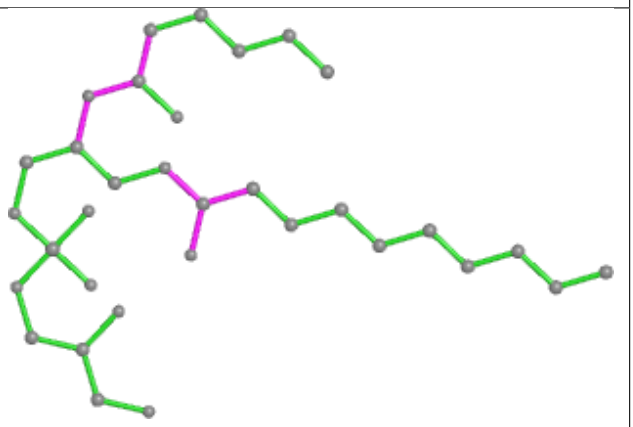


Rings

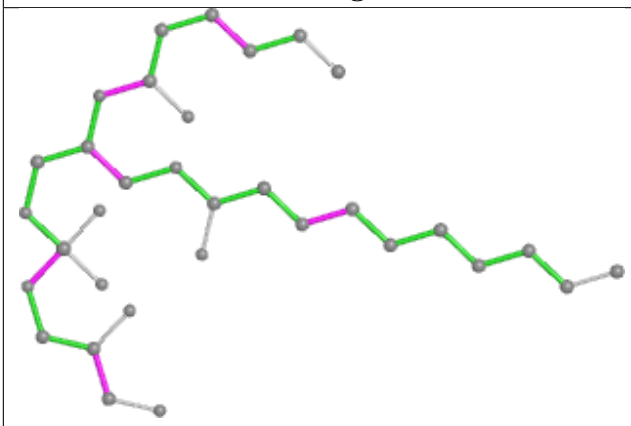
Ligand PGV L 511



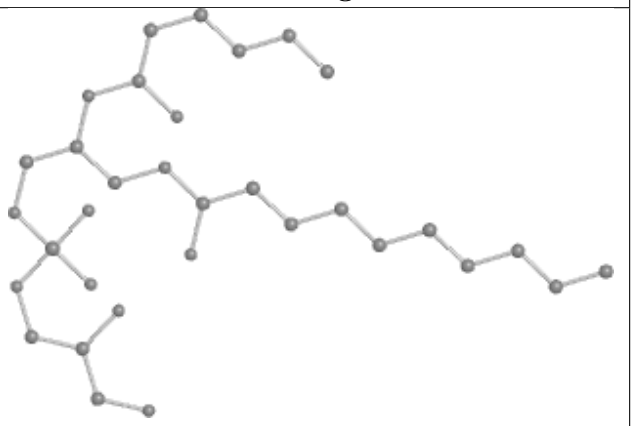
Bond lengths



Bond angles

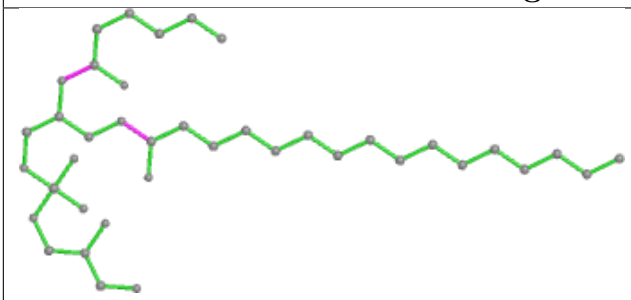


Torsions

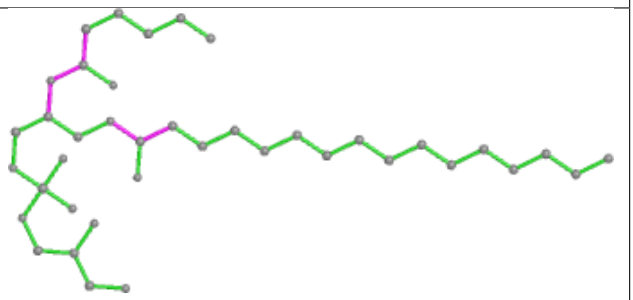


Rings

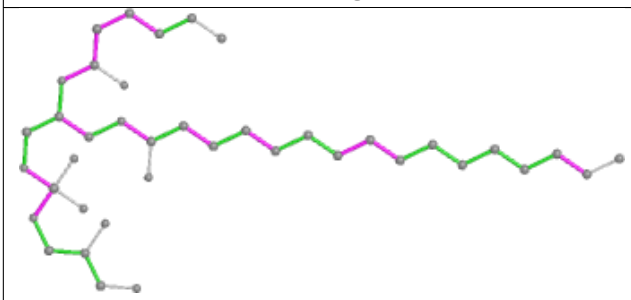
Ligand PGV L 507



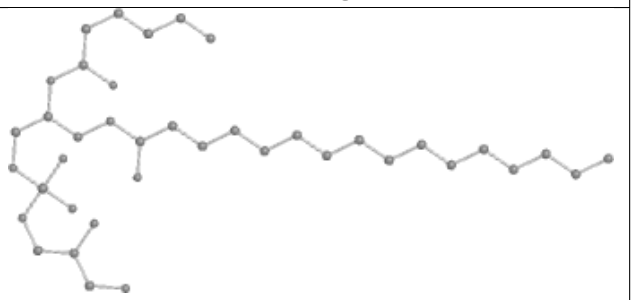
Bond lengths



Bond angles

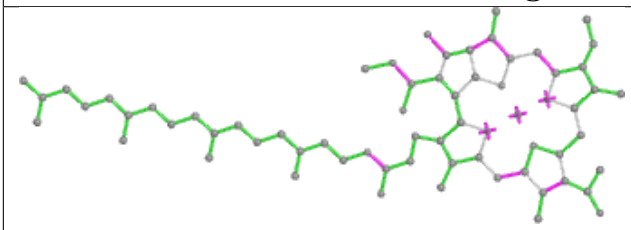


Torsions

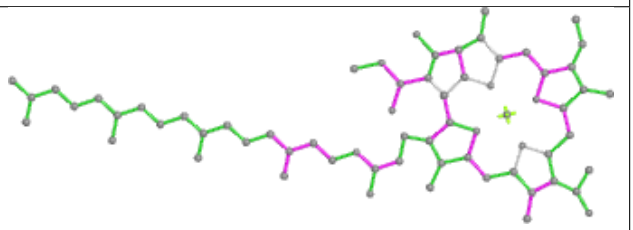


Rings

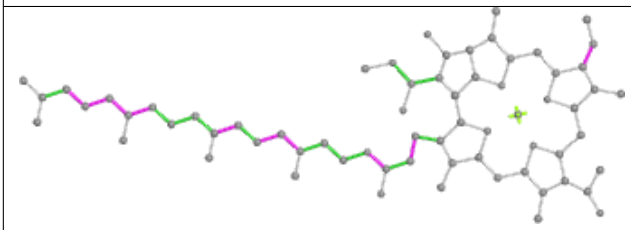
Ligand BCL U 101



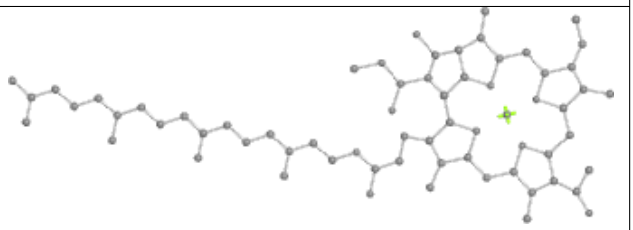
Bond lengths



Bond angles

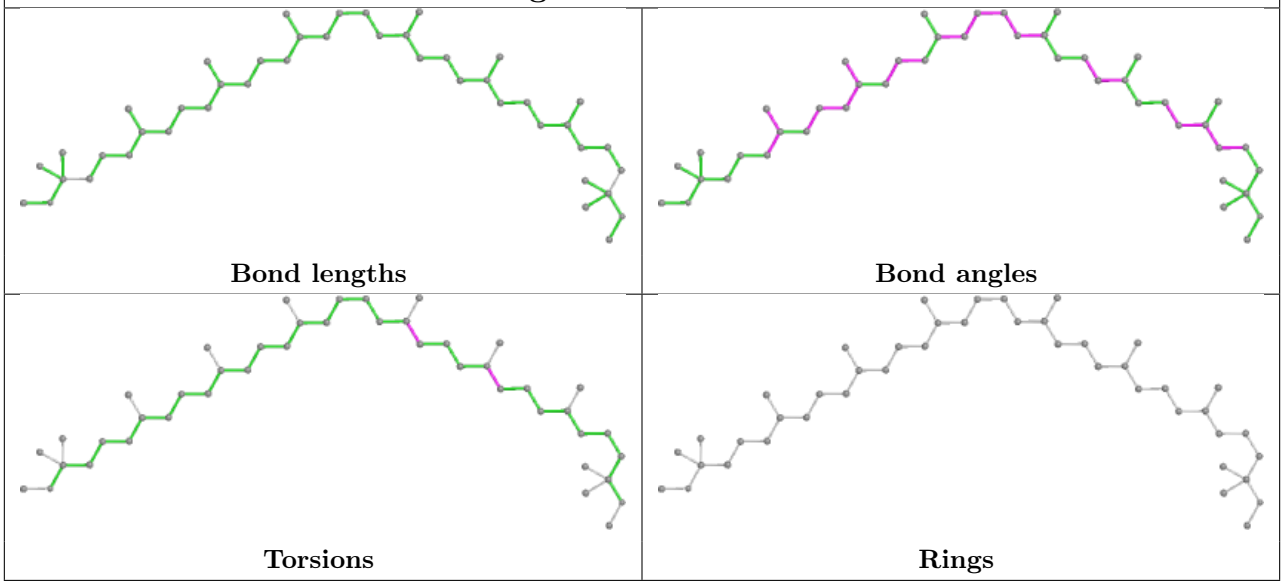


Torsions

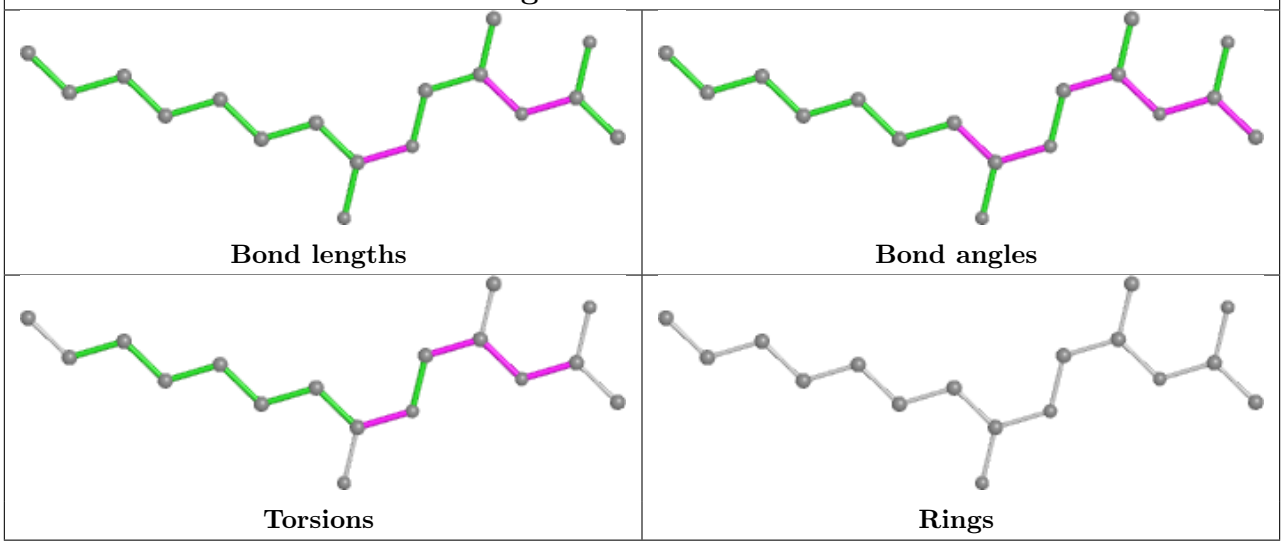


Rings

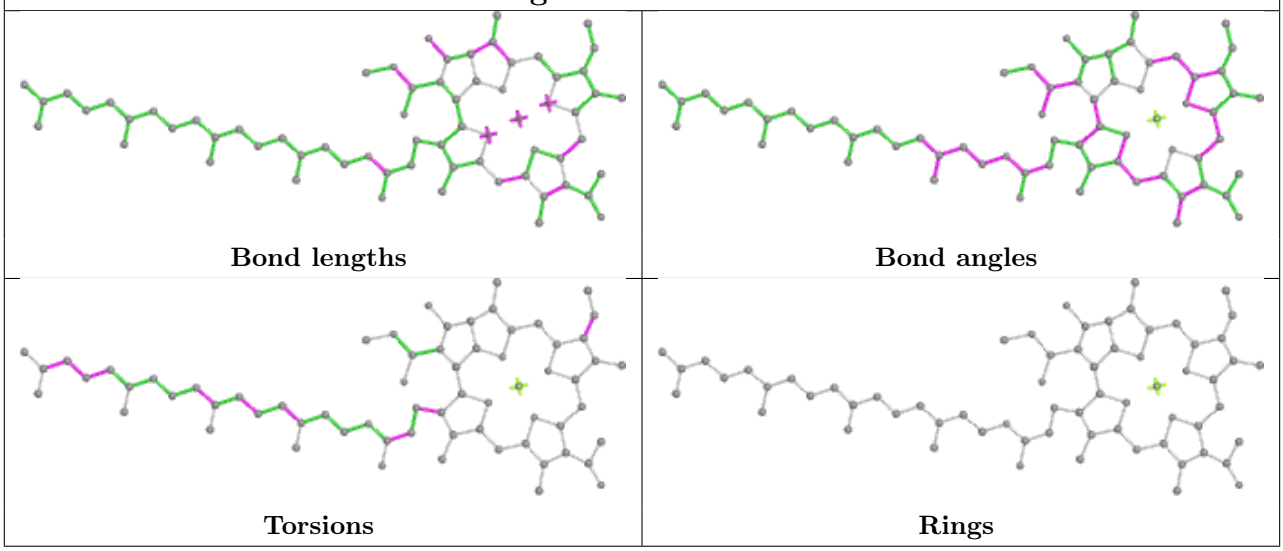
Ligand CRT 7 102



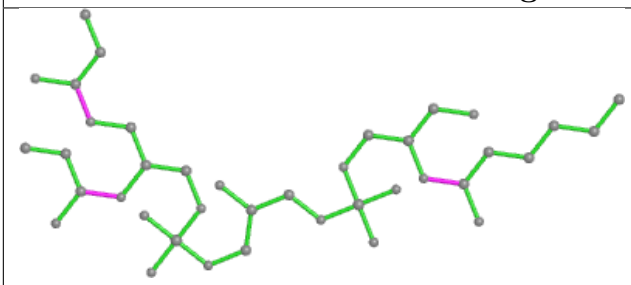
Ligand DGA C 506



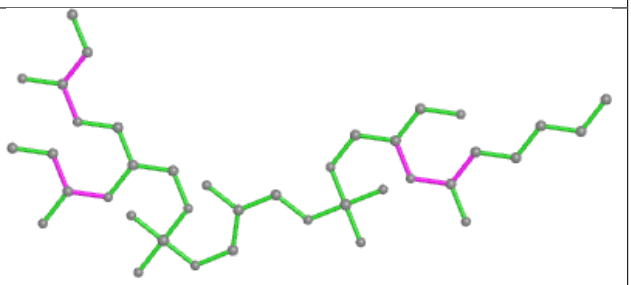
Ligand BCL 2 102



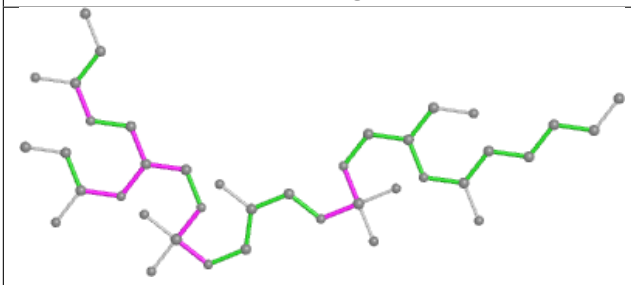
Ligand CDL M 408



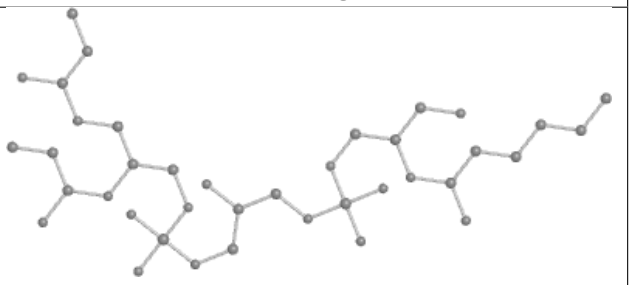
Bond lengths



Bond angles

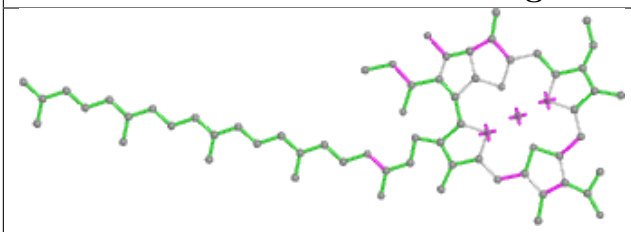


Torsions

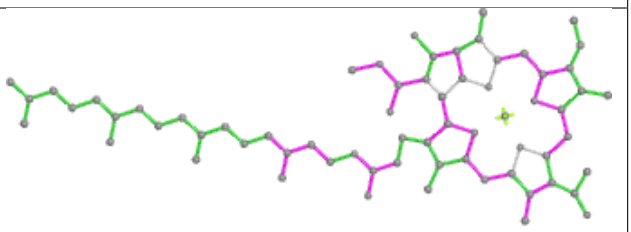


