Full wwPDB EM Validation Report

Sep 15, 2021 – 01:33 pm BST

PDB ID	:	7OY8
EMDB ID	:	EMD-13110
Title	:	Cryo-EM structure of the Rhodospirillum rubrum RC-LH1 complex
Authors	:	Qian, P.; Croll, T.I.; Castro, H.P.; Moriarty, N.W.; sader, K.; Hunter, C.N.
Deposited on	:	2021-06-23
Resolution	:	2.50 Å(reported)
Based on initial models	:	1LGH, 3I4D

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

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

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

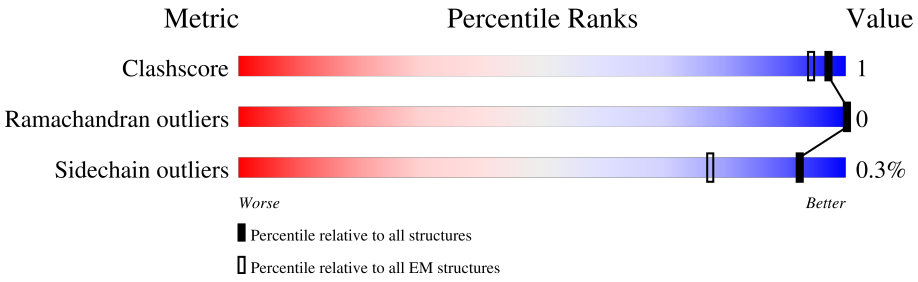
EMDB validation analysis	:	0.0.0.dev97
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.1

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 2.50 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	1	54	81% 19%
1	3	54	81% 19%
1	5	54	81% 19%
1	7	54	80% 19%
1	9	54	85% 15%
1	I	54	80% 19%
1	K	54	83% 17%
1	O	54	81% 19%

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Mol	Chain	Length	Quality of chain
1	Q	54	87% 13%
1	S	54	83% 17%
1	U	54	81% 19%
1	W	54	81% 19%
1	Y	54	76% 20%
1	d	54	81% 19%
1	m	54	83% 17%
1	n	54	81% 19%
2	2	50	92% 8%
2	4	50	6% 94% 6%
2	6	50	90% 6%
2	8	50	94%
2	A	50	86% 6% 8%
2	D	50	90% 6%
2	E	50	90% 8%
2	F	50	92% 6%
2	G	50	94% 6%
2	J	50	90% 8%
2	N	50	90% 8%
2	T	50	94% 6%
2	V	50	92% 8%
2	X	50	92% 6%
2	Z	50	94% 6%
3	H	257	100%
4	L	276	96%

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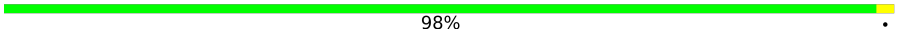
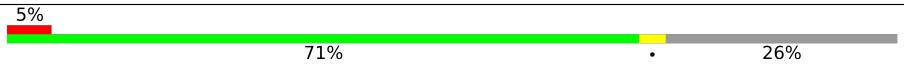
Mol	Chain	Length	Quality of chain
5	M	306	
6	R	62	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	07D	1	1001	X	-	-	-
7	07D	2	1001	X	-	-	-
7	07D	3	102	X	-	-	-
7	07D	4	1001	X	-	-	-
7	07D	5	102	X	-	-	-
7	07D	6	1001	X	-	-	-
7	07D	7	102	X	-	-	-
7	07D	8	1001	X	-	-	-
7	07D	9	102	X	-	-	-
7	07D	A	101	X	-	-	-
7	07D	D	1001	X	-	-	-
7	07D	E	1001	X	-	-	-
7	07D	F	1001	X	-	-	-
7	07D	G	1001	X	-	-	-
7	07D	H	301	X	-	-	-
7	07D	I	102	X	-	-	-
7	07D	J	1001	X	-	-	-
7	07D	K	102	X	-	-	-
7	07D	L	1004	X	-	-	-
7	07D	L	1005	X	-	-	-
7	07D	M	404	X	-	-	-
7	07D	M	405	X	-	-	-
7	07D	N	1002	X	-	-	-
7	07D	O	102	X	-	-	-
7	07D	Q	102	X	-	-	-
7	07D	R	101	X	-	-	-
7	07D	S	102	X	-	-	-
7	07D	T	101	X	-	-	-
7	07D	U	1001	X	-	-	-
7	07D	V	1001	X	-	-	-
7	07D	W	1001	X	-	-	-
7	07D	X	1001	X	-	-	-
7	07D	Y	102	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	07D	Z	1001	X	-	-	-
7	07D	d	1002	X	-	-	-
7	07D	m	102	X	-	-	-
7	07D	n	102	X	-	-	-

2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 22902 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Light-harvesting protein B-870 beta chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	1	44	Total	C	N	O	0	0
			360	247	57	56		
1	3	44	Total	C	N	O	0	0
			360	247	57	56		
1	5	44	Total	C	N	O	0	0
			360	247	57	56		
1	7	44	Total	C	N	O	0	0
			360	247	57	56		
1	9	46	Total	C	N	O	0	0
			370	252	59	59		
1	I	44	Total	C	N	O	0	0
			360	247	57	56		
1	K	45	Total	C	N	O	0	0
			364	249	58	57		
1	O	44	Total	C	N	O	0	0
			360	247	57	56		
1	Q	47	Total	C	N	O	0	0
			378	258	60	60		
1	S	45	Total	C	N	O	0	0
			364	249	58	57		
1	U	44	Total	C	N	O	0	0
			360	247	57	56		
1	W	44	Total	C	N	O	0	0
			360	247	57	56		
1	Y	43	Total	C	N	O	0	0
			352	241	56	55		
1	d	44	Total	C	N	O	0	0
			360	247	57	56		
1	m	45	Total	C	N	O	0	0
			364	249	58	57		
1	n	44	Total	C	N	O	0	0
			360	247	57	56		

- Molecule 2 is a protein called Antenna complex, alpha/beta subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	46	Total	C	N	O	S	0	0
			388	263	63	61	1		
2	4	47	Total	C	N	O	S	0	0
			397	269	65	62	1		
2	6	47	Total	C	N	O	S	0	0
			397	269	65	62	1		
2	8	48	Total	C	N	O	S	0	0
			404	274	66	63	1		
2	A	46	Total	C	N	O	S	0	0
			388	263	63	61	1		
2	D	47	Total	C	N	O	S	0	0
			397	269	65	62	1		
2	E	46	Total	C	N	O	S	0	0
			388	263	63	61	1		
2	F	47	Total	C	N	O	S	0	0
			397	269	65	62	1		
2	G	47	Total	C	N	O	S	0	0
			397	269	65	62	1		
2	J	46	Total	C	N	O	S	0	0
			388	263	63	61	1		
2	N	46	Total	C	N	O	S	0	0
			388	263	63	61	1		
2	T	47	Total	C	N	O	S	0	0
			397	269	65	62	1		
2	V	46	Total	C	N	O	S	0	0
			388	263	63	61	1		
2	X	47	Total	C	N	O	S	0	0
			397	269	65	62	1		
2	Z	47	Total	C	N	O	S	0	0
			397	269	65	62	1		

- Molecule 3 is a protein called Photosynthetic reaction center, H-chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	257	Total	C	N	O	S	0	0
			1972	1263	343	362	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	L	274	Total	C	N	O	S	0	0
			2164	1456	344	354	10		

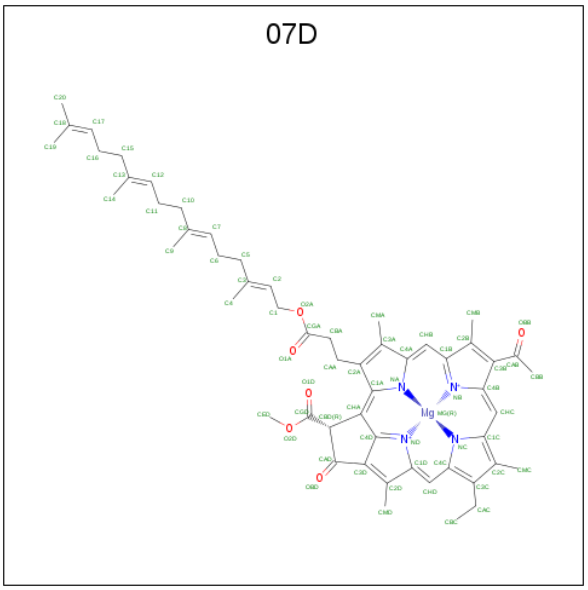
- Molecule 5 is a protein called Reaction center protein M chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	M	305	Total	C	N	O	S	0	0
			2424	1619	398	398	9		

- Molecule 6 is a protein called Antenna complex, alpha/beta subunit.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	R	46	Total	C	N	O	0	0
			387	263	64	60		

- Molecule 7 is Trans-Geranyl BACTERIOCHLOROPHYLL A (three-letter code: 07D) (formula: $C_{55}H_{64}MgN_4O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
7	1	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	2	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	3	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	4	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	5	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	6	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	7	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
7	8	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	9	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	A	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	D	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	E	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	F	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	G	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	H	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	I	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	J	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	K	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	L	1	Total	C	Mg	N	O	0
			132	110	2	8	12	
7	L	1	Total	C	Mg	N	O	0
			132	110	2	8	12	
7	M	1	Total	C	Mg	N	O	0
			132	110	2	8	12	
7	M	1	Total	C	Mg	N	O	0
			132	110	2	8	12	
7	N	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	O	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	Q	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	R	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	S	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	T	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

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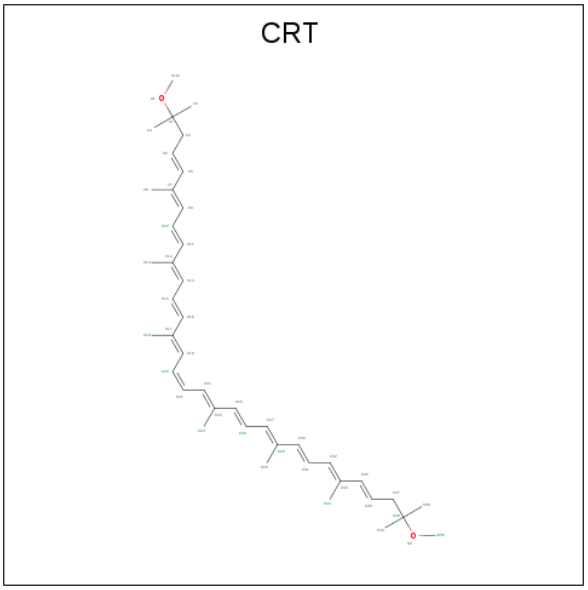
Mol	Chain	Residues	Atoms					AltConf
7	U	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	V	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	W	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	X	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	Y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	Z	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	d	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	m	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	n	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

- Molecule 8 is SPIRILLOXANTHIN (three-letter code: CRT) (formula: $C_{42}H_{60}O_2$).



Mol	Chain	Residues	Atoms			AltConf
8	1	1	Total	C	O	0
			44	42	2	
8	3	1	Total	C	O	0
			44	42	2	

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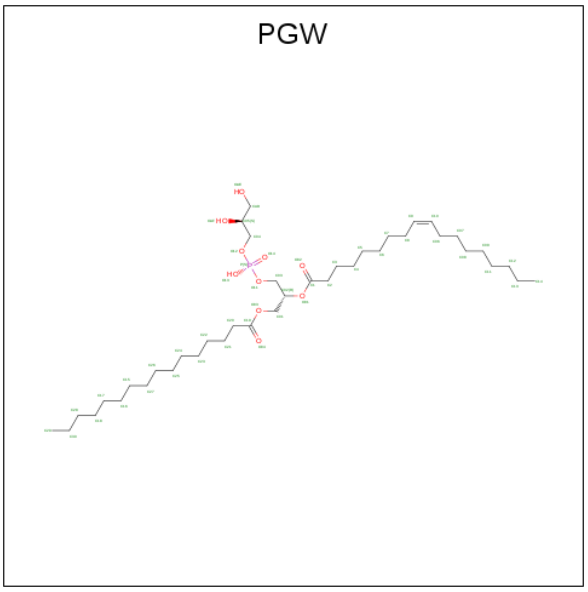
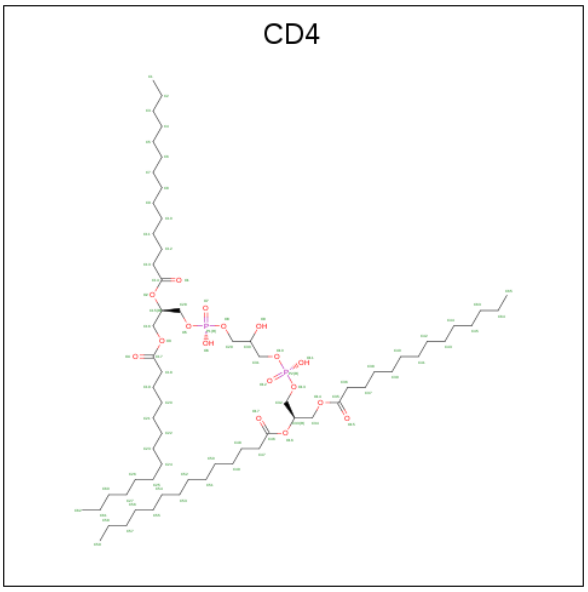
Mol	Chain	Residues	Atoms			AltConf
8	5	1	Total	C	O	0
			44	42	2	
8	7	1	Total	C	O	0
			44	42	2	
8	9	1	Total	C	O	0
			44	42	2	
8	I	1	Total	C	O	0
			44	42	2	
8	J	1	Total	C	O	0
			44	42	2	
8	K	1	Total	C	O	0
			44	42	2	
8	M	1	Total	C	O	0
			44	42	2	
8	N	1	Total	C	O	0
			44	42	2	
8	O	1	Total	C	O	0
			44	42	2	
8	Q	1	Total	C	O	0
			44	42	2	
8	S	1	Total	C	O	0
			44	42	2	
8	Y	1	Total	C	O	0
			44	42	2	
8	d	1	Total	C	O	0
			44	42	2	
8	m	1	Total	C	O	0
			44	42	2	
8	n	1	Total	C	O	0
			44	42	2	

- Molecule 9 is (1R)-2-{[(S)-{[(2S)-2,3-dihydroxypropyl]oxy}(hydroxy)phosphoryl]oxy}-1-[(hexadecanoyloxy)methyl]ethyl (9Z)-octadec-9-enoate (three-letter code: PGW) (formula: $C_{40}H_{77}O_{10}P$).



Mol	Chain	Residues	Atoms				AltConf
9	H	1	Total	C	O	P	0
			102	80	20	2	
9	H	1	Total	C	O	P	0
			102	80	20	2	

- Molecule 10 is (2R,5R,11R,14R)-5,8,11-trihydroxy-5,11-dioxido-17-oxo-2,14-bis(tetradecanoyloxy)-4,6,10,12,16-pentaoxa-5,11-diphosphatriacont-1-yl tetradecanoate (three-letter code: CD4) (formula: $C_{65}H_{126}O_{17}P_2$).



Mol	Chain	Residues	Atoms				AltConf
10	H	1	Total	C	O	P	0
			84	65	17	2	

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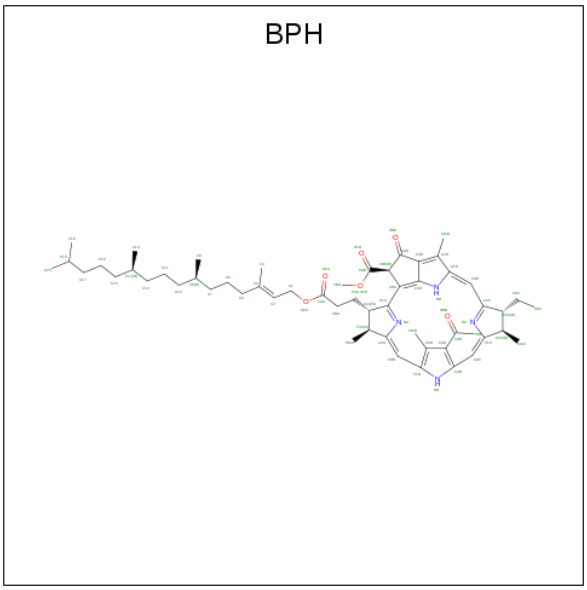
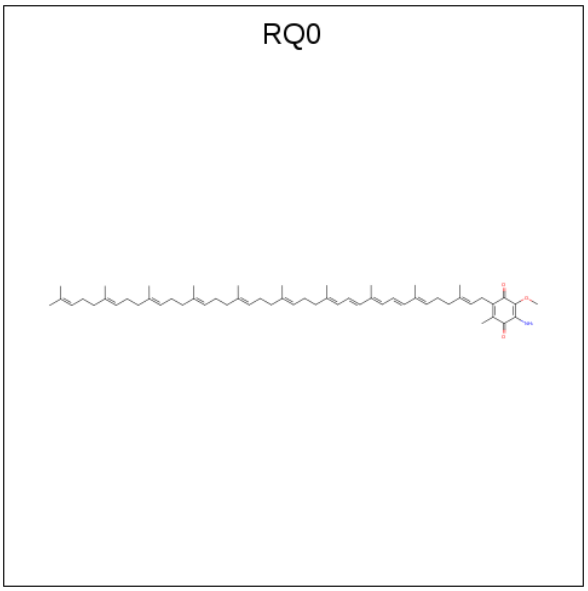
Mol	Chain	Residues	Atoms				AltConf
10	M	1	Total	C	O	P	0
			84	65	17	2	

- Molecule 11 is BACTERIOPHEOPHYTIN A (three-letter code: BPH) (formula: $C_{55}H_{76}N_4O_6$) (labeled as "Ligand of Interest" by depositor).



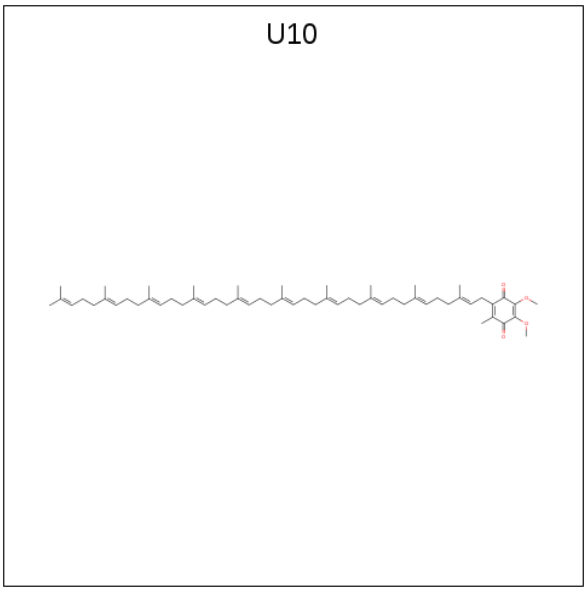
Mol	Chain	Residues	Atoms				AltConf
11	L	1	Total	C	N	O	0
			65	55	4	6	
11	M	1	Total	C	N	O	0
			65	55	4	6	

- Molecule 12 is 2-azanyl-5-[(2 {E},6 {E},8 {E},10 {E},12 {E},14 {E},18 {E},22 {E},26 {E},30 {E},34 {E})-3,7,11,15,19,23,27,31,35,39-decamethyltetraconta-2,6,8,10,12,14,18,22,26,30,34,38-dodecaenyl]-3-methoxy-6-methyl-cyclohexa-2,5-diene-1,4-dione (three-letter code: RQ0) (formula: $C_{58}H_{85}NO_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
12	L	1	Total	C	N	O	0
			62	58	1	3	

- Molecule 13 is UBIQUINONE-10 (three-letter code: U10) (formula: $C_{59}H_{90}O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
13	L	1	Total	C	O	0
			126	118	8	
13	L	1	Total	C	O	0
			126	118	8	

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

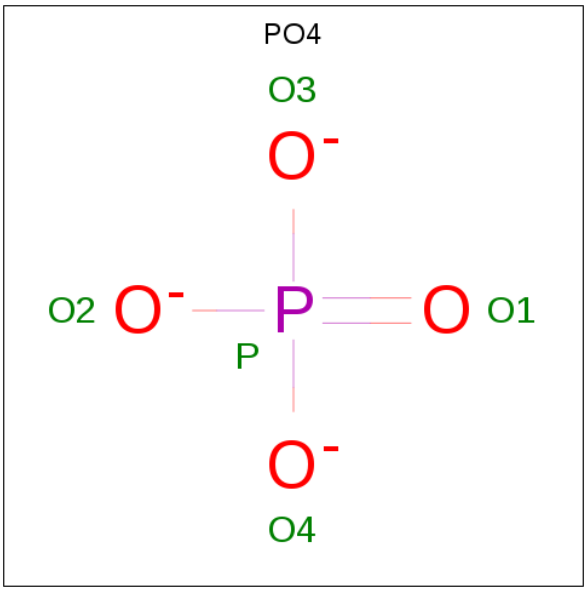
- Molecule 14 is FE (III) ION (three-letter code: FE) (formula: Fe).

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

- Molecule 15 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

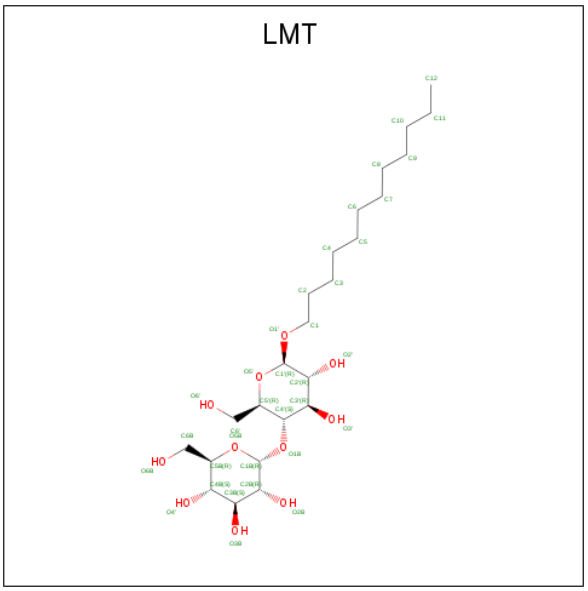
Mol	Chain	Residues	Atoms	AltConf
15	M	1	Total Cl 1 1	0

- Molecule 16 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms	AltConf
16	M	1	Total O P 5 4 1	0

- Molecule 17 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms	AltConf
17	R	1	Total C O 35 24 11	0

- Molecule 18 is water.

Mol	Chain	Residues	Atoms	AltConf
18	2	1	Total O 1 1	0
18	3	1	Total O 1 1	0
18	4	11	Total O 11 11	0
18	5	2	Total O 2 2	0
18	6	8	Total O 8 8	0
18	7	1	Total O 1 1	0
18	8	6	Total O 6 6	0
18	9	1	Total O 1 1	0
18	A	8	Total O 8 8	0
18	D	6	Total O 6 6	0
18	E	5	Total O 5 5	0

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Mol	Chain	Residues	Atoms	AltConf
18	F	6	Total O 6 6	0
18	G	8	Total O 8 8	0
18	H	68	Total O 68 68	0
18	I	1	Total O 1 1	0
18	J	3	Total O 3 3	0
18	K	1	Total O 1 1	0
18	L	89	Total O 89 89	0
18	M	86	Total O 86 86	0
18	N	14	Total O 14 14	0
18	O	3	Total O 3 3	0
18	Q	2	Total O 2 2	0
18	R	8	Total O 8 8	0
18	S	2	Total O 2 2	0
18	T	4	Total O 4 4	0
18	U	3	Total O 3 3	0
18	V	4	Total O 4 4	0
18	W	1	Total O 1 1	0
18	X	8	Total O 8 8	0
18	Y	1	Total O 1 1	0
18	Z	7	Total O 7 7	0
18	d	2	Total O 2 2	0

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Mol	Chain	Residues	Atoms		AltConf
			Total	O	
18	n	1	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: Light-harvesting protein B-870 beta chain

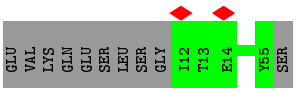
Chain 1:

• Molecule 1: Light-harvesting protein B-870 beta chain

Chain 3:

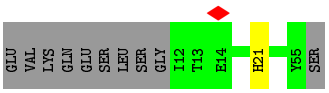
• Molecule 1: Light-harvesting protein B-870 beta chain

Chain 5:



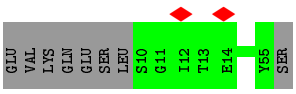
• Molecule 1: Light-harvesting protein B-870 beta chain

Chain 7:



• Molecule 1: Light-harvesting protein B-870 beta chain

Chain 9:



• Molecule 1: Light-harvesting protein B-870 beta chain

Chain I:

• Molecule 1: Light-harvesting protein B-870 beta chain

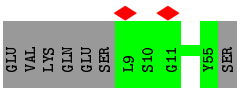
Chain K:

• Molecule 1: Light-harvesting protein B-870 beta chain

Chain O:

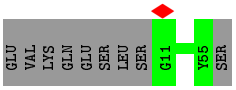
• Molecule 1: Light-harvesting protein B-870 beta chain

Chain Q:



• Molecule 1: Light-harvesting protein B-870 beta chain

Chain S:

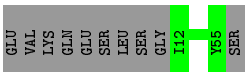


• Molecule 1: Light-harvesting protein B-870 beta chain

Chain U:

• Molecule 1: Light-harvesting protein B-870 beta chain

Chain W:

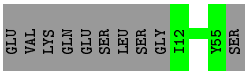


• Molecule 1: Light-harvesting protein B-870 beta chain

Chain Y:

• Molecule 1: Light-harvesting protein B-870 beta chain

Chain d:



• Molecule 1: Light-harvesting protein B-870 beta chain

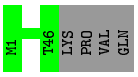
Chain m:

• Molecule 1: Light-harvesting protein B-870 beta chain

Chain n:

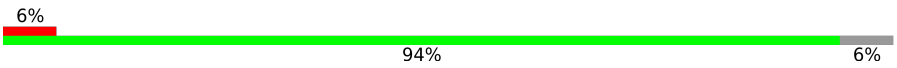
• Molecule 2: Antenna complex, alpha/beta subunit

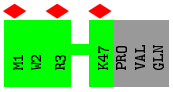
Chain 2:



• Molecule 2: Antenna complex, alpha/beta subunit

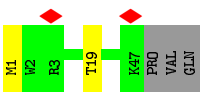
Chain 4:





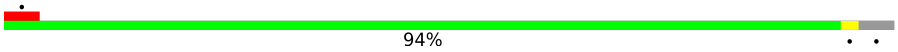
• Molecule 2: Antenna complex, alpha/beta subunit

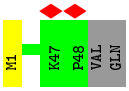
Chain 6:



• Molecule 2: Antenna complex, alpha/beta subunit

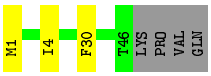
Chain 8:





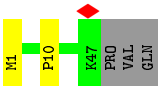
- Molecule 2: Antenna complex, alpha/beta subunit

Chain A:



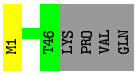
- Molecule 2: Antenna complex, alpha/beta subunit

Chain D:



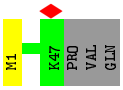
- Molecule 2: Antenna complex, alpha/beta subunit

Chain E:



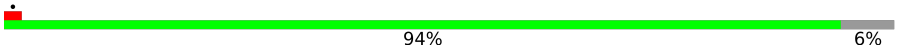
- Molecule 2: Antenna complex, alpha/beta subunit

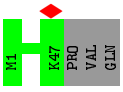
Chain F:



- Molecule 2: Antenna complex, alpha/beta subunit

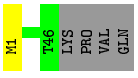
Chain G:





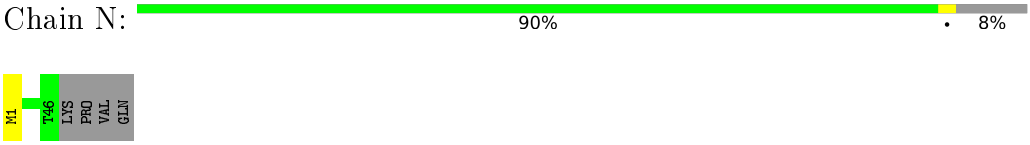
- Molecule 2: Antenna complex, alpha/beta subunit

Chain J:



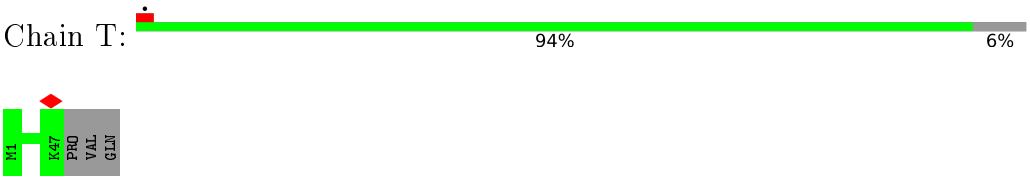
• Molecule 2: Antenna complex, alpha/beta subunit

Chain N:



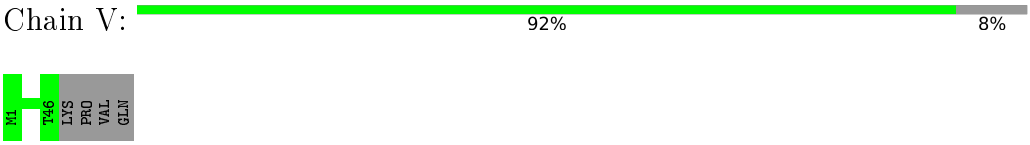
• Molecule 2: Antenna complex, alpha/beta subunit

Chain T:



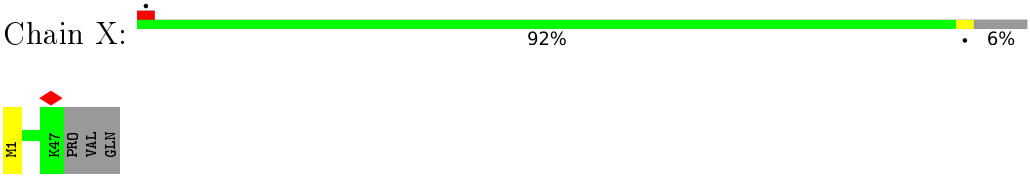
• Molecule 2: Antenna complex, alpha/beta subunit

Chain V:



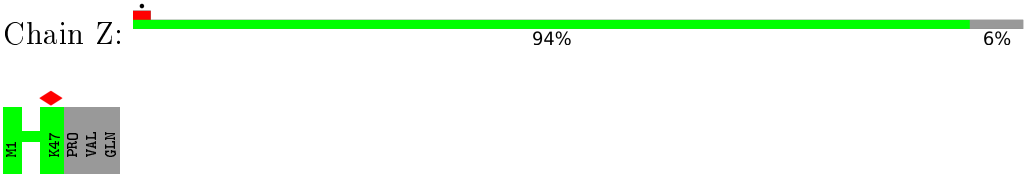
• Molecule 2: Antenna complex, alpha/beta subunit

Chain X:



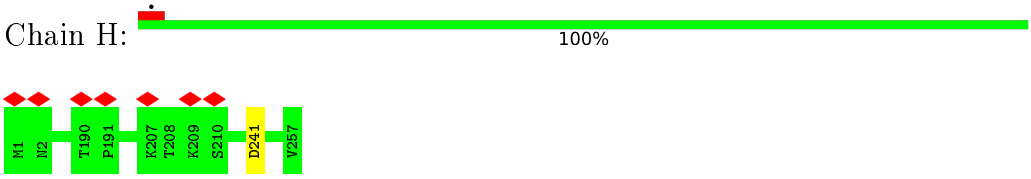
• Molecule 2: Antenna complex, alpha/beta subunit

Chain Z:



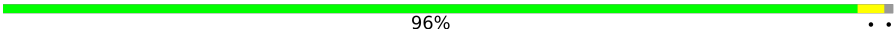
• Molecule 3: Photosynthetic reaction center, H-chain

Chain H:



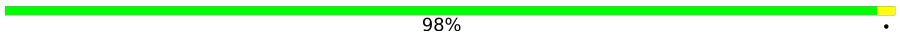
• Molecule 4: Photosynthetic reaction center L subunit

Chain L:



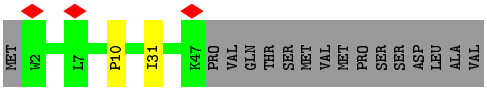
- Molecule 5: Reaction center protein M chain

Chain M:



- Molecule 6: Antenna complex, alpha/beta subunit

Chain R:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	519005	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	45	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	120000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.161	Depositor
Minimum map value	-0.071	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.0165	Depositor
Map size (Å)	332.8, 332.8, 332.8	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.3, 1.3, 1.3	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 07D, PO4, FME, U10, CL, RQ0, FE, CD4, LMT, BPH, PGW, CRT

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	1	0.26	0/376	0.40	0/514
1	3	0.26	0/376	0.41	0/514
1	5	0.26	0/376	0.43	0/514
1	7	0.26	0/376	0.42	0/514
1	9	0.27	0/386	0.43	0/527
1	I	0.26	0/376	0.41	0/514
1	K	0.26	0/380	0.40	0/519
1	O	0.26	0/376	0.40	0/514
1	Q	0.25	0/394	0.44	0/538
1	S	0.26	0/380	0.42	0/519
1	U	0.26	0/376	0.41	0/514
1	W	0.26	0/376	0.41	0/514
1	Y	0.27	0/368	0.46	0/503
1	d	0.25	0/376	0.41	0/514
1	m	0.26	0/380	0.44	0/519
1	n	0.26	0/376	0.42	0/514
2	2	0.26	0/390	0.54	0/532
2	4	0.26	0/399	0.54	0/543
2	6	0.26	0/399	0.56	0/543
2	8	0.25	0/407	0.55	0/555
2	A	0.26	0/390	0.54	0/532
2	D	0.25	0/399	0.52	0/543
2	E	0.26	0/390	0.54	0/532
2	F	0.26	0/399	0.53	0/543
2	G	0.26	0/399	0.51	0/543
2	J	0.25	0/390	0.52	0/532
2	N	0.26	0/390	0.54	0/532
2	T	0.26	0/399	0.54	0/543
2	V	0.26	0/390	0.53	0/532
2	X	0.26	0/399	0.53	0/543
2	Z	0.26	0/399	0.54	0/543
3	H	0.25	0/2014	0.59	0/2739

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
4	L	0.25	0/2248	0.51	0/3077
5	M	0.26	0/2515	0.52	0/3429
6	R	0.26	0/399	0.55	0/543
All	All	0.26	0/19163	0.50	0/26144

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	360	0	350	0	0
1	3	360	0	350	0	0
1	5	360	0	350	0	0
1	7	360	0	350	1	0
1	9	370	0	358	0	0
1	I	360	0	350	1	0
1	K	364	0	353	0	0
1	O	360	0	350	0	0
1	Q	378	0	369	0	0
1	S	364	0	353	0	0
1	U	360	0	350	0	0
1	W	360	0	350	0	0
1	Y	352	0	339	2	0
1	d	360	0	350	0	0
1	m	364	0	353	0	0
1	n	360	0	350	0	0
2	2	388	0	394	0	0
2	4	397	0	407	0	0
2	6	397	0	407	2	0
2	8	404	0	414	0	0
2	A	388	0	394	2	0
2	D	397	0	407	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	388	0	394	0	0
2	F	397	0	407	0	0
2	G	397	0	407	0	0
2	J	388	0	394	0	0
2	N	388	0	394	0	0
2	T	397	0	407	0	0
2	V	388	0	394	0	0
2	X	397	0	407	0	0
2	Z	397	0	407	0	0
3	H	1972	0	2023	0	0
4	L	2164	0	2126	4	0
5	M	2424	0	2365	3	0
6	R	387	0	396	2	0
7	1	66	0	0	0	0
7	2	66	0	0	0	0
7	3	66	0	0	0	0
7	4	66	0	0	0	0
7	5	66	0	0	0	0
7	6	66	0	0	0	0
7	7	66	0	0	0	0
7	8	66	0	0	0	0
7	9	66	0	0	0	0
7	A	66	0	0	0	0
7	D	66	0	0	0	0
7	E	66	0	0	0	0
7	F	66	0	0	0	0
7	G	66	0	0	0	0
7	H	66	0	0	0	0
7	I	66	0	0	0	0
7	J	66	0	0	0	0
7	K	66	0	0	0	0
7	L	132	0	0	0	0
7	M	132	0	0	0	0
7	N	66	0	0	0	0
7	O	66	0	0	0	0
7	Q	66	0	0	0	0
7	R	66	0	0	0	0
7	S	66	0	0	0	0
7	T	66	0	0	0	0
7	U	66	0	0	0	0
7	V	66	0	0	0	0
7	W	66	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	X	66	0	0	0	0
7	Y	66	0	0	0	0
7	Z	66	0	0	0	0
7	d	66	0	0	0	0
7	m	66	0	0	0	0
7	n	66	0	0	0	0
8	1	44	0	60	0	0
8	3	44	0	60	0	0
8	5	44	0	60	3	0
8	7	44	0	60	0	0
8	9	44	0	60	0	0
8	I	44	0	60	1	0
8	J	44	0	60	1	0
8	K	44	0	60	0	0
8	M	44	0	60	2	0
8	N	44	0	60	1	0
8	O	44	0	60	0	0
8	Q	44	0	60	0	0
8	S	44	0	60	0	0
8	Y	44	0	60	1	0
8	d	44	0	60	0	0
8	m	44	0	60	0	0
8	n	44	0	60	0	0
9	H	102	0	152	0	0
10	H	84	0	124	0	0
10	M	84	0	124	0	0
11	L	65	0	76	1	0
11	M	65	0	76	1	0
12	L	62	0	0	0	0
13	L	126	0	180	3	0
13	M	63	0	90	1	0
14	M	1	0	0	0	0
15	M	1	0	0	0	0
16	M	5	0	0	0	0
17	R	35	0	45	0	0
18	2	1	0	0	0	0
18	3	1	0	0	0	0
18	4	11	0	0	0	0
18	5	2	0	0	0	0
18	6	8	0	0	0	0
18	7	1	0	0	0	0
18	8	6	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	9	1	0	0	0	0
18	A	8	0	0	0	0
18	D	6	0	0	0	0
18	E	5	0	0	0	0
18	F	6	0	0	0	0
18	G	8	0	0	0	0
18	H	68	0	0	0	0
18	I	1	0	0	0	0
18	J	3	0	0	0	0
18	K	1	0	0	0	0
18	L	89	0	0	0	0
18	M	86	0	0	0	0
18	N	14	0	0	0	0
18	O	3	0	0	0	0
18	Q	2	0	0	0	0
18	R	8	0	0	0	0
18	S	2	0	0	0	0
18	T	4	0	0	0	0
18	U	3	0	0	0	0
18	V	4	0	0	0	0
18	W	1	0	0	0	0
18	X	8	0	0	0	0
18	Y	1	0	0	0	0
18	Z	7	0	0	0	0
18	d	2	0	0	0	0
18	n	1	0	0	0	0
All	All	22902	0	20456	23	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 1.