Rings

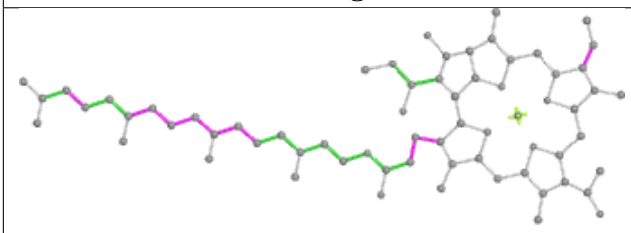
Ligand BCL B 102



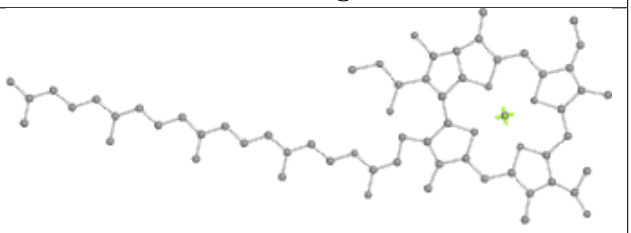
Bond lengths



Bond angles

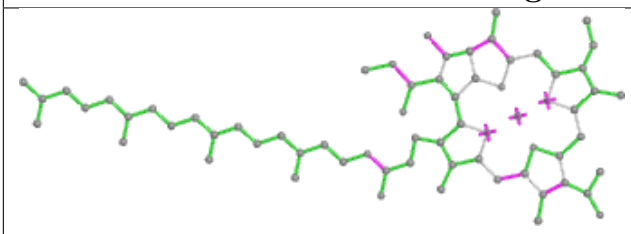


Torsions

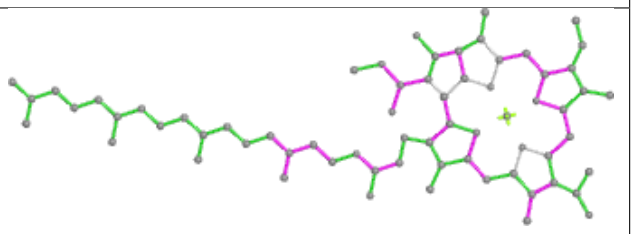


Rings

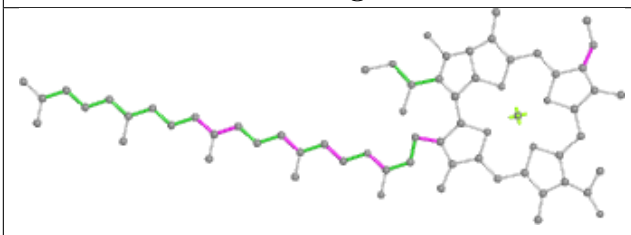
Ligand BCL R 101



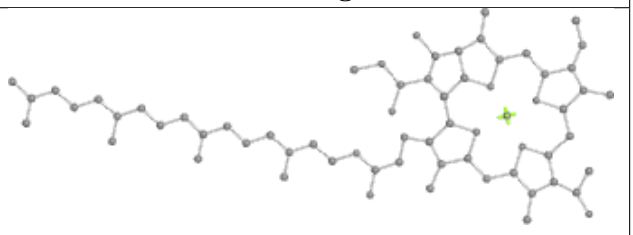
Bond lengths



Bond angles

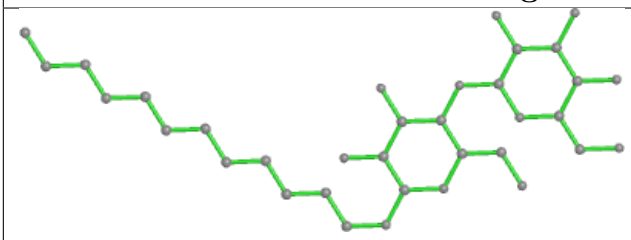


Torsions

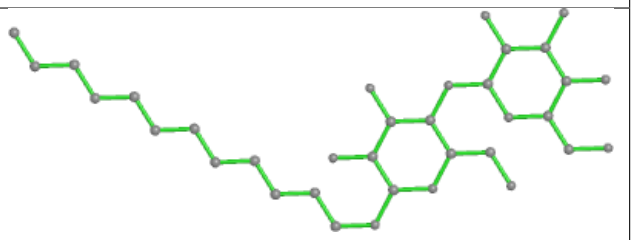


Rings

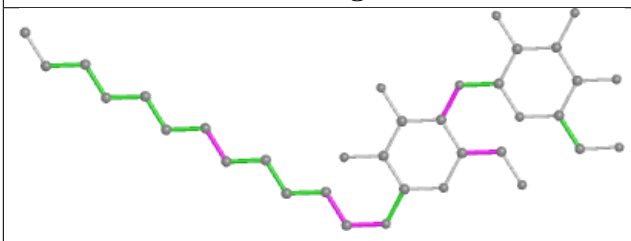
Ligand LMT V 101



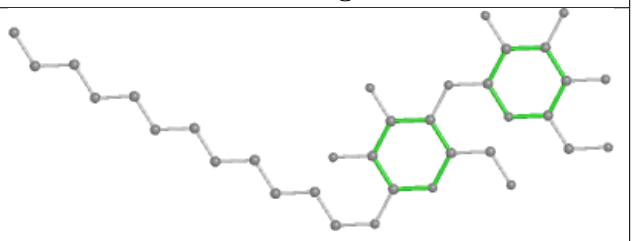
Bond lengths



Bond angles

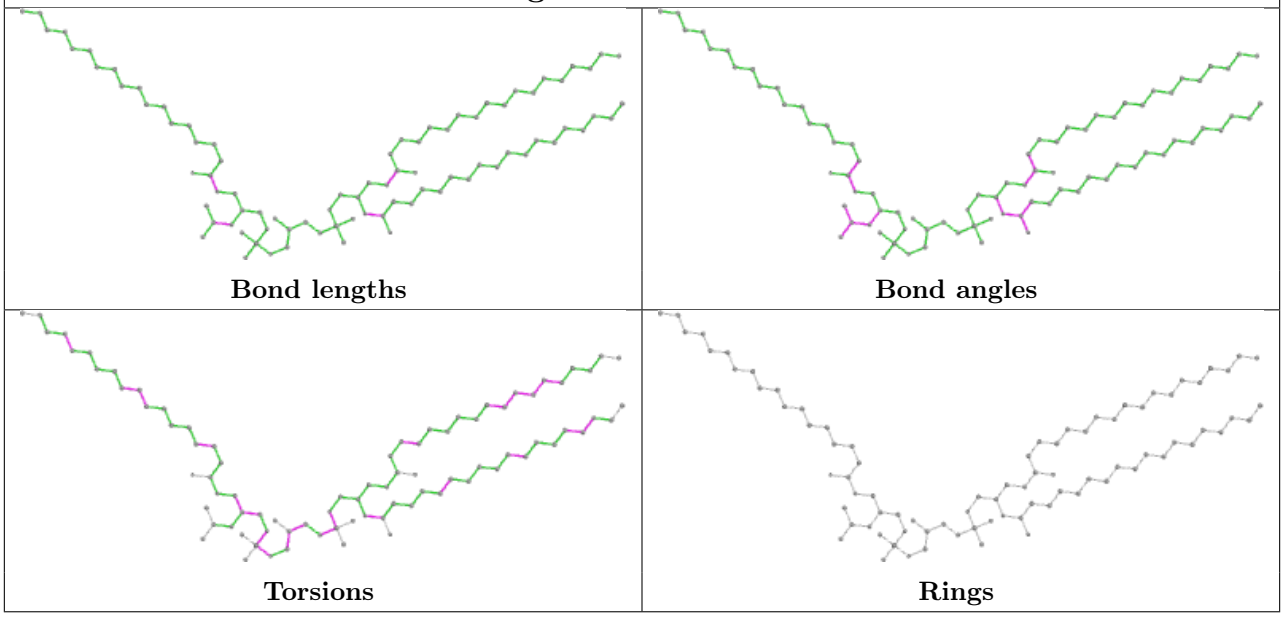


Torsions

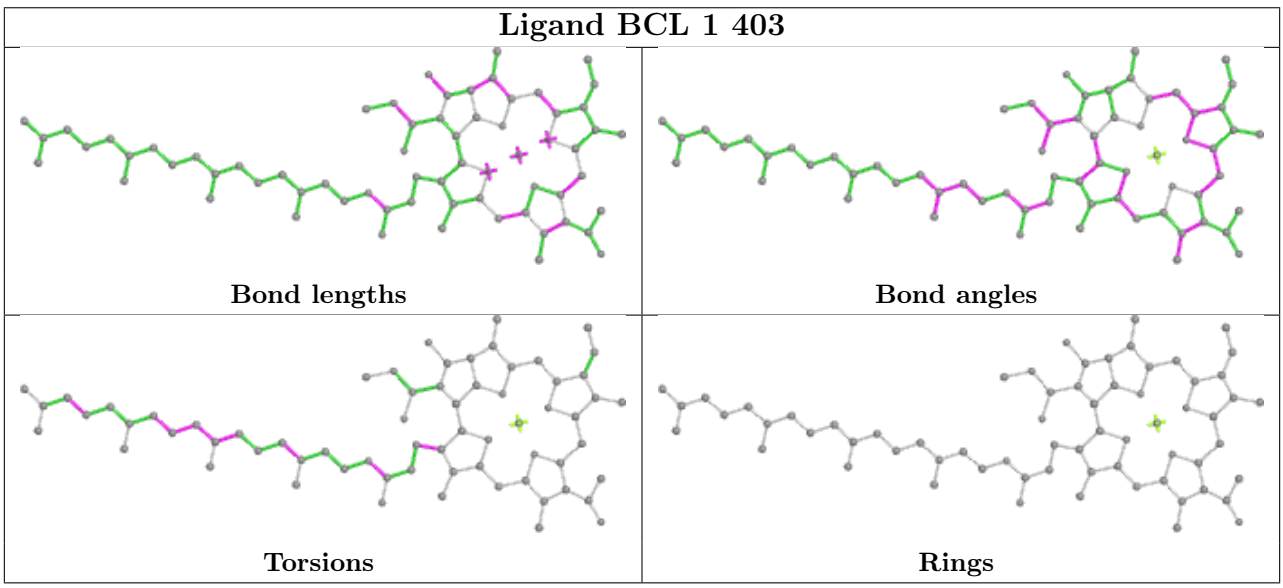


Rings

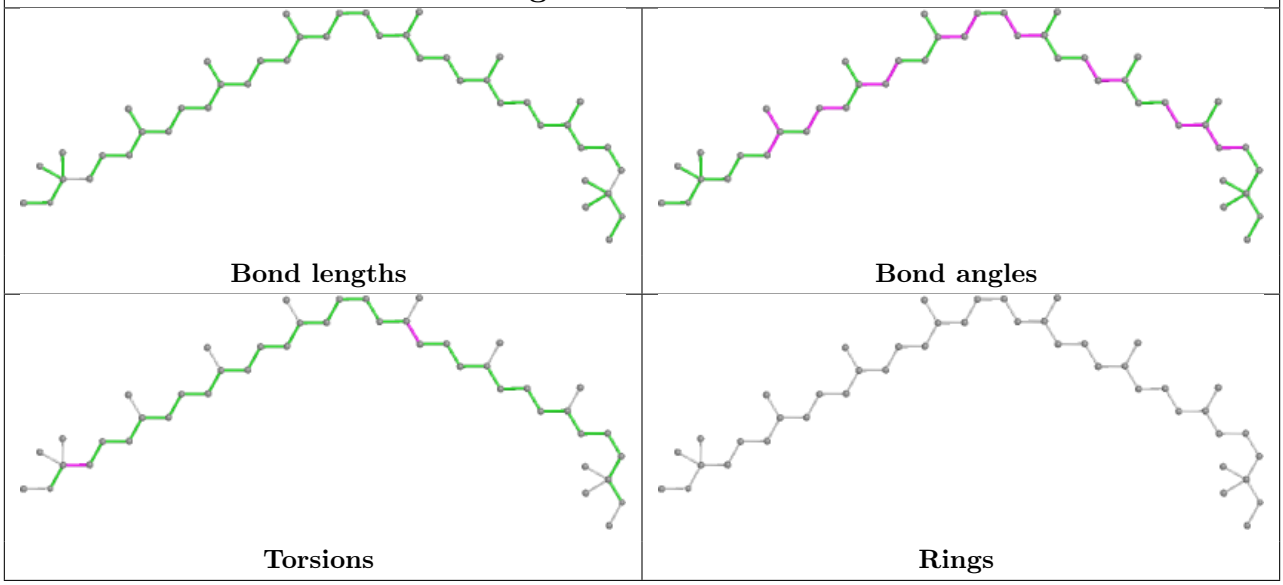
Ligand CDL L 510



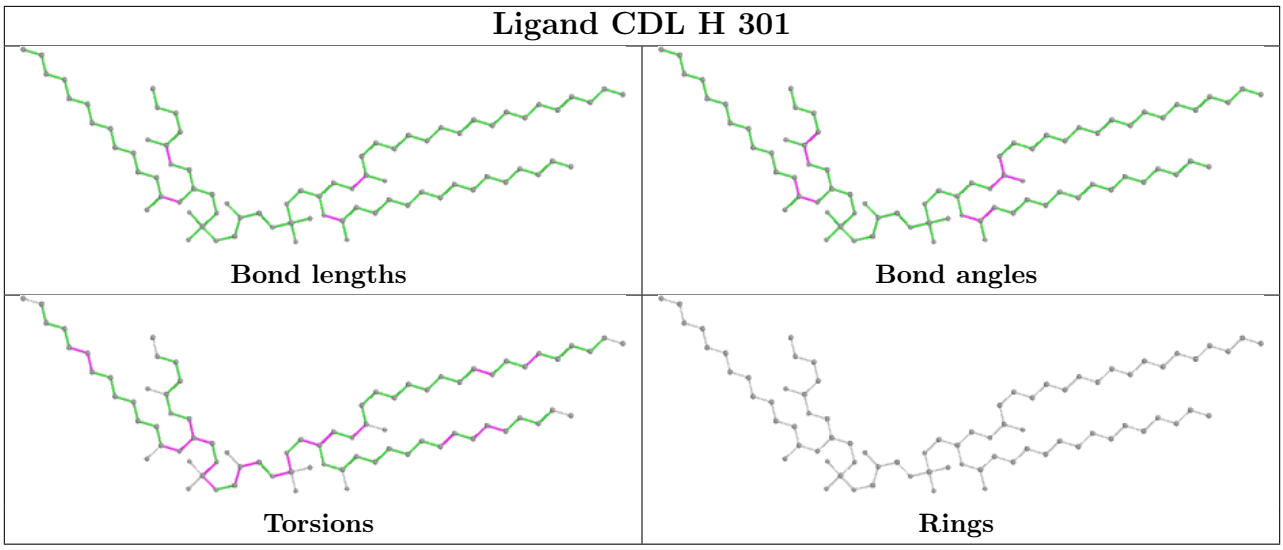
Ligand BCL 1 403



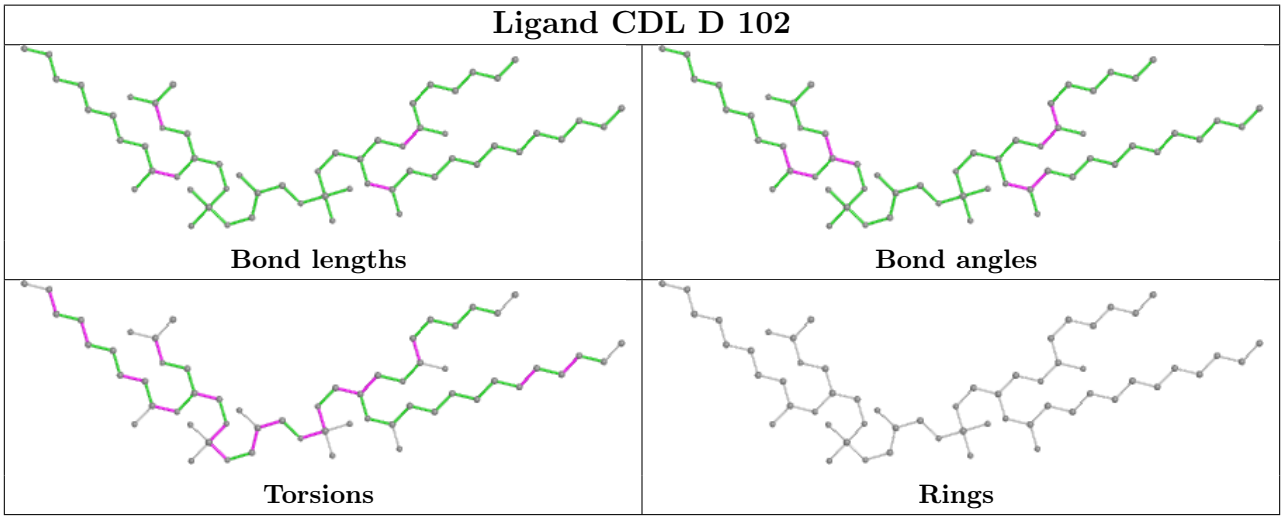
Ligand CRT 4 103



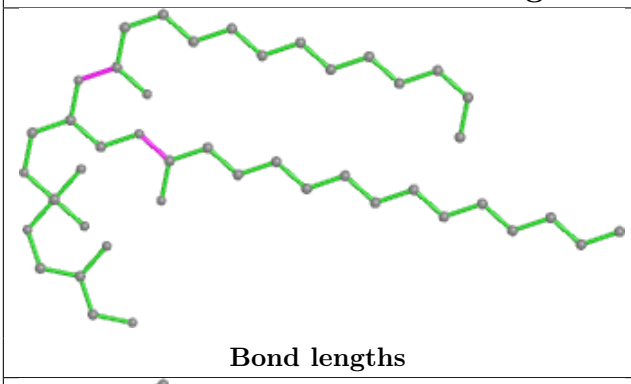
Ligand CDL H 301



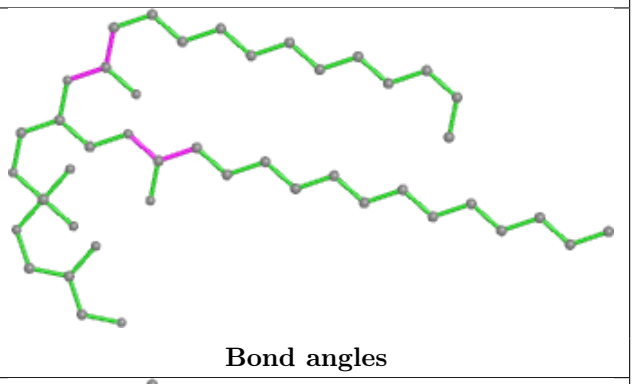
Ligand CDL D 102



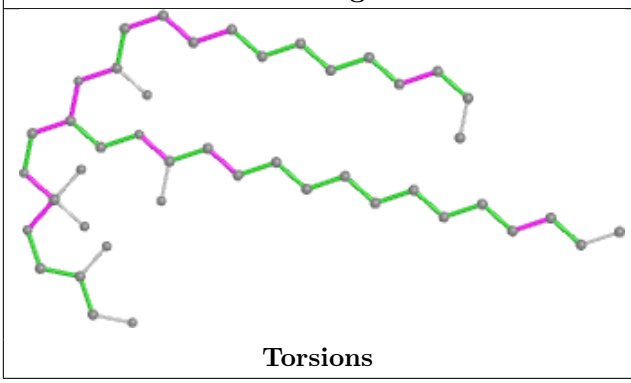
Ligand PGV 5 101



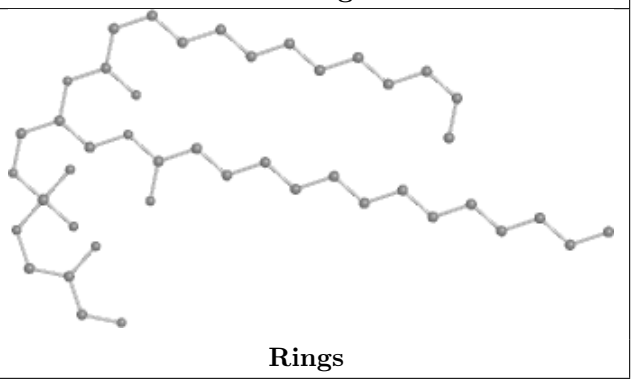
Bond lengths



Bond angles

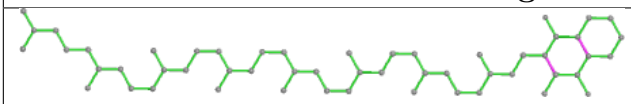


Torsions

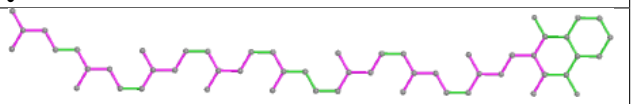


Rings

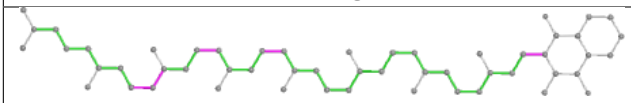
Ligand MQ8 M 406



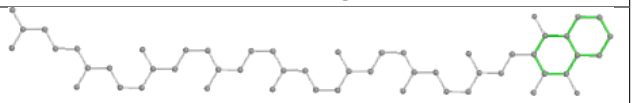
Bond lengths



Bond angles

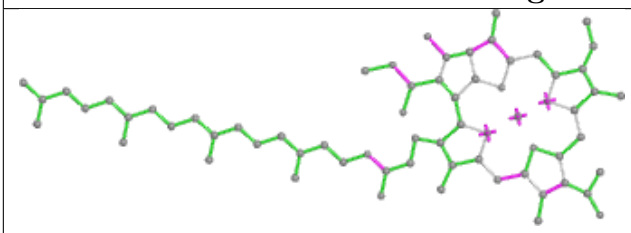


Torsions

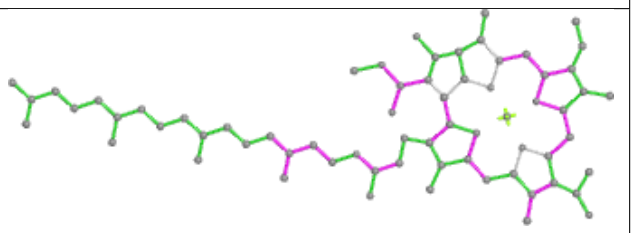


Rings

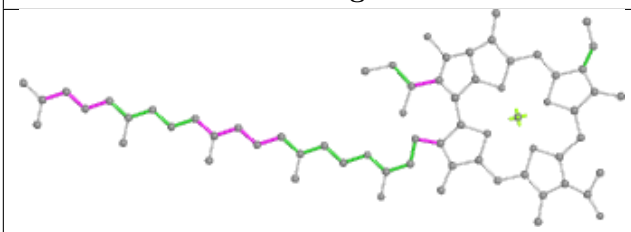
Ligand BCL L 508



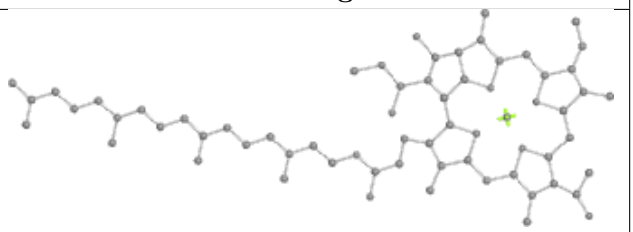
Bond lengths



Bond angles

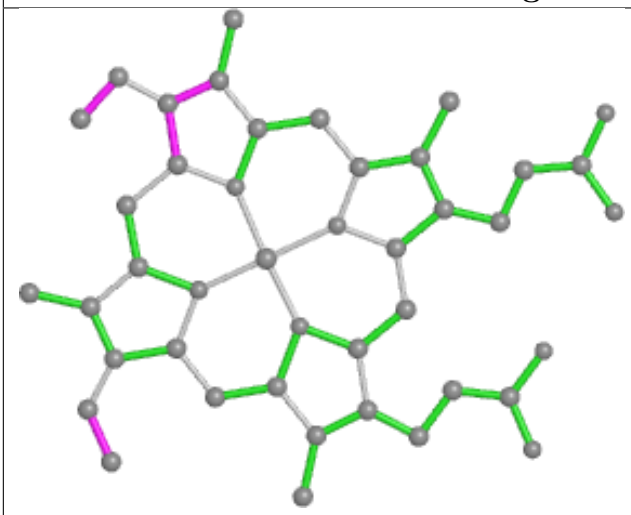


Torsions

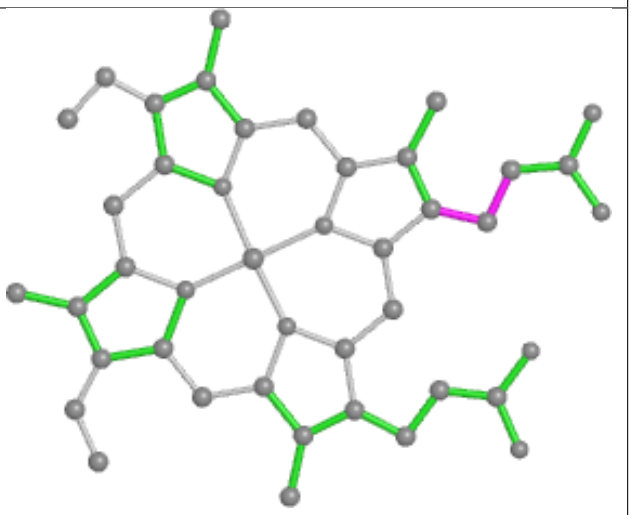


Rings

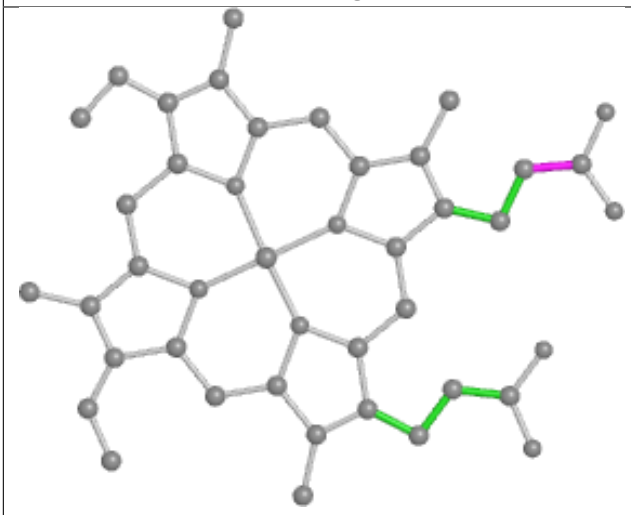
Ligand HEC C 501



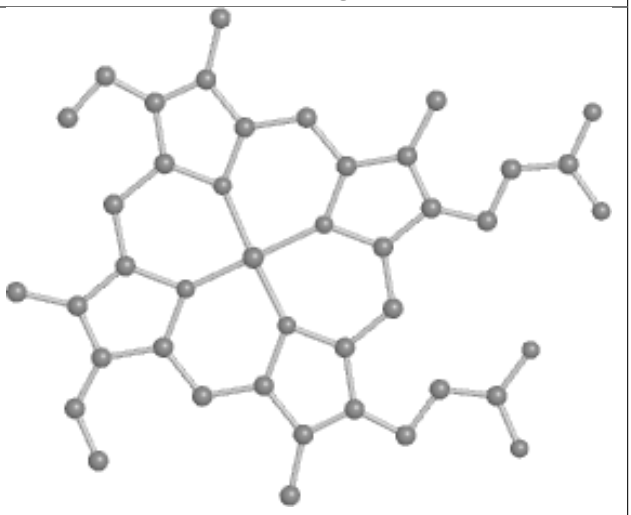
Bond lengths



Bond angles

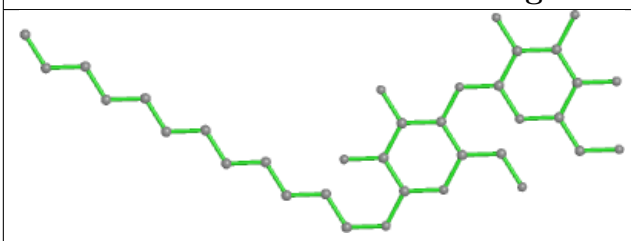


Torsions

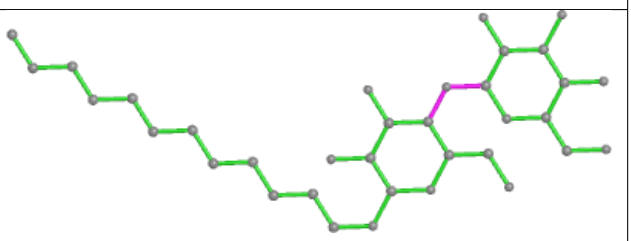


Rings

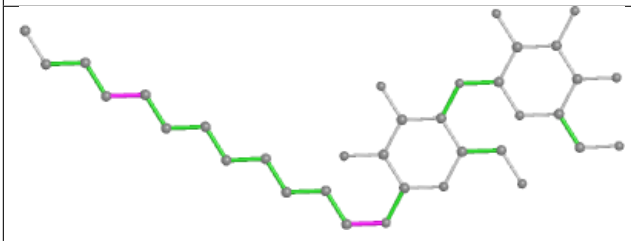
Ligand LMT 8 101



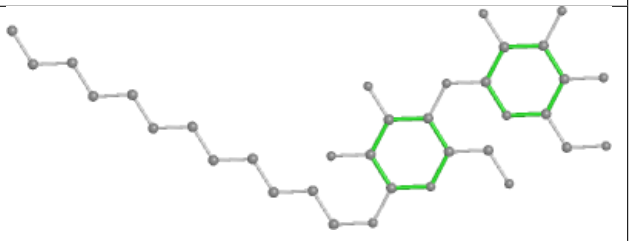
Bond lengths



Bond angles

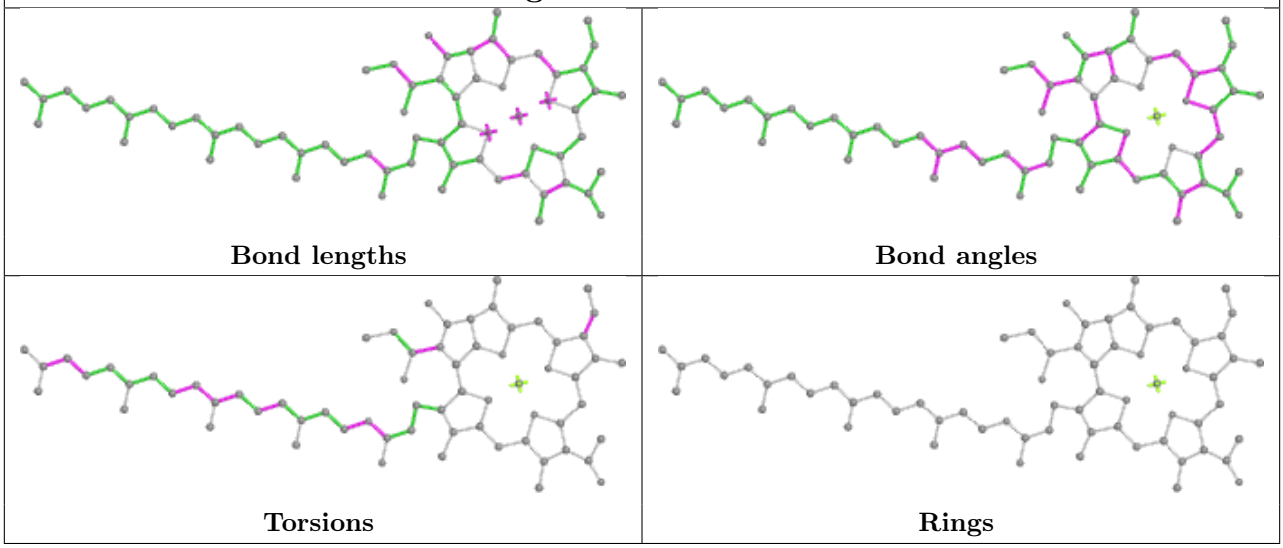


Torsions

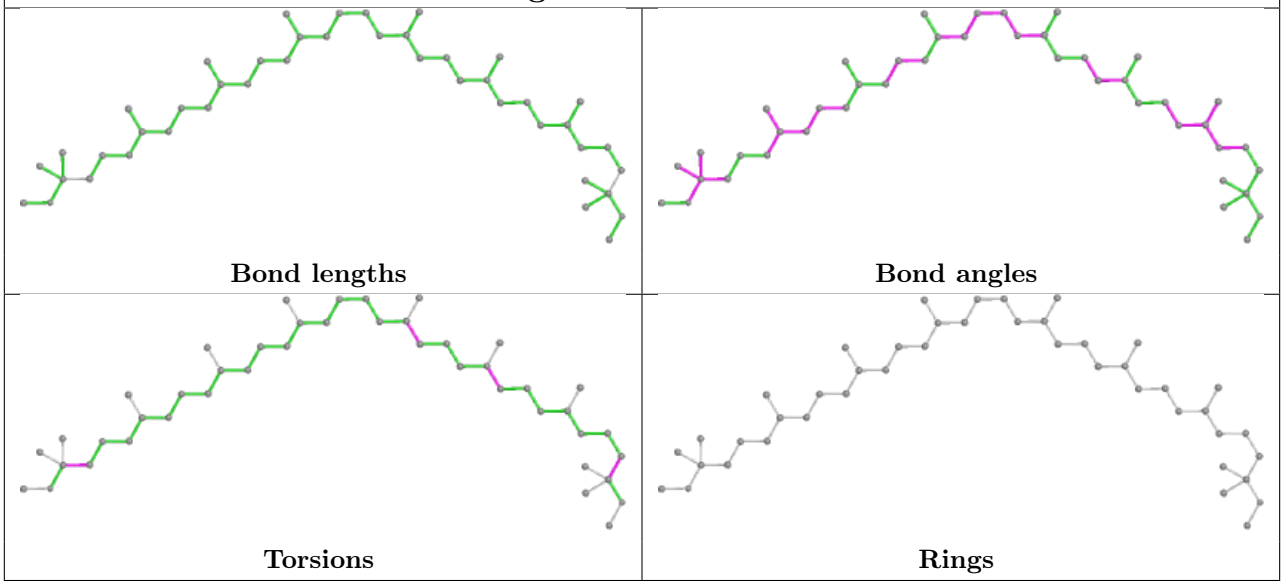


Rings

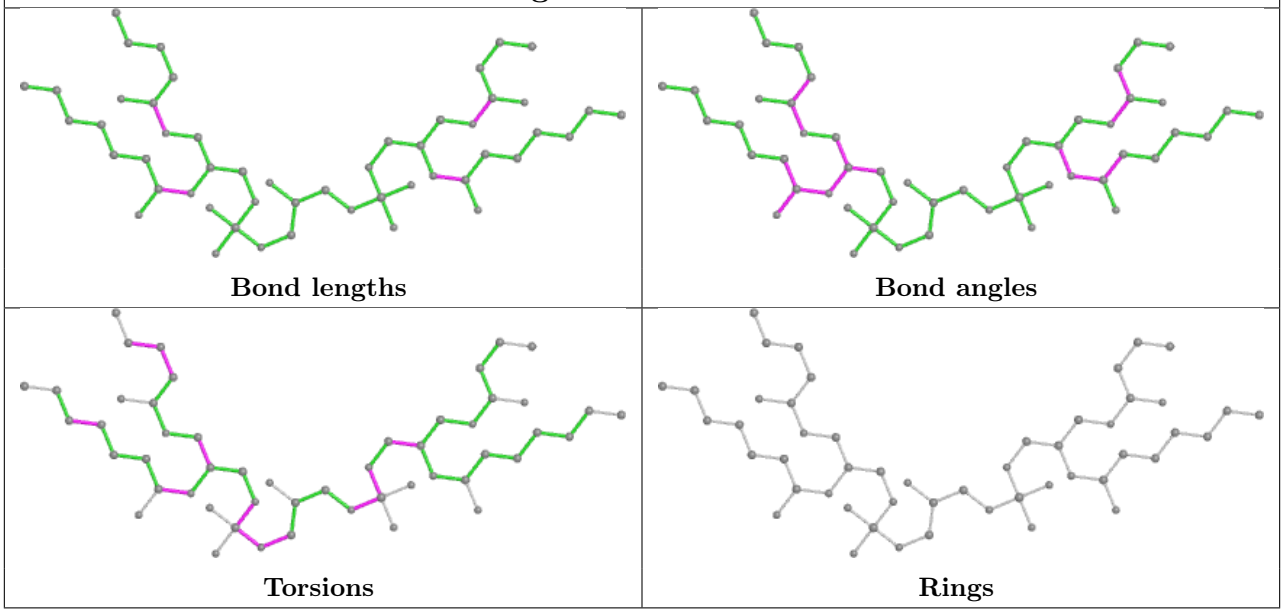
Ligand BCL O 502



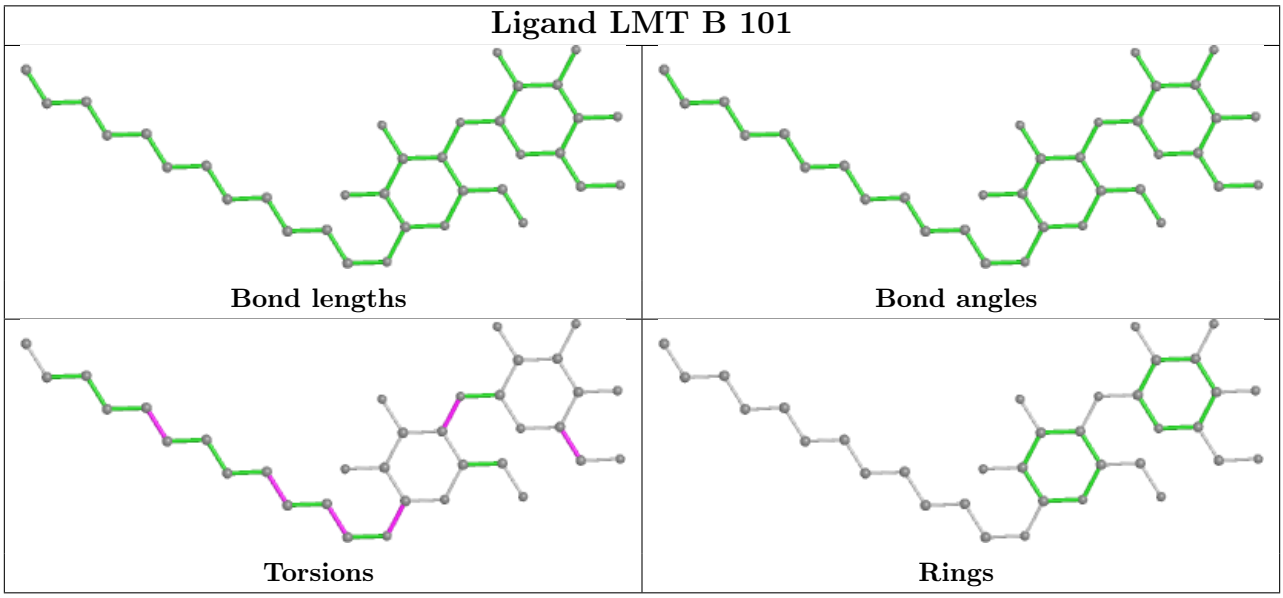