All (23) 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)
13:L:1006:U10:H3M3	6:R:31:ILE:HA	1.84	0.59
4:L:133:VAL:HG23	4:L:134:VAL:HG23	1.91	0.52
2:6:19:THR:HG23	5:M:58:LEU:HD23	1.92	0.52
4:L:174:HIS:CE1	4:L:178:ILE:HD11	2.44	0.51
4:L:44:VAL:HG21	13:M:403:U10:H551	1.93	0.50
5:M:160:GLY:HA3	8:M:406:CRT:H292	1.94	0.49
2:A:4:ILE:HD11	8:J:1002:CRT:H82	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:201:HIS:CE1	5:M:205:ILE:HD11	2.50	0.46
13:L:1006:U10:H103	13:L:1006:U10:H1M1	1.98	0.46
11:L:1001:BPH:HHC	11:L:1001:BPH:CBB	2.46	0.46
4:L:76:LEU:HA	4:L:143:TRP:CD1	2.54	0.43
11:M:402:BPH:HHD	11:M:402:BPH:HBC3	2.02	0.42
8:N:1001:CRT:H31	8:N:1001:CRT:H291	1.95	0.42
8:5:101:CRT:H26	8:5:101:CRT:H241	1.95	0.42
6:R:10:PRO:HB3	1:Y:20:PHE:CE2	2.55	0.41
1:Y:28:ILE:HG22	8:Y:101:CRT:C19	2.50	0.41
2:A:30:PHE:CD1	13:L:1006:U10:H71	2.56	0.41
2:6:1:FME:HB2	1:7:21:HIS:CE1	2.55	0.41
8:5:101:CRT:H31	8:5:101:CRT:H291	1.98	0.41
2:D:10:PRO:HB3	1:I:20:PHE:CE1	2.56	0.41
8:M:406:CRT:H10	8:M:406:CRT:H81	1.95	0.40
8:I:101:CRT:H26	8:I:101:CRT:H241	1.89	0.40
8:5:101:CRT:H36	8:5:101:CRT:H341	1.96	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	42/54 (78%)	41 (98%)	1 (2%)	0	100	100
1	3	42/54 (78%)	41 (98%)	1 (2%)	0	100	100
1	5	42/54 (78%)	42 (100%)	0	0	100	100
1	7	42/54 (78%)	41 (98%)	1 (2%)	0	100	100
1	9	44/54 (82%)	44 (100%)	0	0	100	100
1	I	42/54 (78%)	41 (98%)	1 (2%)	0	100	100
1	K	43/54 (80%)	42 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	O	42/54 (78%)	41 (98%)	1 (2%)	0	100	100
1	Q	45/54 (83%)	45 (100%)	0	0	100	100
1	S	43/54 (80%)	43 (100%)	0	0	100	100
1	U	42/54 (78%)	41 (98%)	1 (2%)	0	100	100
1	W	42/54 (78%)	42 (100%)	0	0	100	100
1	Y	41/54 (76%)	40 (98%)	1 (2%)	0	100	100
1	d	42/54 (78%)	42 (100%)	0	0	100	100
1	m	43/54 (80%)	42 (98%)	1 (2%)	0	100	100
1	n	42/54 (78%)	42 (100%)	0	0	100	100
2	2	44/50 (88%)	44 (100%)	0	0	100	100
2	4	45/50 (90%)	43 (96%)	2 (4%)	0	100	100
2	6	45/50 (90%)	43 (96%)	2 (4%)	0	100	100
2	8	46/50 (92%)	45 (98%)	1 (2%)	0	100	100
2	A	44/50 (88%)	44 (100%)	0	0	100	100
2	D	45/50 (90%)	44 (98%)	1 (2%)	0	100	100
2	E	44/50 (88%)	43 (98%)	1 (2%)	0	100	100
2	F	45/50 (90%)	45 (100%)	0	0	100	100
2	G	45/50 (90%)	43 (96%)	2 (4%)	0	100	100
2	J	44/50 (88%)	43 (98%)	1 (2%)	0	100	100
2	N	44/50 (88%)	43 (98%)	1 (2%)	0	100	100
2	T	45/50 (90%)	44 (98%)	1 (2%)	0	100	100
2	V	44/50 (88%)	43 (98%)	1 (2%)	0	100	100
2	X	45/50 (90%)	45 (100%)	0	0	100	100
2	Z	45/50 (90%)	44 (98%)	1 (2%)	0	100	100
3	H	255/257 (99%)	246 (96%)	9 (4%)	0	100	100
4	L	272/276 (99%)	264 (97%)	8 (3%)	0	100	100
5	M	303/306 (99%)	292 (96%)	11 (4%)	0	100	100
6	R	44/62 (71%)	43 (98%)	1 (2%)	0	100	100
All	All	2223/2515 (88%)	2171 (98%)	52 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	36/45 (80%)	36 (100%)	0	100	100
1	3	36/45 (80%)	36 (100%)	0	100	100
1	5	36/45 (80%)	36 (100%)	0	100	100
1	7	36/45 (80%)	36 (100%)	0	100	100
1	9	37/45 (82%)	37 (100%)	0	100	100
1	I	36/45 (80%)	36 (100%)	0	100	100
1	K	36/45 (80%)	36 (100%)	0	100	100
1	O	36/45 (80%)	36 (100%)	0	100	100
1	Q	38/45 (84%)	38 (100%)	0	100	100
1	S	36/45 (80%)	36 (100%)	0	100	100
1	U	36/45 (80%)	36 (100%)	0	100	100
1	W	36/45 (80%)	36 (100%)	0	100	100
1	Y	35/45 (78%)	35 (100%)	0	100	100
1	d	36/45 (80%)	36 (100%)	0	100	100
1	m	36/45 (80%)	36 (100%)	0	100	100
1	n	36/45 (80%)	36 (100%)	0	100	100
2	2	39/43 (91%)	39 (100%)	0	100	100
2	4	40/43 (93%)	40 (100%)	0	100	100
2	6	40/43 (93%)	40 (100%)	0	100	100
2	8	41/43 (95%)	41 (100%)	0	100	100
2	A	39/43 (91%)	39 (100%)	0	100	100
2	D	40/43 (93%)	40 (100%)	0	100	100
2	E	39/43 (91%)	39 (100%)	0	100	100
2	F	40/43 (93%)	40 (100%)	0	100	100
2	G	40/43 (93%)	40 (100%)	0	100	100
2	J	39/43 (91%)	39 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	N	39/43 (91%)	39 (100%)	0	100 100
2	T	40/43 (93%)	40 (100%)	0	100 100
2	V	39/43 (91%)	39 (100%)	0	100 100
2	X	40/43 (93%)	40 (100%)	0	100 100
2	Z	40/43 (93%)	40 (100%)	0	100 100
3	H	204/204 (100%)	203 (100%)	1 (0%)	88 96
4	L	219/220 (100%)	217 (99%)	2 (1%)	78 92
5	M	239/240 (100%)	237 (99%)	2 (1%)	81 93
6	R	40/55 (73%)	40 (100%)	0	100 100
All	All	1875/2084 (90%)	1870 (100%)	5 (0%)	92 97

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	H	241	ASP
4	L	248	CYS
4	L	273	TRP
5	M	195	PHE
5	M	215	PHE

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

Mol	Chain	Res	Type
3	H	216	GLN
2	T	12	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

15 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	$\#\|Z\| > 2$
2	FME	6	1	2	8,9,10	0.95	0	7,9,11	0.93	0
2	FME	A	1	2	8,9,10	0.88	0	7,9,11	1.13	1 (14%)
2	FME	2	1	2	8,9,10	0.92	0	7,9,11	1.01	0
2	FME	Z	1	2	8,9,10	0.94	0	7,9,11	0.88	0
2	FME	N	1	2	8,9,10	0.91	0	7,9,11	1.06	1 (14%)
2	FME	E	1	2	8,9,10	0.94	0	7,9,11	1.12	1 (14%)
2	FME	V	1	2	8,9,10	0.93	0	7,9,11	1.02	0
2	FME	X	1	2	8,9,10	0.94	0	7,9,11	1.08	1 (14%)
2	FME	4	1	2	8,9,10	0.91	0	7,9,11	0.89	0
2	FME	T	1	2	8,9,10	0.92	0	7,9,11	1.02	0
2	FME	D	1	2	8,9,10	0.91	0	7,9,11	1.09	1 (14%)
2	FME	J	1	2	8,9,10	0.91	0	7,9,11	1.18	1 (14%)
2	FME	8	1	2	8,9,10	0.92	0	7,9,11	1.06	1 (14%)
2	FME	F	1	2	8,9,10	0.90	0	7,9,11	1.13	1 (14%)
2	FME	G	1	2	8,9,10	0.94	0	7,9,11	1.10	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FME	6	1	2	-	1/7/9/11	-
2	FME	A	1	2	-	1/7/9/11	-
2	FME	2	1	2	-	0/7/9/11	-
2	FME	Z	1	2	-	0/7/9/11	-
2	FME	N	1	2	-	0/7/9/11	-
2	FME	E	1	2	-	2/7/9/11	-
2	FME	V	1	2	-	1/7/9/11	-
2	FME	X	1	2	-	2/7/9/11	-
2	FME	4	1	2	-	1/7/9/11	-
2	FME	T	1	2	-	1/7/9/11	-
2	FME	D	1	2	-	1/7/9/11	-
2	FME	J	1	2	-	1/7/9/11	-
2	FME	8	1	2	-	3/7/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FME	F	1	2	-	1/7/9/11	-
2	FME	G	1	2	-	3/7/9/11	-

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	J	1	FME	C-CA-N	2.57	114.38	109.73
2	E	1	FME	C-CA-N	2.46	114.16	109.73
2	X	1	FME	C-CA-N	2.38	114.03	109.73
2	F	1	FME	C-CA-N	2.37	114.00	109.73
2	A	1	FME	C-CA-N	2.23	113.77	109.73
2	N	1	FME	C-CA-N	2.18	113.67	109.73
2	D	1	FME	C-CA-N	2.09	113.51	109.73
2	8	1	FME	C-CA-N	2.09	113.50	109.73

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	8	1	FME	O-C-CA-CB
2	D	1	FME	O-C-CA-CB
2	G	1	FME	CB-CA-N-CN
2	G	1	FME	O-C-CA-CB
2	J	1	FME	C-CA-CB-CG
2	T	1	FME	O-C-CA-CB
2	A	1	FME	N-CA-CB-CG
2	X	1	FME	N-CA-CB-CG
2	4	1	FME	C-CA-CB-CG
2	8	1	FME	C-CA-CB-CG
2	E	1	FME	N-CA-CB-CG
2	E	1	FME	CB-CG-SD-CE
2	F	1	FME	C-CA-CB-CG
2	G	1	FME	C-CA-CB-CG
2	X	1	FME	CB-CG-SD-CE
2	6	1	FME	CB-CG-SD-CE
2	8	1	FME	CB-CA-N-CN
2	V	1	FME	CB-CA-N-CN

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	6	1	FME	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 68 ligands modelled in this entry, 2 are monoatomic - leaving 66 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
8	CRT	M	406	-	41,43,43	0.54	0	50,54,54	0.85	1 (2%)
7	07D	3	102	-	65,74,74	1.95	10 (15%)	65,115,115	3.26	15 (23%)
7	07D	X	1001	-	65,74,74	1.94	10 (15%)	65,115,115	3.18	15 (23%)
8	CRT	N	1001	-	41,43,43	0.60	0	50,54,54	0.88	2 (4%)
8	CRT	n	101	-	41,43,43	0.58	0	50,54,54	0.85	1 (2%)
7	07D	Q	102	-	65,74,74	1.94	10 (15%)	65,115,115	3.21	14 (21%)
7	07D	4	1001	-	65,74,74	1.94	10 (15%)	65,115,115	3.20	15 (23%)
7	07D	W	1001	-	65,74,74	1.94	10 (15%)	65,115,115	3.23	15 (23%)
8	CRT	3	101	-	41,43,43	0.63	0	50,54,54	0.69	0
7	07D	I	102	-	65,74,74	1.94	10 (15%)	65,115,115	3.24	14 (21%)
7	07D	T	101	-	65,74,74	1.94	10 (15%)	65,115,115	3.23	15 (23%)
7	07D	n	102	-	65,74,74	1.94	10 (15%)	65,115,115	3.28	14 (21%)
7	07D	L	1005	-	65,74,74	1.98	10 (15%)	65,115,115	3.24	14 (21%)
8	CRT	K	101	-	41,43,43	0.57	0	50,54,54	0.75	0
8	CRT	1	1002	-	41,43,43	0.62	0	50,54,54	0.85	0
8	CRT	O	101	-	41,43,43	0.59	0	50,54,54	0.69	0
13	U10	L	1006	-	63,63,63	0.16	0	76,79,79	0.68	1 (1%)
13	U10	L	1003	-	63,63,63	0.19	0	76,79,79	0.46	0
17	LMT	R	102	-	36,36,36	1.10	5 (13%)	47,47,47	0.84	2 (4%)
8	CRT	d	1001	-	41,43,43	0.64	0	50,54,54	1.02	4 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
8	CRT	I	101	-	41,43,43	0.57	0	50,54,54	0.76	0
7	07D	6	1001	-	65,74,74	1.94	10 (15%)	65,115,115	3.17	15 (23%)
7	07D	7	102	-	65,74,74	1.94	10 (15%)	65,115,115	3.28	13 (20%)
7	07D	M	404	-	65,74,74	2.00	11 (16%)	65,115,115	3.16	15 (23%)
7	07D	U	1001	-	65,74,74	1.94	10 (15%)	65,115,115	3.22	14 (21%)
7	07D	2	1001	-	65,74,74	1.96	10 (15%)	65,115,115	3.10	15 (23%)
13	U10	M	403	-	63,63,63	0.15	0	76,79,79	0.54	0
7	07D	Z	1001	-	65,74,74	1.95	10 (15%)	65,115,115	3.11	15 (23%)
16	PO4	M	409	-	4,4,4	0.98	0	6,6,6	0.45	0
9	PGW	H	303	7	50,50,50	0.45	0	53,56,56	0.82	2 (3%)
7	07D	R	101	-	65,74,74	1.94	10 (15%)	65,115,115	3.12	16 (24%)
7	07D	1	1001	-	65,74,74	1.94	10 (15%)	65,115,115	3.26	14 (21%)
8	CRT	J	1002	-	41,43,43	0.57	0	50,54,54	0.76	0
7	07D	O	102	-	65,74,74	1.94	10 (15%)	65,115,115	3.23	14 (21%)
7	07D	F	1001	-	65,74,74	1.94	9 (13%)	65,115,115	3.19	15 (23%)
7	07D	J	1001	-	65,74,74	1.94	10 (15%)	65,115,115	3.22	15 (23%)
7	07D	N	1002	-	65,74,74	1.95	10 (15%)	65,115,115	3.17	15 (23%)
8	CRT	9	101	-	41,43,43	0.63	0	50,54,54	1.13	5 (10%)
7	07D	9	102	-	65,74,74	1.93	10 (15%)	65,115,115	3.28	14 (21%)
8	CRT	S	101	-	41,43,43	0.57	0	50,54,54	0.76	0
7	07D	H	301	9	65,74,74	1.96	10 (15%)	65,115,115	3.04	14 (21%)
7	07D	L	1004	-	65,74,74	1.96	10 (15%)	65,115,115	3.23	15 (23%)
7	07D	K	102	-	65,74,74	1.94	10 (15%)	65,115,115	3.25	14 (21%)
7	07D	E	1001	-	65,74,74	1.94	10 (15%)	65,115,115	3.23	15 (23%)
9	PGW	H	302	-	50,50,50	0.47	0	53,56,56	0.92	3 (5%)
10	CD4	H	304	-	83,83,83	0.48	0	89,95,95	0.88	2 (2%)
8	CRT	Q	101	-	41,43,43	0.58	0	50,54,54	0.78	0
7	07D	d	1002	-	65,74,74	1.95	10 (15%)	65,115,115	3.28	14 (21%)
7	07D	m	102	-	65,74,74	1.97	11 (16%)	65,115,115	3.31	15 (23%)
7	07D	M	405	-	65,74,74	1.99	11 (16%)	65,115,115	3.08	16 (24%)
8	CRT	7	101	-	41,43,43	0.59	0	50,54,54	0.74	0
7	07D	S	102	-	65,74,74	1.94	10 (15%)	65,115,115	3.28	15 (23%)
10	CD4	M	407	-	83,83,83	0.47	0	89,95,95	0.89	3 (3%)
7	07D	Y	102	-	65,74,74	1.94	10 (15%)	65,115,115	3.27	16 (24%)
8	CRT	5	101	-	41,43,43	0.60	0	50,54,54	0.74	0
7	07D	A	101	-	65,74,74	1.95	9 (13%)	65,115,115	3.22	15 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
8	CRT	m	101	-	41,43,43	0.60	0	50,54,54	0.78	0
12	RQ0	L	1002	-	62,62,62	1.58	7 (11%)	69,78,78	1.31	5 (7%)
11	BPH	L	1001	-	64,70,70	0.85	3 (4%)	76,101,101	1.10	6 (7%)
8	CRT	Y	101	-	41,43,43	0.62	0	50,54,54	0.92	1 (2%)
11	BPH	M	402	-	64,70,70	0.85	3 (4%)	76,101,101	1.17	6 (7%)
7	07D	8	1001	-	65,74,74	1.96	10 (15%)	65,115,115	3.08	15 (23%)
7	07D	G	1001	-	65,74,74	1.96	10 (15%)	65,115,115	3.08	14 (21%)
7	07D	V	1001	-	65,74,74	1.94	10 (15%)	65,115,115	3.21	14 (21%)
7	07D	D	1001	-	65,74,74	1.94	9 (13%)	65,115,115	3.16	15 (23%)
7	07D	5	102	-	65,74,74	1.93	10 (15%)	65,115,115	3.26	14 (21%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	CRT	M	406	-	-	8/51/51/51	-
7	07D	3	102	-	1/1/21/28	8/41/137/137	-
7	07D	X	1001	-	1/1/21/28	10/41/137/137	-
8	CRT	N	1001	-	-	4/51/51/51	-
8	CRT	n	101	-	-	2/51/51/51	-
7	07D	Q	102	-	1/1/21/28	5/41/137/137	-
7	07D	4	1001	-	1/1/21/28	7/41/137/137	-
7	07D	W	1001	-	1/1/21/28	6/41/137/137	-
8	CRT	3	101	-	-	6/51/51/51	-
7	07D	I	102	-	1/1/21/28	4/41/137/137	-
7	07D	T	101	-	1/1/21/28	6/41/137/137	-
7	07D	n	102	-	1/1/21/28	11/41/137/137	-
7	07D	L	1005	-	1/1/21/28	10/41/137/137	-
8	CRT	K	101	-	-	3/51/51/51	-
8	CRT	1	1002	-	-	4/51/51/51	-
8	CRT	O	101	-	-	7/51/51/51	-
13	U10	L	1006	-	-	7/63/87/87	0/1/1/1
13	U10	L	1003	-	-	10/63/87/87	0/1/1/1
17	LMT	R	102	-	-	2/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	CRT	d	1001	-	-	2/51/51/51	-
8	CRT	I	101	-	-	2/51/51/51	-
7	07D	6	1001	-	1/1/21/28	8/41/137/137	-
7	07D	7	102	-	1/1/21/28	8/41/137/137	-
7	07D	M	404	-	1/1/21/28	8/41/137/137	-
7	07D	U	1001	-	1/1/21/28	4/41/137/137	-
7	07D	2	1001	-	1/1/21/28	6/41/137/137	-
13	U10	M	403	-	-	8/63/87/87	0/1/1/1
7	07D	Z	1001	-	1/1/21/28	7/41/137/137	-
9	PGW	H	303	7	-	8/55/55/55	-
7	07D	R	101	-	1/1/21/28	10/41/137/137	-
7	07D	1	1001	-	1/1/21/28	6/41/137/137	-
8	CRT	J	1002	-	-	0/51/51/51	-
7	07D	O	102	-	1/1/21/28	5/41/137/137	-
7	07D	F	1001	-	1/1/21/28	12/41/137/137	-
7	07D	J	1001	-	1/1/21/28	6/41/137/137	-
7	07D	N	1002	-	1/1/21/28	5/41/137/137	-
8	CRT	9	101	-	-	6/51/51/51	-
7	07D	9	102	-	1/1/21/28	4/41/137/137	-
8	CRT	S	101	-	-	4/51/51/51	-
7	07D	H	301	9	1/1/21/28	15/41/137/137	-
7	07D	L	1004	-	1/1/21/28	7/41/137/137	-
7	07D	K	102	-	1/1/21/28	3/41/137/137	-
7	07D	E	1001	-	1/1/21/28	8/41/137/137	-
9	PGW	H	302	-	-	13/55/55/55	-
10	CD4	H	304	-	-	11/94/94/94	-
8	CRT	Q	101	-	-	2/51/51/51	-
7	07D	d	1002	-	1/1/21/28	11/41/137/137	-
7	07D	m	102	-	1/1/21/28	5/41/137/137	-
7	07D	M	405	-	1/1/21/28	6/41/137/137	-
8	CRT	7	101	-	-	2/51/51/51	-
7	07D	S	102	-	1/1/21/28	4/41/137/137	-
10	CD4	M	407	-	-	14/94/94/94	-
7	07D	Y	102	-	1/1/21/28	7/41/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	CRT	5	101	-	-	4/51/51/51	-
7	07D	A	101	-	1/1/21/28	9/41/137/137	-
8	CRT	m	101	-	-	3/51/51/51	-
12	RQ0	L	1002	-	-	18/61/85/85	0/1/1/1
11	BPH	L	1001	-	-	5/54/105/105	0/5/6/6
8	CRT	Y	101	-	-	1/51/51/51	-
11	BPH	M	402	-	-	4/54/105/105	0/5/6/6
7	07D	8	1001	-	1/1/21/28	7/41/137/137	-
7	07D	G	1001	-	1/1/21/28	7/41/137/137	-
7	07D	V	1001	-	1/1/21/28	10/41/137/137	-
7	07D	D	1001	-	1/1/21/28	6/41/137/137	-
7	07D	5	102	-	1/1/21/28	10/41/137/137	-

All (388) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	L	1002	RQ0	C11-C07	7.68	1.54	1.34
12	L	1002	RQ0	C18-C14	7.64	1.54	1.34
7	M	404	07D	C1C-NC	-6.38	1.29	1.35
7	L	1005	07D	C1C-NC	-6.34	1.29	1.35
7	d	1002	07D	C1C-NC	-6.26	1.29	1.35
7	A	101	07D	C1C-NC	-6.25	1.29	1.35
7	E	1001	07D	C1C-NC	-6.24	1.29	1.35
7	J	1001	07D	C1C-NC	-6.24	1.29	1.35
7	V	1001	07D	C1C-NC	-6.24	1.29	1.35
7	1	1001	07D	C1C-NC	-6.23	1.29	1.35
7	X	1001	07D	C1C-NC	-6.23	1.29	1.35
7	G	1001	07D	C1C-NC	-6.23	1.29	1.35
7	D	1001	07D	C1C-NC	-6.22	1.29	1.35
7	4	1001	07D	C1C-NC	-6.22	1.29	1.35
7	8	1001	07D	C1C-NC	-6.22	1.29	1.35
7	N	1002	07D	C1C-NC	-6.21	1.29	1.35
7	Z	1001	07D	C1C-NC	-6.21	1.29	1.35
7	I	102	07D	C1C-NC	-6.21	1.29	1.35
7	U	1001	07D	C1C-NC	-6.21	1.29	1.35
7	2	1001	07D	C1C-NC	-6.21	1.29	1.35
7	F	1001	07D	C1C-NC	-6.21	1.29	1.35
7	6	1001	07D	C1C-NC	-6.21	1.29	1.35
7	T	101	07D	C1C-NC	-6.20	1.29	1.35
7	5	102	07D	C1C-NC	-6.20	1.29	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	L	1004	07D	C1C-NC	-6.20	1.29	1.35
7	S	102	07D	C1C-NC	-6.20	1.29	1.35
7	W	1001	07D	C1C-NC	-6.19	1.29	1.35
7	7	102	07D	C1C-NC	-6.19	1.29	1.35
7	m	102	07D	C1C-NC	-6.18	1.29	1.35
7	n	102	07D	C1C-NC	-6.18	1.29	1.35
7	Y	102	07D	C1C-NC	-6.18	1.29	1.35
7	M	405	07D	C1C-NC	-6.18	1.29	1.35
7	Q	102	07D	C1C-NC	-6.17	1.29	1.35
7	K	102	07D	C1C-NC	-6.17	1.29	1.35
7	R	101	07D	C1C-NC	-6.17	1.29	1.35
7	3	102	07D	C1C-NC	-6.16	1.29	1.35
7	9	102	07D	C1C-NC	-6.16	1.29	1.35
7	O	102	07D	C1C-NC	-6.15	1.29	1.35
7	H	301	07D	C1C-NC	-6.14	1.29	1.35
7	L	1005	07D	C2A-C3A	5.88	1.55	1.37
7	M	405	07D	C3C-C2C	5.87	1.55	1.37
7	D	1001	07D	C3C-C2C	5.86	1.55	1.37
7	M	405	07D	C2A-C3A	5.86	1.55	1.37
7	M	404	07D	C3C-C2C	5.85	1.55	1.37
7	X	1001	07D	C3C-C2C	5.85	1.55	1.37
7	Z	1001	07D	C3C-C2C	5.85	1.55	1.37
7	T	101	07D	C3C-C2C	5.85	1.55	1.37
7	F	1001	07D	C3C-C2C	5.85	1.55	1.37
7	J	1001	07D	C3C-C2C	5.85	1.55	1.37
7	4	1001	07D	C3C-C2C	5.85	1.55	1.37
7	H	301	07D	C3C-C2C	5.85	1.55	1.37
7	G	1001	07D	C3C-C2C	5.85	1.55	1.37
7	8	1001	07D	C3C-C2C	5.85	1.55	1.37
7	L	1005	07D	C3C-C2C	5.84	1.55	1.37
7	E	1001	07D	C3C-C2C	5.84	1.55	1.37
7	L	1004	07D	C3C-C2C	5.84	1.55	1.37
7	6	1001	07D	C3C-C2C	5.84	1.55	1.37
7	V	1001	07D	C3C-C2C	5.84	1.55	1.37
7	N	1002	07D	C3C-C2C	5.84	1.55	1.37
7	2	1001	07D	C3C-C2C	5.84	1.55	1.37
7	R	101	07D	C3C-C2C	5.84	1.55	1.37
7	A	101	07D	C3C-C2C	5.83	1.55	1.37
7	K	102	07D	C3C-C2C	5.83	1.54	1.37
7	7	102	07D	C3C-C2C	5.83	1.54	1.37
7	O	102	07D	C3C-C2C	5.83	1.54	1.37
7	d	1002	07D	C3C-C2C	5.83	1.54	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	1	1001	07D	C3C-C2C	5.83	1.54	1.37
7	5	102	07D	C3C-C2C	5.83	1.54	1.37
7	Y	102	07D	C3C-C2C	5.82	1.54	1.37
7	n	102	07D	C3C-C2C	5.82	1.54	1.37
7	I	102	07D	C3C-C2C	5.82	1.54	1.37
7	W	1001	07D	C3C-C2C	5.82	1.54	1.37
7	S	102	07D	C3C-C2C	5.82	1.54	1.37
7	9	102	07D	C3C-C2C	5.82	1.54	1.37
7	U	1001	07D	C3C-C2C	5.82	1.54	1.37
7	3	102	07D	C3C-C2C	5.82	1.54	1.37
7	m	102	07D	C3C-C2C	5.82	1.54	1.37
7	Q	102	07D	C3C-C2C	5.81	1.54	1.37
7	L	1004	07D	C2A-C3A	5.79	1.54	1.37
7	M	404	07D	C2A-C3A	5.77	1.54	1.37
7	n	102	07D	C2A-C3A	5.77	1.54	1.37
7	K	102	07D	C2A-C3A	5.77	1.54	1.37
7	d	1002	07D	C2A-C3A	5.77	1.54	1.37
7	2	1001	07D	C2A-C3A	5.76	1.54	1.37
7	8	1001	07D	C2A-C3A	5.75	1.54	1.37
7	m	102	07D	C2A-C3A	5.75	1.54	1.37
7	9	102	07D	C2A-C3A	5.75	1.54	1.37
7	R	101	07D	C2A-C3A	5.75	1.54	1.37
7	O	102	07D	C2A-C3A	5.75	1.54	1.37
7	A	101	07D	C2A-C3A	5.74	1.54	1.37
7	V	1001	07D	C2A-C3A	5.74	1.54	1.37
7	N	1002	07D	C2A-C3A	5.74	1.54	1.37
7	S	102	07D	C2A-C3A	5.74	1.54	1.37
7	X	1001	07D	C2A-C3A	5.74	1.54	1.37
7	Y	102	07D	C2A-C3A	5.74	1.54	1.37
7	1	1001	07D	C2A-C3A	5.73	1.54	1.37
7	4	1001	07D	C2A-C3A	5.73	1.54	1.37
7	G	1001	07D	C2A-C3A	5.73	1.54	1.37
7	7	102	07D	C2A-C3A	5.73	1.54	1.37
7	T	101	07D	C2A-C3A	5.73	1.54	1.37
7	F	1001	07D	C2A-C3A	5.73	1.54	1.37
7	J	1001	07D	C2A-C3A	5.73	1.54	1.37
7	3	102	07D	C2A-C3A	5.72	1.54	1.37
7	U	1001	07D	C2A-C3A	5.72	1.54	1.37
7	I	102	07D	C2A-C3A	5.72	1.54	1.37
7	W	1001	07D	C2A-C3A	5.72	1.54	1.37
7	6	1001	07D	C2A-C3A	5.72	1.54	1.37
7	M	404	07D	C4C-NC	5.72	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	5	102	07D	C2A-C3A	5.72	1.54	1.37
7	Q	102	07D	C2A-C3A	5.72	1.54	1.37
7	T	101	07D	C4C-NC	5.71	1.40	1.35
7	D	1001	07D	C2A-C3A	5.71	1.54	1.37
7	A	101	07D	C4C-NC	5.71	1.40	1.35
7	L	1004	07D	C4C-NC	5.71	1.40	1.35
7	V	1001	07D	C4C-NC	5.70	1.40	1.35
7	E	1001	07D	C2A-C3A	5.70	1.54	1.37
7	Z	1001	07D	C2A-C3A	5.70	1.54	1.37
7	D	1001	07D	C4C-NC	5.70	1.40	1.35
7	H	301	07D	C4C-NC	5.69	1.40	1.35
7	N	1002	07D	C4C-NC	5.69	1.40	1.35
7	Z	1001	07D	C4C-NC	5.69	1.40	1.35
7	8	1001	07D	C4C-NC	5.69	1.40	1.35
7	6	1001	07D	C4C-NC	5.68	1.40	1.35
7	R	101	07D	C4C-NC	5.68	1.40	1.35
7	4	1001	07D	C4C-NC	5.67	1.40	1.35
7	E	1001	07D	C4C-NC	5.67	1.40	1.35
7	W	1001	07D	C4C-NC	5.67	1.40	1.35
7	K	102	07D	C4C-NC	5.67	1.40	1.35
7	9	102	07D	C4C-NC	5.66	1.40	1.35
7	U	1001	07D	C4C-NC	5.66	1.40	1.35
7	Q	102	07D	C4C-NC	5.66	1.40	1.35
7	5	102	07D	C4C-NC	5.66	1.40	1.35
7	7	102	07D	C4C-NC	5.66	1.40	1.35
7	F	1001	07D	C4C-NC	5.66	1.40	1.35
7	O	102	07D	C4C-NC	5.66	1.40	1.35
7	I	102	07D	C4C-NC	5.65	1.40	1.35
7	2	1001	07D	C4C-NC	5.65	1.40	1.35
7	X	1001	07D	C4C-NC	5.65	1.40	1.35
7	Y	102	07D	C4C-NC	5.64	1.40	1.35
7	n	102	07D	C4C-NC	5.64	1.40	1.35
7	J	1001	07D	C4C-NC	5.64	1.40	1.35
7	3	102	07D	C4C-NC	5.64	1.40	1.35
7	m	102	07D	C4C-NC	5.63	1.40	1.35
7	d	1002	07D	C4C-NC	5.63	1.40	1.35
7	H	301	07D	C2A-C3A	5.63	1.54	1.37
7	G	1001	07D	C4C-NC	5.63	1.40	1.35
7	1	1001	07D	C4C-NC	5.62	1.40	1.35
7	S	102	07D	C4C-NC	5.62	1.40	1.35
7	L	1005	07D	C4C-NC	5.60	1.40	1.35
7	M	405	07D	C4C-NC	5.57	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	Q	102	07D	C3D-C4D	-4.73	1.32	1.43
7	S	102	07D	C3D-C4D	-4.73	1.32	1.43
7	U	1001	07D	C3D-C4D	-4.73	1.32	1.43
7	M	405	07D	C3D-C4D	-4.73	1.32	1.43
7	n	102	07D	C3D-C4D	-4.72	1.32	1.43
7	Y	102	07D	C3D-C4D	-4.72	1.32	1.43
7	3	102	07D	C3D-C4D	-4.72	1.32	1.43
7	5	102	07D	C3D-C4D	-4.72	1.32	1.43
7	W	1001	07D	C3D-C4D	-4.72	1.32	1.43
7	9	102	07D	C3D-C4D	-4.72	1.32	1.43
7	O	102	07D	C3D-C4D	-4.72	1.32	1.43
7	N	1002	07D	C3D-C4D	-4.72	1.32	1.43
7	K	102	07D	C3D-C4D	-4.72	1.32	1.43
7	d	1002	07D	C3D-C4D	-4.72	1.32	1.43
7	1	1001	07D	C3D-C4D	-4.72	1.32	1.43
7	R	101	07D	C3D-C4D	-4.71	1.32	1.43
7	L	1005	07D	C3D-C4D	-4.71	1.32	1.43
7	E	1001	07D	C3D-C4D	-4.71	1.32	1.43
7	T	101	07D	C3D-C4D	-4.71	1.32	1.43
7	A	101	07D	C3D-C4D	-4.71	1.32	1.43
7	J	1001	07D	C3D-C4D	-4.71	1.32	1.43
7	7	102	07D	C3D-C4D	-4.71	1.32	1.43
7	4	1001	07D	C3D-C4D	-4.71	1.32	1.43
7	D	1001	07D	C3D-C4D	-4.71	1.32	1.43
7	F	1001	07D	C3D-C4D	-4.70	1.32	1.43
7	6	1001	07D	C3D-C4D	-4.70	1.32	1.43
7	m	102	07D	C3D-C4D	-4.70	1.32	1.43
7	M	404	07D	C3D-C4D	-4.70	1.32	1.43
7	2	1001	07D	C3D-C4D	-4.70	1.32	1.43
7	I	102	07D	C3D-C4D	-4.70	1.32	1.43
7	Z	1001	07D	C3D-C4D	-4.70	1.32	1.43
7	8	1001	07D	C3D-C4D	-4.70	1.32	1.43
7	X	1001	07D	C3D-C4D	-4.70	1.32	1.43
7	G	1001	07D	C3D-C4D	-4.69	1.32	1.43
7	V	1001	07D	C3D-C4D	-4.69	1.32	1.43
7	H	301	07D	C3D-C4D	-4.68	1.32	1.43
7	L	1004	07D	C3D-C4D	-4.67	1.32	1.43
7	M	404	07D	C1A-C2A	4.61	1.53	1.42
7	H	301	07D	C1A-C2A	4.53	1.52	1.42
7	L	1004	07D	C1A-C2A	4.53	1.52	1.42
7	8	1001	07D	C1A-C2A	4.39	1.52	1.42
7	M	405	07D	C1A-C2A	4.39	1.52	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	1001	07D	C1A-C2A	4.36	1.52	1.42
7	R	101	07D	C1A-C2A	4.31	1.52	1.42
7	2	1001	07D	C1A-C2A	4.31	1.52	1.42
7	Z	1001	07D	C1A-C2A	4.29	1.52	1.42
7	A	101	07D	C1A-C2A	4.29	1.52	1.42
7	3	102	07D	C1A-C2A	4.28	1.52	1.42
7	N	1002	07D	C1A-C2A	4.28	1.52	1.42
7	L	1005	07D	C1A-C2A	4.27	1.52	1.42
7	m	102	07D	C1A-C2A	4.25	1.52	1.42
7	X	1001	07D	C1A-C2A	4.25	1.52	1.42
7	6	1001	07D	C1A-C2A	4.24	1.52	1.42
7	L	1005	07D	CHD-C1D	4.21	1.45	1.35
7	T	101	07D	C1A-C2A	4.20	1.52	1.42
7	V	1001	07D	C1A-C2A	4.20	1.52	1.42
7	O	102	07D	C1A-C2A	4.19	1.52	1.42
7	E	1001	07D	C1A-C2A	4.18	1.52	1.42
7	4	1001	07D	C1A-C2A	4.18	1.52	1.42
7	Q	102	07D	C1A-C2A	4.16	1.52	1.42
7	D	1001	07D	C1A-C2A	4.15	1.52	1.42
7	n	102	07D	C1A-C2A	4.15	1.52	1.42
7	M	405	07D	CHD-C1D	4.13	1.45	1.35
7	F	1001	07D	C1A-C2A	4.13	1.51	1.42
7	J	1001	07D	C1A-C2A	4.13	1.51	1.42
7	S	102	07D	C1A-C2A	4.12	1.51	1.42
7	7	102	07D	C1A-C2A	4.12	1.51	1.42
7	1	1001	07D	C1A-C2A	4.12	1.51	1.42
7	W	1001	07D	C1A-C2A	4.11	1.51	1.42
7	K	102	07D	C1A-C2A	4.11	1.51	1.42
7	I	102	07D	C1A-C2A	4.11	1.51	1.42
7	U	1001	07D	C1A-C2A	4.11	1.51	1.42
7	M	404	07D	CHD-C1D	4.09	1.45	1.35
7	Y	102	07D	C1A-C2A	4.09	1.51	1.42
7	d	1002	07D	C1A-C2A	4.07	1.51	1.42
7	W	1001	07D	CHD-C1D	4.06	1.45	1.35
7	K	102	07D	CHD-C1D	4.06	1.45	1.35
7	Z	1001	07D	CHD-C1D	4.05	1.45	1.35
7	7	102	07D	CHD-C1D	4.05	1.45	1.35
7	D	1001	07D	CHD-C1D	4.04	1.45	1.35
7	F	1001	07D	CHD-C1D	4.03	1.45	1.35
7	X	1001	07D	CHD-C1D	4.03	1.45	1.35
7	R	101	07D	CHD-C1D	4.03	1.45	1.35
7	n	102	07D	CHD-C1D	4.02	1.45	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	8	1001	07D	CHD-C1D	4.02	1.45	1.35
7	L	1004	07D	CHD-C1D	4.02	1.45	1.35
7	Q	102	07D	CHD-C1D	4.02	1.45	1.35
7	H	301	07D	CHD-C1D	4.02	1.45	1.35
7	2	1001	07D	CHD-C1D	4.01	1.45	1.35
7	T	101	07D	CHD-C1D	4.01	1.45	1.35
7	E	1001	07D	CHD-C1D	4.01	1.45	1.35
7	N	1002	07D	CHD-C1D	4.01	1.45	1.35
7	Y	102	07D	CHD-C1D	4.01	1.45	1.35
7	5	102	07D	C1A-C2A	4.01	1.51	1.42
7	3	102	07D	C1D-C2D	-4.01	1.36	1.44
7	A	101	07D	CHD-C1D	4.01	1.45	1.35
7	6	1001	07D	CHD-C1D	4.00	1.45	1.35
7	S	102	07D	CHD-C1D	4.00	1.45	1.35
7	m	102	07D	CHD-C1D	4.00	1.45	1.35
7	9	102	07D	CHD-C1D	3.99	1.45	1.35
7	9	102	07D	C1A-C2A	3.99	1.51	1.42
7	J	1001	07D	CHD-C1D	3.99	1.45	1.35
7	4	1001	07D	CHD-C1D	3.99	1.45	1.35
7	O	102	07D	C1D-C2D	-3.99	1.36	1.44
7	1	1001	07D	CHD-C1D	3.99	1.45	1.35
7	5	102	07D	CHD-C1D	3.99	1.45	1.35
7	I	102	07D	CHD-C1D	3.98	1.45	1.35
7	d	1002	07D	C1D-C2D	-3.97	1.36	1.44
7	U	1001	07D	CHD-C1D	3.97	1.45	1.35
7	V	1001	07D	C4A-C3A	3.97	1.51	1.42
7	V	1001	07D	CHD-C1D	3.96	1.45	1.35
7	N	1002	07D	C4A-C3A	3.96	1.51	1.42
7	S	102	07D	C4A-C3A	3.96	1.51	1.42
7	3	102	07D	CHD-C1D	3.96	1.45	1.35
7	O	102	07D	CHD-C1D	3.96	1.45	1.35
7	Q	102	07D	C4A-C3A	3.96	1.51	1.42
7	n	102	07D	C4A-C3A	3.95	1.51	1.42
7	K	102	07D	C4A-C3A	3.95	1.51	1.42
7	2	1001	07D	C4A-C3A	3.95	1.51	1.42
7	Z	1001	07D	C4A-C3A	3.95	1.51	1.42
7	F	1001	07D	C4A-C3A	3.95	1.51	1.42
7	T	101	07D	C4A-C3A	3.95	1.51	1.42
7	U	1001	07D	C4A-C3A	3.95	1.51	1.42
7	J	1001	07D	C4A-C3A	3.95	1.51	1.42
7	d	1002	07D	CHD-C1D	3.95	1.45	1.35
7	4	1001	07D	C4A-C3A	3.95	1.51	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	E	1001	07D	C4A-C3A	3.95	1.51	1.42
7	A	101	07D	C4A-C3A	3.95	1.51	1.42
7	X	1001	07D	C4A-C3A	3.95	1.51	1.42
7	D	1001	07D	C4A-C3A	3.95	1.51	1.42
7	R	101	07D	C4A-C3A	3.95	1.51	1.42
7	7	102	07D	C4A-C3A	3.94	1.51	1.42
7	G	1001	07D	C4A-C3A	3.94	1.51	1.42
7	I	102	07D	C4A-C3A	3.94	1.51	1.42
7	5	102	07D	C4A-C3A	3.94	1.51	1.42
7	L	1005	07D	C4A-C3A	3.94	1.51	1.42
7	d	1002	07D	C4A-C3A	3.94	1.51	1.42
7	I	102	07D	C1D-C2D	-3.94	1.36	1.44
7	O	102	07D	C4A-C3A	3.94	1.51	1.42
7	1	1001	07D	C4A-C3A	3.94	1.51	1.42
7	3	102	07D	C4A-C3A	3.94	1.51	1.42
7	W	1001	07D	C4A-C3A	3.93	1.51	1.42
7	8	1001	07D	C4A-C3A	3.93	1.51	1.42
7	9	102	07D	C4A-C3A	3.93	1.51	1.42
7	M	404	07D	C4A-C3A	3.93	1.51	1.42
7	Y	102	07D	C4A-C3A	3.92	1.51	1.42
7	6	1001	07D	C4A-C3A	3.92	1.51	1.42
7	m	102	07D	C4A-C3A	3.92	1.51	1.42
7	M	405	07D	C4A-C3A	3.92	1.51	1.42
7	L	1004	07D	C4A-C3A	3.91	1.51	1.42
7	H	301	07D	C4A-C3A	3.91	1.51	1.42
7	G	1001	07D	CHD-C1D	3.91	1.45	1.35
7	S	102	07D	C1D-C2D	-3.90	1.37	1.44
7	U	1001	07D	C1D-C2D	-3.90	1.37	1.44
7	1	1001	07D	C1D-C2D	-3.89	1.37	1.44
7	Q	102	07D	C1D-C2D	-3.88	1.37	1.44
7	m	102	07D	C1D-C2D	-3.87	1.37	1.44
7	n	102	07D	C1D-C2D	-3.86	1.37	1.44
7	K	102	07D	C1D-C2D	-3.84	1.37	1.44
7	5	102	07D	C1D-C2D	-3.84	1.37	1.44
7	7	102	07D	C1D-C2D	-3.83	1.37	1.44
7	G	1001	07D	C1D-C2D	-3.81	1.37	1.44
7	9	102	07D	C1D-C2D	-3.79	1.37	1.44
7	W	1001	07D	C1D-C2D	-3.79	1.37	1.44
7	Y	102	07D	C1D-C2D	-3.76	1.37	1.44
7	H	301	07D	C1D-C2D	-3.75	1.37	1.44
7	8	1001	07D	C1D-C2D	-3.71	1.37	1.44
7	2	1001	07D	C1D-C2D	-3.68	1.37	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	L	1004	07D	C1D-C2D	-3.67	1.37	1.44
7	L	1005	07D	C1D-C2D	-3.67	1.37	1.44
7	J	1001	07D	C1D-C2D	-3.66	1.37	1.44
7	M	405	07D	C1D-C2D	-3.62	1.37	1.44
7	M	404	07D	C1D-C2D	-3.62	1.37	1.44
7	6	1001	07D	C1D-C2D	-3.62	1.37	1.44
7	T	101	07D	C1D-C2D	-3.61	1.37	1.44
7	N	1002	07D	C1D-C2D	-3.59	1.37	1.44
7	A	101	07D	C1D-C2D	-3.59	1.37	1.44
7	E	1001	07D	C1D-C2D	-3.59	1.37	1.44
7	Z	1001	07D	C1D-C2D	-3.59	1.37	1.44
7	V	1001	07D	C1D-C2D	-3.56	1.37	1.44
7	D	1001	07D	C1D-C2D	-3.55	1.37	1.44
7	4	1001	07D	C1D-C2D	-3.54	1.37	1.44
7	R	101	07D	C1D-C2D	-3.54	1.37	1.44
7	X	1001	07D	C1D-C2D	-3.53	1.37	1.44
7	F	1001	07D	C1D-C2D	-3.50	1.37	1.44
7	M	405	07D	CAA-C2A	3.13	1.57	1.52
7	M	404	07D	CAA-C2A	2.81	1.57	1.52
7	m	102	07D	CAA-C2A	2.77	1.57	1.52
17	R	102	LMT	O3'-C3'	-2.72	1.36	1.43
12	L	1002	RQ0	C56-C55	-2.71	1.35	1.39
11	M	402	BPH	C3D-CAD	-2.68	1.41	1.47
11	L	1001	BPH	C3D-CAD	-2.67	1.41	1.47
12	L	1002	RQ0	C07-C19	2.53	1.51	1.45
12	L	1002	RQ0	C14-C23	2.51	1.51	1.45
7	L	1005	07D	CAA-C2A	2.48	1.56	1.52
12	L	1002	RQ0	C11-C25	2.43	1.51	1.43
11	M	402	BPH	C1B-C2B	-2.35	1.40	1.45
17	R	102	LMT	O2B-C2B	-2.34	1.37	1.43
12	L	1002	RQ0	C18-C27	2.34	1.50	1.43
17	R	102	LMT	O3B-C3B	-2.33	1.37	1.43
17	R	102	LMT	O2'-C2'	-2.26	1.37	1.43
11	L	1001	BPH	C1B-C2B	-2.22	1.41	1.45
11	M	402	BPH	CHC-C1C	2.20	1.41	1.36
11	L	1001	BPH	CHC-C1C	2.16	1.41	1.36
17	R	102	LMT	O4'-C4B	-2.14	1.37	1.43
7	G	1001	07D	C4C-CHD	-2.13	1.35	1.41
7	m	102	07D	C4C-CHD	-2.12	1.35	1.41
7	Y	102	07D	C4C-CHD	-2.12	1.35	1.41
7	I	102	07D	C4C-CHD	-2.11	1.35	1.41
7	d	1002	07D	C4C-CHD	-2.11	1.35	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	1	1001	07D	C4C-CHD	-2.11	1.35	1.41
7	3	102	07D	C4C-CHD	-2.10	1.35	1.41
7	O	102	07D	C4C-CHD	-2.10	1.35	1.41
7	L	1004	07D	C4C-CHD	-2.09	1.35	1.41
7	n	102	07D	C4C-CHD	-2.09	1.35	1.41
7	U	1001	07D	C4C-CHD	-2.09	1.35	1.41
7	2	1001	07D	C4C-CHD	-2.08	1.35	1.41
7	S	102	07D	C4C-CHD	-2.08	1.35	1.41
7	E	1001	07D	C4C-CHD	-2.07	1.35	1.41
7	6	1001	07D	C4C-CHD	-2.07	1.35	1.41
7	H	301	07D	C4C-CHD	-2.07	1.35	1.41
7	7	102	07D	C4C-CHD	-2.07	1.35	1.41
7	V	1001	07D	C4C-CHD	-2.06	1.35	1.41
7	5	102	07D	C4C-CHD	-2.06	1.35	1.41
7	M	405	07D	C1C-CHC	2.06	1.46	1.41
7	Q	102	07D	C4C-CHD	-2.06	1.35	1.41
7	K	102	07D	C4C-CHD	-2.06	1.35	1.41
7	9	102	07D	C4C-CHD	-2.06	1.35	1.41
7	8	1001	07D	C4C-CHD	-2.05	1.35	1.41
7	T	101	07D	C4C-CHD	-2.05	1.35	1.41
7	J	1001	07D	C4C-CHD	-2.04	1.35	1.41
7	N	1002	07D	C4C-CHD	-2.04	1.35	1.41
7	W	1001	07D	C4C-CHD	-2.04	1.35	1.41
7	4	1001	07D	C4C-CHD	-2.04	1.35	1.41
7	M	404	07D	C4C-CHD	-2.03	1.35	1.41
7	Z	1001	07D	C4C-CHD	-2.02	1.35	1.41
7	R	101	07D	C4C-CHD	-2.02	1.35	1.41
7	X	1001	07D	C4C-CHD	-2.02	1.35	1.41