Ligand CRT S 104



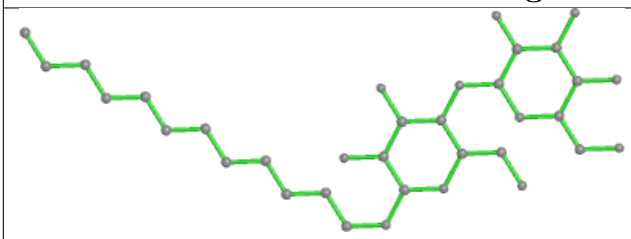
Ligand CDL I 101



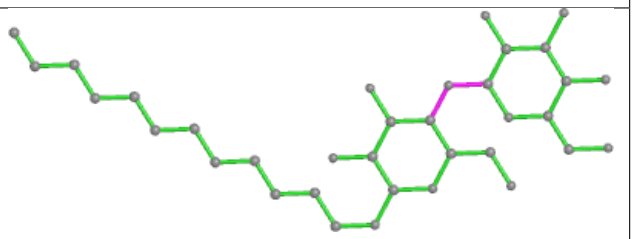
Ligand LMT B 101



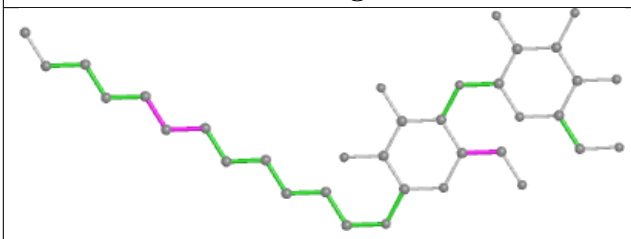
Ligand LMT 4 101



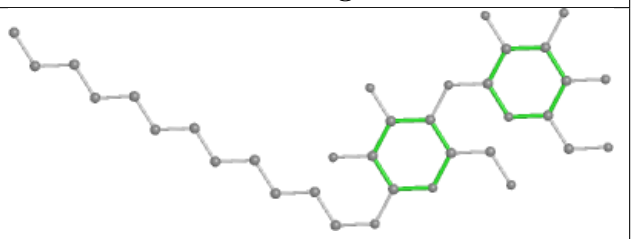
Bond lengths



Bond angles

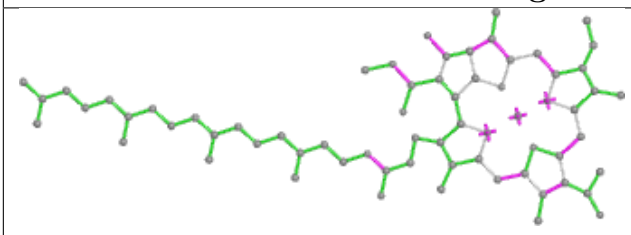


Torsions

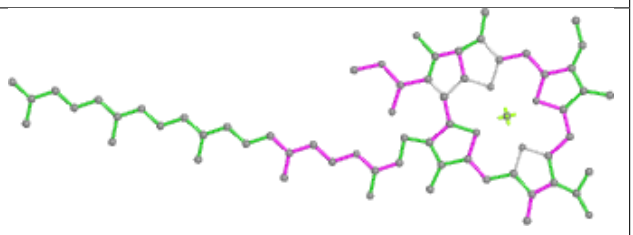


Rings

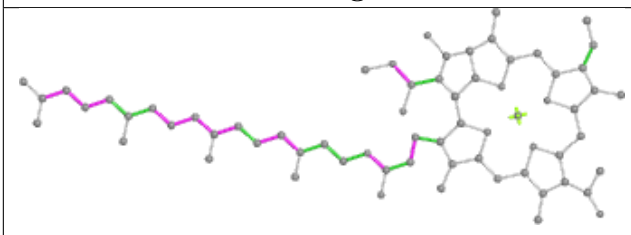
Ligand BCL 5 102



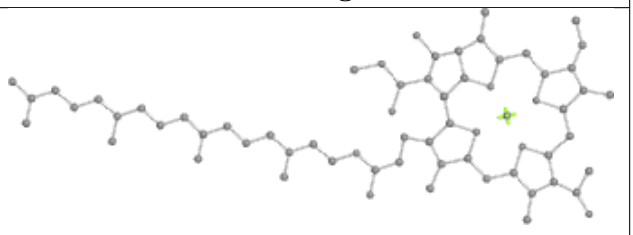
Bond lengths



Bond angles

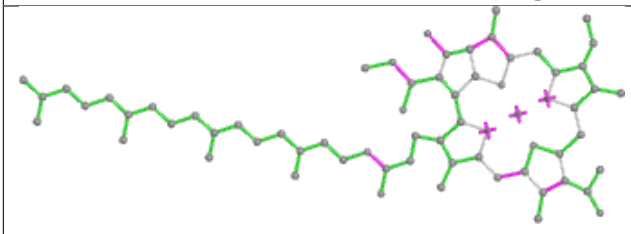


Torsions

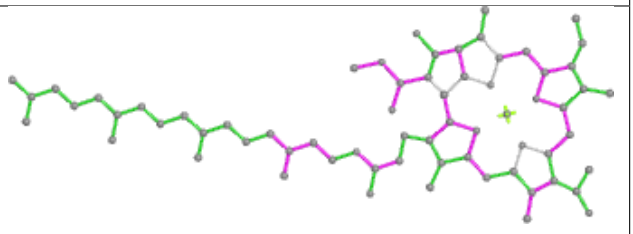


Rings

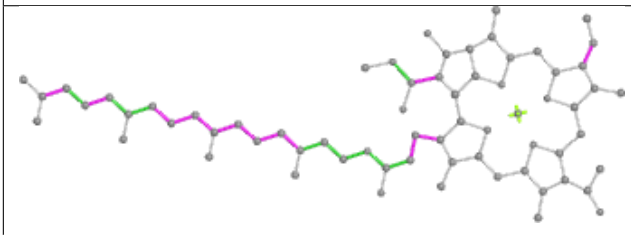
Ligand BCL 8 102



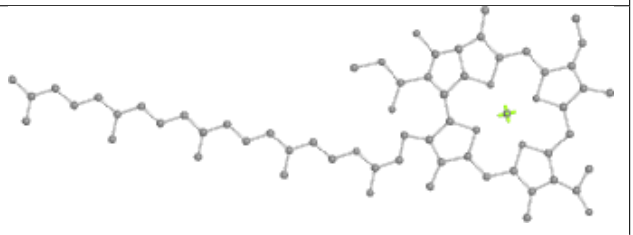
Bond lengths



Bond angles

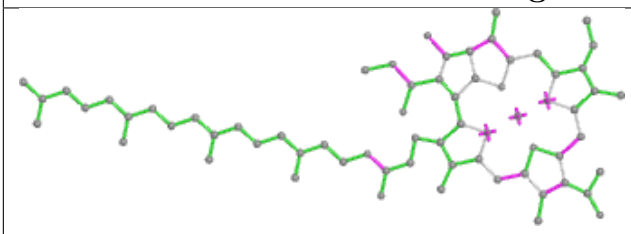


Torsions

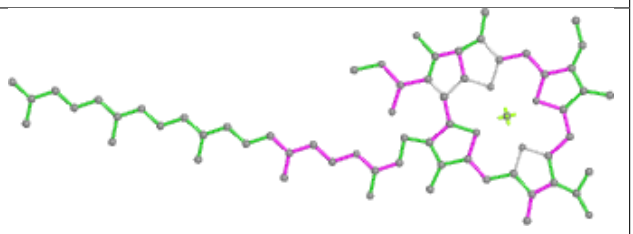


Rings

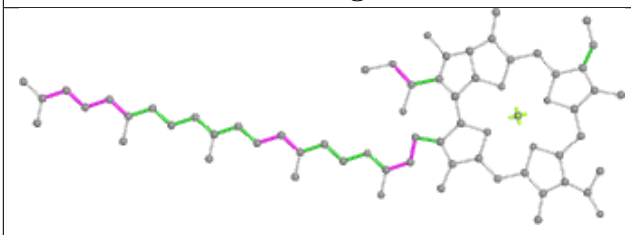
Ligand BCL J 102



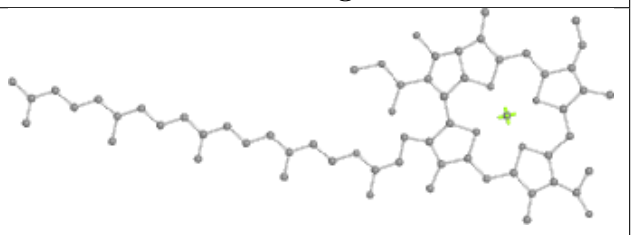
Bond lengths



Bond angles

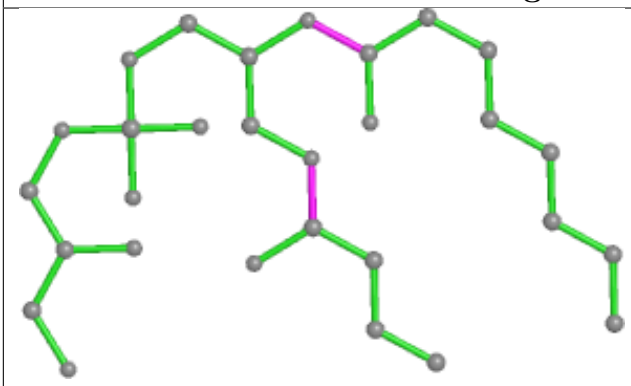


Torsions

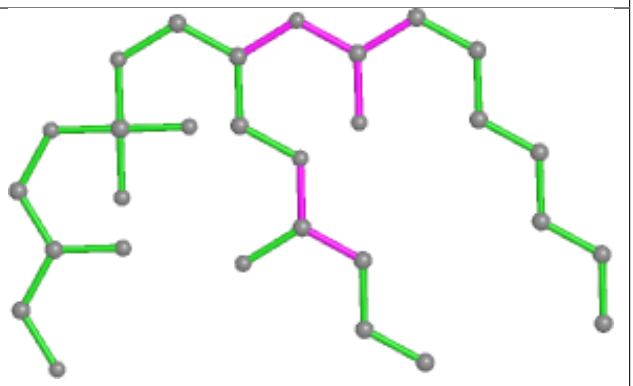


Rings

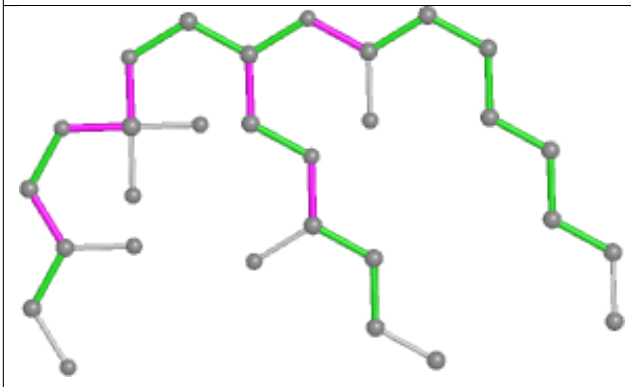
Ligand PGV L 506