All (586) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	m	102	07D	CAA-C2A-C1A	-16.84	109.18	127.48
7	9	102	07D	CAA-C2A-C1A	-16.80	109.23	127.48
7	d	1002	07D	CAA-C2A-C1A	-16.51	109.54	127.48
7	S	102	07D	CAA-C2A-C1A	-16.39	109.67	127.48
7	Y	102	07D	CAA-C2A-C1A	-16.33	109.73	127.48
7	1	1001	07D	CAA-C2A-C1A	-16.31	109.76	127.48
7	5	102	07D	CAA-C2A-C1A	-16.21	109.86	127.48
7	n	102	07D	CAA-C2A-C1A	-16.21	109.87	127.48
7	7	102	07D	CAA-C2A-C1A	-16.21	109.87	127.48
7	K	102	07D	CAA-C2A-C1A	-16.13	109.96	127.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	I	102	07D	CAA-C2A-C1A	-16.03	110.06	127.48
7	O	102	07D	CAA-C2A-C1A	-15.97	110.12	127.48
7	T	101	07D	CAA-C2A-C1A	-15.95	110.15	127.48
7	W	1001	07D	CAA-C2A-C1A	-15.94	110.16	127.48
7	E	1001	07D	CAA-C2A-C1A	-15.84	110.27	127.48
7	3	102	07D	CAA-C2A-C1A	-15.77	110.34	127.48
7	V	1001	07D	CAA-C2A-C1A	-15.77	110.35	127.48
7	U	1001	07D	CAA-C2A-C1A	-15.72	110.40	127.48
7	Q	102	07D	CAA-C2A-C1A	-15.66	110.46	127.48
7	4	1001	07D	CAA-C2A-C1A	-15.57	110.56	127.48
7	F	1001	07D	CAA-C2A-C1A	-15.54	110.59	127.48
7	J	1001	07D	CAA-C2A-C1A	-15.46	110.68	127.48
7	A	101	07D	CAA-C2A-C1A	-15.24	110.92	127.48
7	X	1001	07D	CAA-C2A-C1A	-15.17	110.99	127.48
7	6	1001	07D	CAA-C2A-C1A	-15.07	111.11	127.48
7	N	1002	07D	CAA-C2A-C1A	-15.04	111.14	127.48
7	D	1001	07D	CAA-C2A-C1A	-14.92	111.27	127.48
7	L	1004	07D	CAA-C2A-C1A	-14.88	111.31	127.48
7	R	101	07D	CAA-C2A-C1A	-14.21	112.04	127.48
7	2	1001	07D	CAA-C2A-C1A	-14.16	112.10	127.48
7	Z	1001	07D	CAA-C2A-C1A	-14.03	112.23	127.48
7	G	1001	07D	CAA-C2A-C1A	-13.52	112.79	127.48
7	8	1001	07D	CAA-C2A-C1A	-13.49	112.82	127.48
7	L	1005	07D	CAA-C2A-C1A	-13.30	113.03	127.48
7	M	405	07D	CAA-C2A-C1A	-12.12	114.31	127.48
7	M	404	07D	CAA-C2A-C1A	-11.80	114.66	127.48
7	M	405	07D	CMC-C2C-C1C	-11.41	110.92	128.46
7	H	301	07D	CMC-C2C-C1C	-11.40	110.94	128.46
7	M	404	07D	CMC-C2C-C1C	-11.28	111.12	128.46
7	L	1005	07D	CMC-C2C-C1C	-11.27	111.14	128.46
7	L	1004	07D	CMC-C2C-C1C	-11.09	111.42	128.46
7	G	1001	07D	CMC-C2C-C1C	-10.76	111.93	128.46
7	J	1001	07D	CMC-C2C-C1C	-10.74	111.95	128.46
7	H	301	07D	CAA-C2A-C1A	-10.74	115.81	127.48
7	D	1001	07D	CMC-C2C-C1C	-10.71	112.01	128.46
7	T	101	07D	CMC-C2C-C1C	-10.64	112.11	128.46
7	7	102	07D	CMC-C2C-C1C	-10.62	112.15	128.46
7	5	102	07D	CMC-C2C-C1C	-10.61	112.15	128.46
7	R	101	07D	CMC-C2C-C1C	-10.61	112.15	128.46
7	6	1001	07D	CMC-C2C-C1C	-10.61	112.16	128.46
7	X	1001	07D	CMC-C2C-C1C	-10.61	112.16	128.46
7	4	1001	07D	CMC-C2C-C1C	-10.60	112.18	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	N	1002	07D	CMC-C2C-C1C	-10.59	112.18	128.46
7	n	102	07D	CMC-C2C-C1C	-10.59	112.18	128.46
7	Z	1001	07D	CMC-C2C-C1C	-10.57	112.22	128.46
7	d	1002	07D	CMC-C2C-C1C	-10.55	112.25	128.46
7	E	1001	07D	CMC-C2C-C1C	-10.54	112.26	128.46
7	2	1001	07D	CMC-C2C-C1C	-10.52	112.29	128.46
7	A	101	07D	CMC-C2C-C1C	-10.47	112.38	128.46
7	8	1001	07D	CMC-C2C-C1C	-10.43	112.43	128.46
7	Y	102	07D	CMC-C2C-C1C	-10.42	112.45	128.46
7	1	1001	07D	CMC-C2C-C1C	-10.40	112.48	128.46
7	W	1001	07D	CMC-C2C-C1C	-10.39	112.49	128.46
7	F	1001	07D	CMC-C2C-C1C	-10.38	112.51	128.46
7	V	1001	07D	CMC-C2C-C1C	-10.38	112.51	128.46
7	O	102	07D	CMC-C2C-C1C	-10.38	112.51	128.46
7	3	102	07D	CMC-C2C-C1C	-10.34	112.58	128.46
7	K	102	07D	CMC-C2C-C1C	-10.30	112.63	128.46
7	I	102	07D	CMC-C2C-C1C	-10.30	112.64	128.46
7	U	1001	07D	CMC-C2C-C1C	-10.24	112.73	128.46
7	S	102	07D	CMC-C2C-C1C	-10.22	112.76	128.46
7	Q	102	07D	CMC-C2C-C1C	-10.21	112.77	128.46
7	9	102	07D	CMC-C2C-C1C	-10.20	112.78	128.46
7	m	102	07D	CMC-C2C-C1C	-10.20	112.79	128.46
7	M	404	07D	C1C-C2C-C3C	-9.05	100.70	107.00
7	L	1005	07D	C1C-C2C-C3C	-8.90	100.80	107.00
7	L	1005	07D	C4D-ND-C1D	8.48	110.52	106.71
7	M	405	07D	C4D-ND-C1D	8.45	110.50	106.71
7	H	301	07D	C4D-ND-C1D	7.81	110.22	106.71
7	L	1004	07D	C1C-C2C-C3C	-7.67	101.66	107.00
7	M	404	07D	C4D-ND-C1D	7.50	110.08	106.71
7	A	101	07D	C1C-C2C-C3C	-7.36	101.87	107.00
7	7	102	07D	C1C-C2C-C3C	-7.31	101.91	107.00
7	d	1002	07D	C1C-C2C-C3C	-7.25	101.95	107.00
7	n	102	07D	C1C-C2C-C3C	-7.25	101.95	107.00
7	m	102	07D	C1C-C2C-C3C	-7.21	101.98	107.00
7	9	102	07D	C1C-C2C-C3C	-7.20	101.99	107.00
7	5	102	07D	C1C-C2C-C3C	-7.19	101.99	107.00
7	S	102	07D	C1C-C2C-C3C	-7.16	102.01	107.00
7	Y	102	07D	C1C-C2C-C3C	-7.16	102.02	107.00
7	U	1001	07D	C1C-C2C-C3C	-7.15	102.02	107.00
7	Q	102	07D	C1C-C2C-C3C	-7.15	102.03	107.00
7	3	102	07D	C1C-C2C-C3C	-7.14	102.03	107.00
7	K	102	07D	C1C-C2C-C3C	-7.13	102.03	107.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	X	1001	07D	C1C-C2C-C3C	-7.13	102.04	107.00
7	O	102	07D	C1C-C2C-C3C	-7.10	102.06	107.00
7	3	102	07D	C4D-ND-C1D	7.10	109.90	106.71
7	E	1001	07D	C1C-C2C-C3C	-7.08	102.07	107.00
7	I	102	07D	C1C-C2C-C3C	-7.06	102.08	107.00
7	Z	1001	07D	C1C-C2C-C3C	-7.06	102.08	107.00
7	n	102	07D	C4D-ND-C1D	7.06	109.88	106.71
7	T	101	07D	C1C-C2C-C3C	-7.05	102.09	107.00
7	1	1001	07D	C1C-C2C-C3C	-7.04	102.10	107.00
7	K	102	07D	C4D-ND-C1D	7.03	109.87	106.71
7	6	1001	07D	C1C-C2C-C3C	-7.03	102.11	107.00
7	H	301	07D	C1C-C2C-C3C	-7.03	102.11	107.00
7	N	1002	07D	C1C-C2C-C3C	-7.02	102.11	107.00
7	V	1001	07D	C1C-C2C-C3C	-7.02	102.11	107.00
7	W	1001	07D	C1C-C2C-C3C	-7.01	102.12	107.00
7	F	1001	07D	C1C-C2C-C3C	-7.01	102.12	107.00
7	7	102	07D	C4D-ND-C1D	6.96	109.83	106.71
7	S	102	07D	C4D-ND-C1D	6.94	109.83	106.71
7	G	1001	07D	C1C-C2C-C3C	-6.94	102.17	107.00
7	4	1001	07D	C1C-C2C-C3C	-6.88	102.21	107.00
7	D	1001	07D	C1C-C2C-C3C	-6.87	102.22	107.00
7	8	1001	07D	C1C-C2C-C3C	-6.86	102.22	107.00
7	Y	102	07D	C4D-ND-C1D	6.86	109.79	106.71
7	R	101	07D	C1C-C2C-C3C	-6.83	102.25	107.00
7	O	102	07D	C4D-ND-C1D	6.82	109.77	106.71
7	1	1001	07D	C4D-ND-C1D	6.82	109.77	106.71
7	d	1002	07D	C4D-ND-C1D	6.81	109.77	106.71
7	2	1001	07D	C1C-C2C-C3C	-6.80	102.26	107.00
7	U	1001	07D	C4D-ND-C1D	6.79	109.76	106.71
7	J	1001	07D	C1C-C2C-C3C	-6.79	102.27	107.00
7	8	1001	07D	C4D-ND-C1D	6.75	109.74	106.71
7	Q	102	07D	C4D-ND-C1D	6.74	109.74	106.71
7	J	1001	07D	C4D-ND-C1D	6.74	109.73	106.71
7	W	1001	07D	C4D-ND-C1D	6.70	109.72	106.71
7	Z	1001	07D	C4D-ND-C1D	6.67	109.70	106.71
7	Q	102	07D	CMC-C2C-C3C	-6.62	112.45	124.94
7	I	102	07D	C4D-ND-C1D	6.62	109.68	106.71
7	K	102	07D	CMC-C2C-C3C	-6.62	112.47	124.94
7	9	102	07D	CMC-C2C-C3C	-6.60	112.49	124.94
7	I	102	07D	CMC-C2C-C3C	-6.59	112.51	124.94
7	Y	102	07D	CMC-C2C-C3C	-6.54	112.61	124.94
7	m	102	07D	C4D-ND-C1D	6.54	109.64	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	1	1001	07D	CMC-C2C-C3C	-6.52	112.64	124.94
7	3	102	07D	CMC-C2C-C3C	-6.52	112.65	124.94
7	5	102	07D	CMC-C2C-C3C	-6.52	112.65	124.94
7	A	101	07D	C4D-ND-C1D	6.50	109.63	106.71
7	5	102	07D	C4D-ND-C1D	6.50	109.63	106.71
7	U	1001	07D	CMC-C2C-C3C	-6.49	112.70	124.94
7	9	102	07D	C4D-ND-C1D	6.48	109.62	106.71
7	n	102	07D	CMC-C2C-C3C	-6.48	112.73	124.94
7	M	405	07D	C1C-C2C-C3C	-6.47	102.49	107.00
7	O	102	07D	CMC-C2C-C3C	-6.44	112.80	124.94
7	L	1004	07D	C4D-ND-C1D	6.44	109.60	106.71
7	R	101	07D	C4D-ND-C1D	6.43	109.60	106.71
7	m	102	07D	CMC-C2C-C3C	-6.42	112.84	124.94
7	W	1001	07D	CMC-C2C-C3C	-6.41	112.85	124.94
7	A	101	07D	CMC-C2C-C3C	-6.41	112.85	124.94
7	7	102	07D	CMC-C2C-C3C	-6.36	112.95	124.94
7	S	102	07D	CMC-C2C-C3C	-6.34	112.98	124.94
7	d	1002	07D	CMC-C2C-C3C	-6.33	113.01	124.94
7	E	1001	07D	C4D-ND-C1D	6.32	109.55	106.71
7	X	1001	07D	C4D-ND-C1D	6.30	109.54	106.71
7	m	102	07D	CMA-C3A-C2A	-6.29	113.08	124.94
7	2	1001	07D	CMC-C2C-C3C	-6.26	113.13	124.94
7	L	1004	07D	CMC-C2C-C3C	-6.25	113.16	124.94
7	M	405	07D	CMC-C2C-C3C	-6.22	113.21	124.94
7	T	101	07D	CMC-C2C-C3C	-6.22	113.21	124.94
7	8	1001	07D	CMC-C2C-C3C	-6.21	113.22	124.94
7	4	1001	07D	CMC-C2C-C3C	-6.21	113.23	124.94
7	6	1001	07D	C4D-ND-C1D	6.21	109.50	106.71
7	F	1001	07D	C4D-ND-C1D	6.20	109.49	106.71
7	H	301	07D	CMA-C3A-C2A	-6.18	113.28	124.94
7	J	1001	07D	CMC-C2C-C3C	-6.18	113.28	124.94
7	V	1001	07D	C4D-ND-C1D	6.18	109.48	106.71
7	2	1001	07D	C4D-ND-C1D	6.17	109.48	106.71
7	M	404	07D	CMC-C2C-C3C	-6.16	113.33	124.94
7	L	1005	07D	CMC-C2C-C3C	-6.15	113.34	124.94
7	E	1001	07D	CMC-C2C-C3C	-6.15	113.35	124.94
7	D	1001	07D	C4D-ND-C1D	6.13	109.46	106.71
7	H	301	07D	CMC-C2C-C3C	-6.12	113.40	124.94
7	G	1001	07D	C4D-ND-C1D	6.12	109.46	106.71
7	G	1001	07D	CMC-C2C-C3C	-6.12	113.41	124.94
7	R	101	07D	CMC-C2C-C3C	-6.10	113.45	124.94
7	N	1002	07D	CMC-C2C-C3C	-6.09	113.47	124.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	6	1001	07D	CMC-C2C-C3C	-6.08	113.49	124.94
7	V	1001	07D	CMC-C2C-C3C	-6.07	113.50	124.94
7	N	1002	07D	C4D-ND-C1D	6.03	109.42	106.71
7	F	1001	07D	CMC-C2C-C3C	-6.02	113.59	124.94
7	X	1001	07D	CMC-C2C-C3C	-6.02	113.59	124.94
7	D	1001	07D	CMC-C2C-C3C	-6.02	113.60	124.94
7	Z	1001	07D	CMC-C2C-C3C	-6.01	113.61	124.94
7	T	101	07D	C4D-ND-C1D	5.98	109.39	106.71
7	U	1001	07D	CMA-C3A-C2A	-5.93	113.76	124.94
7	H	301	07D	CBD-CHA-C4D	-5.91	101.89	108.54
7	L	1004	07D	CBD-CHA-C4D	-5.90	101.89	108.54
7	M	404	07D	CBD-CHA-C4D	-5.90	101.90	108.54
7	K	102	07D	CMA-C3A-C2A	-5.89	113.83	124.94
7	I	102	07D	CMA-C3A-C2A	-5.88	113.85	124.94
7	5	102	07D	CMA-C3A-C2A	-5.88	113.86	124.94
7	X	1001	07D	CMA-C3A-C2A	-5.86	113.89	124.94
7	J	1001	07D	CMA-C3A-C2A	-5.82	113.96	124.94
7	4	1001	07D	C4D-ND-C1D	5.81	109.32	106.71
7	V	1001	07D	CMA-C3A-C2A	-5.81	113.99	124.94
12	L	1002	RQ0	C11-C07-C19	-5.81	110.11	126.42
7	Q	102	07D	CMA-C3A-C2A	-5.79	114.02	124.94
7	9	102	07D	CMA-C3A-C2A	-5.76	114.07	124.94
7	6	1001	07D	CMA-C3A-C2A	-5.76	114.08	124.94
7	7	102	07D	CMA-C3A-C2A	-5.74	114.12	124.94
7	F	1001	07D	CMA-C3A-C2A	-5.72	114.15	124.94
7	d	1002	07D	CMA-C3A-C2A	-5.70	114.20	124.94
7	N	1002	07D	CMA-C3A-C2A	-5.69	114.22	124.94
7	2	1001	07D	CMA-C3A-C2A	-5.68	114.22	124.94
7	H	301	07D	CAA-C2A-C3A	-5.68	110.91	127.25
7	8	1001	07D	CAA-C2A-C3A	-5.67	110.95	127.25
7	A	101	07D	CMA-C3A-C2A	-5.67	114.26	124.94
7	1	1001	07D	CMA-C3A-C2A	-5.65	114.29	124.94
7	Y	102	07D	CMA-C3A-C2A	-5.65	114.30	124.94
7	G	1001	07D	CMA-C3A-C2A	-5.64	114.31	124.94
7	E	1001	07D	CMA-C3A-C2A	-5.63	114.32	124.94
7	A	101	07D	CBD-CHA-C4D	-5.63	102.19	108.54
7	n	102	07D	CMA-C3A-C2A	-5.63	114.32	124.94
7	8	1001	07D	CBD-CHA-C4D	-5.63	102.20	108.54
7	W	1001	07D	CMA-C3A-C2A	-5.62	114.34	124.94
7	M	405	07D	CBD-CHA-C4D	-5.61	102.22	108.54
7	Z	1001	07D	CMA-C3A-C2A	-5.61	114.36	124.94
7	D	1001	07D	CMA-C3A-C2A	-5.60	114.39	124.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	S	102	07D	CMA-C3A-C2A	-5.59	114.41	124.94
7	R	101	07D	CMA-C3A-C2A	-5.59	114.41	124.94
7	O	102	07D	CMA-C3A-C2A	-5.58	114.42	124.94
7	4	1001	07D	CMA-C3A-C2A	-5.57	114.44	124.94
7	M	404	07D	CAA-C2A-C3A	-5.57	111.24	127.25
7	G	1001	07D	CBD-CHA-C4D	-5.56	102.28	108.54
7	L	1005	07D	CMA-C3A-C2A	-5.56	114.47	124.94
7	M	405	07D	CMA-C3A-C2A	-5.53	114.52	124.94
7	T	101	07D	CMA-C3A-C2A	-5.52	114.53	124.94
7	M	404	07D	CMA-C3A-C2A	-5.52	114.53	124.94
7	G	1001	07D	CAA-C2A-C3A	-5.50	111.45	127.25
7	Z	1001	07D	CAA-C2A-C3A	-5.49	111.48	127.25
7	V	1001	07D	CBD-CHA-C4D	-5.47	102.38	108.54
7	6	1001	07D	CBD-CHA-C4D	-5.45	102.40	108.54
7	X	1001	07D	CBD-CHA-C4D	-5.44	102.41	108.54
7	N	1002	07D	CBD-CHA-C4D	-5.43	102.42	108.54
7	2	1001	07D	CBD-CHA-C4D	-5.43	102.42	108.54
7	L	1005	07D	CBD-CHA-C4D	-5.43	102.43	108.54
7	3	102	07D	CMA-C3A-C2A	-5.42	114.73	124.94
7	L	1004	07D	CMA-C3A-C2A	-5.41	114.73	124.94
7	D	1001	07D	CAA-C2A-C3A	-5.41	111.70	127.25
7	8	1001	07D	CMA-C3A-C2A	-5.41	114.74	124.94
7	4	1001	07D	CBD-CHA-C4D	-5.41	102.45	108.54
7	R	101	07D	CAA-C2A-C3A	-5.41	111.70	127.25
7	E	1001	07D	CBD-CHA-C4D	-5.40	102.45	108.54
7	J	1001	07D	CBD-CHA-C4D	-5.39	102.47	108.54
7	I	102	07D	CBD-CHA-C4D	-5.39	102.47	108.54
7	F	1001	07D	CBD-CHA-C4D	-5.38	102.47	108.54
7	3	102	07D	CBD-CHA-C4D	-5.38	102.48	108.54
7	1	1001	07D	CBD-CHA-C4D	-5.37	102.49	108.54
7	D	1001	07D	CBD-CHA-C4D	-5.37	102.49	108.54
7	T	101	07D	CBD-CHA-C4D	-5.36	102.50	108.54
7	O	102	07D	CBD-CHA-C4D	-5.36	102.50	108.54
7	Z	1001	07D	CBD-CHA-C4D	-5.35	102.52	108.54
7	Y	102	07D	CBD-CHA-C4D	-5.34	102.52	108.54
7	m	102	07D	CBD-CHA-C4D	-5.34	102.53	108.54
7	3	102	07D	CAA-C2A-C3A	-5.33	111.93	127.25
7	7	102	07D	CBD-CHA-C4D	-5.33	102.54	108.54
7	S	102	07D	CBD-CHA-C4D	-5.32	102.55	108.54
7	9	102	07D	CBD-CHA-C4D	-5.30	102.57	108.54
7	6	1001	07D	CAA-C2A-C3A	-5.28	112.07	127.25
7	T	101	07D	CAA-C2A-C3A	-5.27	112.11	127.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	W	1001	07D	CBD-CHA-C4D	-5.26	102.62	108.54
7	n	102	07D	CBD-CHA-C4D	-5.25	102.62	108.54
7	R	101	07D	CBD-CHA-C4D	-5.25	102.63	108.54
7	4	1001	07D	CAA-C2A-C3A	-5.24	112.19	127.25
7	U	1001	07D	CBD-CHA-C4D	-5.23	102.65	108.54
7	J	1001	07D	CAA-C2A-C3A	-5.23	112.21	127.25
7	2	1001	07D	CAA-C2A-C3A	-5.22	112.24	127.25
7	Q	102	07D	CBD-CHA-C4D	-5.21	102.67	108.54
7	K	102	07D	CBD-CHA-C4D	-5.20	102.68	108.54
7	A	101	07D	CAA-C2A-C3A	-5.20	112.31	127.25
7	d	1002	07D	CBD-CHA-C4D	-5.19	102.70	108.54
7	V	1001	07D	CAA-C2A-C3A	-5.17	112.40	127.25
7	F	1001	07D	CAA-C2A-C3A	-5.16	112.43	127.25
7	E	1001	07D	CAA-C2A-C3A	-5.15	112.46	127.25
7	n	102	07D	CAA-C2A-C3A	-5.13	112.50	127.25
7	O	102	07D	CAA-C2A-C3A	-5.11	112.57	127.25
7	L	1004	07D	CAA-C2A-C3A	-5.08	112.64	127.25
7	X	1001	07D	CAA-C2A-C3A	-5.08	112.65	127.25
7	5	102	07D	CBD-CHA-C4D	-5.07	102.82	108.54
7	N	1002	07D	CAA-C2A-C3A	-5.07	112.67	127.25
7	1	1001	07D	CAA-C2A-C3A	-5.01	112.86	127.25
7	Q	102	07D	CAA-C2A-C3A	-5.00	112.86	127.25
7	S	102	07D	CAA-C2A-C3A	-5.00	112.87	127.25
7	U	1001	07D	CAA-C2A-C3A	-4.98	112.94	127.25
7	I	102	07D	CAA-C2A-C3A	-4.96	113.00	127.25
7	W	1001	07D	CAA-C2A-C3A	-4.95	113.01	127.25
7	7	102	07D	CAA-C2A-C3A	-4.94	113.05	127.25
7	M	405	07D	CAA-C2A-C3A	-4.93	113.08	127.25
7	d	1002	07D	CAA-C2A-C3A	-4.93	113.09	127.25
7	L	1005	07D	CAA-C2A-C3A	-4.89	113.20	127.25
7	K	102	07D	CAA-C2A-C3A	-4.89	113.20	127.25
7	L	1005	07D	C2D-C1D-ND	-4.88	105.40	109.97
7	S	102	07D	CMB-C2B-C1B	-4.84	117.66	125.04
7	5	102	07D	CAA-C2A-C3A	-4.84	113.34	127.25
7	Y	102	07D	CAA-C2A-C3A	-4.83	113.36	127.25
7	3	102	07D	CMB-C2B-C1B	-4.82	117.70	125.04
7	9	102	07D	CAA-C2A-C3A	-4.80	113.45	127.25
7	M	404	07D	CMB-C2B-C1B	-4.73	117.84	125.04
7	M	405	07D	C2D-C1D-ND	-4.71	105.56	109.97
7	L	1004	07D	CMB-C2B-C1B	-4.64	117.97	125.04
7	M	404	07D	C2D-C1D-ND	-4.63	105.63	109.97
7	W	1001	07D	CMB-C2B-C1B	-4.61	118.02	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	D	1001	07D	CMB-C2B-C1B	-4.54	118.12	125.04
7	U	1001	07D	CMB-C2B-C1B	-4.54	118.13	125.04
7	n	102	07D	CMB-C2B-C1B	-4.50	118.18	125.04
7	T	101	07D	CMB-C2B-C1B	-4.48	118.21	125.04
7	H	301	07D	C2D-C1D-ND	-4.48	105.78	109.97
7	F	1001	07D	CMB-C2B-C1B	-4.48	118.22	125.04
7	d	1002	07D	CMB-C2B-C1B	-4.48	118.22	125.04
7	5	102	07D	CMB-C2B-C1B	-4.47	118.23	125.04
7	R	101	07D	CMB-C2B-C1B	-4.46	118.25	125.04
7	Z	1001	07D	CMB-C2B-C1B	-4.45	118.26	125.04
7	G	1001	07D	CMB-C2B-C1B	-4.44	118.28	125.04
7	E	1001	07D	CMB-C2B-C1B	-4.42	118.31	125.04
7	8	1001	07D	CMB-C2B-C1B	-4.41	118.33	125.04
7	4	1001	07D	CMB-C2B-C1B	-4.40	118.34	125.04
7	H	301	07D	C4A-CHB-C1B	4.40	128.36	122.56
7	I	102	07D	CMB-C2B-C1B	-4.39	118.36	125.04
7	Q	102	07D	CMB-C2B-C1B	-4.39	118.36	125.04
7	1	1001	07D	CMB-C2B-C1B	-4.39	118.36	125.04
7	V	1001	07D	CMB-C2B-C1B	-4.38	118.37	125.04
7	2	1001	07D	CMB-C2B-C1B	-4.37	118.39	125.04
7	7	102	07D	C2D-C1D-ND	-4.36	105.89	109.97
7	X	1001	07D	CMB-C2B-C1B	-4.36	118.40	125.04
7	J	1001	07D	CMB-C2B-C1B	-4.35	118.41	125.04
7	K	102	07D	C2D-C1D-ND	-4.34	105.90	109.97
7	S	102	07D	C2D-C1D-ND	-4.34	105.91	109.97
7	n	102	07D	C2D-C1D-ND	-4.34	105.91	109.97
7	O	102	07D	CMB-C2B-C1B	-4.33	118.44	125.04
7	Q	102	07D	C2D-C1D-ND	-4.32	105.92	109.97
7	Z	1001	07D	C2D-C1D-ND	-4.32	105.92	109.97
7	A	101	07D	C2D-C1D-ND	-4.32	105.92	109.97
7	6	1001	07D	CMB-C2B-C1B	-4.31	118.48	125.04
7	3	102	07D	C2D-C1D-ND	-4.29	105.95	109.97
7	R	101	07D	C2D-C1D-ND	-4.29	105.95	109.97
7	9	102	07D	CMB-C2B-C1B	-4.29	118.51	125.04
7	Y	102	07D	C2D-C1D-ND	-4.29	105.96	109.97
7	U	1001	07D	C2D-C1D-ND	-4.28	105.96	109.97
7	W	1001	07D	C2D-C1D-ND	-4.28	105.97	109.97
7	N	1002	07D	CMB-C2B-C1B	-4.28	118.53	125.04
7	Y	102	07D	CMB-C2B-C1B	-4.27	118.53	125.04
7	d	1002	07D	C2D-C1D-ND	-4.27	105.97	109.97
7	E	1001	07D	C2D-C1D-ND	-4.27	105.97	109.97
7	X	1001	07D	C2D-C1D-ND	-4.26	105.98	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	8	1001	07D	C2D-C1D-ND	-4.26	105.98	109.97
7	1	1001	07D	C2D-C1D-ND	-4.25	105.99	109.97
7	F	1001	07D	C2D-C1D-ND	-4.25	105.99	109.97
7	D	1001	07D	C2D-C1D-ND	-4.25	105.99	109.97
7	J	1001	07D	C2D-C1D-ND	-4.25	105.99	109.97
7	5	102	07D	C2D-C1D-ND	-4.24	106.00	109.97
7	A	101	07D	CMB-C2B-C1B	-4.23	118.59	125.04
7	M	404	07D	C4A-CHB-C1B	4.23	128.14	122.56
7	K	102	07D	CMB-C2B-C1B	-4.22	118.62	125.04
7	m	102	07D	CMB-C2B-C1B	-4.21	118.62	125.04
7	m	102	07D	C2D-C1D-ND	-4.21	106.03	109.97
7	L	1004	07D	C2D-C1D-ND	-4.21	106.03	109.97
7	9	102	07D	C2D-C1D-ND	-4.21	106.03	109.97
7	N	1002	07D	C2D-C1D-ND	-4.20	106.03	109.97
7	T	101	07D	C2D-C1D-ND	-4.20	106.04	109.97
7	M	405	07D	CMB-C2B-C1B	-4.19	118.65	125.04
7	O	102	07D	C2D-C1D-ND	-4.18	106.05	109.97
7	7	102	07D	CMB-C2B-C1B	-4.18	118.68	125.04
7	I	102	07D	C2D-C1D-ND	-4.18	106.06	109.97
7	6	1001	07D	C2D-C1D-ND	-4.15	106.08	109.97
7	4	1001	07D	C4A-CHB-C1B	4.15	128.04	122.56
7	2	1001	07D	C2D-C1D-ND	-4.15	106.09	109.97
7	V	1001	07D	C2D-C1D-ND	-4.15	106.09	109.97
7	4	1001	07D	C2D-C1D-ND	-4.15	106.09	109.97
7	G	1001	07D	C4A-CHB-C1B	4.14	128.02	122.56
12	L	1002	RQ0	C27-C18-C14	-4.12	110.36	123.22
7	2	1001	07D	C4A-CHB-C1B	4.12	127.99	122.56
7	m	102	07D	C4A-CHB-C1B	4.11	127.98	122.56
7	8	1001	07D	C4A-CHB-C1B	4.02	127.86	122.56
7	G	1001	07D	C2D-C1D-ND	-3.97	106.25	109.97
7	L	1004	07D	C4A-CHB-C1B	3.96	127.79	122.56
7	6	1001	07D	C4A-CHB-C1B	3.93	127.75	122.56
7	N	1002	07D	C4A-CHB-C1B	3.93	127.74	122.56
7	L	1005	07D	CMB-C2B-C1B	-3.91	119.09	125.04
7	E	1001	07D	C4A-CHB-C1B	3.86	127.65	122.56
7	R	101	07D	C4A-CHB-C1B	3.84	127.63	122.56
7	V	1001	07D	C4A-CHB-C1B	3.82	127.61	122.56
7	7	102	07D	C4A-CHB-C1B	3.80	127.58	122.56
7	m	102	07D	CAA-C2A-C3A	-3.80	116.33	127.25
7	L	1005	07D	C2B-C1B-NB	-3.78	106.45	110.57
7	D	1001	07D	C4A-CHB-C1B	3.77	127.53	122.56
7	T	101	07D	C4A-CHB-C1B	3.74	127.49	122.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A	101	07D	C4A-CHB-C1B	3.74	127.49	122.56
7	M	405	07D	C2B-C1B-NB	-3.73	106.50	110.57
12	L	1002	RQ0	C18-C14-C23	-3.72	115.97	126.42
7	Z	1001	07D	C4A-CHB-C1B	3.70	127.44	122.56
7	L	1005	07D	C4A-CHB-C1B	3.68	127.42	122.56
7	I	102	07D	C4A-CHB-C1B	3.67	127.41	122.56
7	J	1001	07D	C4A-CHB-C1B	3.66	127.38	122.56
7	1	1001	07D	C4A-CHB-C1B	3.65	127.37	122.56
7	H	301	07D	C2B-C1B-NB	-3.62	106.62	110.57
7	S	102	07D	C2B-C1B-NB	-3.61	106.63	110.57
7	3	102	07D	C2B-C1B-NB	-3.60	106.64	110.57
7	W	1001	07D	C4A-CHB-C1B	3.59	127.29	122.56
7	3	102	07D	C4A-CHB-C1B	3.58	127.28	122.56
7	Y	102	07D	C4A-CHB-C1B	3.56	127.26	122.56
7	5	102	07D	C2B-C1B-NB	-3.56	106.69	110.57
7	n	102	07D	C2B-C1B-NB	-3.56	106.69	110.57
7	5	102	07D	C4A-CHB-C1B	3.54	127.24	122.56
7	F	1001	07D	C4A-CHB-C1B	3.54	127.23	122.56
7	2	1001	07D	C2B-C1B-NB	-3.52	106.72	110.57
7	F	1001	07D	C2B-C1B-NB	-3.51	106.74	110.57
7	K	102	07D	C2B-C1B-NB	-3.50	106.75	110.57
7	7	102	07D	C2B-C1B-NB	-3.49	106.77	110.57
7	6	1001	07D	C2B-C1B-NB	-3.48	106.77	110.57
7	O	102	07D	C2B-C1B-NB	-3.48	106.77	110.57
7	X	1001	07D	C4A-CHB-C1B	3.48	127.15	122.56
7	J	1001	07D	C2B-C1B-NB	-3.48	106.78	110.57
7	Q	102	07D	C4A-CHB-C1B	3.47	127.14	122.56
7	H	301	07D	CMB-C2B-C1B	-3.46	119.77	125.04
7	S	102	07D	C4A-CHB-C1B	3.45	127.12	122.56
7	G	1001	07D	C2B-C1B-NB	-3.44	106.81	110.57
7	9	102	07D	C2B-C1B-NB	-3.44	106.82	110.57
7	M	405	07D	C4A-CHB-C1B	3.44	127.10	122.56
7	d	1002	07D	C2B-C1B-NB	-3.44	106.82	110.57
7	V	1001	07D	C2B-C1B-NB	-3.43	106.83	110.57
7	8	1001	07D	C2B-C1B-NB	-3.42	106.84	110.57
7	I	102	07D	C2B-C1B-NB	-3.42	106.84	110.57
7	N	1002	07D	C2B-C1B-NB	-3.42	106.84	110.57
7	m	102	07D	CBA-CAA-C2A	3.41	118.36	112.60
7	4	1001	07D	C2B-C1B-NB	-3.41	106.85	110.57
7	m	102	07D	C2B-C1B-NB	-3.41	106.85	110.57
7	9	102	07D	C4A-CHB-C1B	3.38	127.03	122.56
7	d	1002	07D	C4A-CHB-C1B	3.38	127.02	122.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	Q	102	07D	C2B-C1B-NB	-3.38	106.89	110.57
7	R	101	07D	C2B-C1B-NB	-3.37	106.89	110.57
7	1	1001	07D	C2B-C1B-NB	-3.37	106.89	110.57
7	W	1001	07D	C2B-C1B-NB	-3.36	106.90	110.57
7	K	102	07D	C4A-CHB-C1B	3.36	126.99	122.56
7	Z	1001	07D	C2B-C1B-NB	-3.35	106.91	110.57
7	Y	102	07D	C2B-C1B-NB	-3.35	106.92	110.57
7	M	404	07D	C2B-C1B-NB	-3.34	106.92	110.57
7	U	1001	07D	C4A-CHB-C1B	3.34	126.97	122.56
11	L	1001	BPH	OBD-CAD-CBD	-3.34	121.12	125.89
7	O	102	07D	C4A-CHB-C1B	3.34	126.96	122.56
7	A	101	07D	C2B-C1B-NB	-3.32	106.95	110.57
7	U	1001	07D	C2B-C1B-NB	-3.31	106.96	110.57
11	M	402	BPH	OBD-CAD-CBD	-3.31	121.17	125.89
7	E	1001	07D	C2B-C1B-NB	-3.30	106.97	110.57
7	T	101	07D	C2B-C1B-NB	-3.29	106.98	110.57
7	X	1001	07D	C2B-C1B-NB	-3.29	106.98	110.57
12	L	1002	RQ0	C42-C41-C46	3.28	120.89	112.05
7	L	1004	07D	C2B-C1B-NB	-3.25	107.02	110.57
7	D	1001	07D	C2B-C1B-NB	-3.23	107.05	110.57
7	n	102	07D	C4A-CHB-C1B	3.22	126.81	122.56
13	L	1006	U10	C8-C7-C6	3.19	120.66	112.05
8	9	101	CRT	C1-C4-C5	3.19	121.50	113.06
8	9	101	CRT	C2-C1-C4	-3.13	106.06	110.86
9	H	302	PGW	C02-O01-C1	3.07	125.36	117.79
12	L	1002	RQ0	C25-C11-C07	-3.05	113.69	123.22
10	M	407	CD4	O2-C14-C13	3.03	118.02	111.50
9	H	303	PGW	O01-C1-C2	3.02	118.02	111.50
10	M	407	CD4	O16-C46-C47	3.02	118.01	111.50
10	H	304	CD4	O2-C14-C13	2.97	117.89	111.50
8	N	1001	CRT	C2-C1-C4	-2.96	106.31	110.86
7	H	301	07D	CBA-CAA-C2A	2.96	117.59	112.60
11	L	1001	BPH	C1-C2-C3	-2.91	121.02	126.04
11	M	402	BPH	C1-C2-C3	2.86	130.99	126.04
11	L	1001	BPH	C1C-NC-C4C	-2.81	108.07	110.54
10	M	407	CD4	O14-C35-C36	2.76	120.57	111.91
8	d	1001	CRT	C1-C4-C5	2.65	120.08	113.06
8	N	1001	CRT	C1-C4-C5	2.57	119.87	113.06
7	S	102	07D	C3B-C2B-C1B	2.57	109.55	105.83
7	3	102	07D	C3B-C2B-C1B	2.56	109.54	105.83
17	R	102	LMT	C3'-C4'-C5'	-2.50	105.19	110.93
7	5	102	07D	C3B-C2B-C1B	2.49	109.44	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	H	302	PGW	O03-C01-C02	2.46	115.59	108.43
8	Y	101	CRT	C31-C32-C33	2.43	130.78	127.31
7	W	1001	07D	C3B-C2B-C1B	2.41	109.32	105.83
7	O	102	07D	C3B-C2B-C1B	2.40	109.31	105.83
9	H	303	PGW	O03-C19-C20	2.40	119.44	111.91
7	n	102	07D	C3B-C2B-C1B	2.40	109.31	105.83
7	L	1004	07D	C3B-C2B-C1B	2.39	109.29	105.83
11	L	1001	BPH	OBB-CAB-CBB	-2.37	114.49	119.73
7	M	404	07D	C3B-C2B-C1B	2.37	109.26	105.83
11	M	402	BPH	CHC-C1C-NC	-2.36	122.40	125.20
7	G	1001	07D	C3B-C2B-C1B	2.34	109.22	105.83
7	9	102	07D	C3B-C2B-C1B	2.33	109.21	105.83
7	L	1005	07D	C3B-C2B-C1B	2.33	109.21	105.83
11	M	402	BPH	C1C-NC-C4C	-2.32	108.50	110.54
8	d	1001	CRT	C20-C21-C22	2.31	128.21	123.47
7	M	404	07D	CMB-C2B-C3B	2.30	132.90	127.61
7	1	1001	07D	C3B-C2B-C1B	2.30	109.16	105.83
7	8	1001	07D	C3B-C2B-C1B	2.30	109.16	105.83
7	m	102	07D	C3B-C2B-C1B	2.30	109.16	105.83
7	7	102	07D	C3B-C2B-C1B	2.30	109.16	105.83
7	2	1001	07D	C3B-C2B-C1B	2.30	109.16	105.83
7	d	1002	07D	C3B-C2B-C1B	2.29	109.15	105.83
8	d	1001	CRT	C31-C32-C33	2.29	130.58	127.31
7	U	1001	07D	C3B-C2B-C1B	2.29	109.15	105.83
7	K	102	07D	C3B-C2B-C1B	2.29	109.14	105.83
7	D	1001	07D	CMB-C2B-C3B	2.29	132.87	127.61
7	4	1001	07D	C3B-C2B-C1B	2.28	109.14	105.83
11	M	402	BPH	CMD-C2D-C3D	2.28	128.95	124.68
11	L	1001	BPH	CHC-C1C-NC	-2.28	122.50	125.20
7	R	101	07D	C3B-C2B-C1B	2.28	109.13	105.83
11	M	402	BPH	C6-C5-C3	2.27	119.42	113.45
7	I	102	07D	C3B-C2B-C1B	2.27	109.12	105.83
7	N	1002	07D	C3B-C2B-C1B	2.27	109.12	105.83
7	Z	1001	07D	C3B-C2B-C1B	2.27	109.12	105.83
11	L	1001	BPH	CMD-C2D-C3D	2.27	128.93	124.68
7	F	1001	07D	C3B-C2B-C1B	2.27	109.12	105.83
7	Q	102	07D	C3B-C2B-C1B	2.27	109.12	105.83
7	6	1001	07D	C3B-C2B-C1B	2.26	109.11	105.83
10	H	304	CD4	O16-C46-C47	2.26	116.37	111.50
7	T	101	07D	C3B-C2B-C1B	2.25	109.09	105.83
7	S	102	07D	CMB-C2B-C3B	2.25	132.78	127.61
7	Y	102	07D	C3B-C2B-C1B	2.24	109.07	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	3	102	07D	CMB-C2B-C3B	2.24	132.76	127.61
7	M	405	07D	C3B-C2B-C1B	2.24	109.07	105.83
7	E	1001	07D	C3B-C2B-C1B	2.23	109.06	105.83
7	L	1004	07D	CMB-C2B-C3B	2.22	132.73	127.61
7	V	1001	07D	C3B-C2B-C1B	2.22	109.05	105.83
7	U	1001	07D	CMB-C2B-C3B	2.22	132.72	127.61
7	T	101	07D	CMB-C2B-C3B	2.21	132.70	127.61
7	M	405	07D	CHD-C1D-C2D	2.21	132.84	126.72
7	J	1001	07D	C3B-C2B-C1B	2.20	109.02	105.83
7	F	1001	07D	CMB-C2B-C3B	2.19	132.66	127.61
7	3	102	07D	CHB-C1B-NB	2.19	127.66	124.20
7	X	1001	07D	C3B-C2B-C1B	2.19	109.00	105.83
7	W	1001	07D	CMB-C2B-C3B	2.19	132.65	127.61
7	D	1001	07D	C3B-C2B-C1B	2.19	109.00	105.83
7	E	1001	07D	CMB-C2B-C3B	2.18	132.62	127.61
7	d	1002	07D	CMB-C2B-C3B	2.18	132.62	127.61
7	R	101	07D	CMB-C2B-C3B	2.18	132.62	127.61
7	A	101	07D	C3B-C2B-C1B	2.17	108.98	105.83
7	Z	1001	07D	CMB-C2B-C3B	2.17	132.62	127.61
7	X	1001	07D	CMB-C2B-C3B	2.16	132.59	127.61
7	V	1001	07D	CMB-C2B-C3B	2.16	132.58	127.61
7	J	1001	07D	CMB-C2B-C3B	2.15	132.56	127.61
8	9	101	CRT	C15-C14-C12	2.13	130.36	127.31
7	4	1001	07D	CMB-C2B-C3B	2.13	132.53	127.61
7	J	1001	07D	CHD-C1D-C2D	2.13	132.63	126.72
7	Q	102	07D	CMB-C2B-C3B	2.13	132.52	127.61
7	I	102	07D	CMB-C2B-C3B	2.13	132.52	127.61
7	8	1001	07D	CMB-C2B-C3B	2.13	132.51	127.61
7	G	1001	07D	CMB-C2B-C3B	2.13	132.51	127.61
7	n	102	07D	CMB-C2B-C3B	2.13	132.51	127.61
7	R	101	07D	CHD-C1D-C2D	2.12	132.60	126.72
8	M	406	CRT	C20-C21-C22	2.12	127.82	123.47
7	F	1001	07D	CHD-C1D-C2D	2.11	132.57	126.72
7	1	1001	07D	CMB-C2B-C3B	2.11	132.48	127.61
7	Z	1001	07D	CHD-C1D-C2D	2.11	132.56	126.72
7	L	1005	07D	CHD-C1D-C2D	2.11	132.56	126.72
7	2	1001	07D	CMB-C2B-C3B	2.10	132.45	127.61
7	M	405	07D	CHB-C1B-NB	2.10	127.52	124.20
17	R	102	LMT	C1-O1'-C1'	2.10	117.32	113.84
7	N	1002	07D	CHD-C1D-C2D	2.10	132.53	126.72
7	X	1001	07D	CHD-C1D-C2D	2.09	132.52	126.72
7	A	101	07D	CMB-C2B-C3B	2.09	132.43	127.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	D	1001	07D	CHD-C1D-C2D	2.09	132.50	126.72
7	6	1001	07D	CMB-C2B-C3B	2.09	132.41	127.61
7	S	102	07D	CHB-C1B-NB	2.08	127.49	124.20
7	Y	102	07D	CMB-C2B-C3B	2.07	132.38	127.61
7	M	404	07D	CHD-C1D-C2D	2.07	132.45	126.72
9	H	302	PGW	O01-C1-C2	2.07	115.96	111.50
7	N	1002	07D	CMB-C2B-C3B	2.06	132.35	127.61
7	H	301	07D	C3B-C2B-C1B	2.06	108.81	105.83
7	4	1001	07D	CHD-C1D-C2D	2.06	132.41	126.72
8	n	101	CRT	C31-C32-C33	2.05	130.24	127.31
7	R	101	07D	CGD-CBD-CAD	-2.05	104.09	110.73
7	A	101	07D	CHD-C1D-C2D	2.05	132.39	126.72
7	6	1001	07D	CHD-C1D-C2D	2.05	132.38	126.72
7	5	102	07D	CMB-C2B-C3B	2.04	132.32	127.61
8	9	101	CRT	C40-C38-C37	-2.04	107.72	110.86
7	8	1001	07D	CHD-C1D-C2D	2.04	132.37	126.72
7	W	1001	07D	CHB-C1B-NB	2.04	127.42	124.20
7	2	1001	07D	CHD-C1D-C2D	2.04	132.35	126.72
8	9	101	CRT	C31-C32-C33	2.03	130.21	127.31
7	Y	102	07D	CHB-C1B-NB	2.03	127.40	124.20
7	9	102	07D	CMB-C2B-C3B	2.03	132.28	127.61
7	M	405	07D	CMB-C2B-C3B	2.03	132.27	127.61
7	E	1001	07D	CHD-C1D-C2D	2.02	132.31	126.72
7	Y	102	07D	CHD-C1D-C2D	2.02	132.31	126.72
8	d	1001	CRT	C20-C19-C17	2.01	130.18	127.31
7	T	101	07D	CHD-C1D-C2D	2.01	132.29	126.72
7	O	102	07D	CMB-C2B-C3B	2.01	132.24	127.61
7	K	102	07D	CMB-C2B-C3B	2.01	132.24	127.61
7	L	1004	07D	CHD-C1D-C2D	2.01	132.28	126.72
7	m	102	07D	CMB-C2B-C3B	2.00	132.22	127.61

All (37) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	1	1001	07D	NA
7	2	1001	07D	NA
7	3	102	07D	NA
7	4	1001	07D	NA
7	5	102	07D	NA
7	6	1001	07D	NA
7	7	102	07D	NA
7	8	1001	07D	NA

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Mol	Chain	Res	Type	Atom
7	9	102	07D	NA
7	A	101	07D	NA
7	D	1001	07D	NA
7	E	1001	07D	NA
7	F	1001	07D	NA
7	G	1001	07D	NA
7	H	301	07D	NA
7	I	102	07D	NA
7	J	1001	07D	NA
7	K	102	07D	NA
7	L	1004	07D	NA
7	L	1005	07D	NA
7	M	404	07D	NA
7	M	405	07D	NA
7	N	1002	07D	NA
7	O	102	07D	NA
7	Q	102	07D	NA
7	R	101	07D	NA
7	S	102	07D	NA
7	T	101	07D	NA
7	U	1001	07D	NA
7	V	1001	07D	NA
7	W	1001	07D	NA
7	X	1001	07D	NA
7	Y	102	07D	NA
7	Z	1001	07D	NA
7	d	1002	07D	NA
7	m	102	07D	NA
7	n	102	07D	NA

All (431) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	1	1001	07D	C1A-C2A-CAA-CBA
7	1	1001	07D	C4C-C3C-CAC-CBC
7	2	1001	07D	C3-C5-C6-C7
7	2	1001	07D	C8-C10-C11-C12
7	2	1001	07D	C4C-C3C-CAC-CBC
7	2	1001	07D	CHA-CBD-CGD-O1D
7	3	102	07D	C1A-C2A-CAA-CBA
7	3	102	07D	C4C-C3C-CAC-CBC
7	4	1001	07D	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
7	4	1001	07D	CHA-CBD-CGD-O1D
7	5	102	07D	C8-C10-C11-C12
7	5	102	07D	C12-C13-C15-C16
7	5	102	07D	C1A-C2A-CAA-CBA
7	5	102	07D	C4C-C3C-CAC-CBC
7	6	1001	07D	C4C-C3C-CAC-CBC
7	7	102	07D	C1A-C2A-CAA-CBA
7	7	102	07D	C4C-C3C-CAC-CBC
7	8	1001	07D	O2A-C1-C2-C3
7	8	1001	07D	C1A-C2A-CAA-CBA
7	8	1001	07D	C4C-C3C-CAC-CBC
7	8	1001	07D	CHA-CBD-CGD-O1D
7	9	102	07D	C13-C15-C16-C17
7	9	102	07D	C1A-C2A-CAA-CBA
7	9	102	07D	C4C-C3C-CAC-CBC
7	A	101	07D	C3A-C2A-CAA-CBA
7	A	101	07D	CHA-CBD-CGD-O1D
7	D	1001	07D	C3-C5-C6-C7
7	D	1001	07D	C4C-C3C-CAC-CBC
7	D	1001	07D	CHA-CBD-CGD-O1D
7	E	1001	07D	C4C-C3C-CAC-CBC
7	E	1001	07D	CHA-CBD-CGD-O1D
7	F	1001	07D	C4C-C3C-CAC-CBC
7	F	1001	07D	CHA-CBD-CGD-O1D
7	G	1001	07D	C4C-C3C-CAC-CBC
7	G	1001	07D	CHA-CBD-CGD-O1D
7	H	301	07D	O2A-C1-C2-C3
7	H	301	07D	C1A-C2A-CAA-CBA
7	H	301	07D	C2B-C3B-CAB-CBB
7	H	301	07D	C4B-C3B-CAB-CBB
7	H	301	07D	C2C-C3C-CAC-CBC
7	I	102	07D	C4C-C3C-CAC-CBC
7	J	1001	07D	C1A-C2A-CAA-CBA
7	J	1001	07D	C3A-C2A-CAA-CBA
7	J	1001	07D	C4C-C3C-CAC-CBC
7	J	1001	07D	CHA-CBD-CGD-O1D
7	K	102	07D	C13-C15-C16-C17
7	K	102	07D	C1A-C2A-CAA-CBA
7	K	102	07D	C4C-C3C-CAC-CBC
7	L	1004	07D	C4C-C3C-CAC-CBC
7	L	1005	07D	C1A-C2A-CAA-CBA
7	L	1005	07D	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
7	L	1005	07D	C2C-C3C-CAC-CBC
7	M	404	07D	C4C-C3C-CAC-CBC
7	M	405	07D	C3A-C2A-CAA-CBA
7	M	405	07D	C4B-C3B-CAB-CBB
7	M	405	07D	C2C-C3C-CAC-CBC
7	N	1002	07D	C4C-C3C-CAC-CBC
7	N	1002	07D	CHA-CBD-CGD-O1D
7	O	102	07D	C1A-C2A-CAA-CBA
7	O	102	07D	C4C-C3C-CAC-CBC
7	Q	102	07D	C1A-C2A-CAA-CBA
7	Q	102	07D	C4C-C3C-CAC-CBC
7	R	101	07D	C12-C13-C15-C16
7	R	101	07D	C4C-C3C-CAC-CBC
7	R	101	07D	CHA-CBD-CGD-O1D
7	R	101	07D	CBD-CGD-O2D-CED
7	S	102	07D	C13-C15-C16-C17
7	S	102	07D	C1A-C2A-CAA-CBA
7	S	102	07D	C4C-C3C-CAC-CBC
7	T	101	07D	C1A-C2A-CAA-CBA
7	T	101	07D	C3A-C2A-CAA-CBA
7	T	101	07D	C4C-C3C-CAC-CBC
7	T	101	07D	CHA-CBD-CGD-O1D
7	U	1001	07D	C1A-C2A-CAA-CBA
7	U	1001	07D	C4C-C3C-CAC-CBC
7	V	1001	07D	C1A-C2A-CAA-CBA
7	V	1001	07D	C3A-C2A-CAA-CBA
7	V	1001	07D	C4C-C3C-CAC-CBC
7	V	1001	07D	CHA-CBD-CGD-O1D
7	W	1001	07D	C8-C10-C11-C12
7	W	1001	07D	C1A-C2A-CAA-CBA
7	W	1001	07D	C4C-C3C-CAC-CBC
7	X	1001	07D	C4C-C3C-CAC-CBC
7	X	1001	07D	CHA-CBD-CGD-O1D
7	Y	102	07D	C1A-C2A-CAA-CBA
7	Y	102	07D	C4C-C3C-CAC-CBC
7	Z	1001	07D	C1A-C2A-CAA-CBA
7	Z	1001	07D	C4C-C3C-CAC-CBC
7	d	1002	07D	C1A-C2A-CAA-CBA
7	d	1002	07D	C4C-C3C-CAC-CBC
7	m	102	07D	O2A-C1-C2-C3
7	m	102	07D	C1A-C2A-CAA-CBA
7	m	102	07D	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
7	m	102	07D	C4C-C3C-CAC-CBC
7	n	102	07D	C1A-C2A-CAA-CBA
7	n	102	07D	C4C-C3C-CAC-CBC
8	1	1002	CRT	C5-C6-C7-C8
8	1	1002	CRT	C5-C6-C7-C9
8	3	101	CRT	C5-C6-C7-C8
8	3	101	CRT	C5-C6-C7-C9
8	5	101	CRT	C5-C6-C7-C8
8	5	101	CRT	C15-C16-C17-C18
8	9	101	CRT	C5-C6-C7-C8
8	I	101	CRT	C5-C6-C7-C8
8	I	101	CRT	C5-C6-C7-C9
8	K	101	CRT	C5-C6-C7-C8
8	K	101	CRT	C5-C6-C7-C9
8	M	406	CRT	C5-C6-C7-C8
8	N	1001	CRT	C5-C6-C7-C8
8	O	101	CRT	C5-C6-C7-C8
8	Q	101	CRT	C5-C6-C7-C8
8	S	101	CRT	C5-C6-C7-C8
8	S	101	CRT	C5-C6-C7-C9
8	d	1001	CRT	C5-C6-C7-C8
8	d	1001	CRT	C5-C6-C7-C9
8	m	101	CRT	C5-C6-C7-C8
8	m	101	CRT	C5-C6-C7-C9
8	n	101	CRT	C5-C6-C7-C8
9	H	302	PGW	C03-O11-P-O14
9	H	303	PGW	C02-C03-O11-P
10	H	304	CD4	C28-O5-P1-O8
10	M	407	CD4	C32-O13-P2-O12
12	L	1002	RQ0	C19-C07-C11-C25
12	L	1002	RQ0	C42-C41-C46-C50
12	L	1002	RQ0	C42-C41-C46-C52
7	R	101	07D	O1D-CGD-O2D-CED
7	5	102	07D	C14-C13-C15-C16
7	Y	102	07D	C4-C3-C5-C6
7	W	1001	07D	C11-C10-C8-C7
7	Y	102	07D	C2-C3-C5-C6
7	7	102	07D	C13-C15-C16-C17
7	9	102	07D	C3-C5-C6-C7
7	G	1001	07D	C3-C5-C6-C7
7	O	102	07D	C13-C15-C16-C17
7	d	1002	07D	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
7	n	102	07D	C8-C10-C11-C12
7	n	102	07D	C13-C15-C16-C17
12	L	1002	RQ0	C33-C28-C29-C35
12	L	1002	RQ0	C31-C30-C34-C43
13	L	1006	U10	C39-C41-C42-C43
11	L	1001	BPH	C15-C16-C17-C18
8	7	101	CRT	C5-C6-C7-C8
8	M	406	CRT	C34-C33-C35-C36
8	N	1001	CRT	C15-C16-C17-C18
8	O	101	CRT	C15-C16-C17-C18
8	S	101	CRT	C15-C16-C17-C18
12	L	1002	RQ0	C18-C14-C23-C44
12	L	1002	RQ0	C11-C07-C19-C27
7	3	102	07D	C2A-CAA-CBA-CGA
12	L	1002	RQ0	C14-C18-C27-C19
7	Q	102	07D	C13-C15-C16-C17
7	Y	102	07D	C8-C10-C11-C12
7	d	1002	07D	C13-C15-C16-C17
12	L	1002	RQ0	C21-C15-C20-C32
13	L	1006	U10	C24-C26-C27-C28
13	L	1006	U10	C34-C36-C37-C38
9	H	302	PGW	C03-O11-P-O12
10	M	407	CD4	C32-O13-P2-O10
7	7	102	07D	C11-C10-C8-C9
10	M	407	CD4	O9-C30-C31-O10
7	7	102	07D	C11-C10-C8-C7
7	8	1001	07D	C11-C10-C8-C7
9	H	303	PGW	C09-C11-C12-C13
12	L	1002	RQ0	C11-C07-C19-C39
9	H	302	PGW	C04-C05-CAD-OAE
8	O	101	CRT	C5-C6-C7-C9
8	Q	101	CRT	C5-C6-C7-C9
12	L	1002	RQ0	C18-C14-C23-C33
7	4	1001	07D	C8-C10-C11-C12
7	m	102	07D	C2A-CAA-CBA-CGA
10	H	304	CD4	C21-C22-C23-C24
7	J	1001	07D	O2A-C1-C2-C3
7	4	1001	07D	C14-C13-C15-C16
7	F	1001	07D	C11-C10-C8-C9
7	F	1001	07D	C11-C10-C8-C7
9	H	303	PGW	O12-C04-C05-OAF
10	H	304	CD4	O8-C29-C30-O9

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Mol	Chain	Res	Type	Atoms
7	N	1002	07D	C4-C3-C5-C6
7	R	101	07D	C14-C13-C15-C16
11	L	1001	BPH	C4-C3-C5-C6
7	4	1001	07D	C12-C13-C15-C16
11	L	1001	BPH	C2-C3-C5-C6
13	L	1003	U10	C12-C11-C9-C8
17	R	102	LMT	C7-C8-C9-C10
13	L	1003	U10	C12-C11-C9-C10
7	3	102	07D	C11-C10-C8-C7
10	M	407	CD4	C5-C6-C7-C8
10	M	407	CD4	C25-C26-C27-C60
9	H	302	PGW	C02-C03-O11-P
12	L	1002	RQ0	C46-C41-C42-C35
7	Z	1001	07D	C11-C10-C8-C9
7	n	102	07D	C11-C10-C8-C7
7	L	1005	07D	C13-C15-C16-C17
8	3	101	CRT	C37-C38-O2-C2M
8	9	101	CRT	C37-C38-O2-C2M
9	H	302	PGW	C02-C01-O03-C19
7	M	405	07D	C2B-C3B-CAB-CBB
7	3	102	07D	C11-C10-C8-C9
13	L	1003	U10	C50-C49-C51-C52
13	L	1003	U10	C48-C49-C51-C52
10	M	407	CD4	C20-C21-C22-C23
7	H	301	07D	CBA-CGA-O2A-C1
8	3	101	CRT	C39-C38-O2-C2M
8	9	101	CRT	C39-C38-O2-C2M
8	9	101	CRT	C40-C38-O2-C2M
8	1	1002	CRT	C2-C1-C4-C5
8	1	1002	CRT	C3-C1-C4-C5
7	d	1002	07D	C14-C13-C15-C16
7	n	102	07D	C11-C10-C8-C9
13	L	1003	U10	C30-C29-C31-C32
7	d	1002	07D	C12-C13-C15-C16
13	L	1003	U10	C28-C29-C31-C32
10	H	304	CD4	C41-C42-C43-C44
8	M	406	CRT	C24-C23-C25-C26
8	5	101	CRT	C5-C6-C7-C9
10	M	407	CD4	C16-C15-C28-O5
7	I	102	07D	C13-C15-C16-C17
7	G	1001	07D	C12-C13-C15-C16
7	L	1004	07D	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
7	Z	1001	07D	C11-C10-C8-C7
7	d	1002	07D	C11-C10-C8-C7
10	H	304	CD4	C30-C31-O10-P2
7	H	301	07D	C2A-CAA-CBA-CGA
7	n	102	07D	C2A-CAA-CBA-CGA
7	V	1001	07D	C4-C3-C5-C6
7	d	1002	07D	C11-C10-C8-C9
9	H	303	PGW	C2-C3-C4-C5
7	3	102	07D	C3-C5-C6-C7
7	n	102	07D	C3-C5-C6-C7
9	H	303	PGW	C05-C04-O12-P
8	M	406	CRT	C32-C33-C35-C36
8	N	1001	CRT	C5-C6-C7-C9
11	M	402	BPH	C10-C11-C12-C13
10	M	407	CD4	O14-C35-C36-C37
7	M	405	07D	CAD-CBD-CGD-O2D
10	H	304	CD4	C52-C53-C54-C55
7	N	1002	07D	C2-C3-C5-C6
7	L	1005	07D	C5-C6-C7-C8
7	R	101	07D	CHA-CBD-CGD-O2D
8	5	101	CRT	C15-C16-C17-C19
8	9	101	CRT	C5-C6-C7-C9
8	O	101	CRT	C15-C16-C17-C19
8	S	101	CRT	C15-C16-C17-C19
9	H	302	PGW	C04-O12-P-O11
7	F	1001	07D	C4-C3-C5-C6
7	F	1001	07D	C14-C13-C15-C16
7	W	1001	07D	C11-C10-C8-C9
7	5	102	07D	C11-C10-C8-C7
9	H	302	PGW	C03-O11-P-O13
9	H	302	PGW	C04-O12-P-O13
10	H	304	CD4	C28-O5-P1-O6
10	M	407	CD4	C28-O5-P1-O7
10	M	407	CD4	C32-O13-P2-O11
7	M	404	07D	CAD-CBD-CGD-O1D
8	m	101	CRT	C1-C4-C5-C6
9	H	302	PGW	C1-C2-C3-C4
10	M	407	CD4	O2-C15-C28-O5
11	M	402	BPH	C6-C7-C8-C10
7	2	1001	07D	C1A-C2A-CAA-CBA
7	4	1001	07D	C1A-C2A-CAA-CBA
7	6	1001	07D	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
7	6	1001	07D	C3A-C2A-CAA-CBA
7	A	101	07D	C1A-C2A-CAA-CBA
7	D	1001	07D	C1A-C2A-CAA-CBA
7	E	1001	07D	C1A-C2A-CAA-CBA
7	F	1001	07D	C1A-C2A-CAA-CBA
7	G	1001	07D	C1A-C2A-CAA-CBA
7	I	102	07D	C1A-C2A-CAA-CBA
7	L	1004	07D	C1A-C2A-CAA-CBA
7	L	1005	07D	C3A-C2A-CAA-CBA
7	M	404	07D	C1A-C2A-CAA-CBA
7	M	405	07D	C1A-C2A-CAA-CBA
7	N	1002	07D	C1A-C2A-CAA-CBA
7	R	101	07D	C1A-C2A-CAA-CBA
7	X	1001	07D	C1A-C2A-CAA-CBA
7	X	1001	07D	C3A-C2A-CAA-CBA
9	H	303	PGW	C5-C6-C7-C8
7	M	404	07D	CAA-CBA-CGA-O2A
7	E	1001	07D	C11-C10-C8-C9
7	3	102	07D	C13-C15-C16-C17
8	O	101	CRT	C37-C38-O2-C2M
9	H	302	PGW	C3-C4-C5-C6
10	H	304	CD4	C3-C4-C5-C6
8	3	101	CRT	C15-C16-C17-C18
7	7	102	07D	C10-C11-C12-C13
13	L	1003	U10	C5-C4-O4-C4M
12	L	1002	RQ0	C12-C08-C17-C38
7	R	101	07D	CBA-CGA-O2A-C1
13	M	403	U10	C40-C39-C41-C42
8	3	101	CRT	C40-C38-O2-C2M
8	O	101	CRT	C39-C38-O2-C2M
8	O	101	CRT	C40-C38-O2-C2M
9	H	303	PGW	C04-O12-P-O11
10	M	407	CD4	C28-O5-P1-O8
7	M	404	07D	C4-C3-C5-C6
7	d	1002	07D	C10-C11-C12-C13
8	M	406	CRT	O1-C1-C4-C5
8	n	101	CRT	C5-C6-C7-C9
7	G	1001	07D	C14-C13-C15-C16
7	n	102	07D	C10-C11-C12-C13
7	8	1001	07D	C8-C10-C11-C12
7	L	1005	07D	C4-C3-C5-C6
7	F	1001	07D	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
13	M	403	U10	C38-C39-C41-C42
7	S	102	07D	C2-C1-O2A-CGA
10	M	407	CD4	O15-C35-C36-C37
13	M	403	U10	C5-C4-O4-C4M
7	X	1001	07D	C11-C10-C8-C9
12	L	1002	RQ0	C39-C19-C27-C18
17	R	102	LMT	O1'-C1-C2-C3
7	1	1001	07D	O2A-C1-C2-C3
8	Y	101	CRT	C5-C6-C7-C8
8	N	1001	CRT	C15-C16-C17-C19
9	H	302	PGW	C01-C02-O01-C1
10	H	304	CD4	C16-C15-O2-C14
10	H	304	CD4	C28-C15-O2-C14
7	5	102	07D	C11-C10-C8-C9
7	V	1001	07D	C11-C10-C8-C9
13	L	1006	U10	C25-C24-C26-C27
7	E	1001	07D	C11-C10-C8-C7
13	M	403	U10	C33-C34-C36-C37
13	L	1006	U10	C3-C4-O4-C4M
13	M	403	U10	C50-C49-C51-C52
12	L	1002	RQ0	C07-C19-C27-C18
7	M	404	07D	C8-C10-C11-C12
7	Y	102	07D	C3-C5-C6-C7
7	A	101	07D	C14-C13-C15-C16
7	L	1004	07D	C11-C10-C8-C9
7	1	1001	07D	C2A-CAA-CBA-CGA
7	F	1001	07D	C12-C13-C15-C16
7	L	1005	07D	C2-C3-C5-C6
7	M	404	07D	C2-C3-C5-C6
7	O	102	07D	C2A-CAA-CBA-CGA
7	V	1001	07D	C2-C3-C5-C6
7	H	301	07D	C15-C16-C17-C18
7	1	1001	07D	C4-C3-C5-C6
7	5	102	07D	C4-C3-C5-C6
7	J	1001	07D	C14-C13-C15-C16
7	d	1002	07D	C4-C3-C5-C6
13	L	1003	U10	C40-C39-C41-C42
13	M	403	U10	C35-C34-C36-C37
7	1	1001	07D	C2-C3-C5-C6
12	L	1002	RQ0	C12-C08-C17-C24
13	L	1006	U10	C5-C4-O4-C4M
7	H	301	07D	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
7	L	1004	07D	C4-C3-C5-C6
7	W	1001	07D	C4-C3-C5-C6
12	L	1002	RQ0	C34-C30-C31-C48
7	Z	1001	07D	C8-C10-C11-C12
13	L	1006	U10	C23-C24-C26-C27
7	A	101	07D	CAA-CBA-CGA-O2A
7	A	101	07D	C4C-C3C-CAC-CBC
7	H	301	07D	C4C-C3C-CAC-CBC
7	L	1005	07D	C4C-C3C-CAC-CBC
7	6	1001	07D	C14-C13-C15-C16
7	Z	1001	07D	C14-C13-C15-C16
10	H	304	CD4	C29-O8-P1-O5
11	M	402	BPH	C6-C7-C8-C9
7	E	1001	07D	CAA-CBA-CGA-O2A
7	L	1004	07D	CAD-CBD-CGD-O2D
7	L	1005	07D	CAD-CBD-CGD-O2D
11	L	1001	BPH	CAD-CBD-CGD-O2D
7	7	102	07D	C2-C1-O2A-CGA
7	E	1001	07D	C14-C13-C15-C16
7	L	1004	07D	C11-C10-C8-C7
7	V	1001	07D	C11-C10-C8-C7
7	X	1001	07D	C11-C10-C8-C7
7	d	1002	07D	C2-C3-C5-C6
12	L	1002	RQ0	C34-C30-C31-C32
13	M	403	U10	C48-C49-C51-C52
7	6	1001	07D	CAA-CBA-CGA-O2A
8	M	406	CRT	C5-C6-C7-C9
8	M	406	CRT	C22-C23-C25-C26
7	A	101	07D	C2C-C3C-CAC-CBC
13	L	1003	U10	C31-C32-C33-C34
7	3	102	07D	O2A-C1-C2-C3
7	4	1001	07D	O2A-C1-C2-C3
7	7	102	07D	O2A-C1-C2-C3
7	O	102	07D	O2A-C1-C2-C3
7	Q	102	07D	O2A-C1-C2-C3
7	U	1001	07D	O2A-C1-C2-C3
7	n	102	07D	O2A-C1-C2-C3
11	L	1001	BPH	O2A-C1-C2-C3
11	M	402	BPH	O2A-C1-C2-C3
7	2	1001	07D	CHA-CBD-CGD-O2D
7	5	102	07D	CHA-CBD-CGD-O1D
7	6	1001	07D	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
7	8	1001	07D	CHA-CBD-CGD-O2D
7	A	101	07D	CHA-CBD-CGD-O2D
7	F	1001	07D	CHA-CBD-CGD-O2D
7	G	1001	07D	CHA-CBD-CGD-O2D
7	H	301	07D	CHA-CBD-CGD-O1D
7	H	301	07D	CHA-CBD-CGD-O2D
7	M	404	07D	CHA-CBD-CGD-O1D
7	T	101	07D	CHA-CBD-CGD-O2D
7	V	1001	07D	CHA-CBD-CGD-O2D
7	X	1001	07D	CHA-CBD-CGD-O2D
7	Z	1001	07D	CHA-CBD-CGD-O1D
9	H	302	PGW	OAF-C05-CAD-OAE
10	M	407	CD4	C18-C19-C20-C21
9	H	302	PGW	O03-C19-C20-C21
13	L	1003	U10	C46-C47-C48-C49
13	M	403	U10	C41-C42-C43-C44
7	Q	102	07D	C2A-CAA-CBA-CGA
7	U	1001	07D	C2A-CAA-CBA-CGA
7	E	1001	07D	CAA-CBA-CGA-O1A
7	F	1001	07D	CAA-CBA-CGA-O2A
9	H	303	PGW	C11-C12-C13-C14
7	H	301	07D	CAA-CBA-CGA-O1A
8	9	101	CRT	C15-C16-C17-C19
7	T	101	07D	CAA-CBA-CGA-O1A
7	6	1001	07D	CAA-CBA-CGA-O1A
7	A	101	07D	CAA-CBA-CGA-O1A
7	X	1001	07D	C4-C3-C5-C6
7	X	1001	07D	CAA-CBA-CGA-O1A
7	F	1001	07D	CAA-CBA-CGA-O1A
7	I	102	07D	C11-C10-C8-C9
7	5	102	07D	CAD-CBD-CGD-O1D
7	6	1001	07D	CAD-CBD-CGD-O1D
7	n	102	07D	CAD-CBD-CGD-O1D
7	X	1001	07D	CAA-CBA-CGA-O2A
8	M	406	CRT	C1-C4-C5-C6
7	Y	102	07D	C2A-CAA-CBA-CGA
8	7	101	CRT	C5-C6-C7-C9
8	K	101	CRT	C15-C16-C17-C19
7	V	1001	07D	CAA-CBA-CGA-O1A
7	R	101	07D	CAA-CBA-CGA-O1A
7	D	1001	07D	C13-C15-C16-C17
7	H	301	07D	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
7	H	301	07D	CAA-CBA-CGA-O2A
7	D	1001	07D	CAA-CBA-CGA-O1A

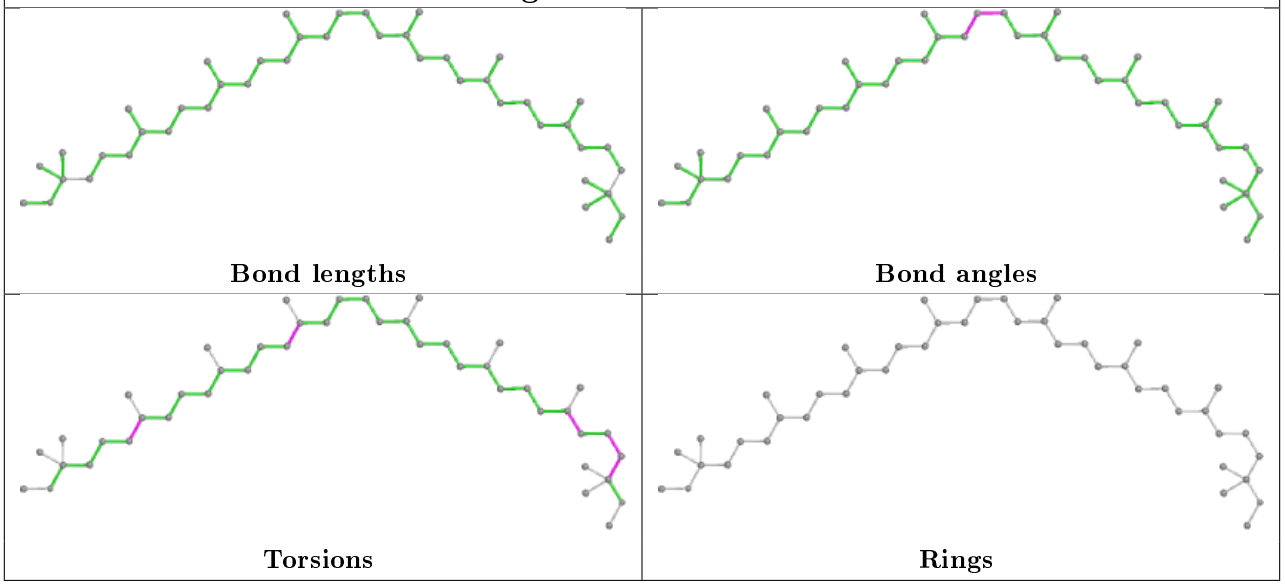
There are no ring outliers.

10 monomers are involved in 15 short contacts:

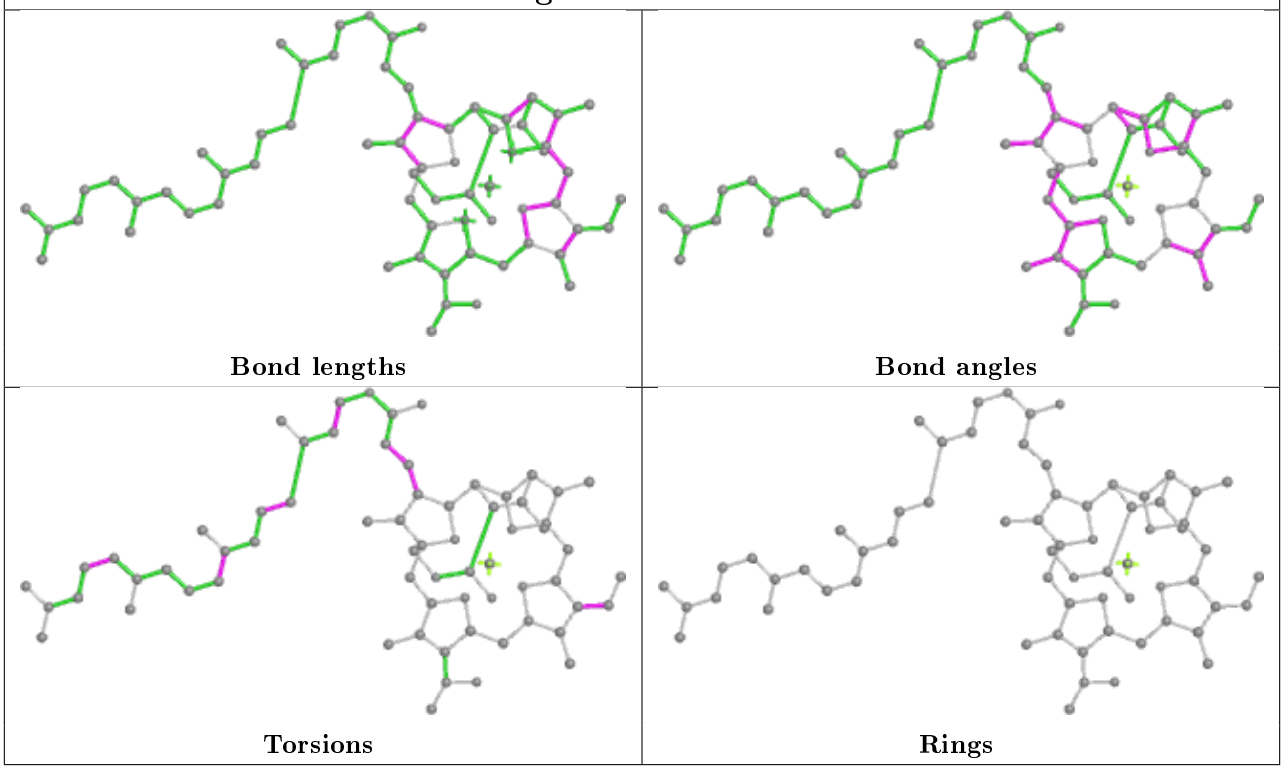
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	M	406	CRT	2	0
8	N	1001	CRT	1	0
13	L	1006	U10	3	0
8	I	101	CRT	1	0
13	M	403	U10	1	0
8	J	1002	CRT	1	0
8	5	101	CRT	3	0
11	L	1001	BPH	1	0
8	Y	101	CRT	1	0
11	M	402	BPH	1	0

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

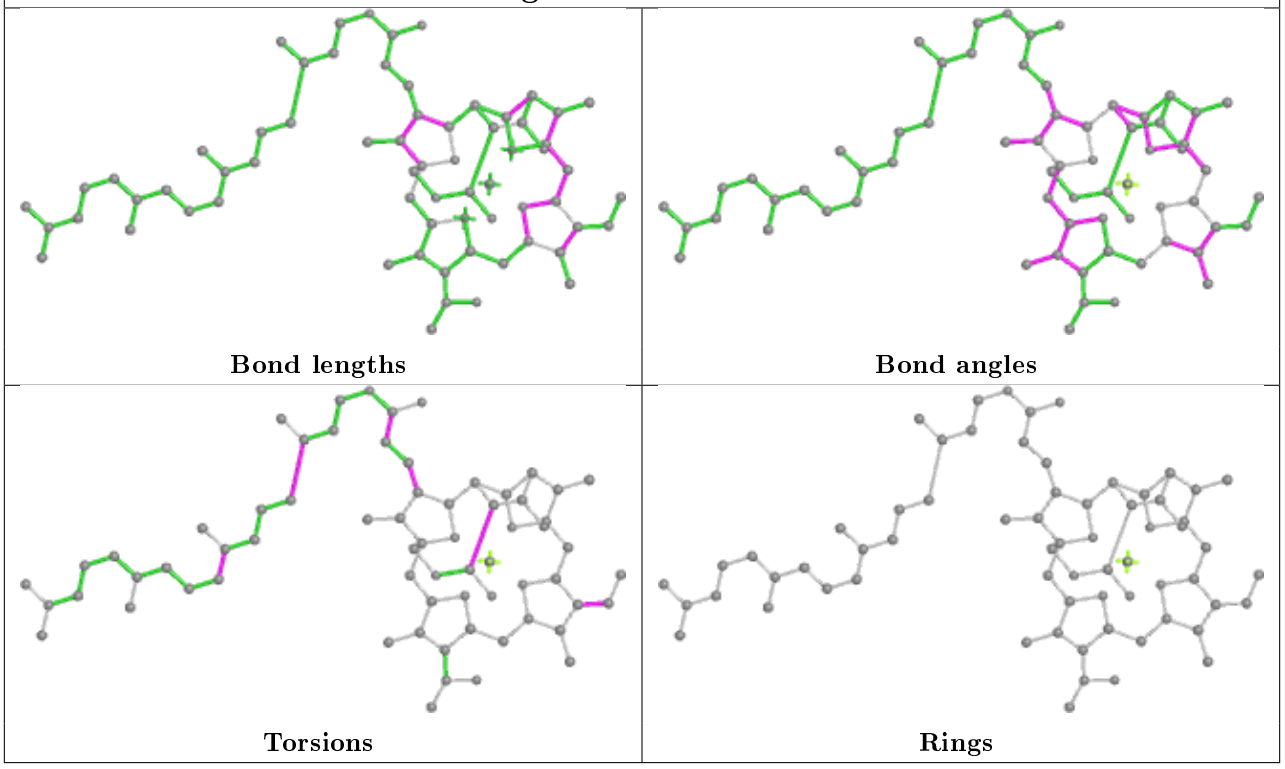
Ligand CRT M 406



Ligand 07D 3 102



Ligand 07D X 1001



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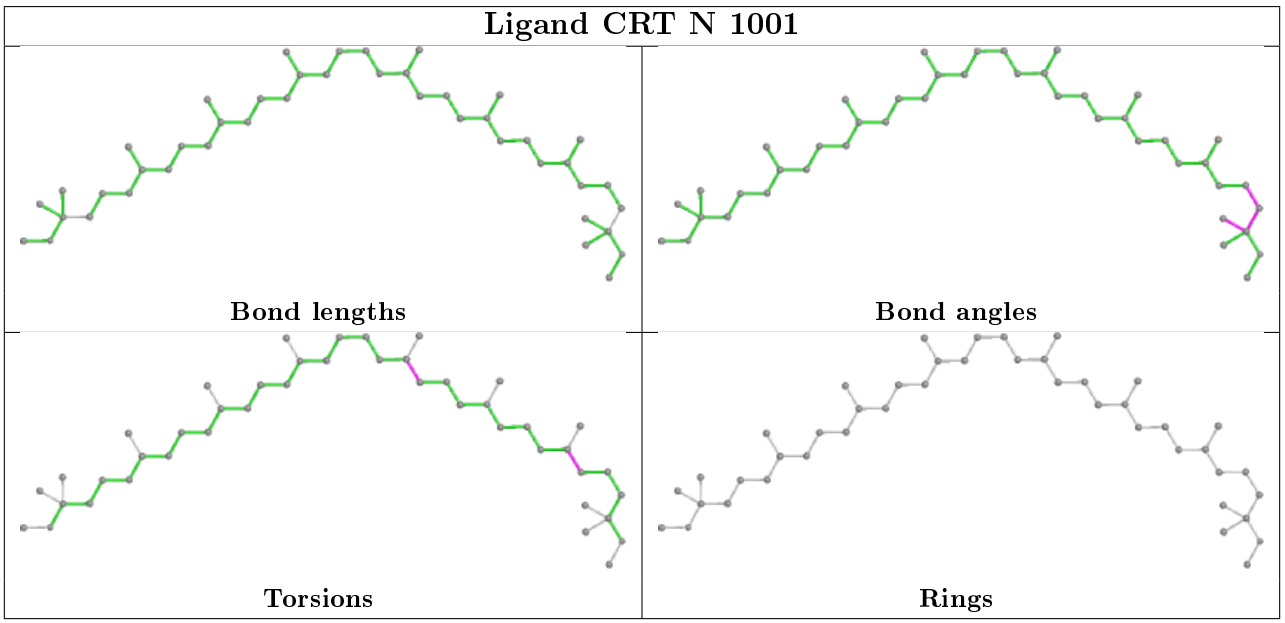

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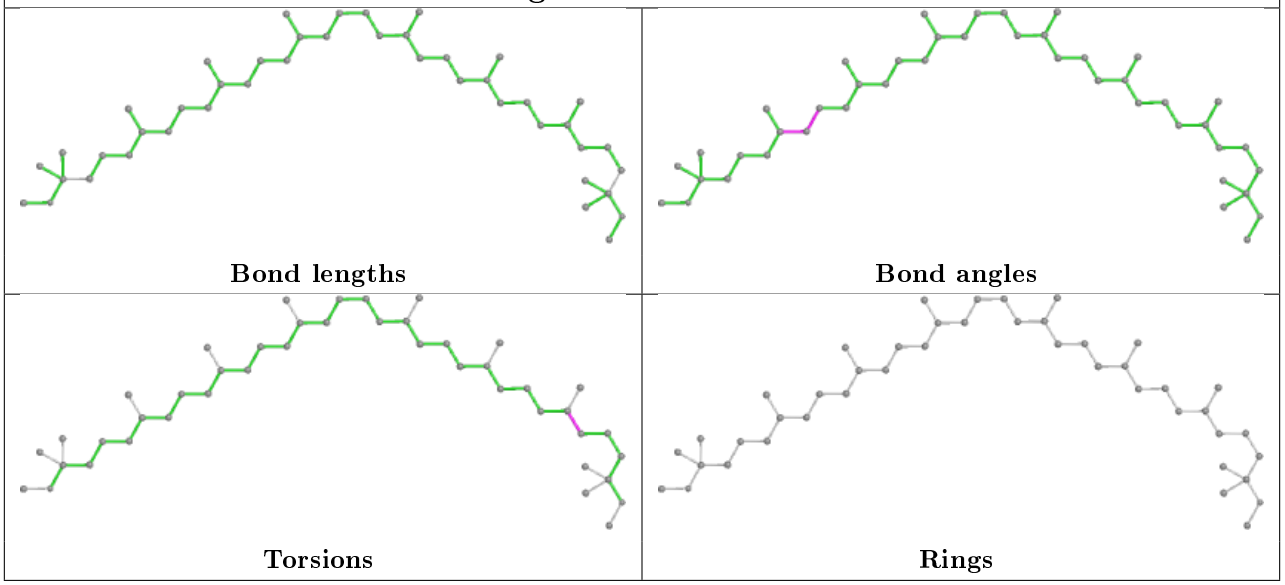
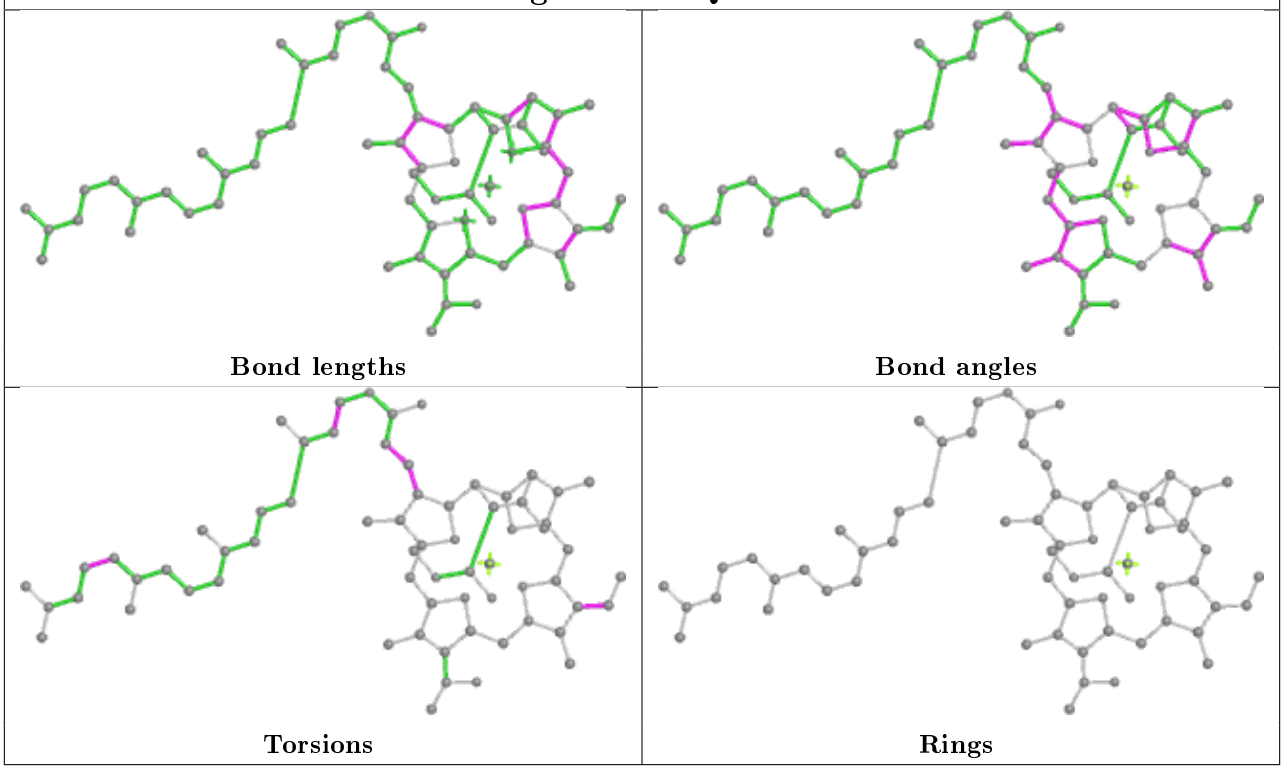


Ligand 07D Q 102



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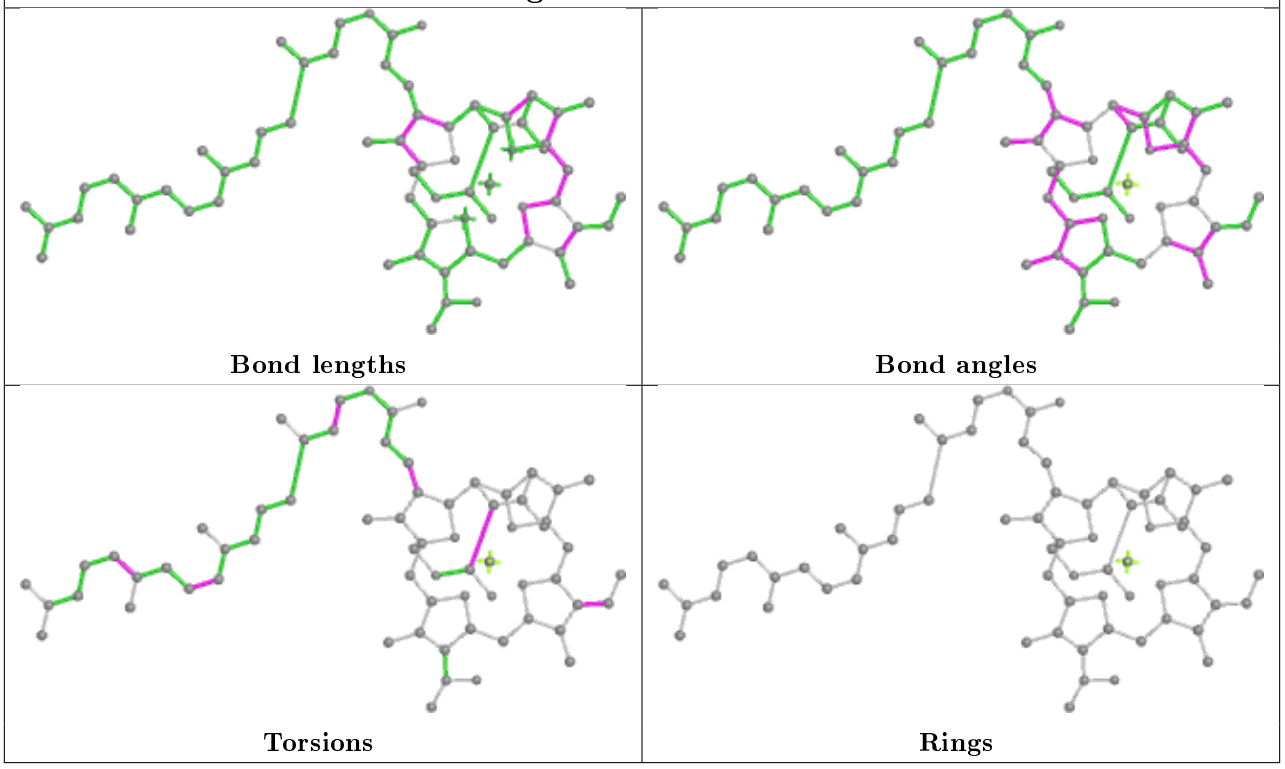

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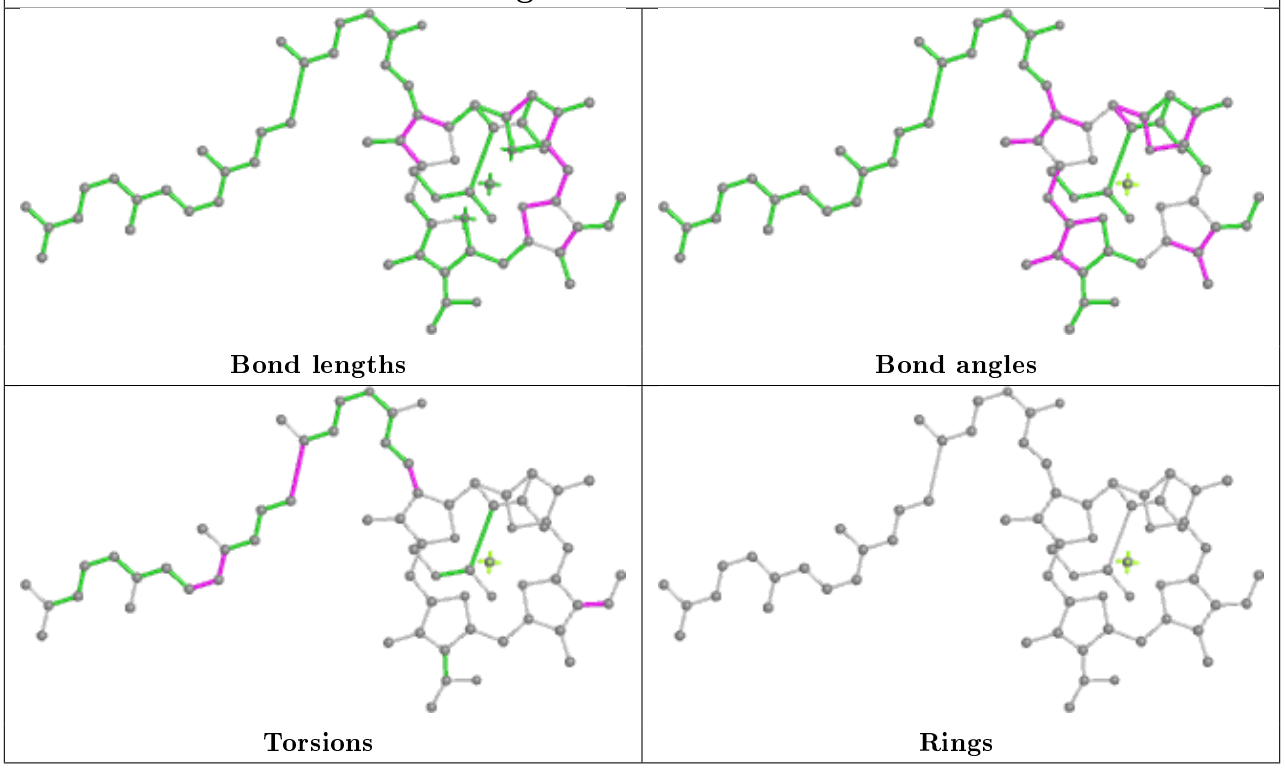