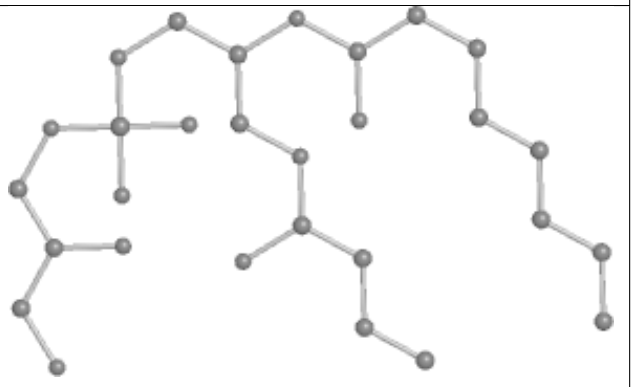
Bond lengths



Bond angles

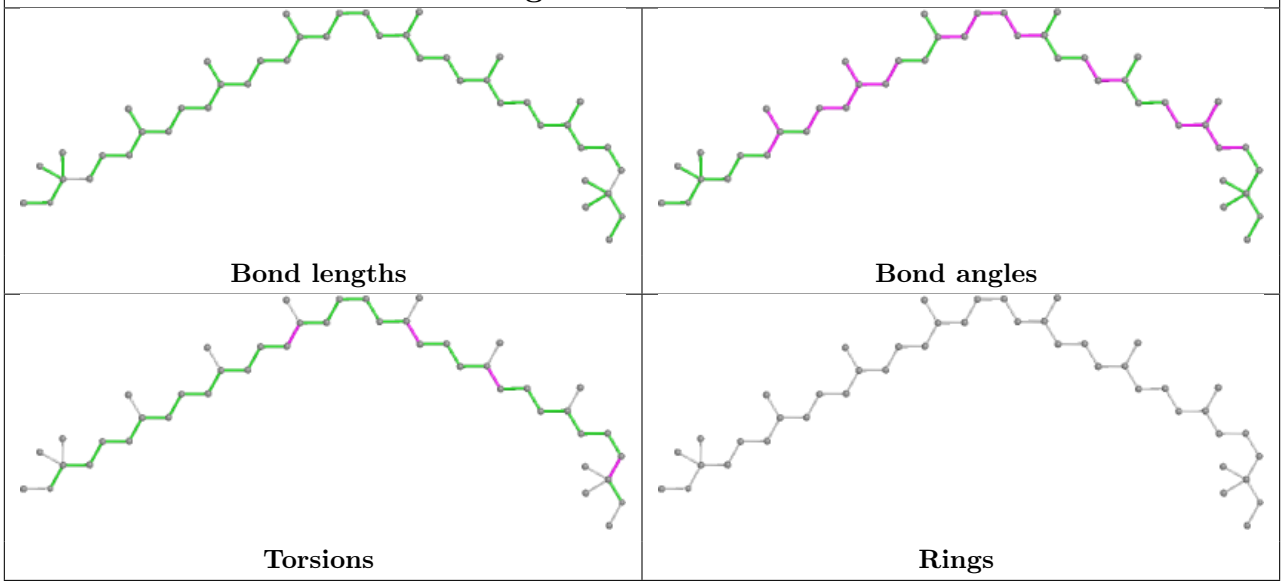


Torsions

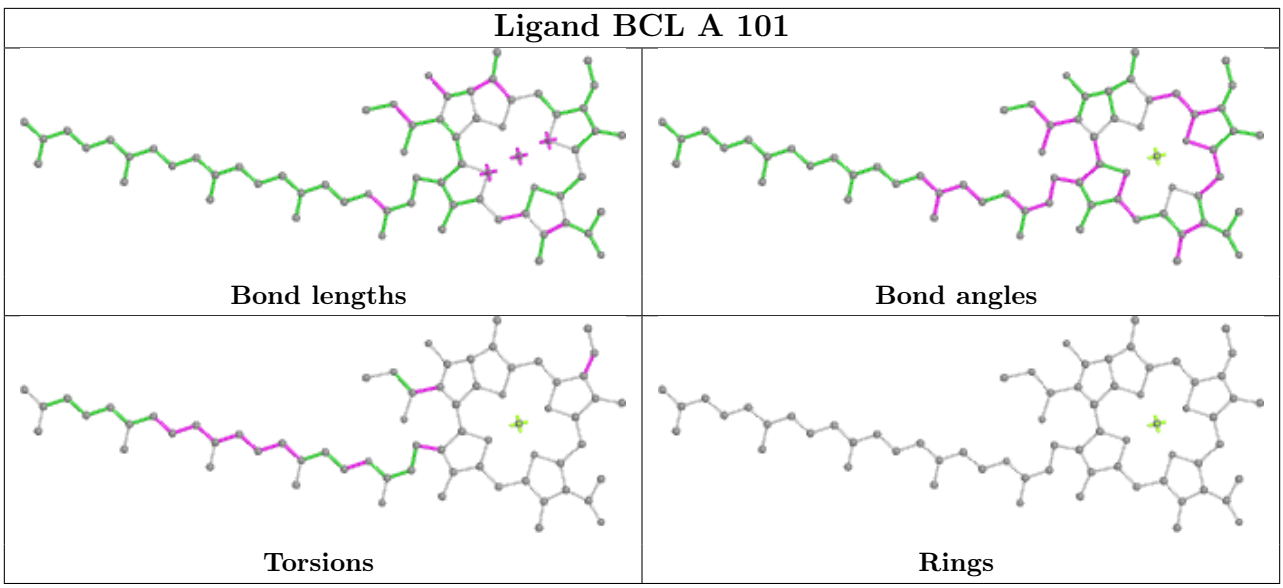


Rings

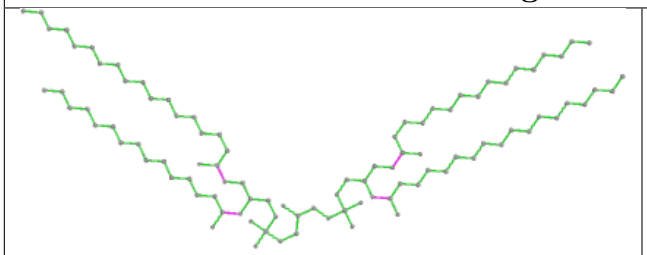
Ligand CRT B 103



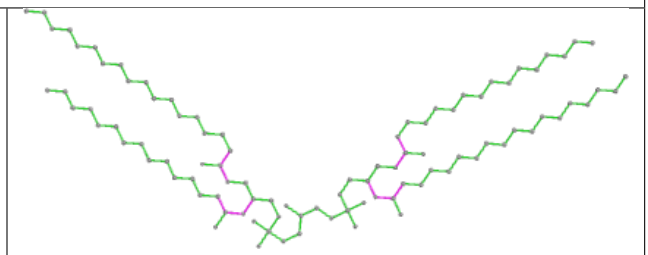
Ligand BCL A 101



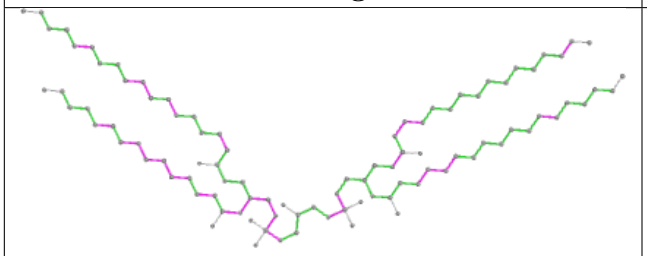
Ligand CDL M 410



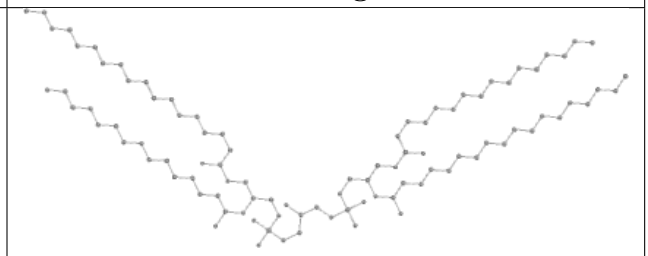
Bond lengths



Bond angles

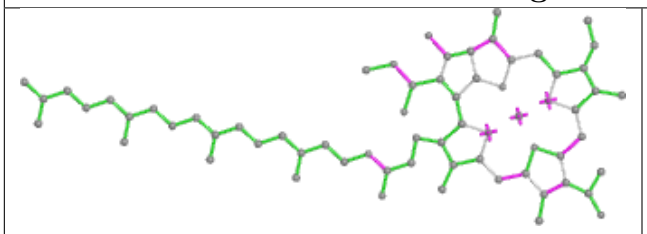


Torsions

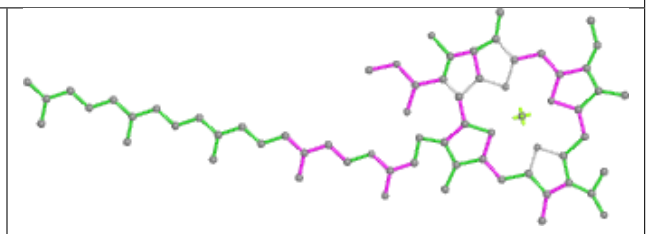


Rings

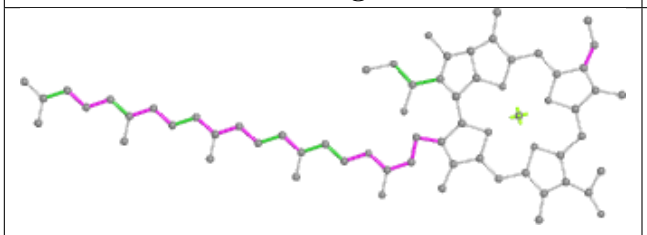
Ligand BCL 4 102



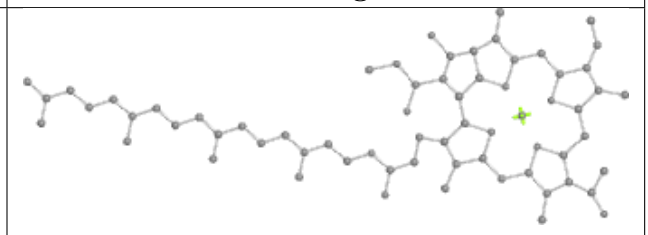
Bond lengths



Bond angles

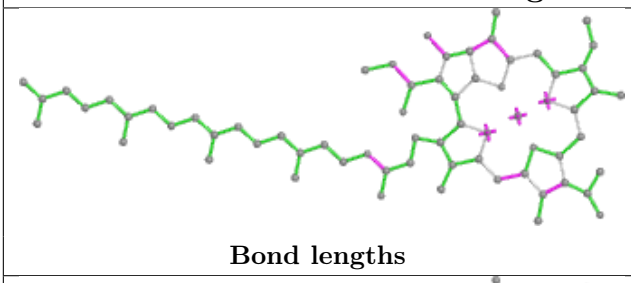


Torsions

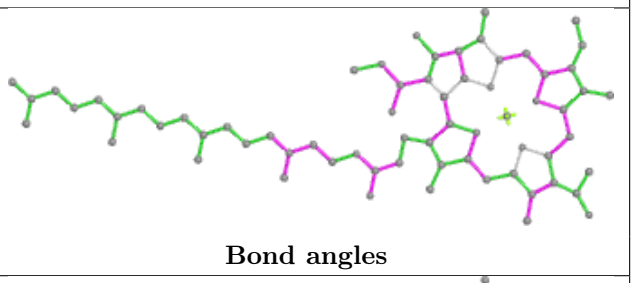


Rings

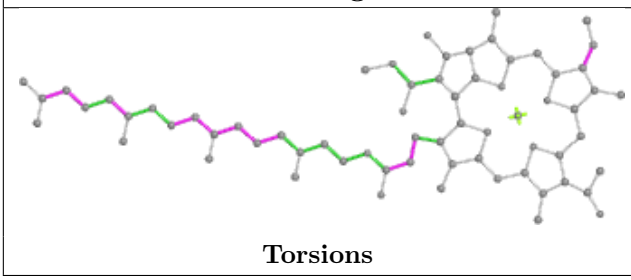
Ligand BCL E 102



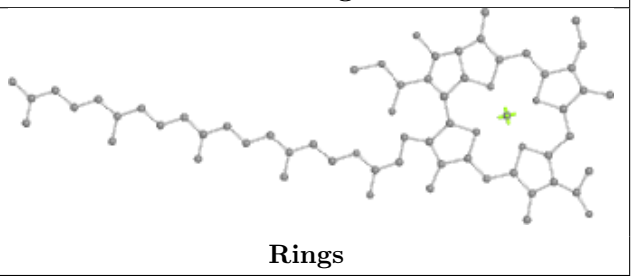
Bond lengths



Bond angles

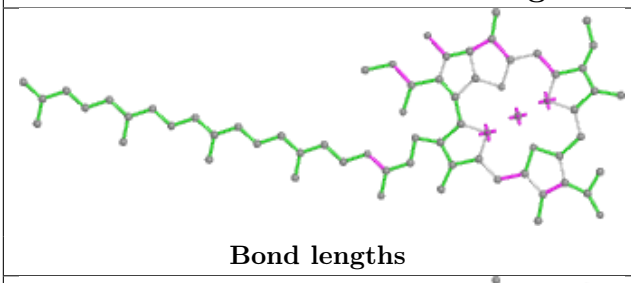


Torsions

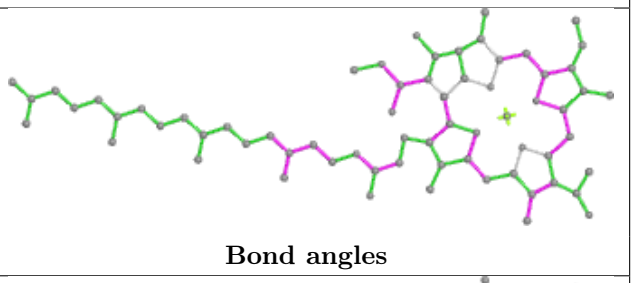


Rings

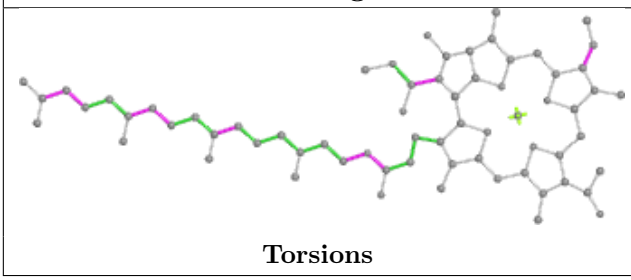
Ligand BCL S 102



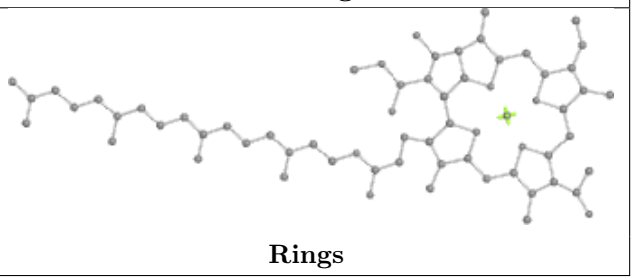
Bond lengths



Bond angles

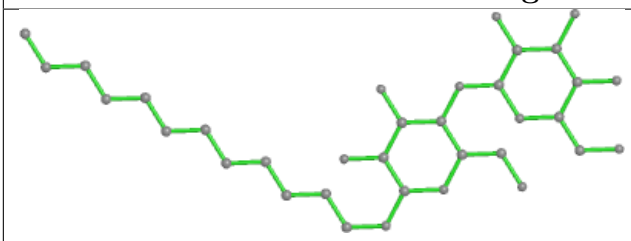