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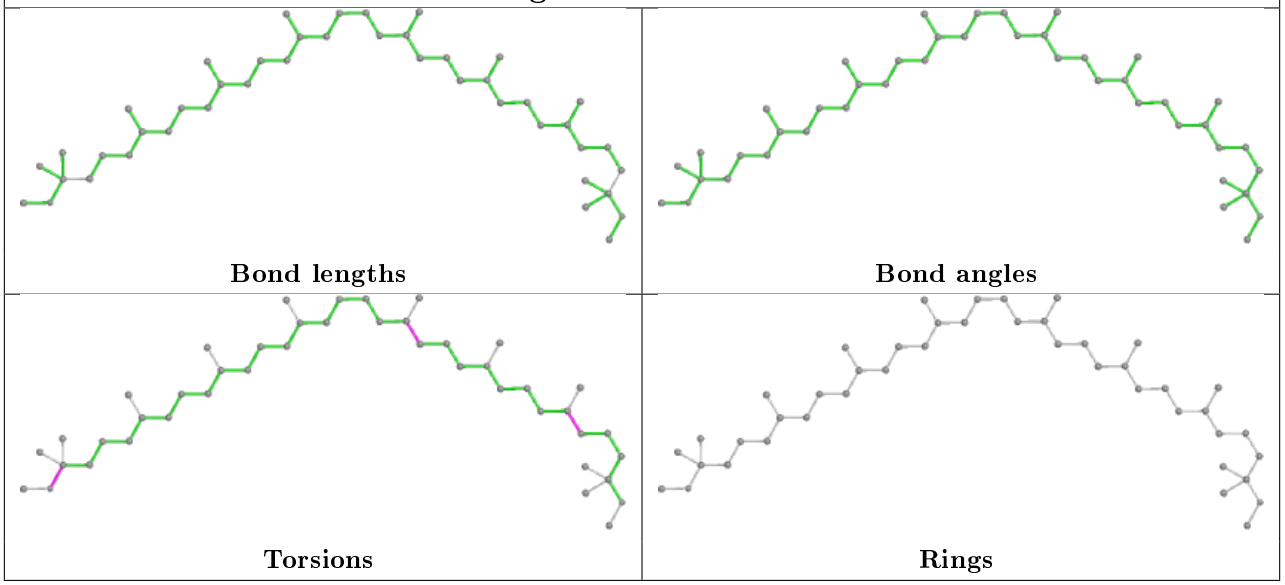
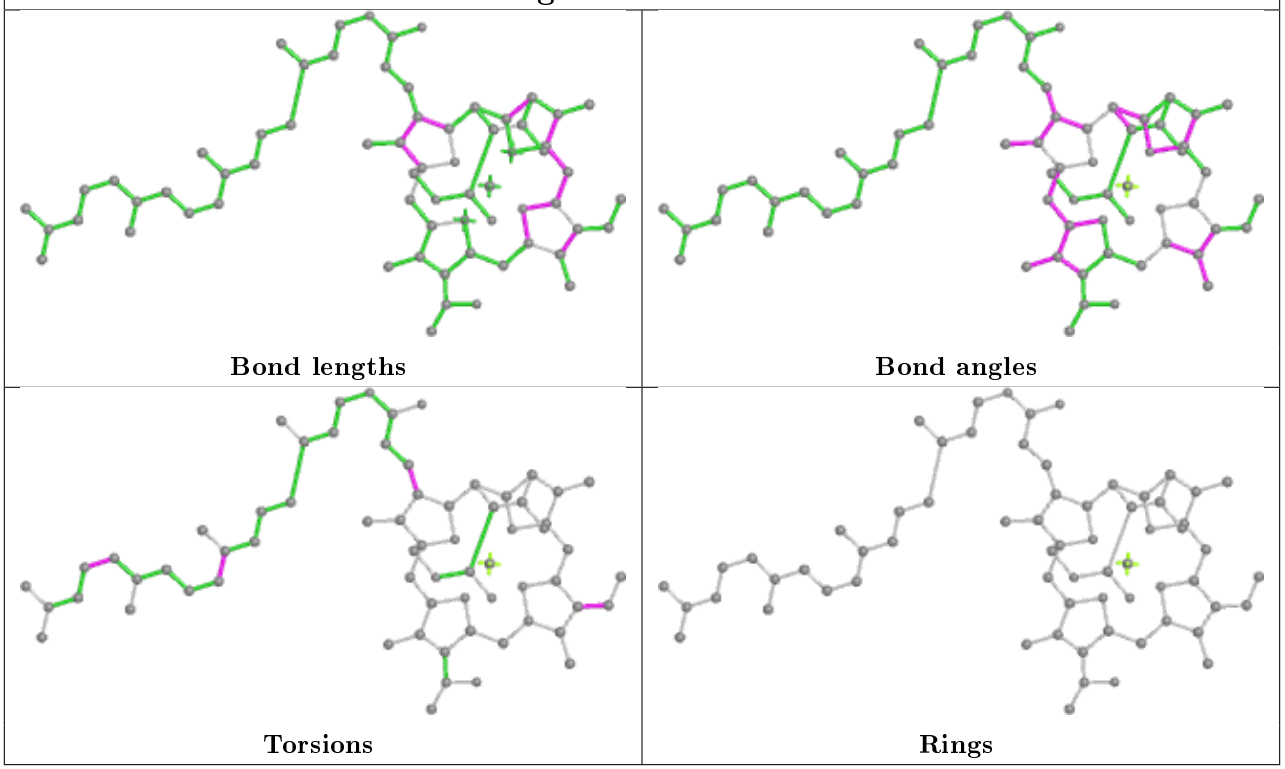


Ligand 07D I 102



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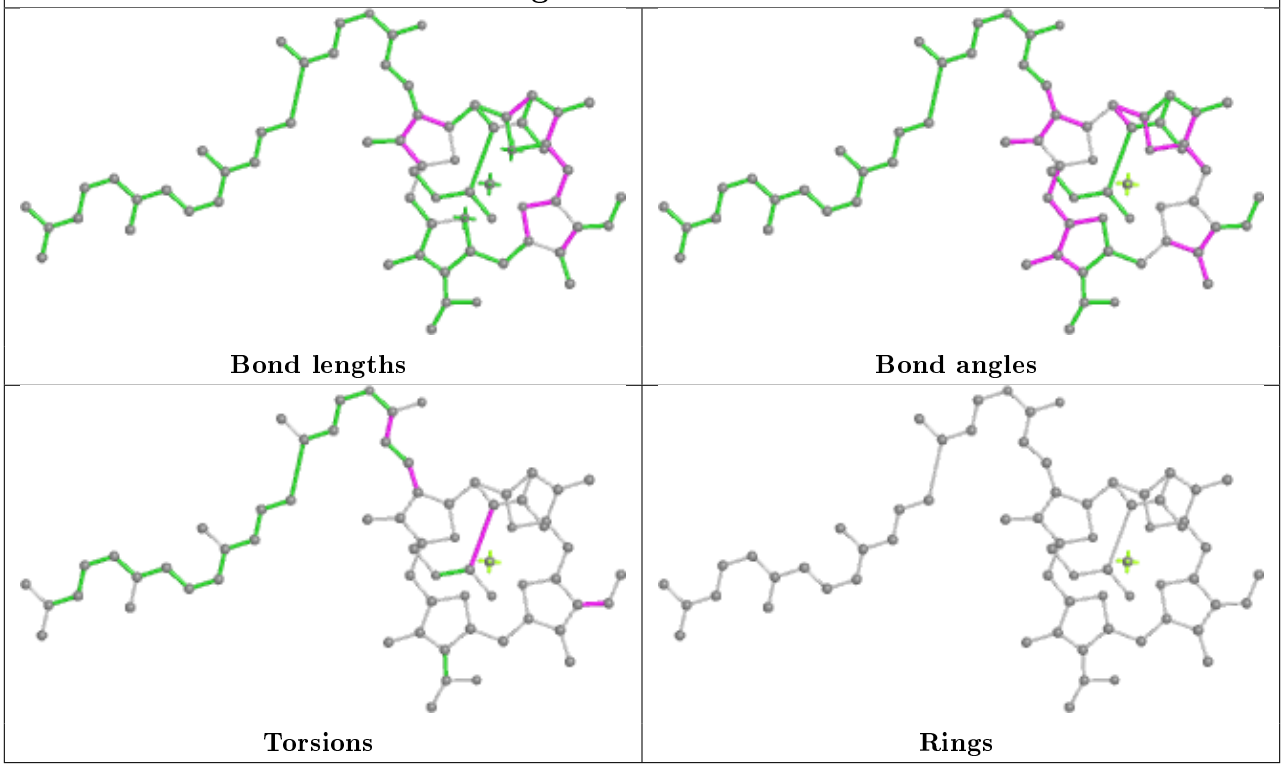

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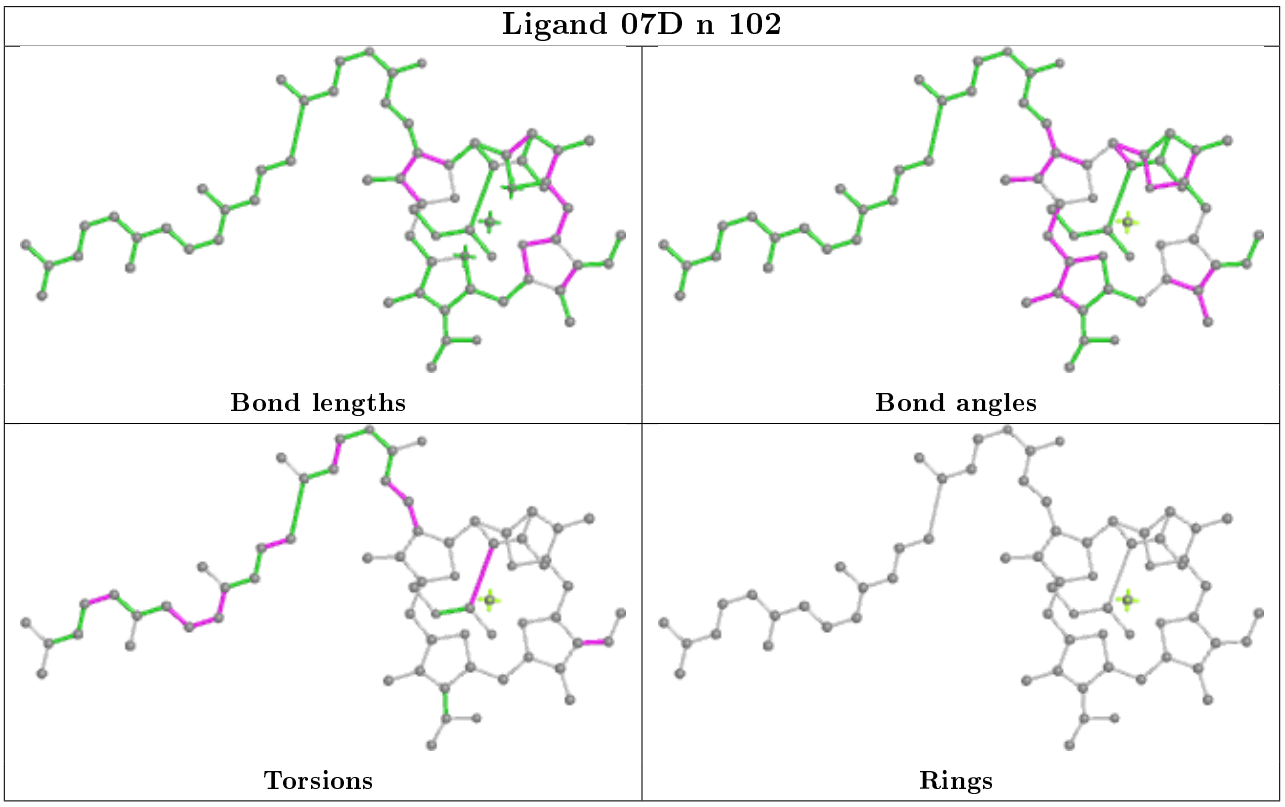
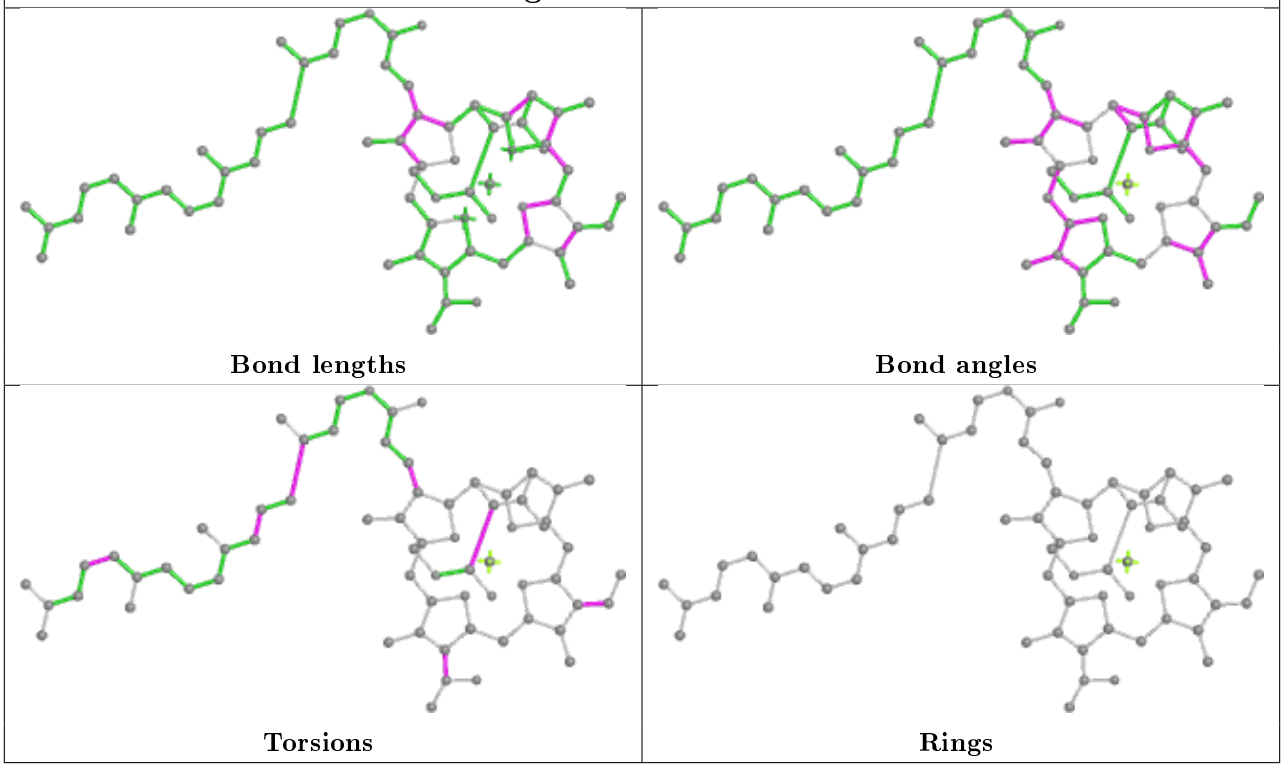
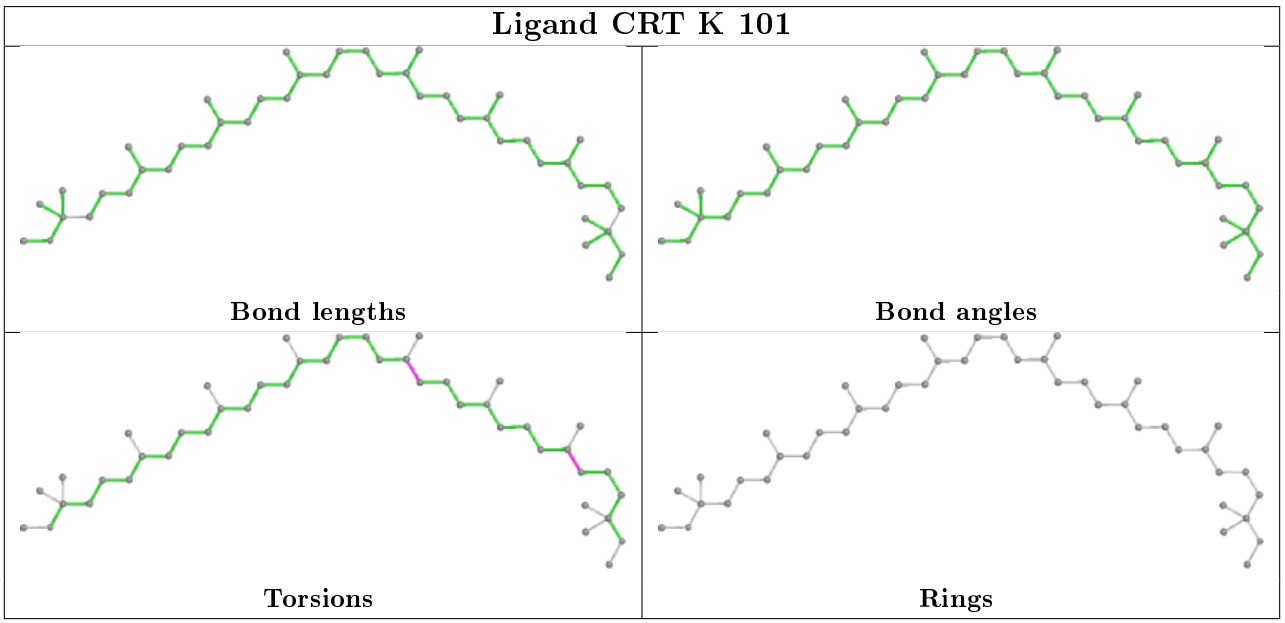


Ligand 07D L 1005



Ligand CRT K 101



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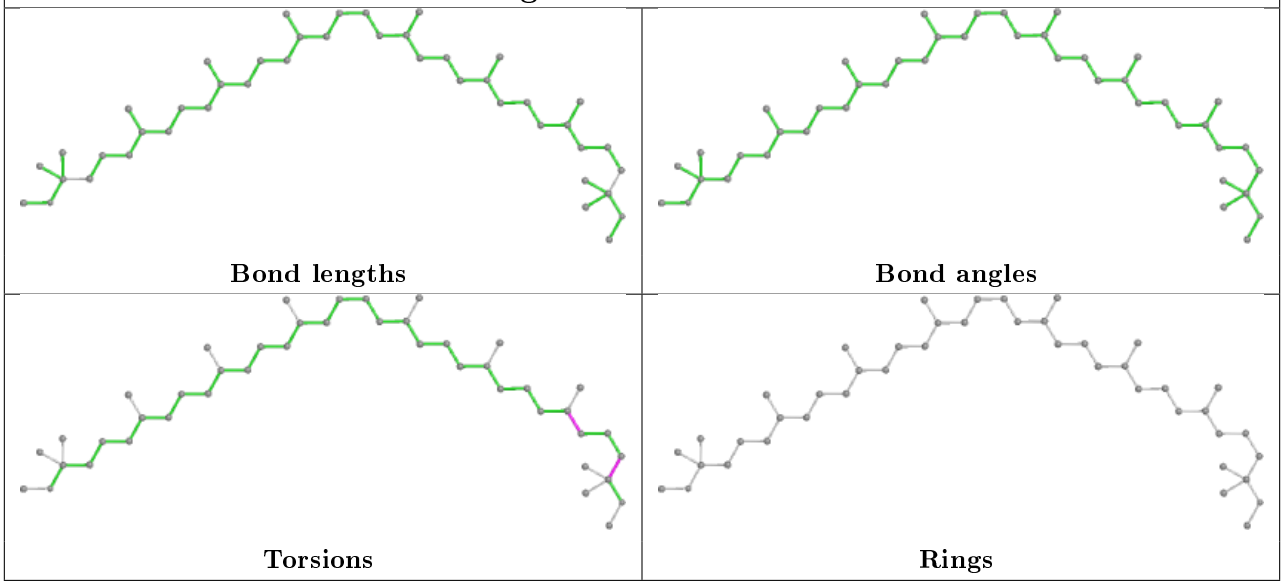
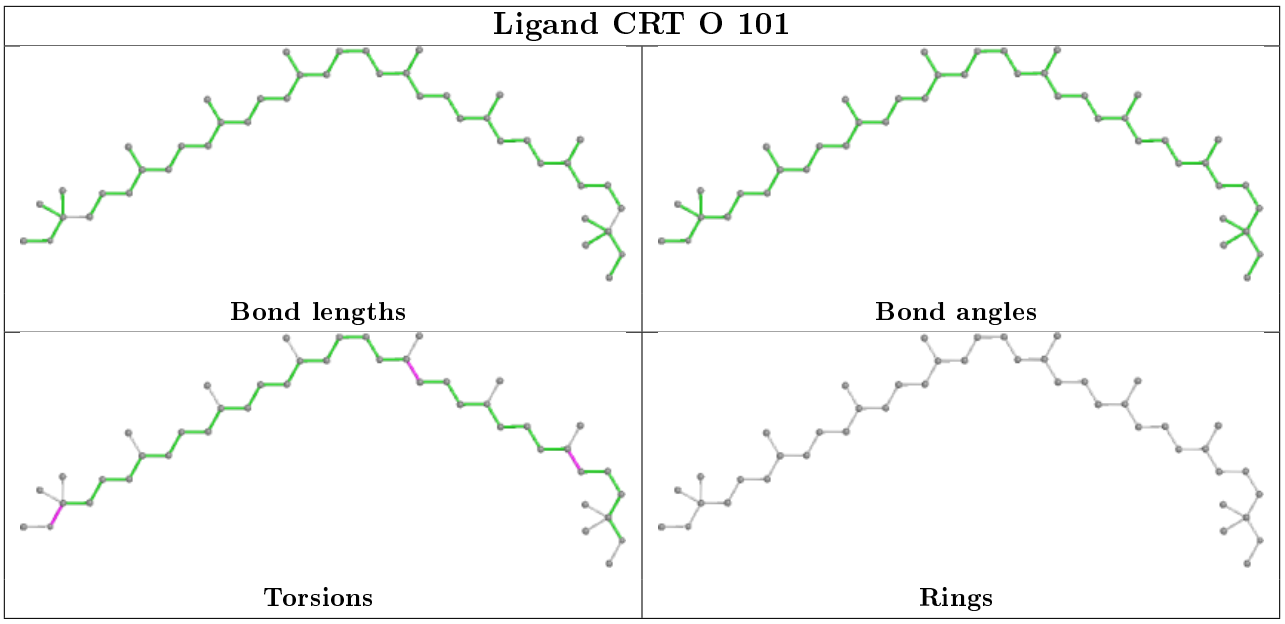
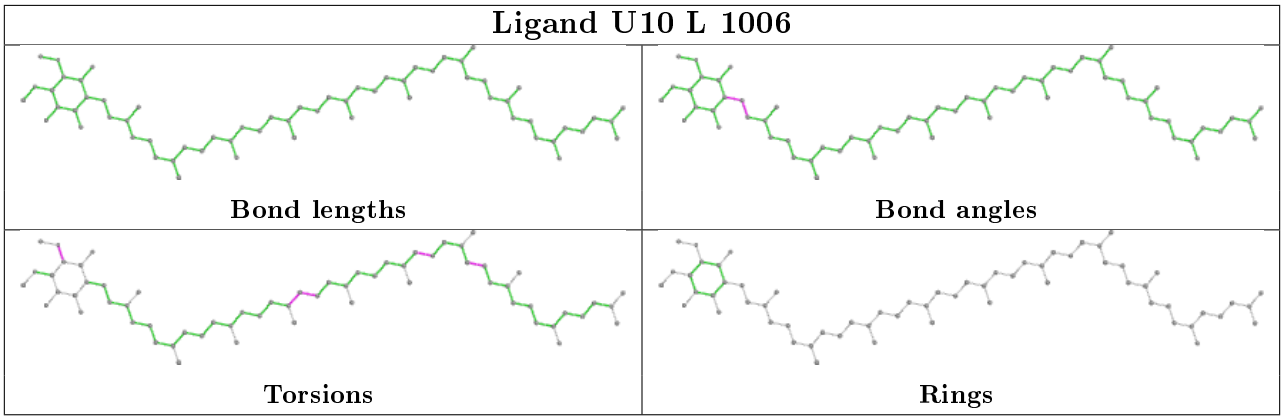


Ligand CRT O 101



Ligand U10 L 1006



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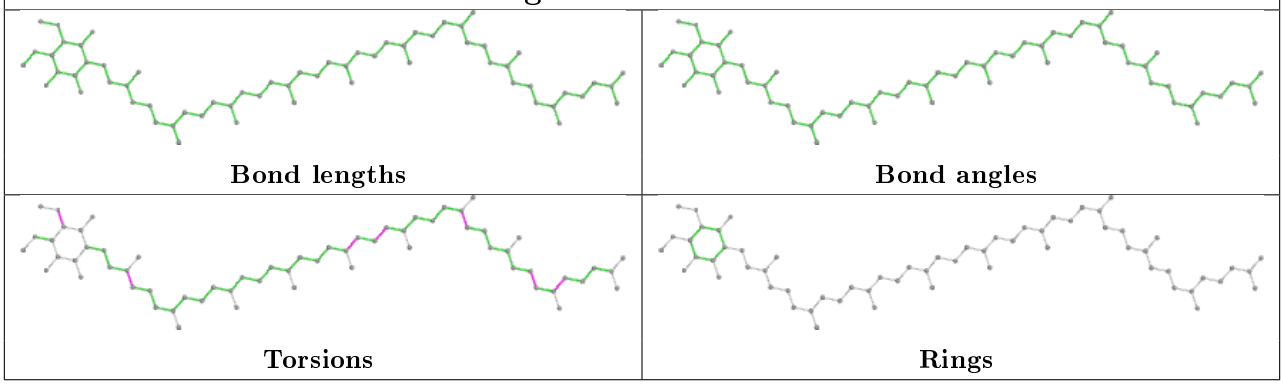
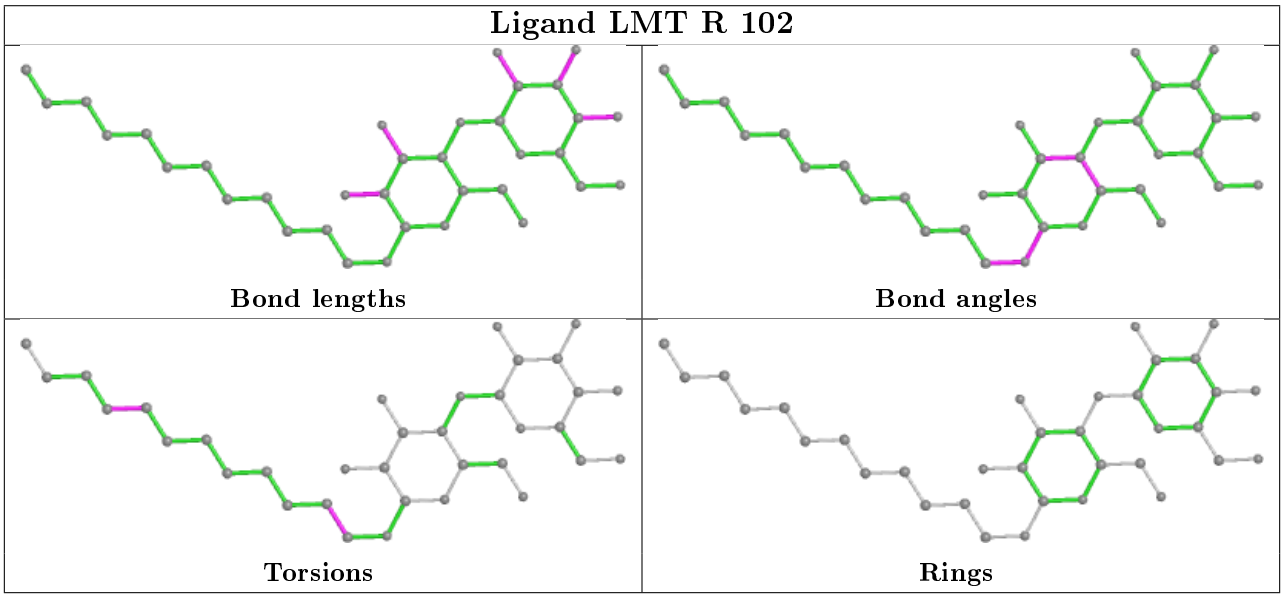
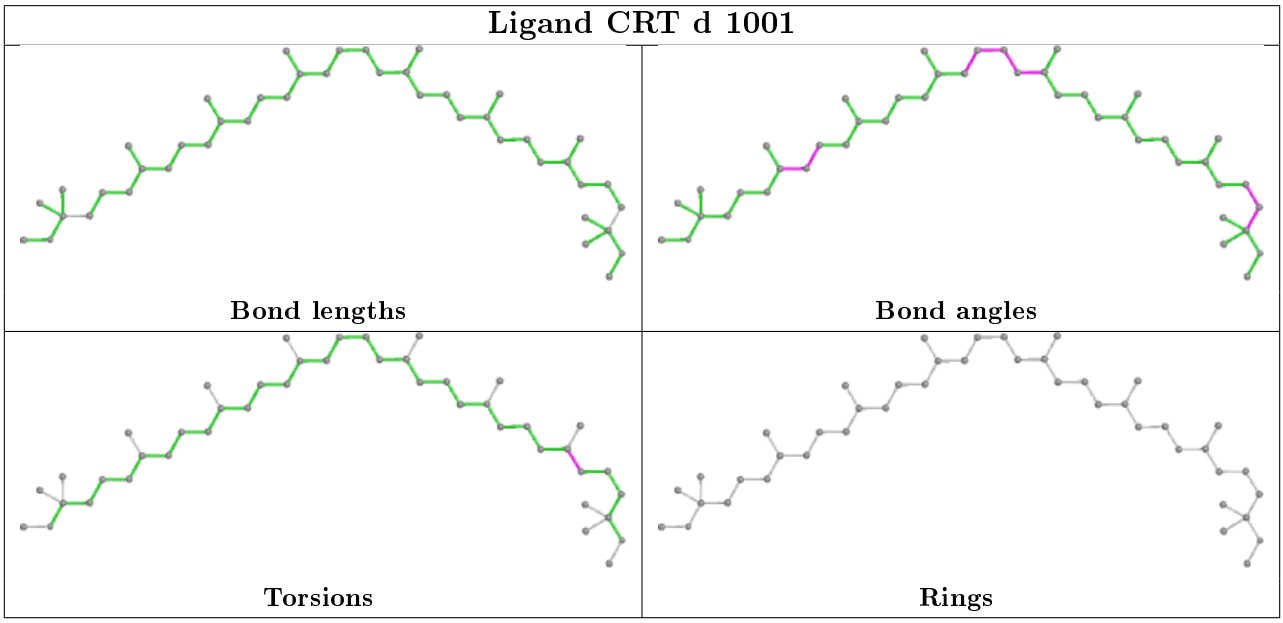


Ligand LMT R 102



Ligand CRT d 1001



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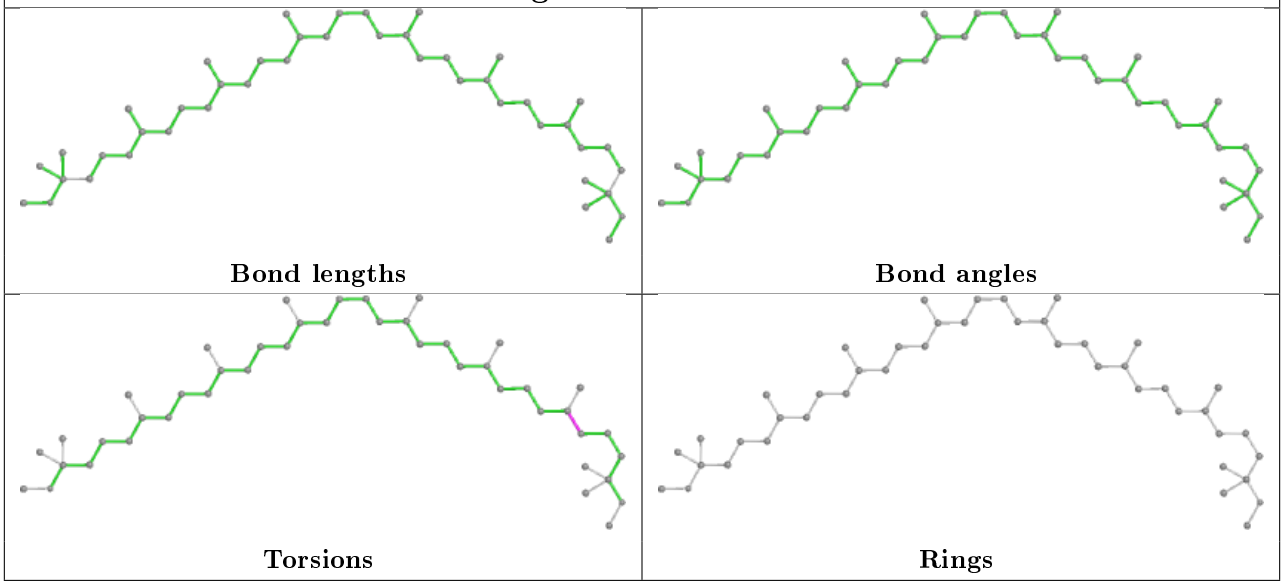

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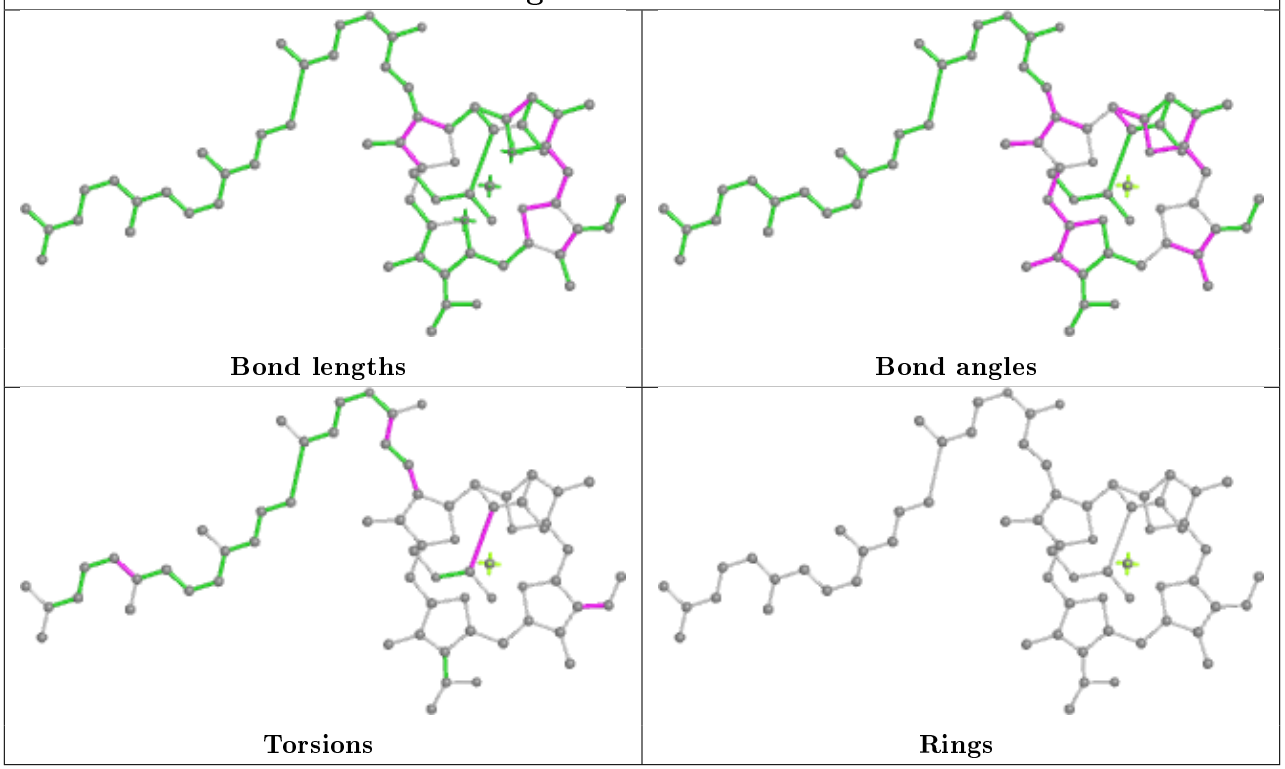
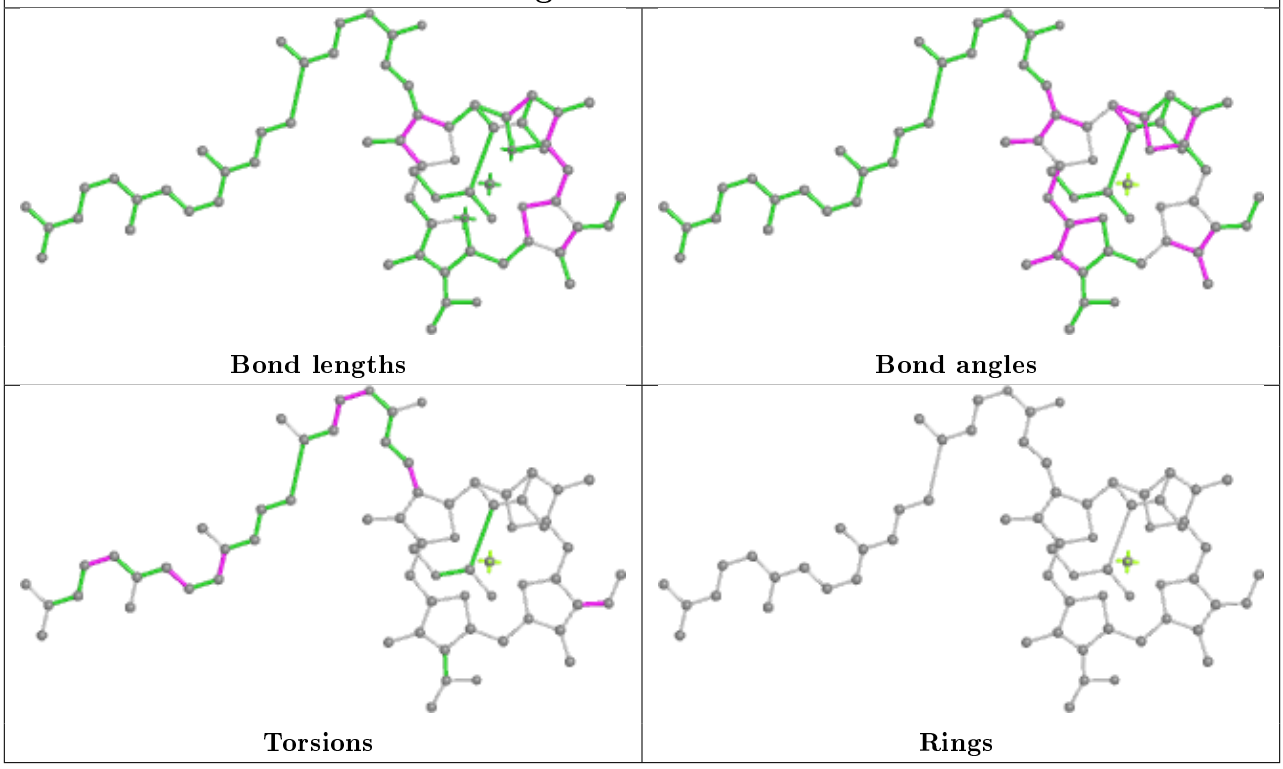
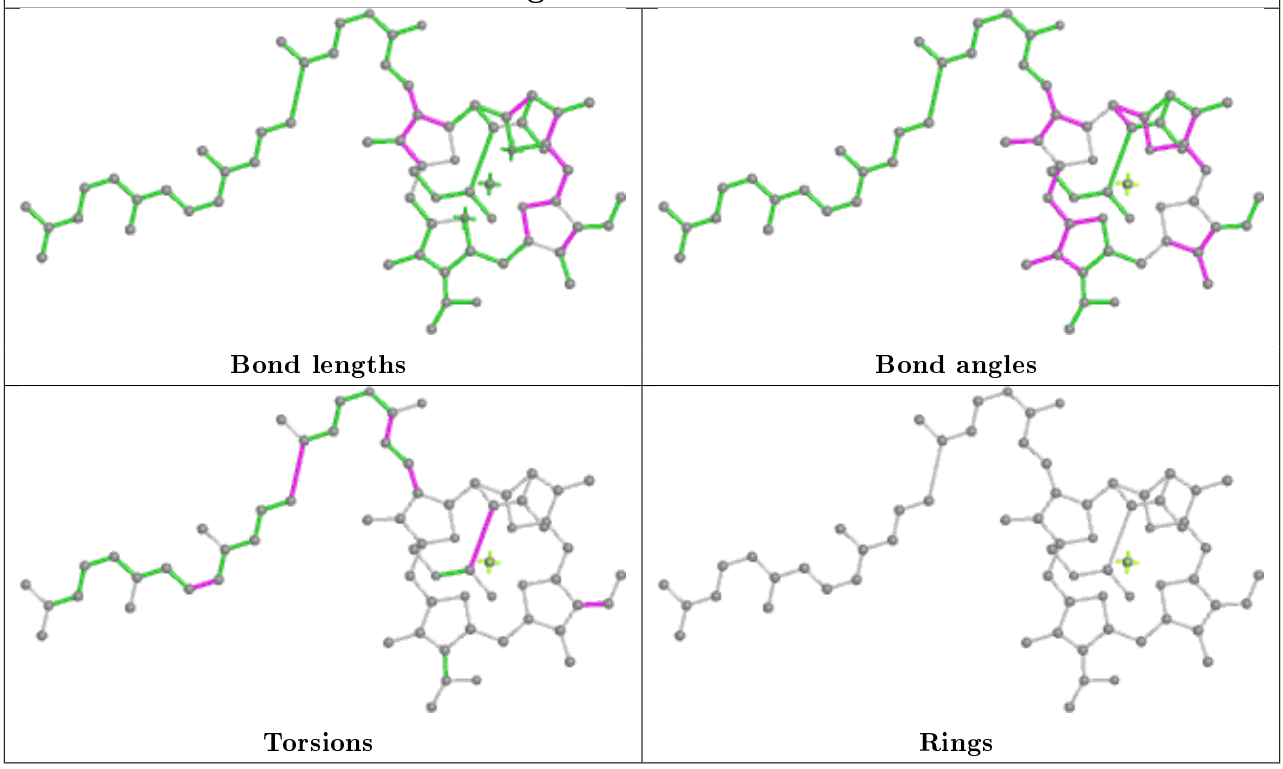


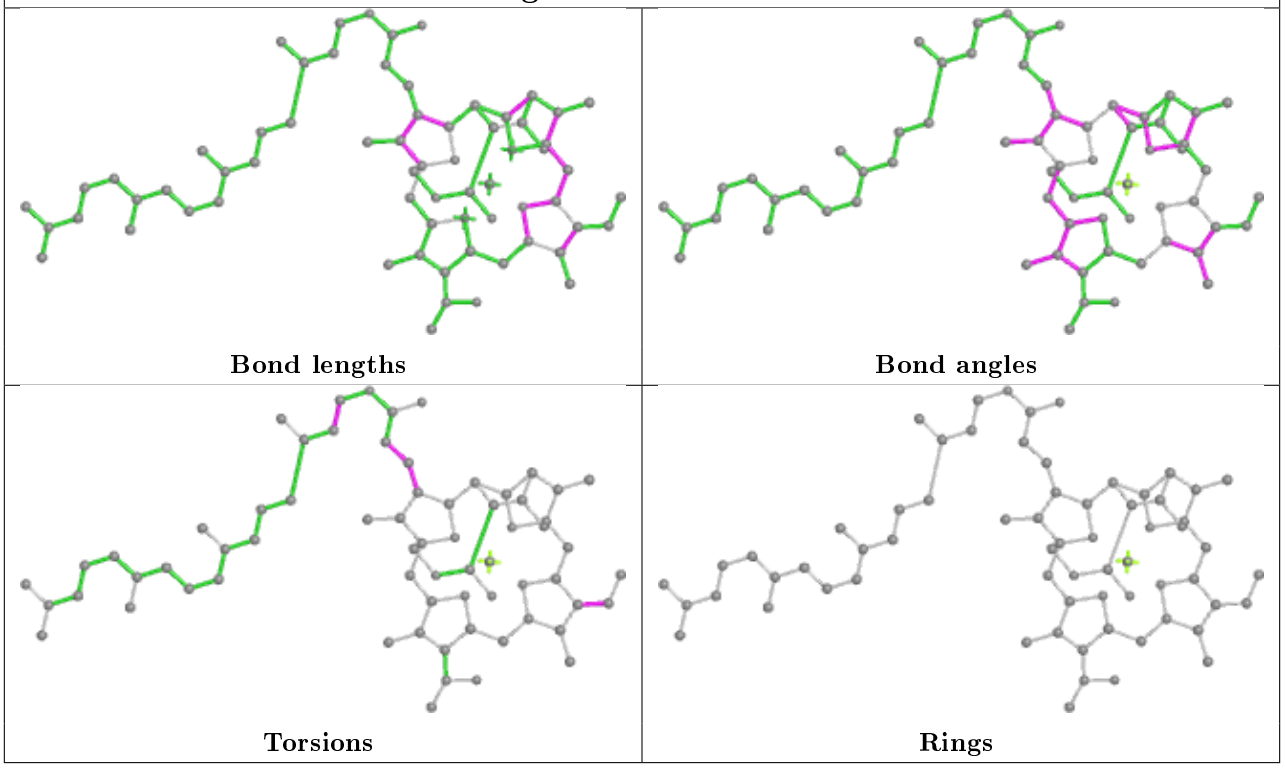
Ligand 07D 7 102



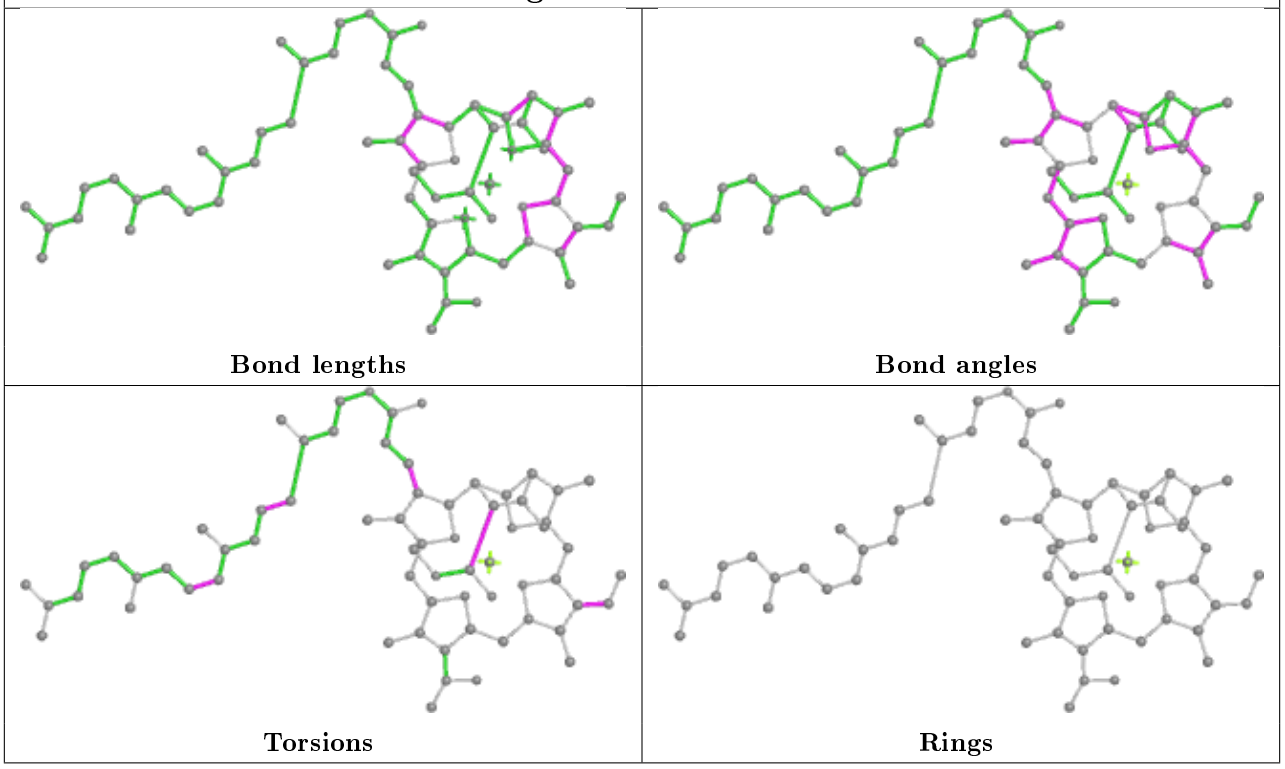
Ligand 07D M 404



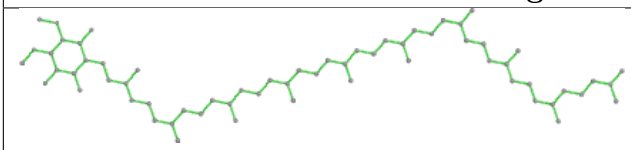
Ligand 07D U 1001



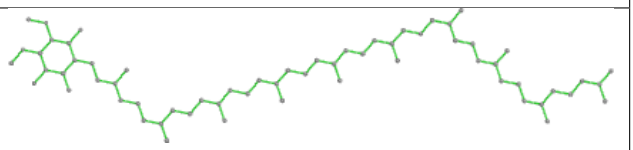
Ligand 07D 2 1001



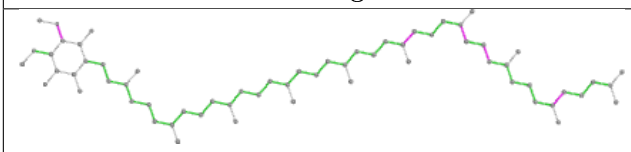
Ligand U10 M 403



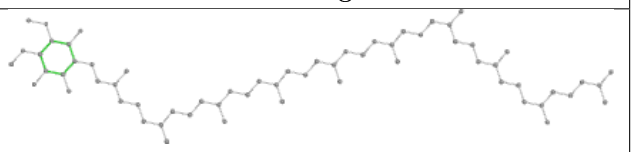
Bond lengths



Bond angles

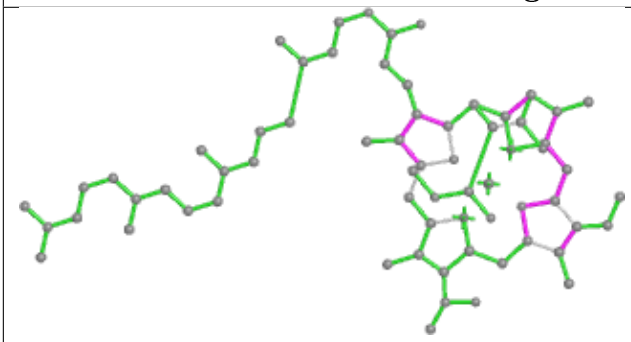


Torsions

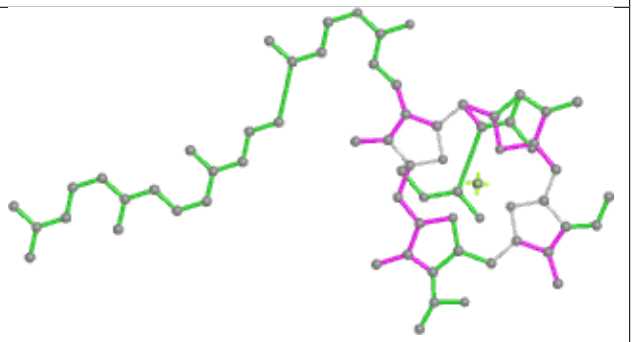


Rings

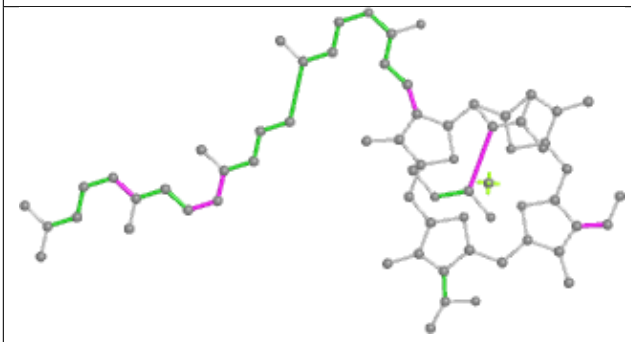
Ligand 07D Z 1001



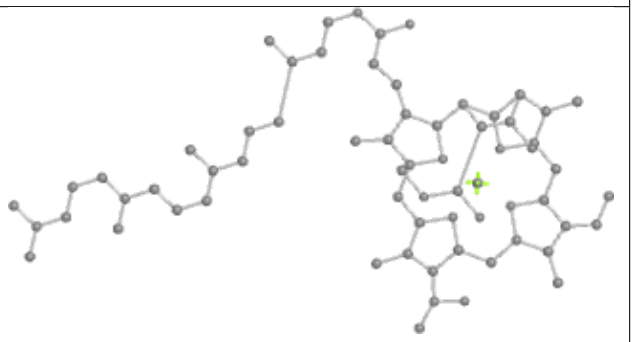
Bond lengths



Bond angles

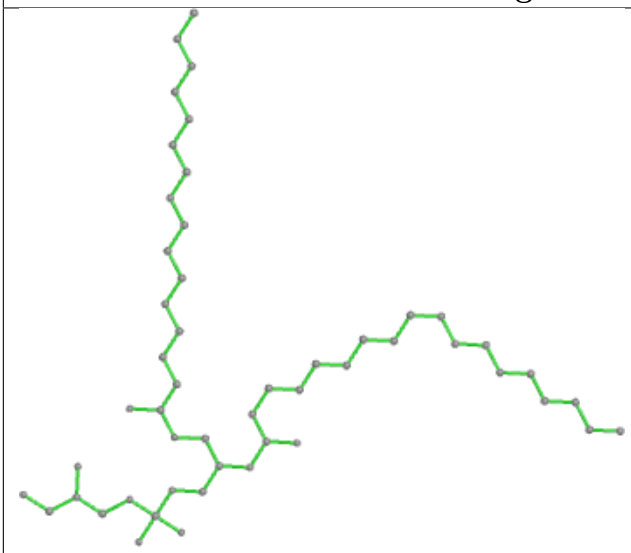


Torsions

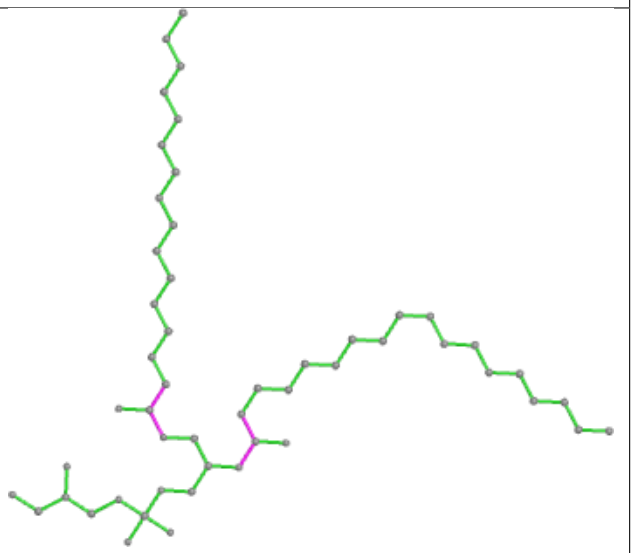


Rings

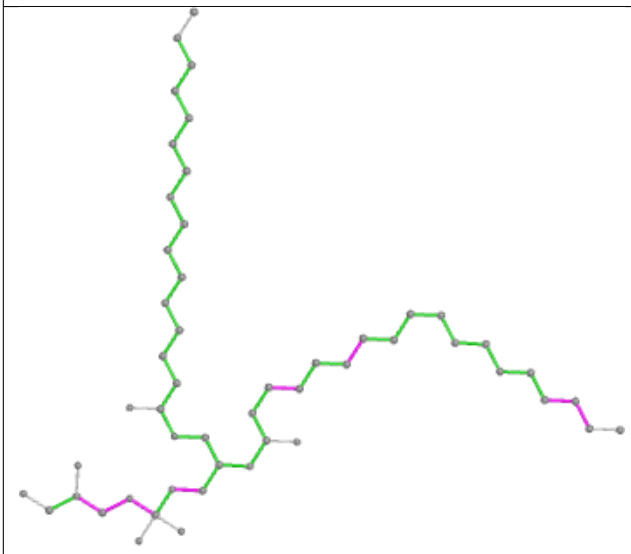
Ligand PGW H 303



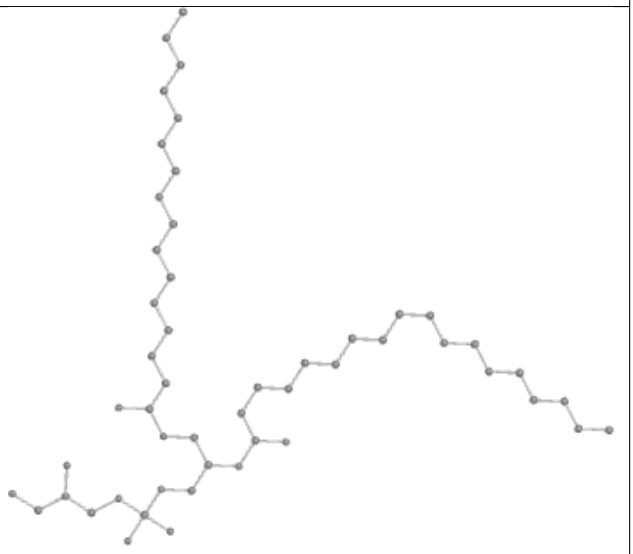
Bond lengths



Bond angles

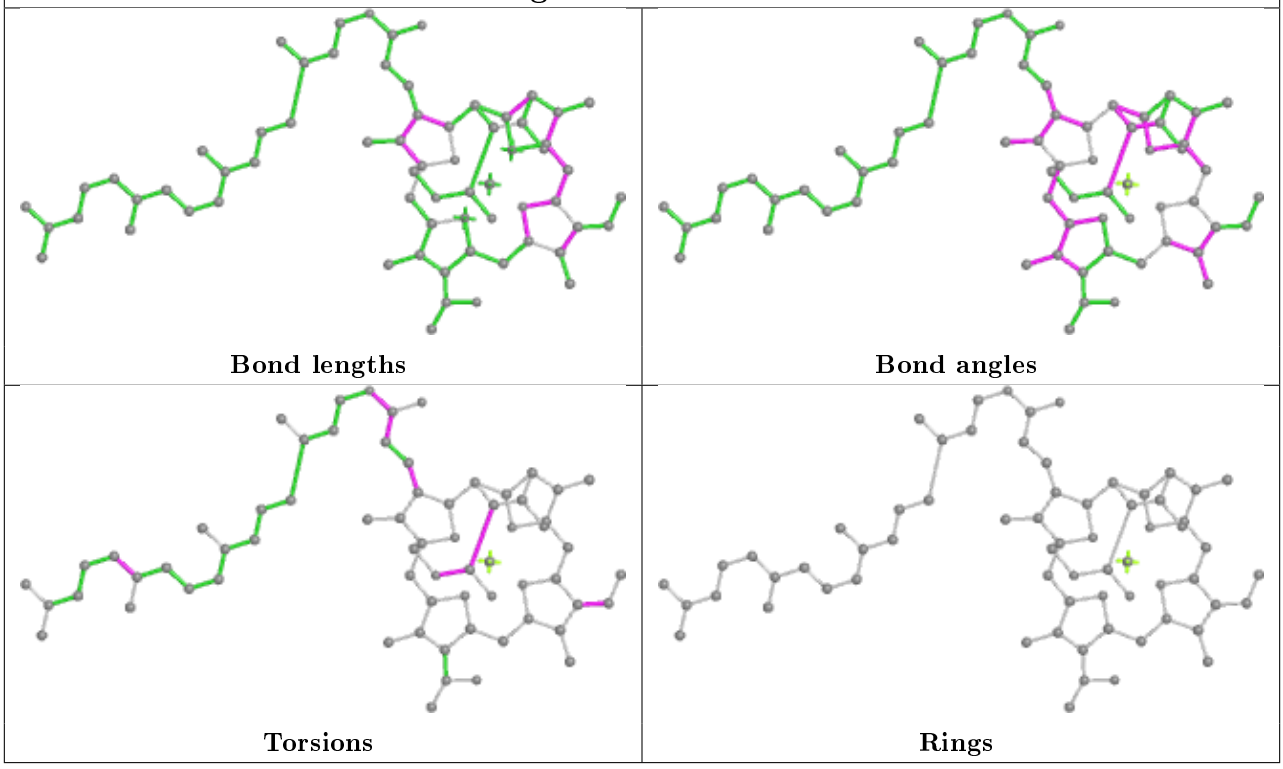


Torsions

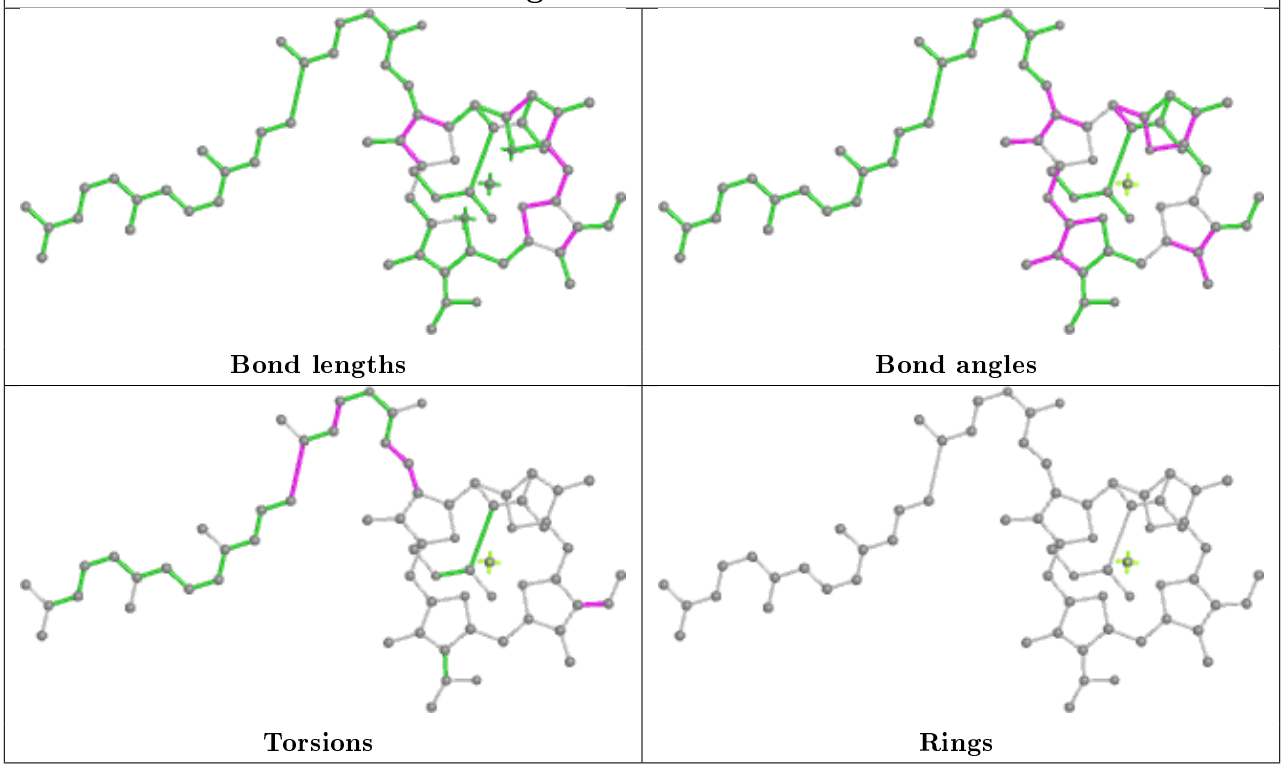


Rings

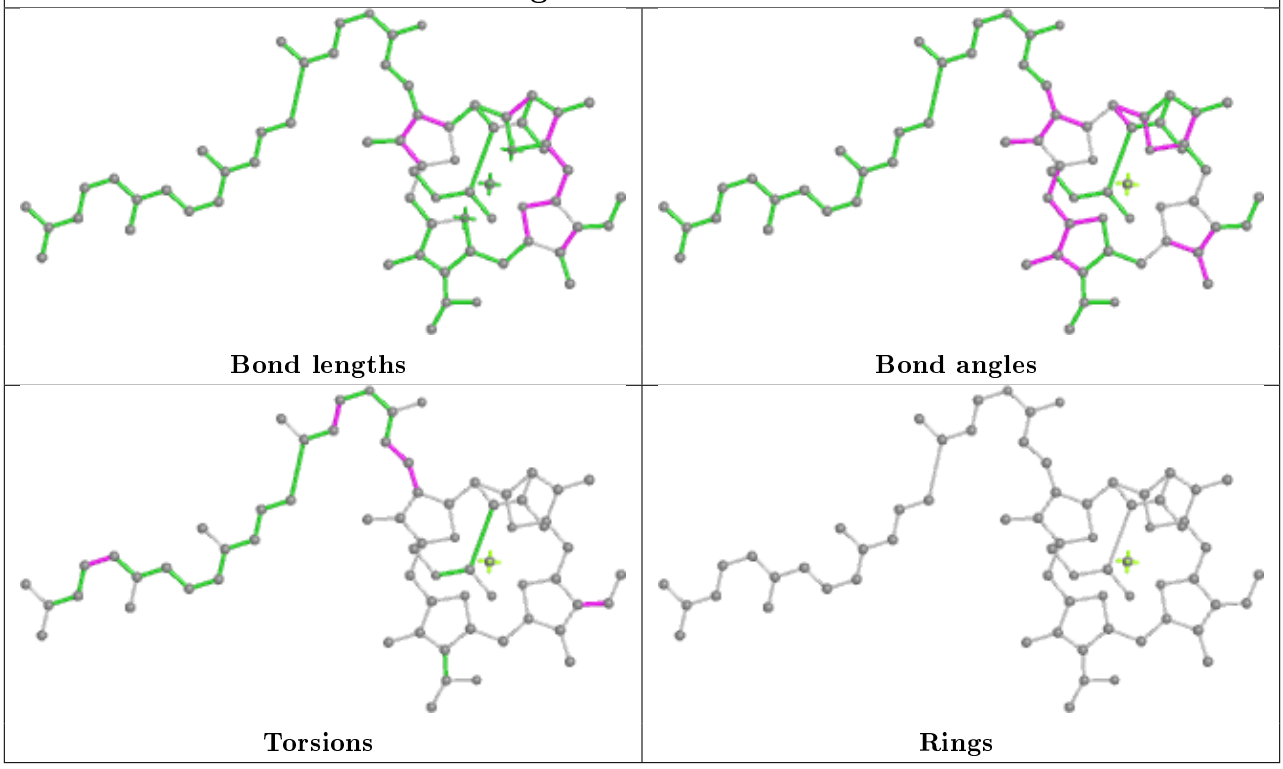
Ligand 07D R 101



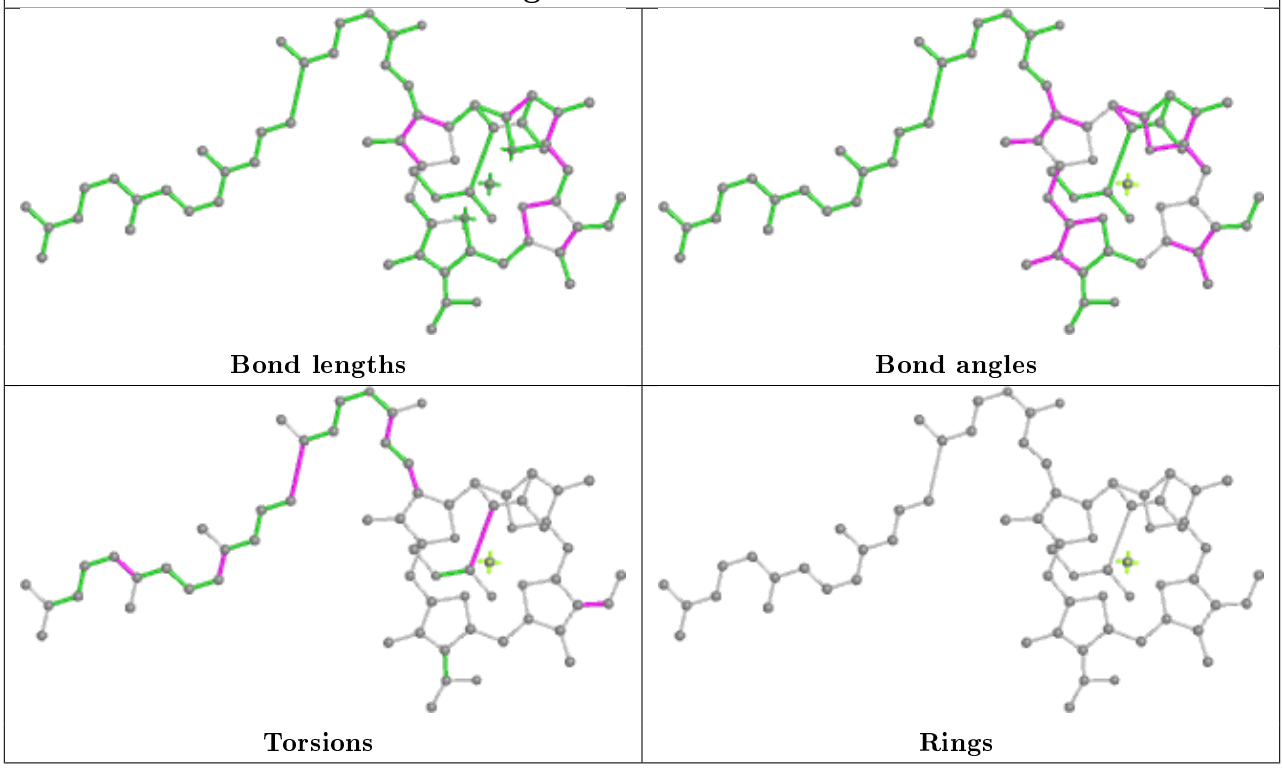
Ligand 07D 1 1001



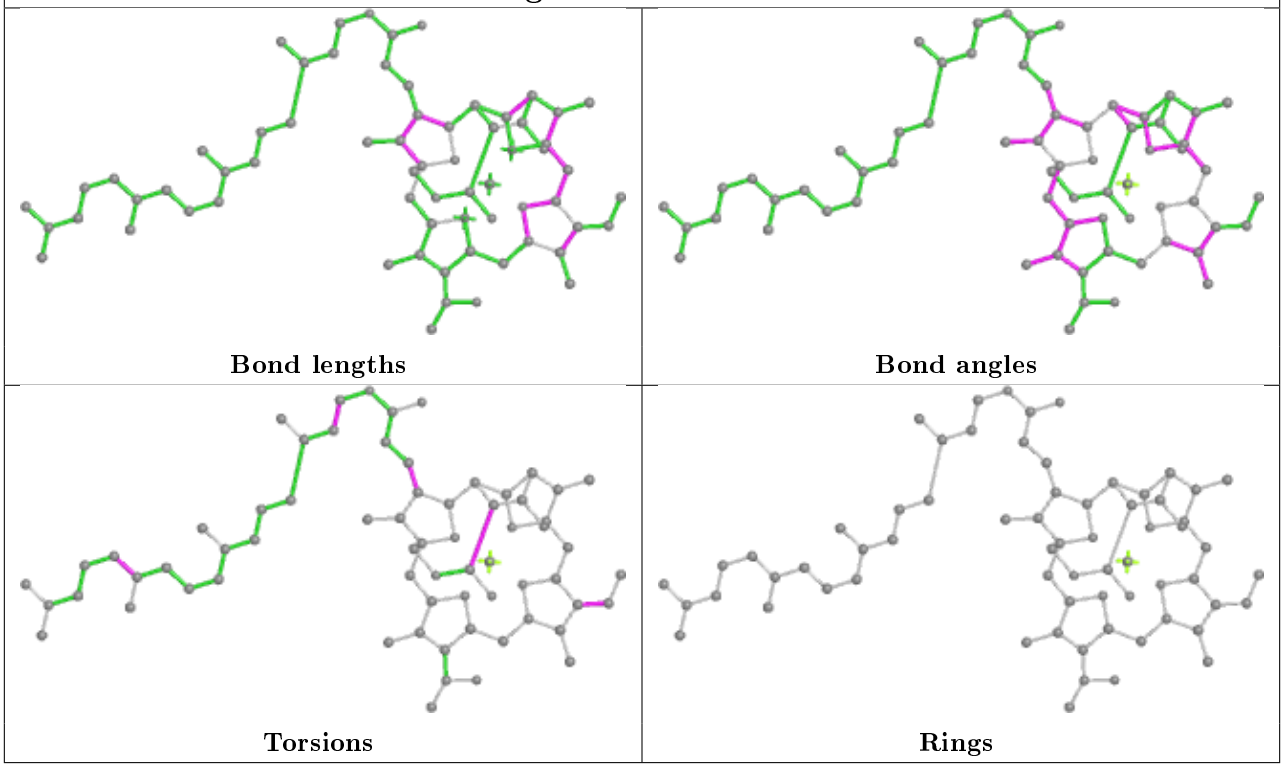
Ligand 07D O 102



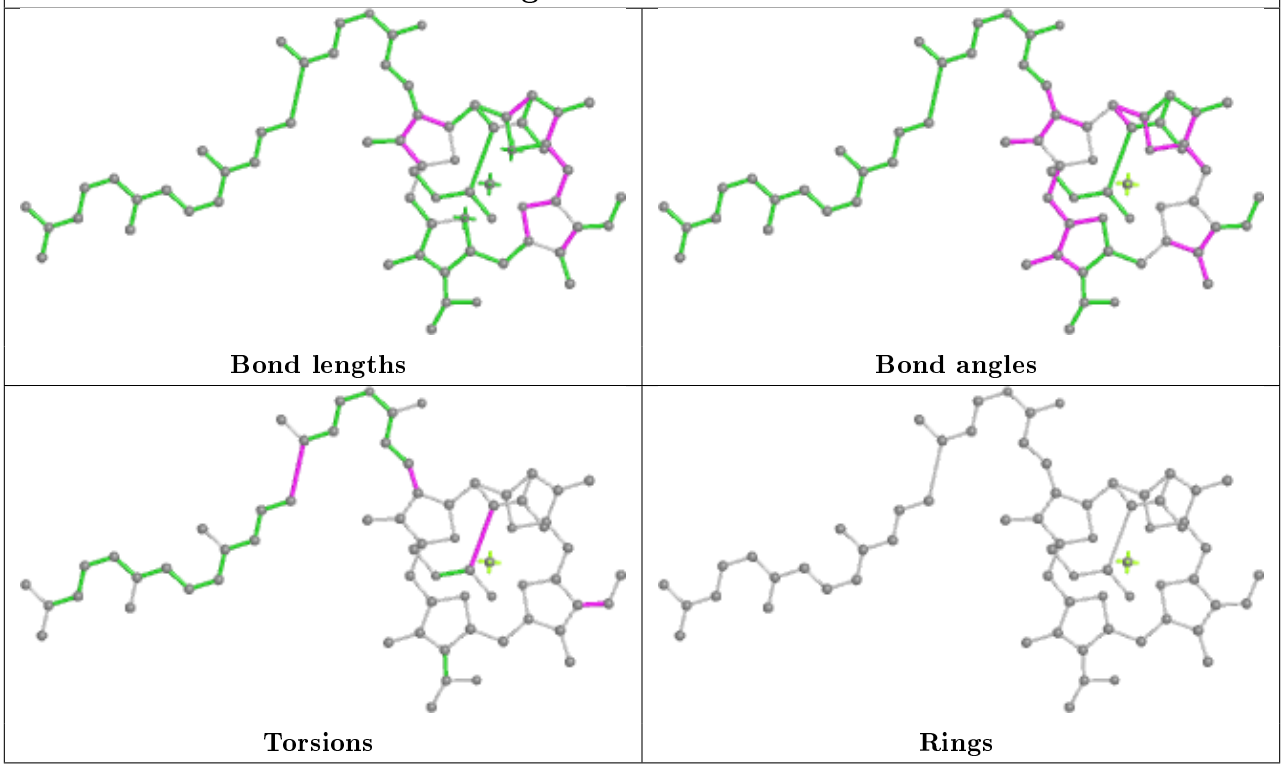
Ligand 07D F 1001



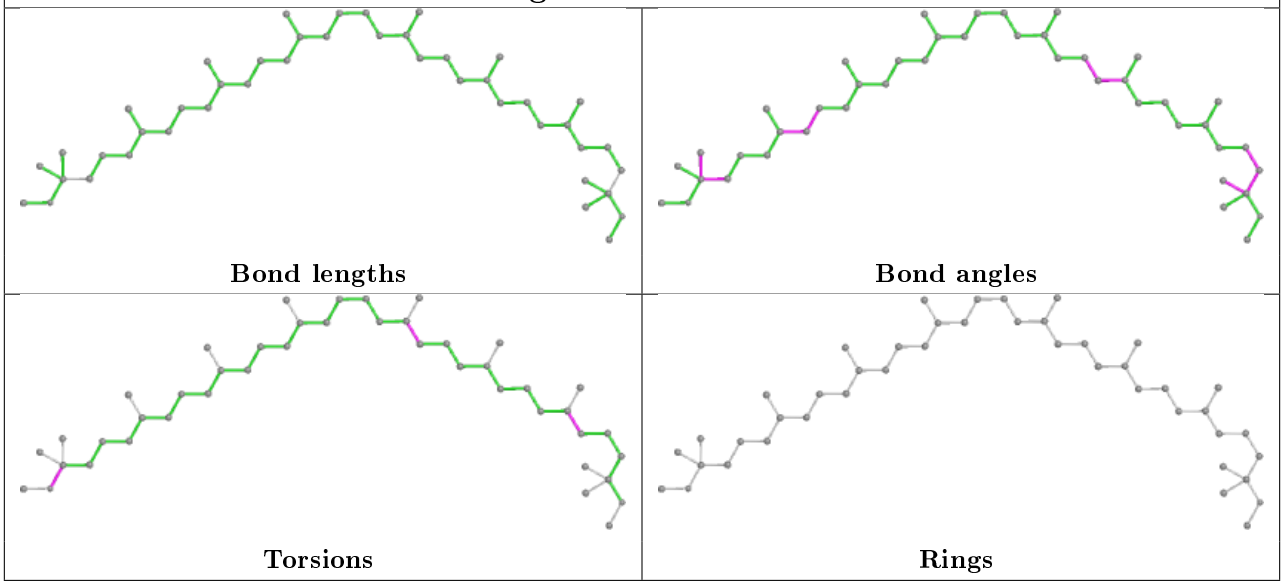
Ligand 07D J 1001



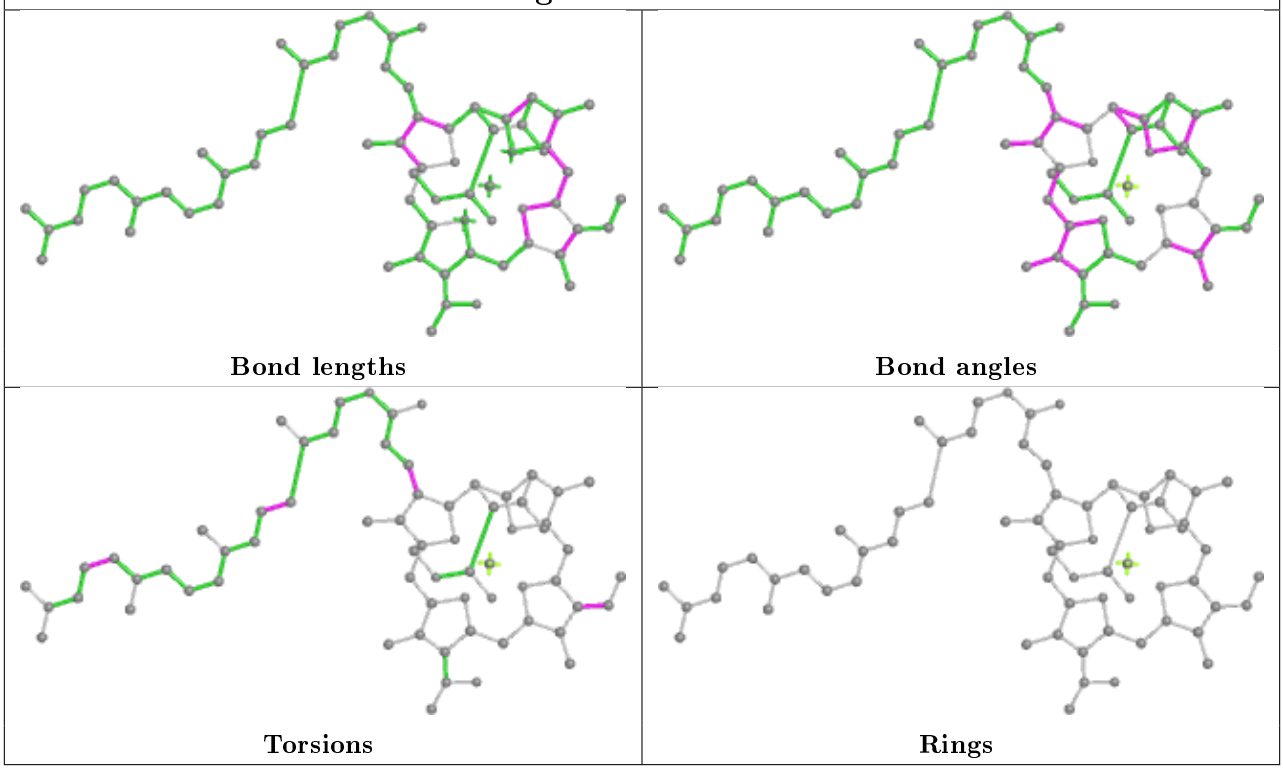