Torsions

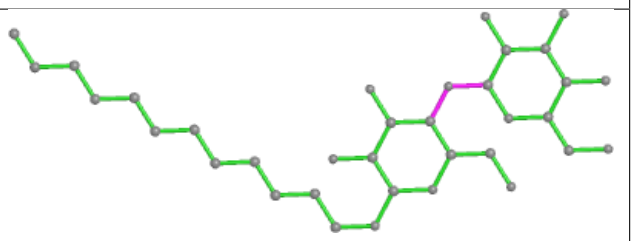


Rings

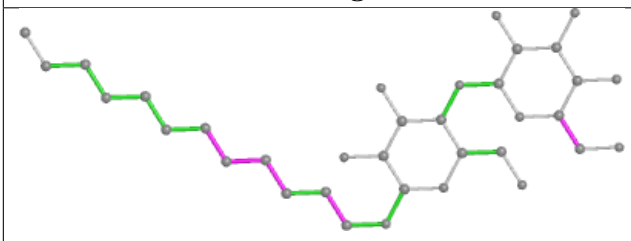
Ligand LMT T 101



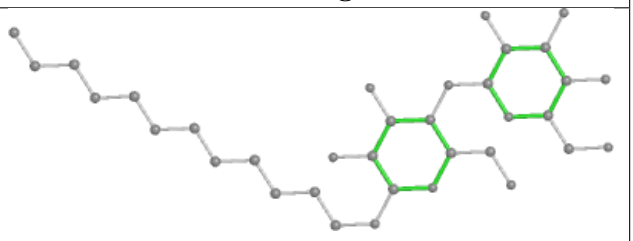
Bond lengths



Bond angles

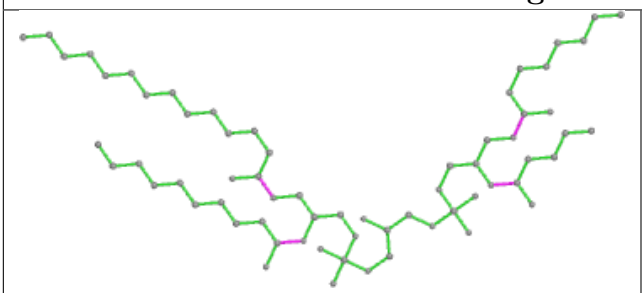


Torsions

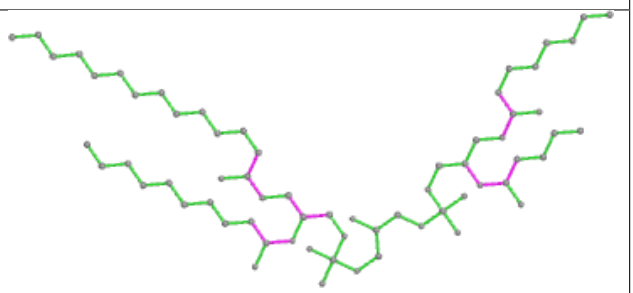


Rings

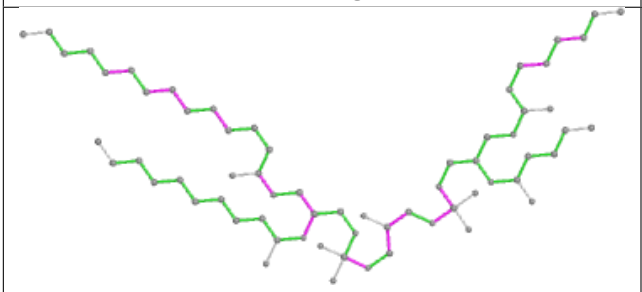
Ligand CDL S 101



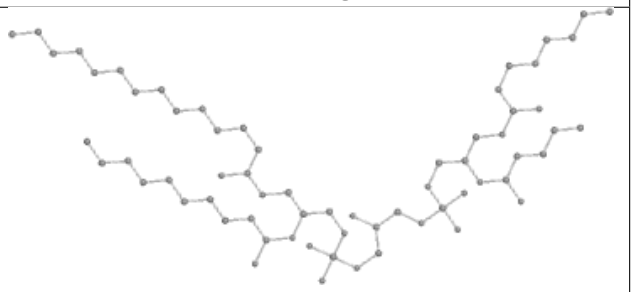
Bond lengths



Bond angles

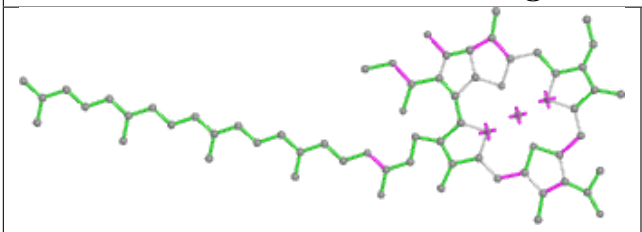


Torsions

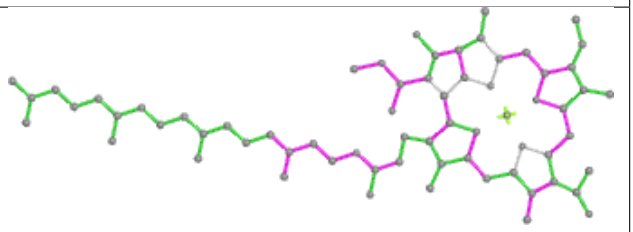


Rings

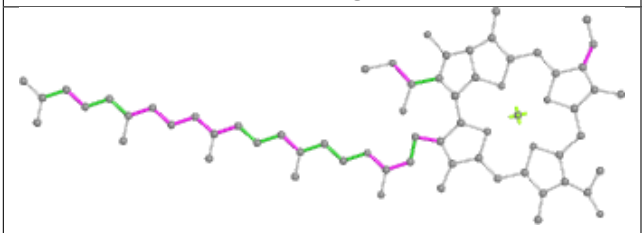
Ligand BCL X 102



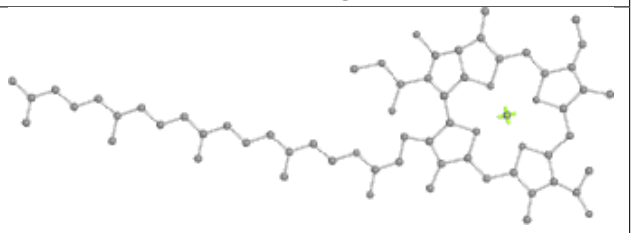
Bond lengths



Bond angles

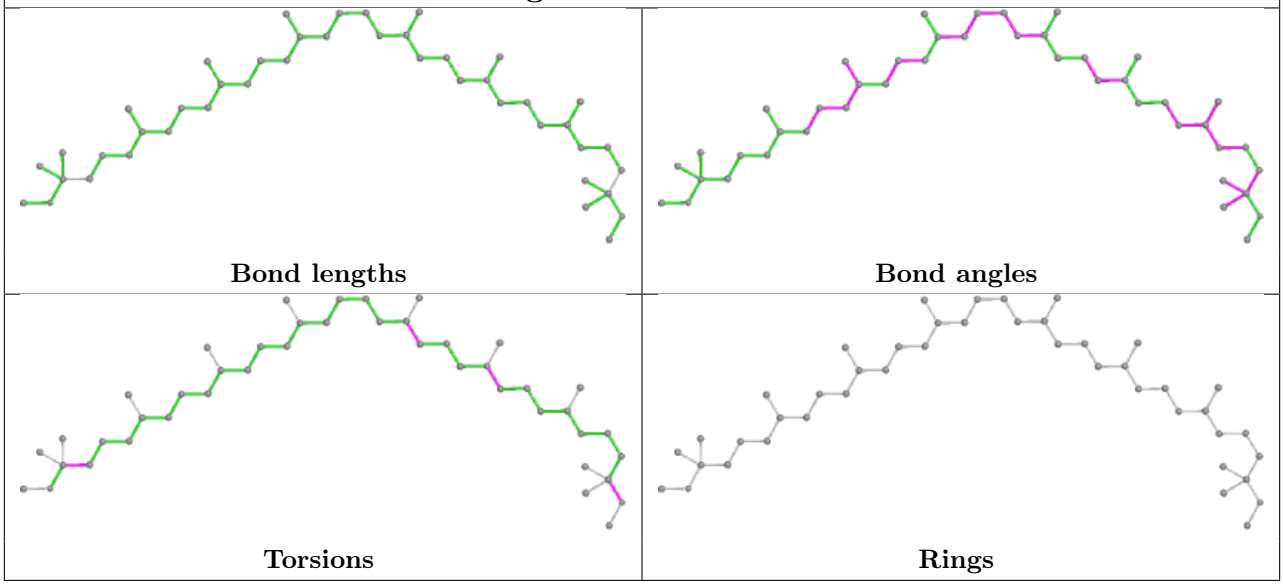


Torsions

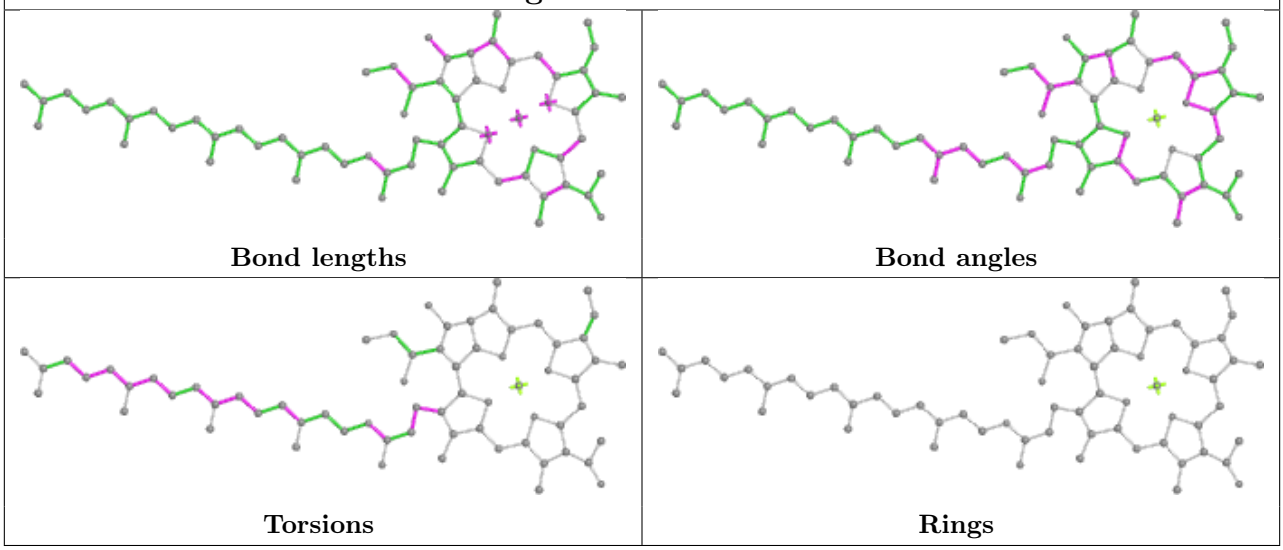


Rings

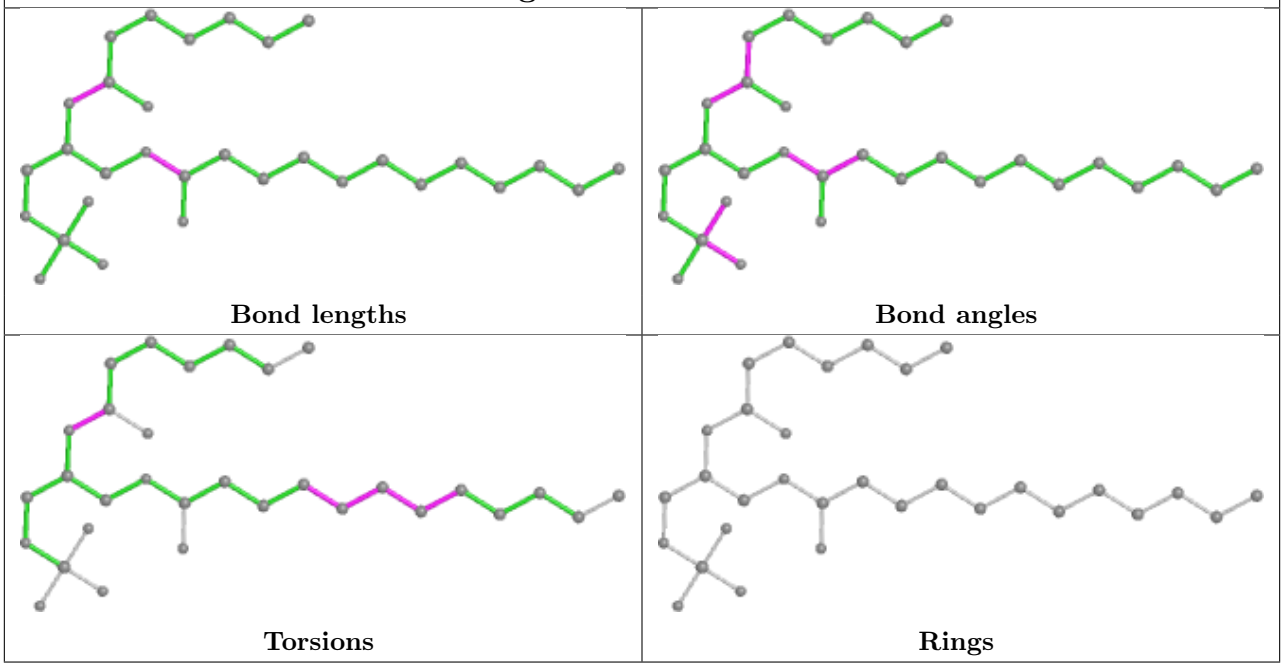
Ligand CRT P 102



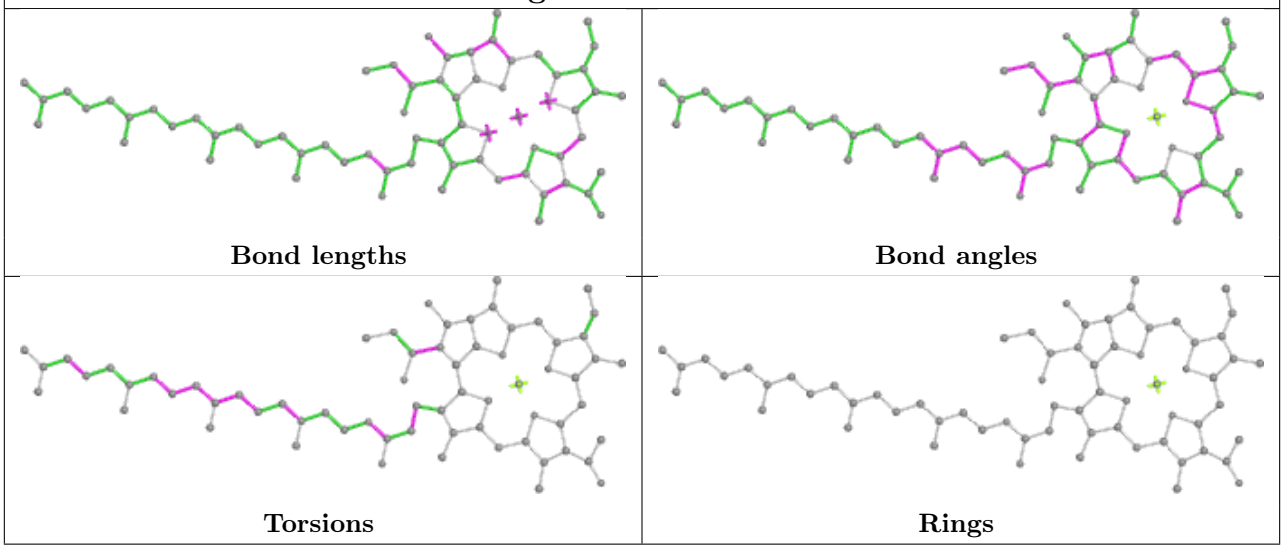
Ligand BCL Y 101



Ligand PGV M 409



Ligand BCL L 502



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

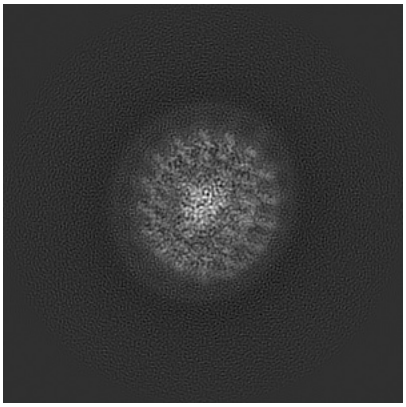
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-32100. These allow visual inspection of the internal detail of the map and identification of artifacts.

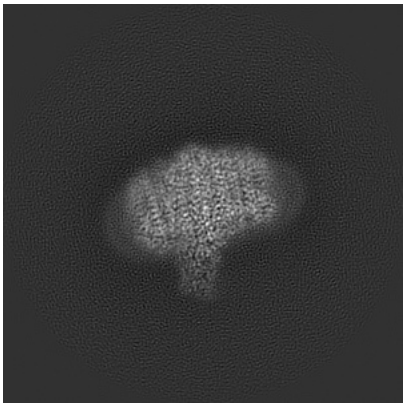
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

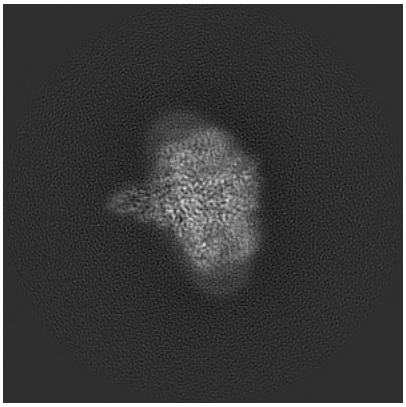
6.1.1 Primary map



X



Y

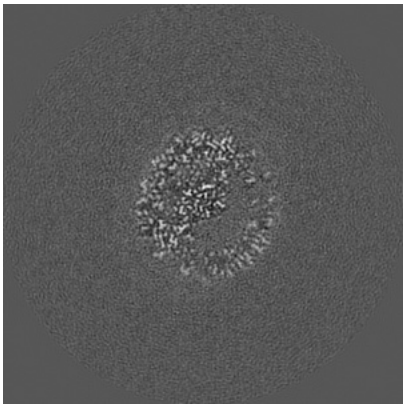


Z

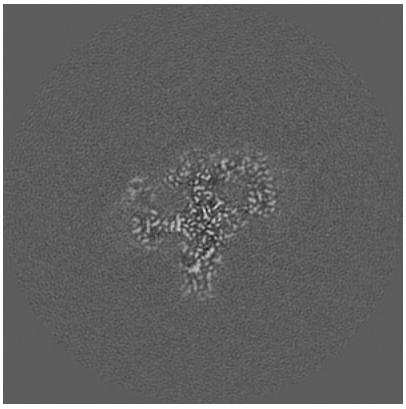
The images above show the map projected in three orthogonal directions.

6.2 Central slices

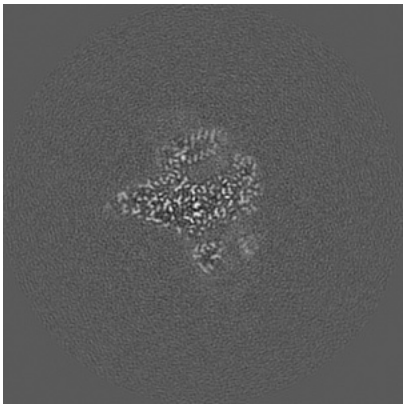
6.2.1 Primary map



X Index: 200



Y Index: 200

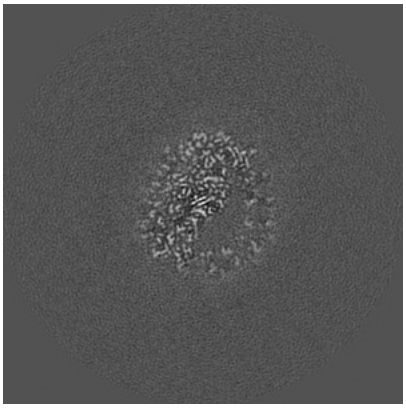


Z Index: 200

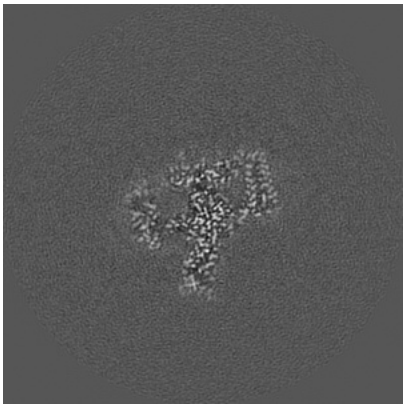
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

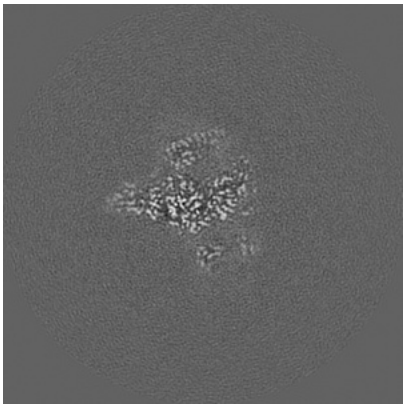
6.3.1 Primary map



X Index: 193



Y Index: 203



Z Index: 205

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 0.0134. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

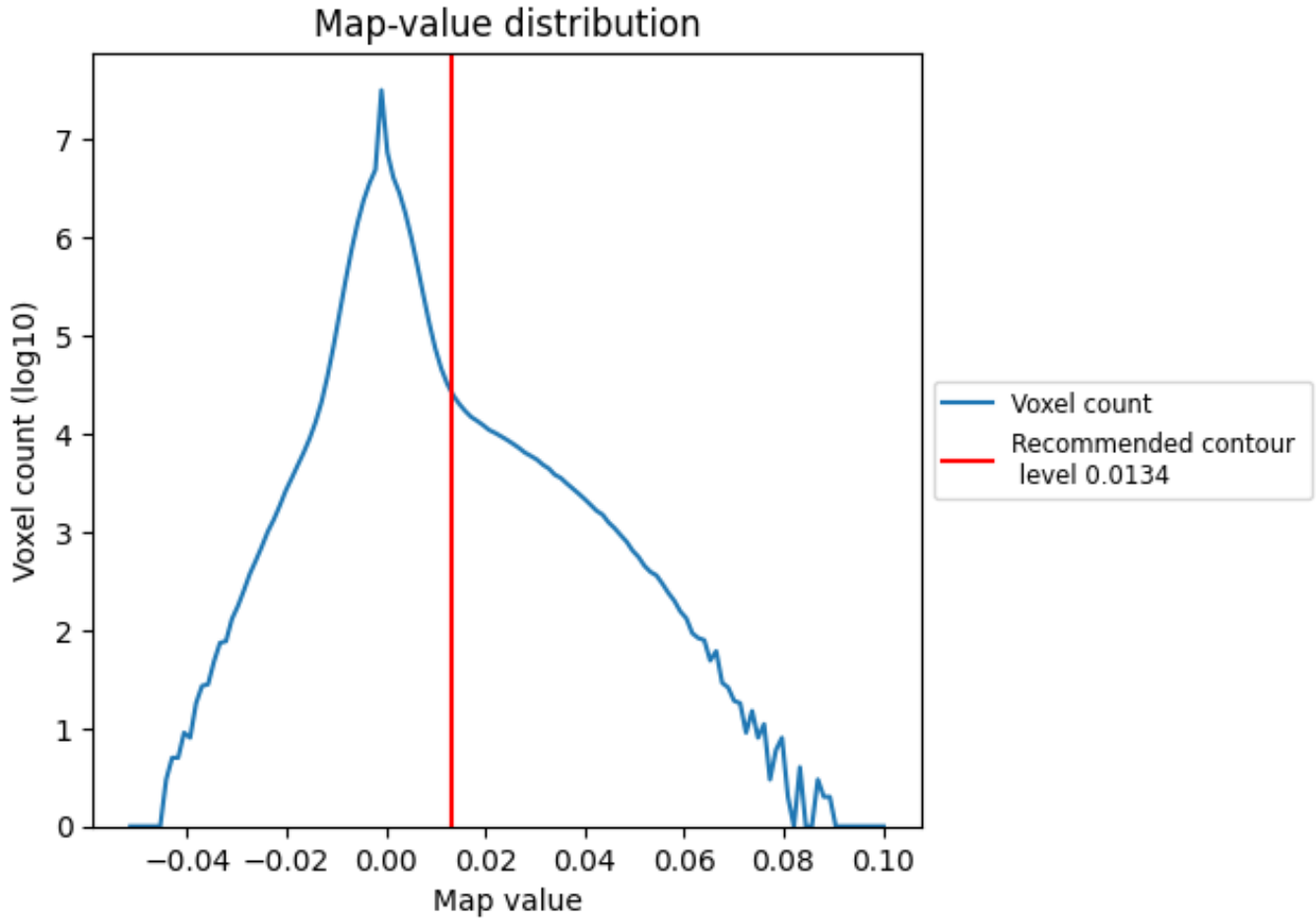
6.5 Mask visualisation (i)

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

7 Map analysis

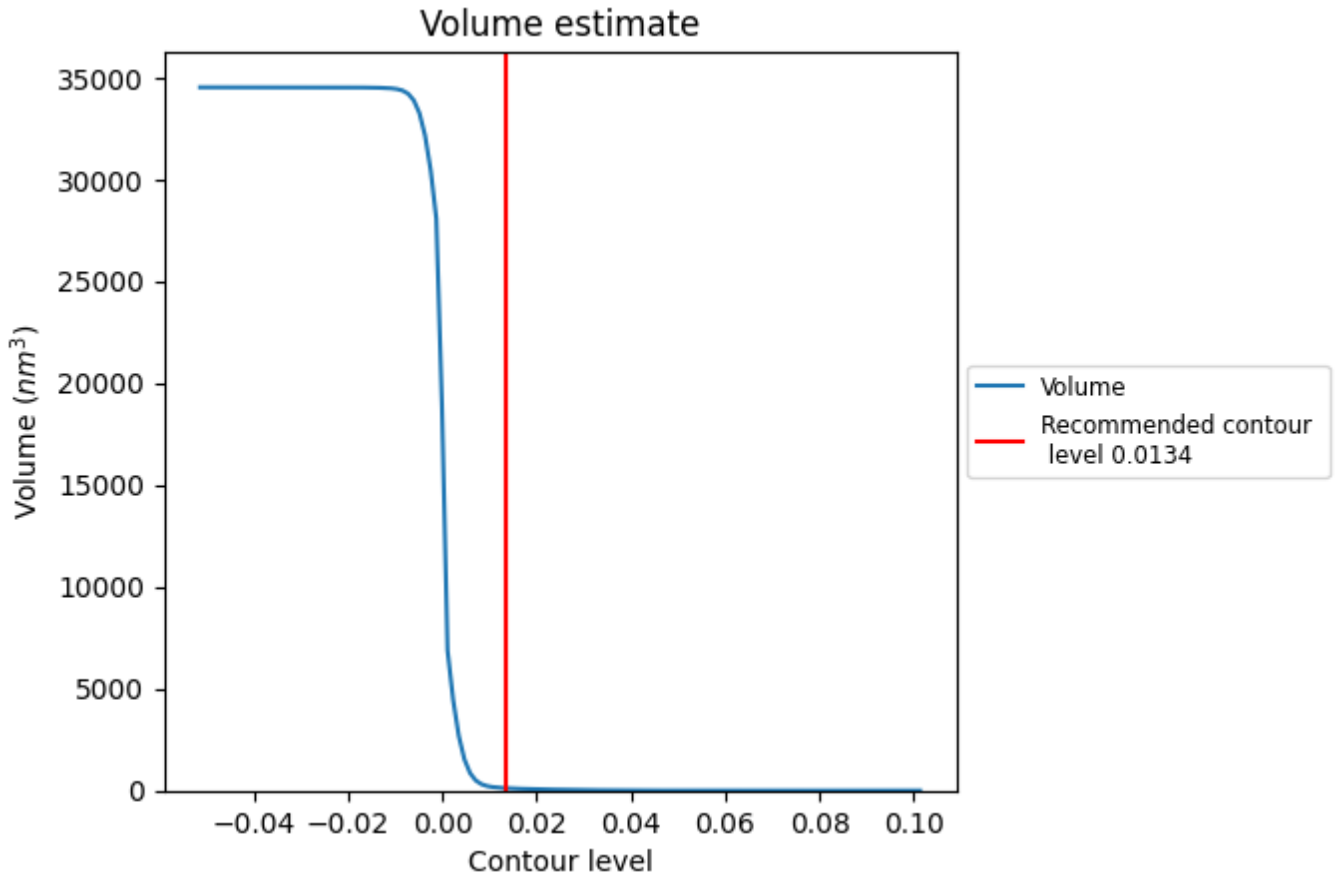
This section contains the results of statistical analysis of the map.

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.

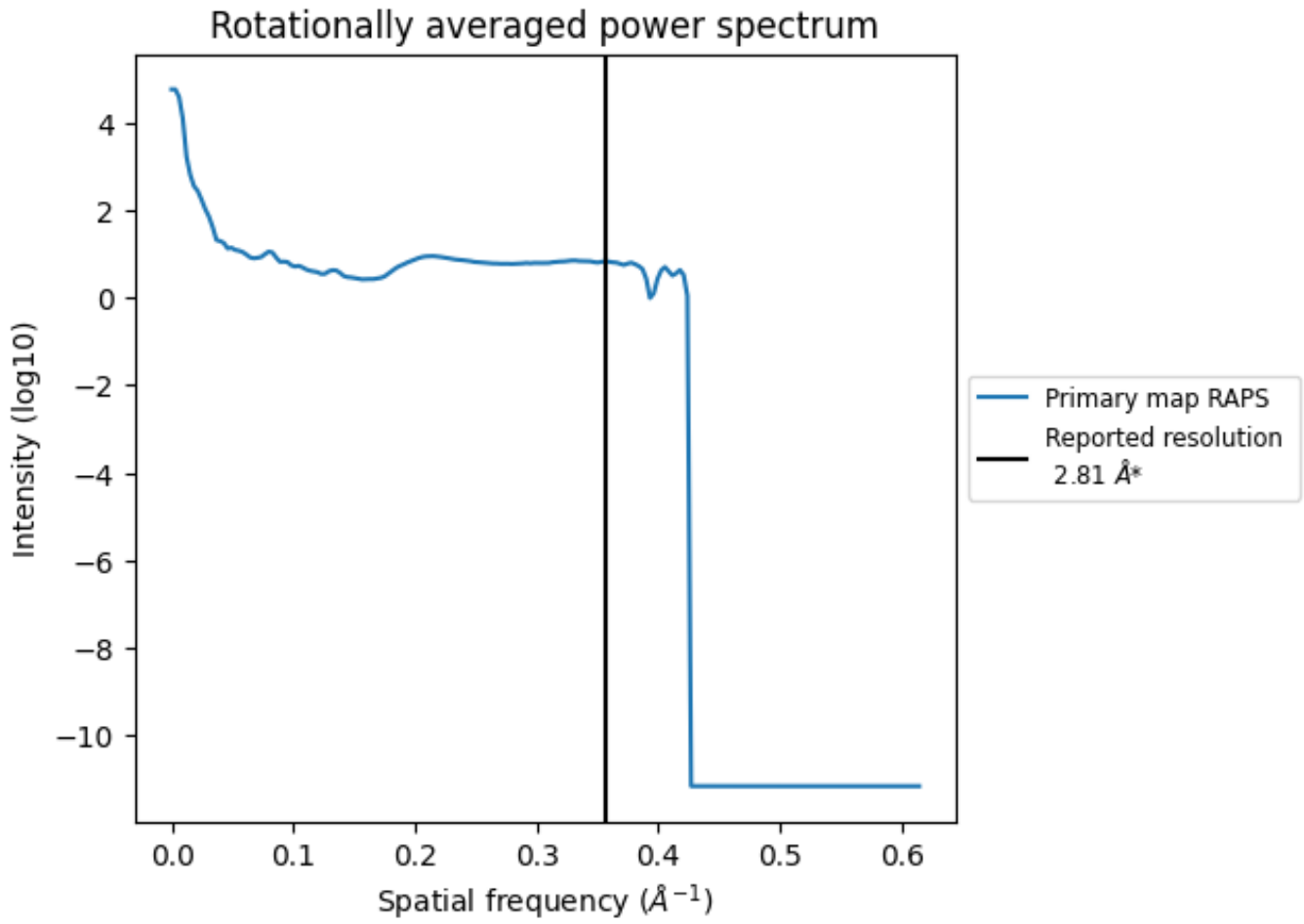
7.2 Volume estimate



The volume at the recommended contour level is 119 nm^3; this corresponds to an approximate mass of 107 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)

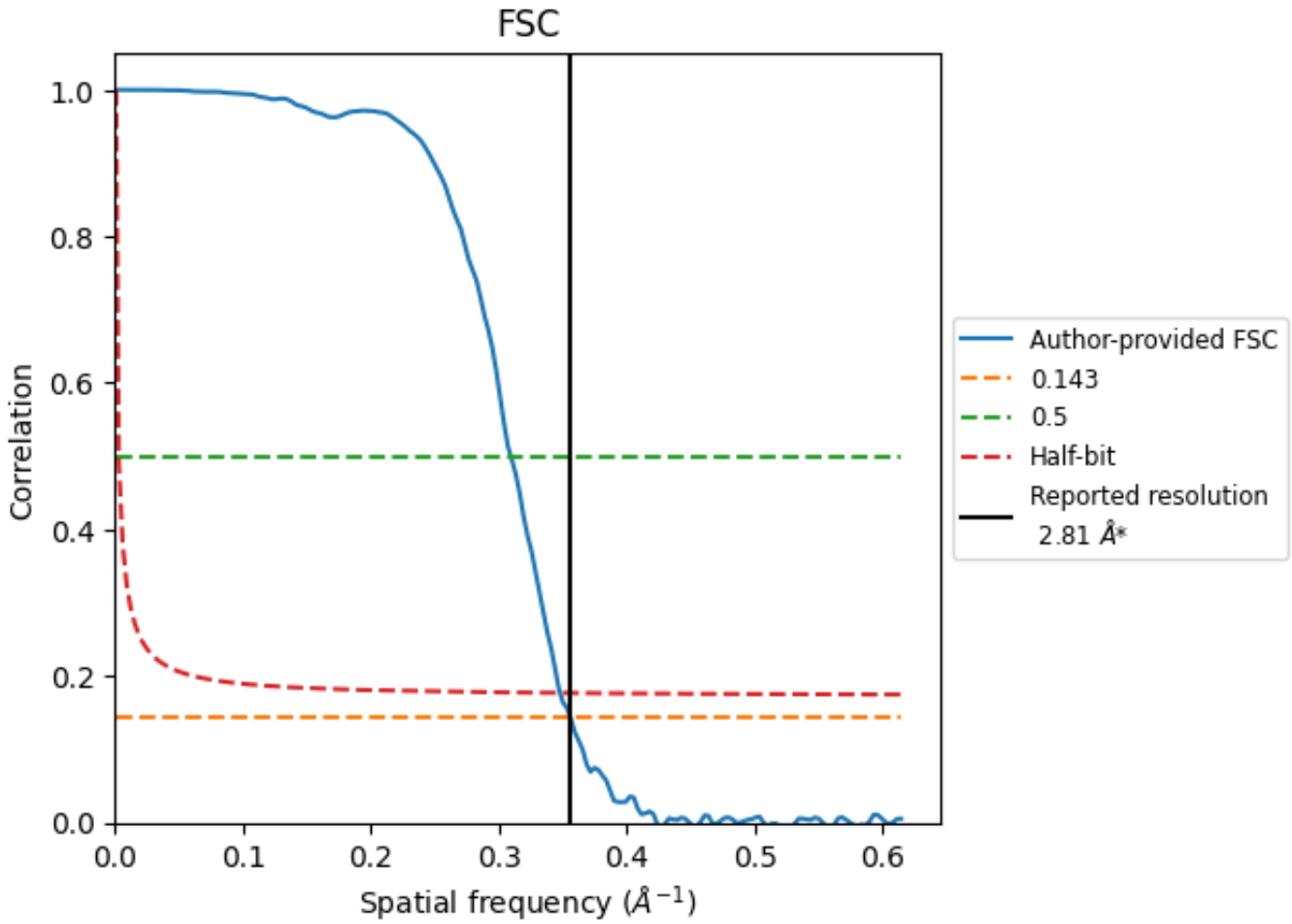


*Reported resolution corresponds to spatial frequency of 0.356 Å^{-1}

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 0.356 Å^{-1}

8.2 Resolution estimates (i)

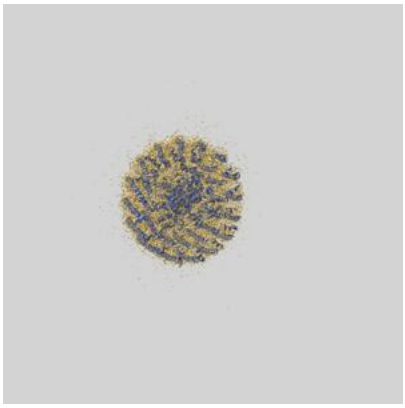
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.81	-	-
Author-provided FSC curve	2.81	3.23	2.88
Unmasked-calculated*	-	-	-

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

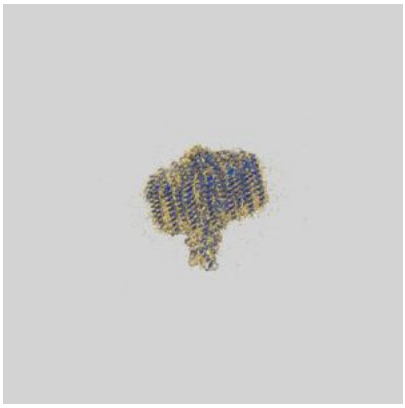
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-32100 and PDB model 7VRJ. Per-residue inclusion information can be found in section 3 on page 20.

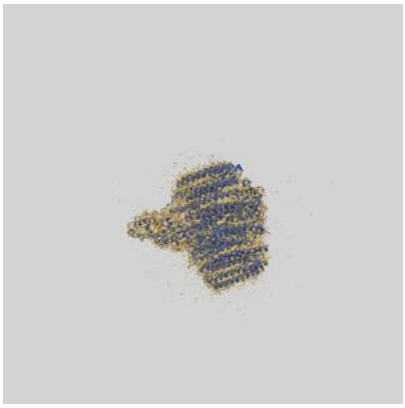
9.1 Map-model overlay



X



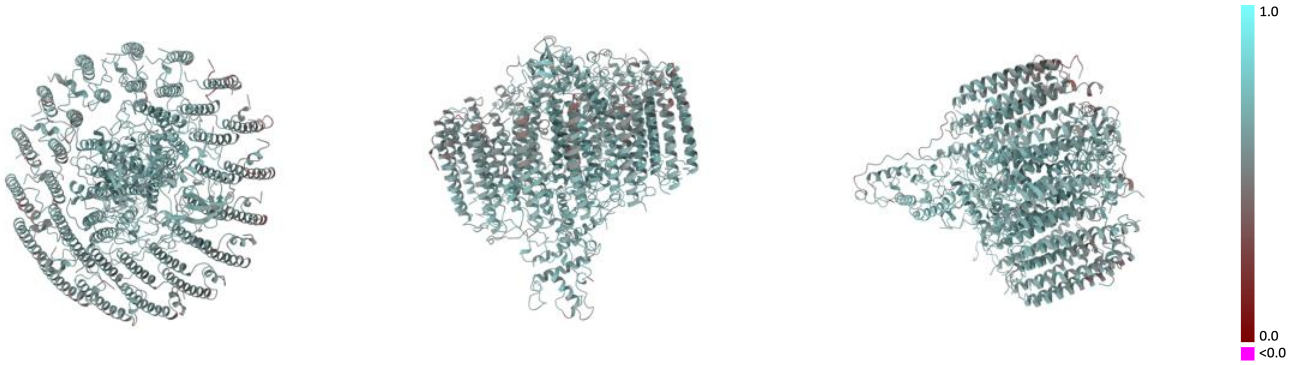
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0134 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.

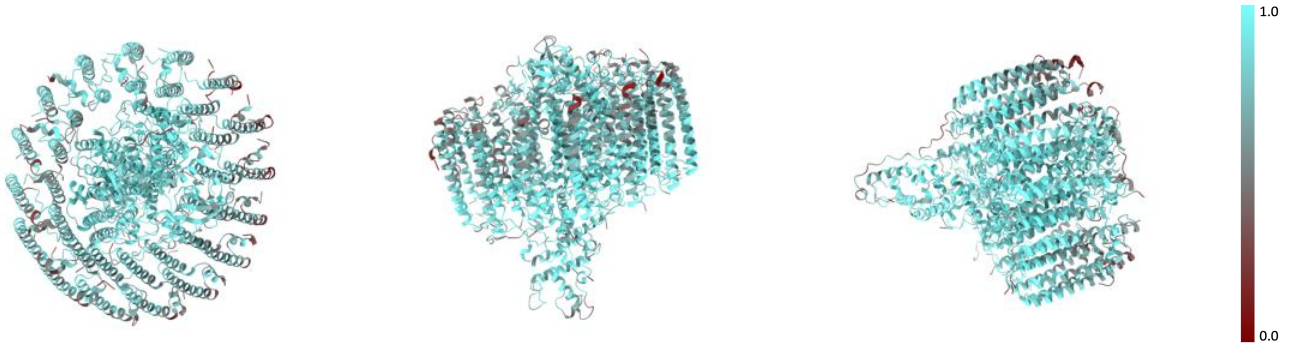
9.2 Q-score mapped to coordinate model (i)



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.

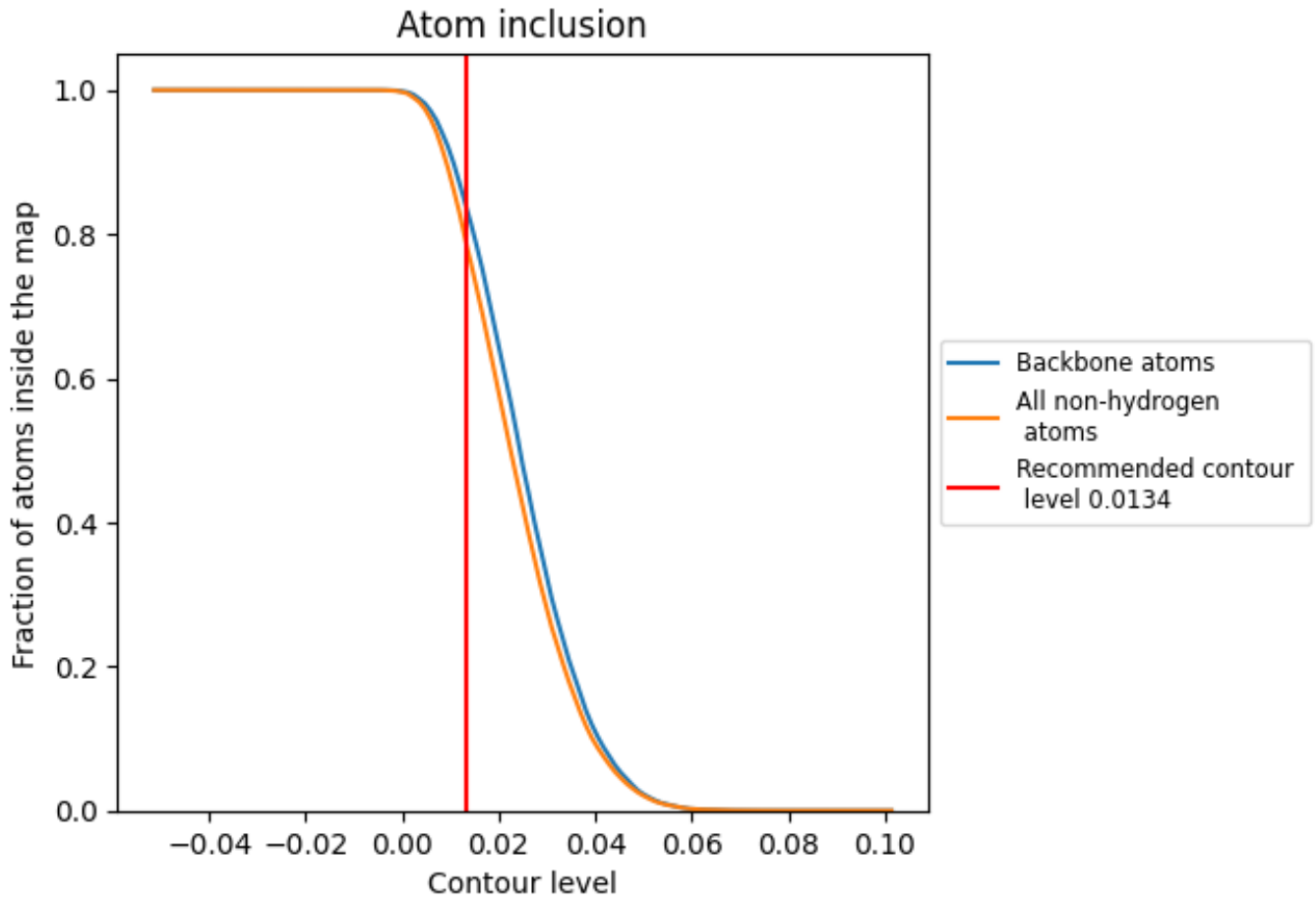
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.0134).

9.4 Atom inclusion (i)



At the recommended contour level, 83% of all backbone atoms, 78% 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 (0.0134) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7827	0.6010
0	0.7689	0.5950
1	0.6795	0.5680
2	0.6653	0.5520
3	0.6908	0.5680
4	0.5988	0.5280
5	0.6989	0.5870
6	0.6580	0.5420
7	0.7352	0.5770
8	0.6942	0.5620
9	0.8361	0.6280
A	0.8483	0.6200
B	0.7556	0.5840
C	0.8854	0.6370
D	0.7804	0.6070
E	0.7607	0.5900
F	0.7746	0.5920
G	0.7149	0.5660
H	0.7567	0.5950
I	0.6829	0.5630
J	0.6534	0.5400
K	0.6723	0.5660
L	0.8893	0.6500
M	0.8854	0.6510
N	0.6689	0.5590
O	0.7648	0.5980
P	0.6965	0.5620
Q	0.8026	0.6110
R	0.7523	0.5790
S	0.7192	0.5810
T	0.7341	0.5790
U	0.7754	0.5870
V	0.7045	0.5640
W	0.7397	0.5890
X	0.6983	0.5650

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Chain	Atom inclusion	Q-score
Y	0.6968	0.5770
Z	0.7028	0.5600