Ligand 07D N 1002



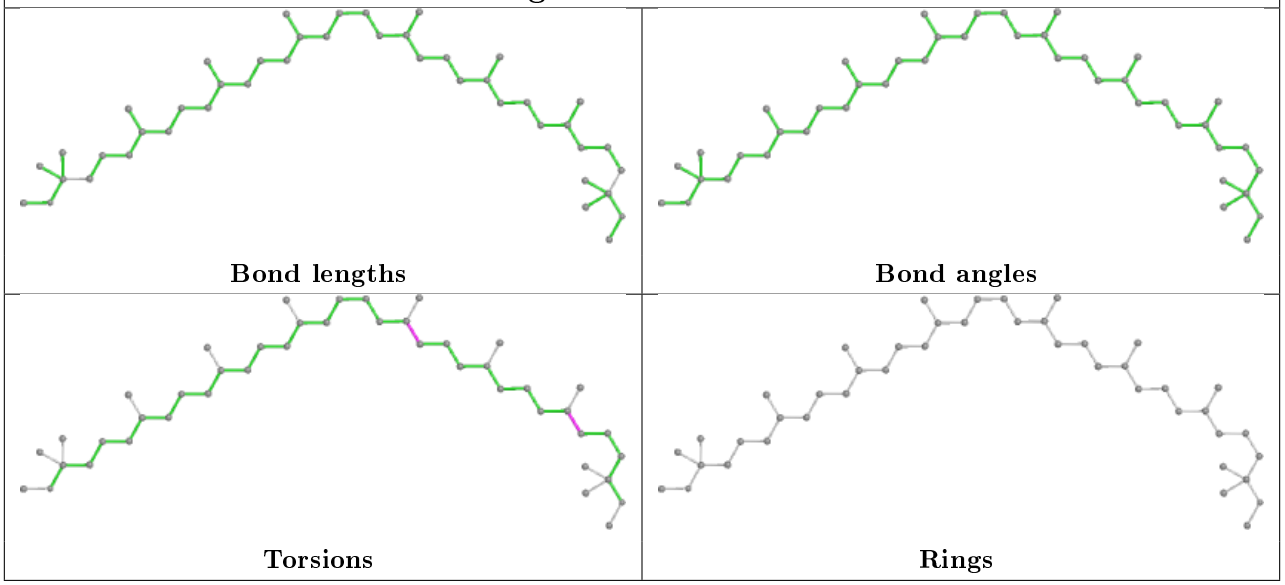
Ligand CRT 9 101



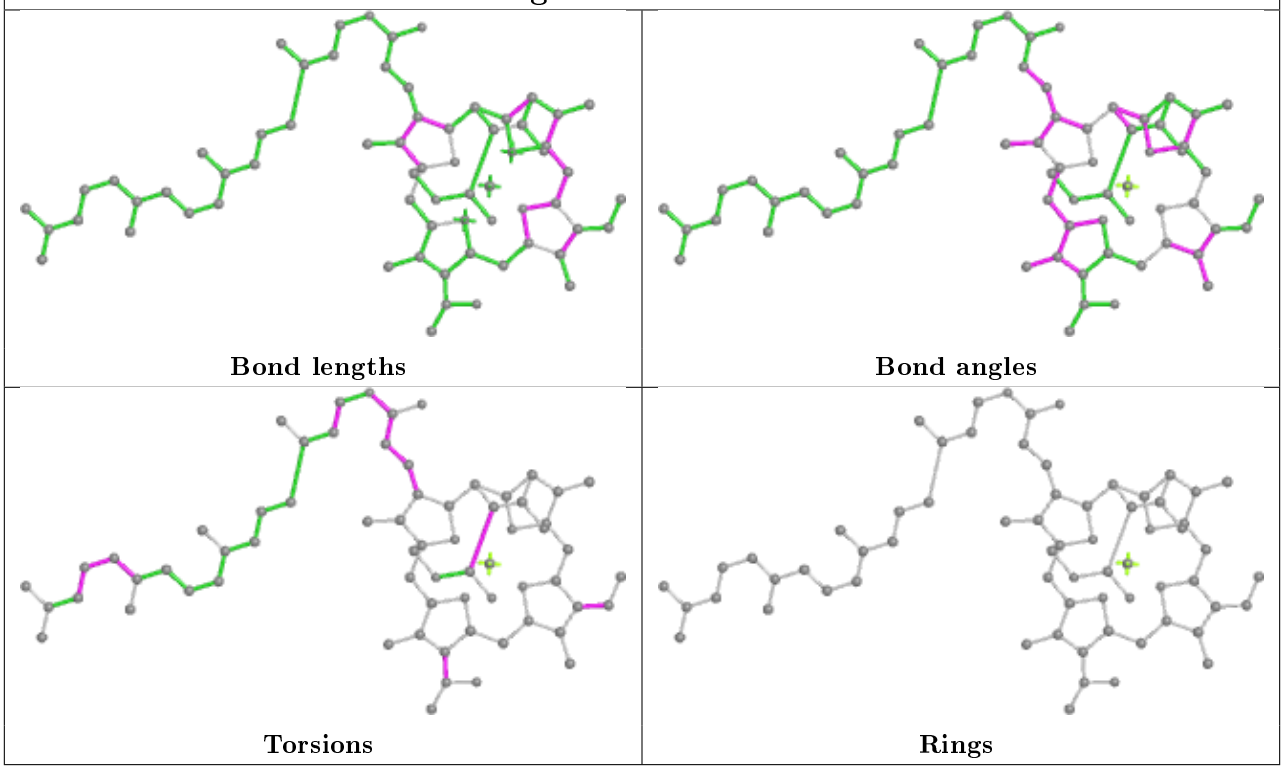
Ligand 07D 9 102



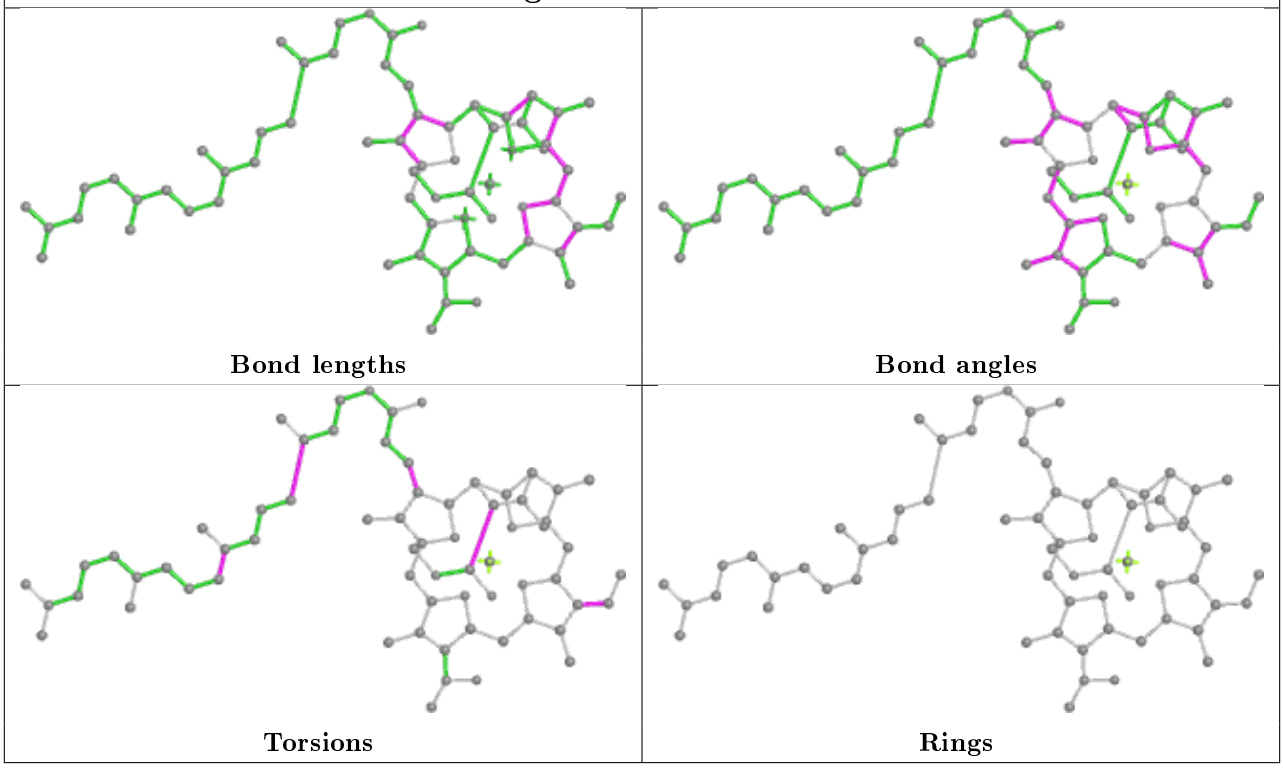
Ligand CRT S 101



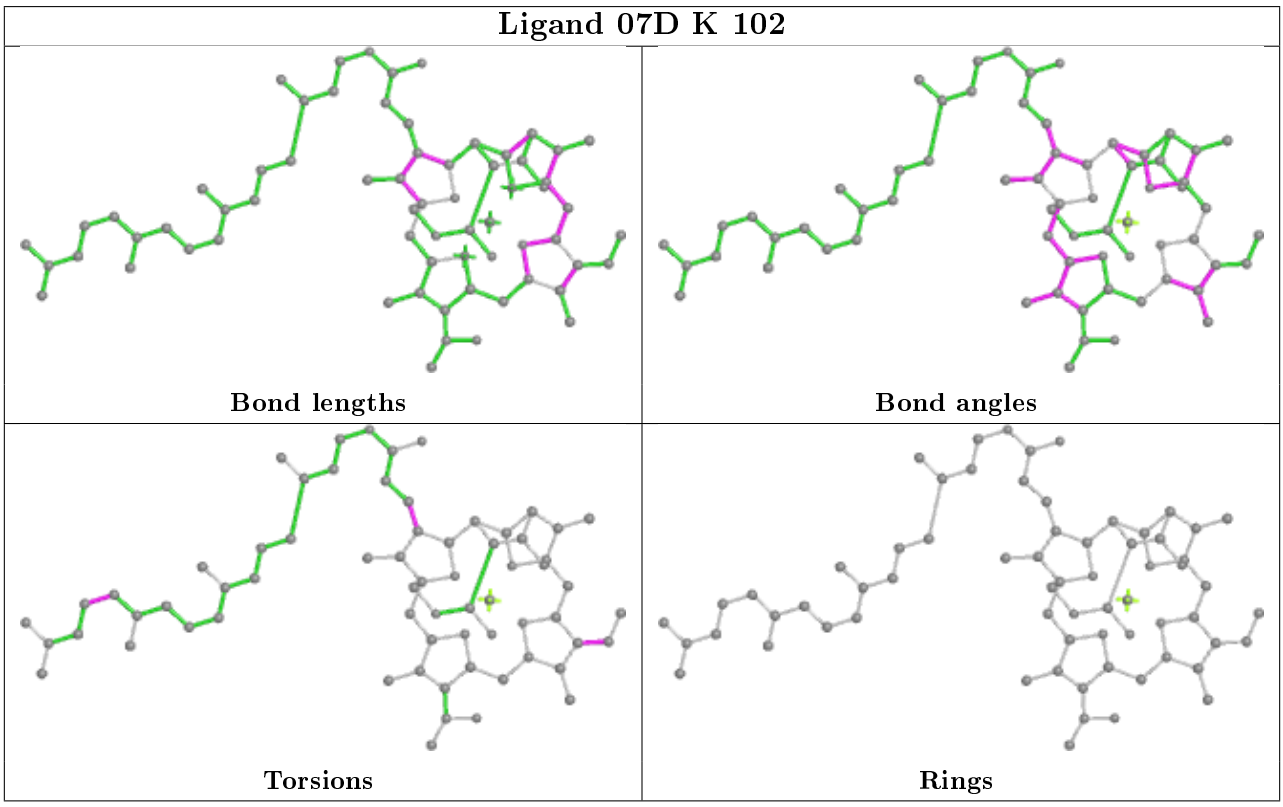
Ligand 07D H 301



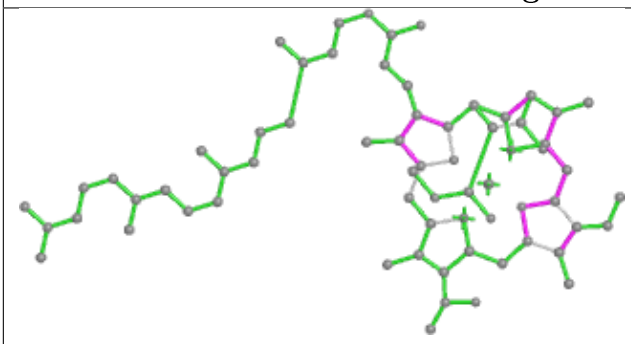
Ligand 07D L 1004



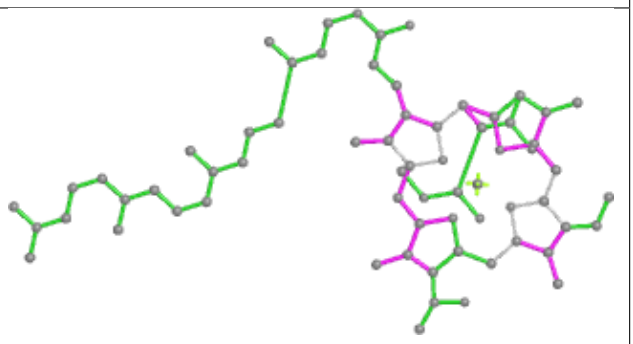
Ligand 07D K 102



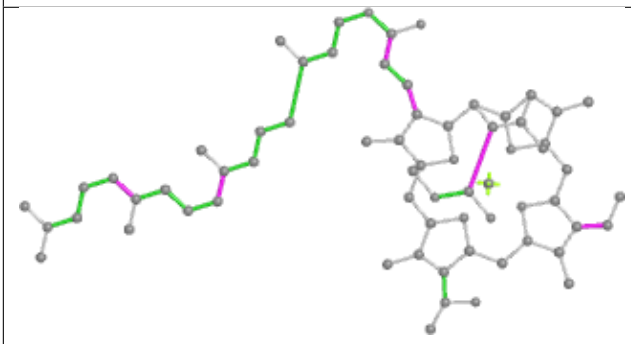
Ligand 07D E 1001



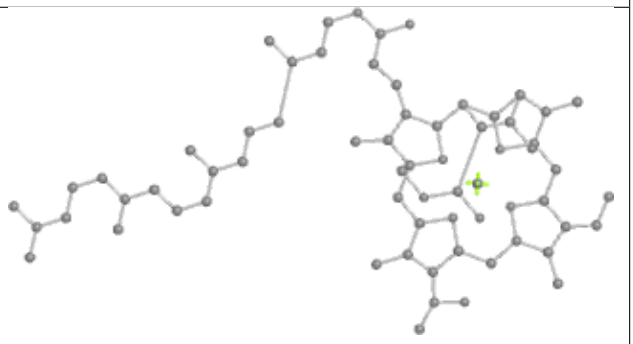
Bond lengths



Bond angles

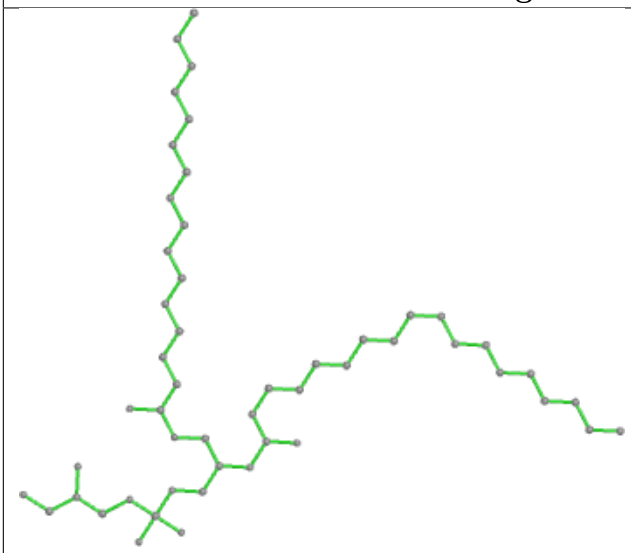


Torsions

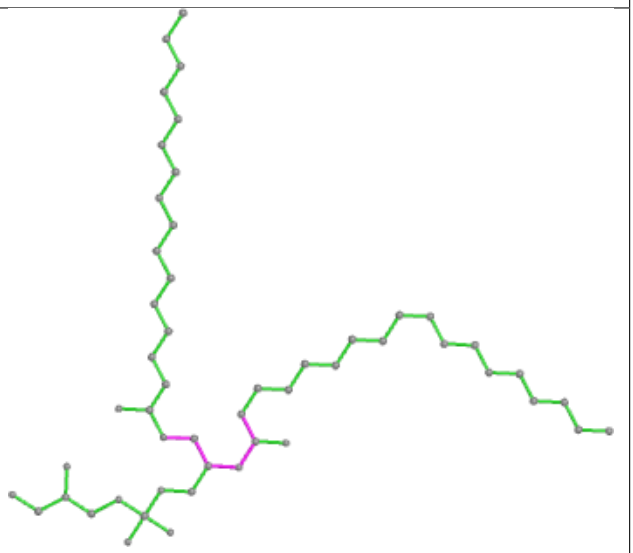


Rings

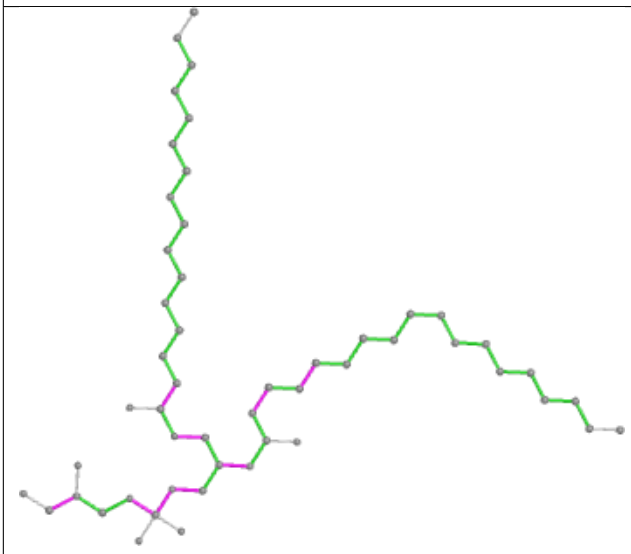
Ligand PGW H 302



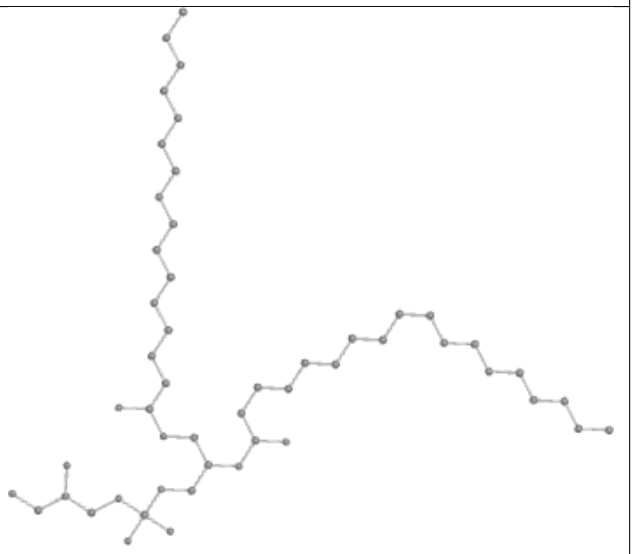
Bond lengths



Bond angles

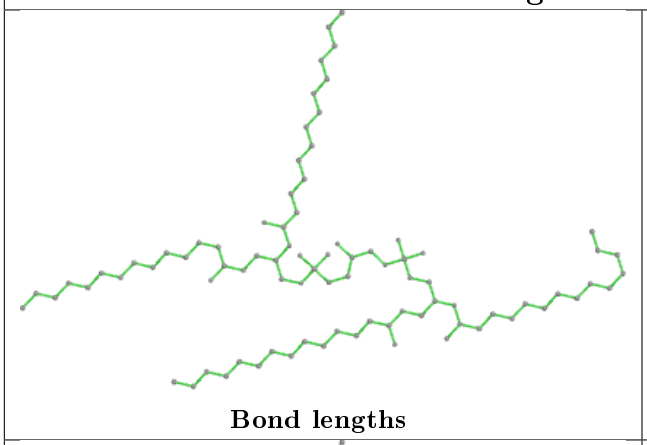


Torsions

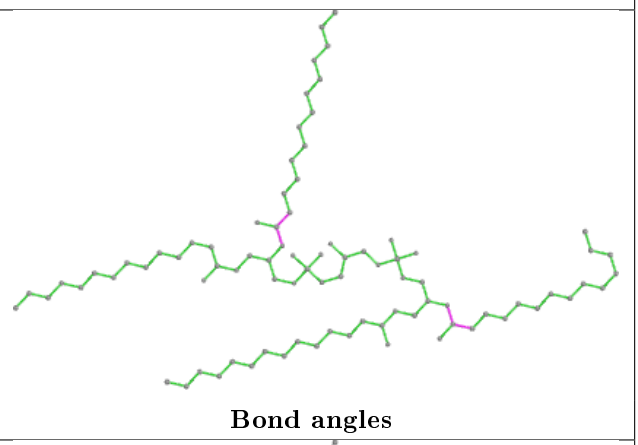


Rings

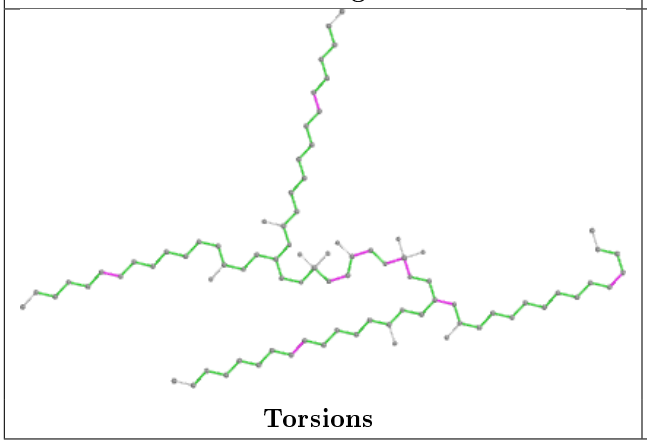
Ligand CD4 H 304



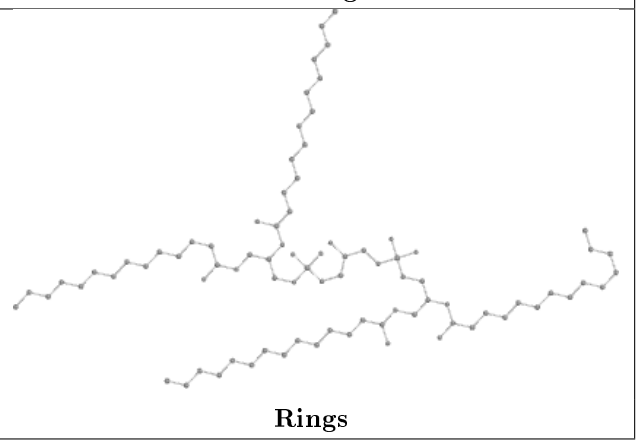
Bond lengths



Bond angles

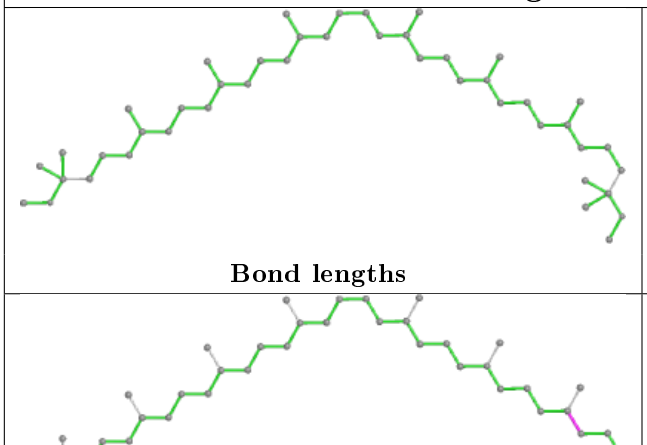


Torsions

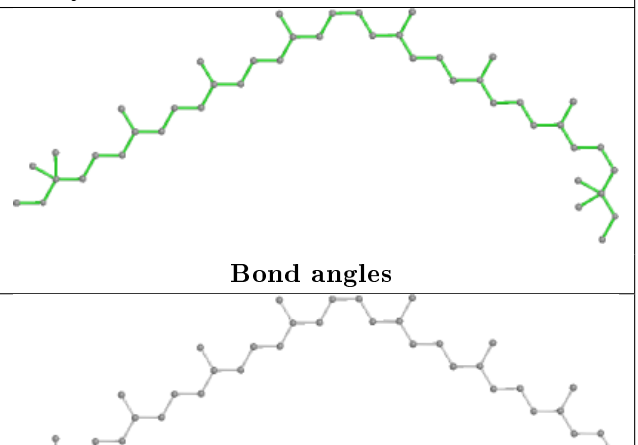


Rings

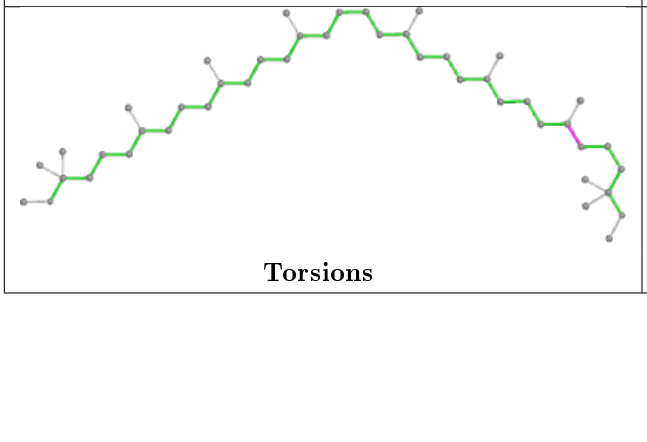
Ligand CRT Q 101



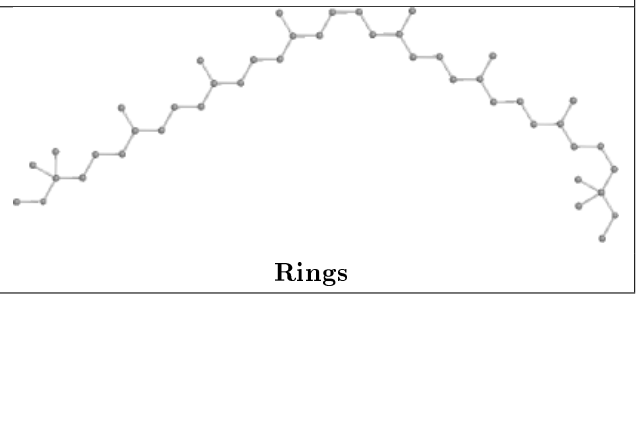
Bond lengths



Bond angles

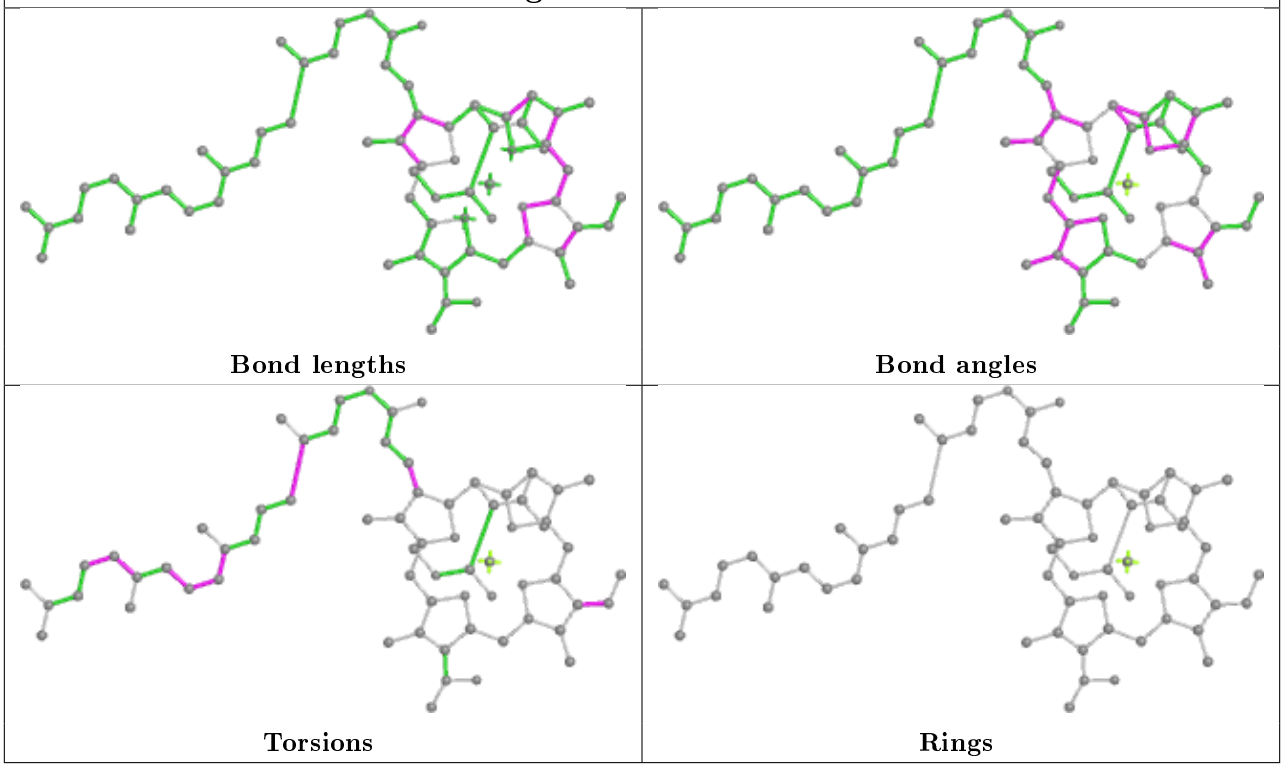


Torsions

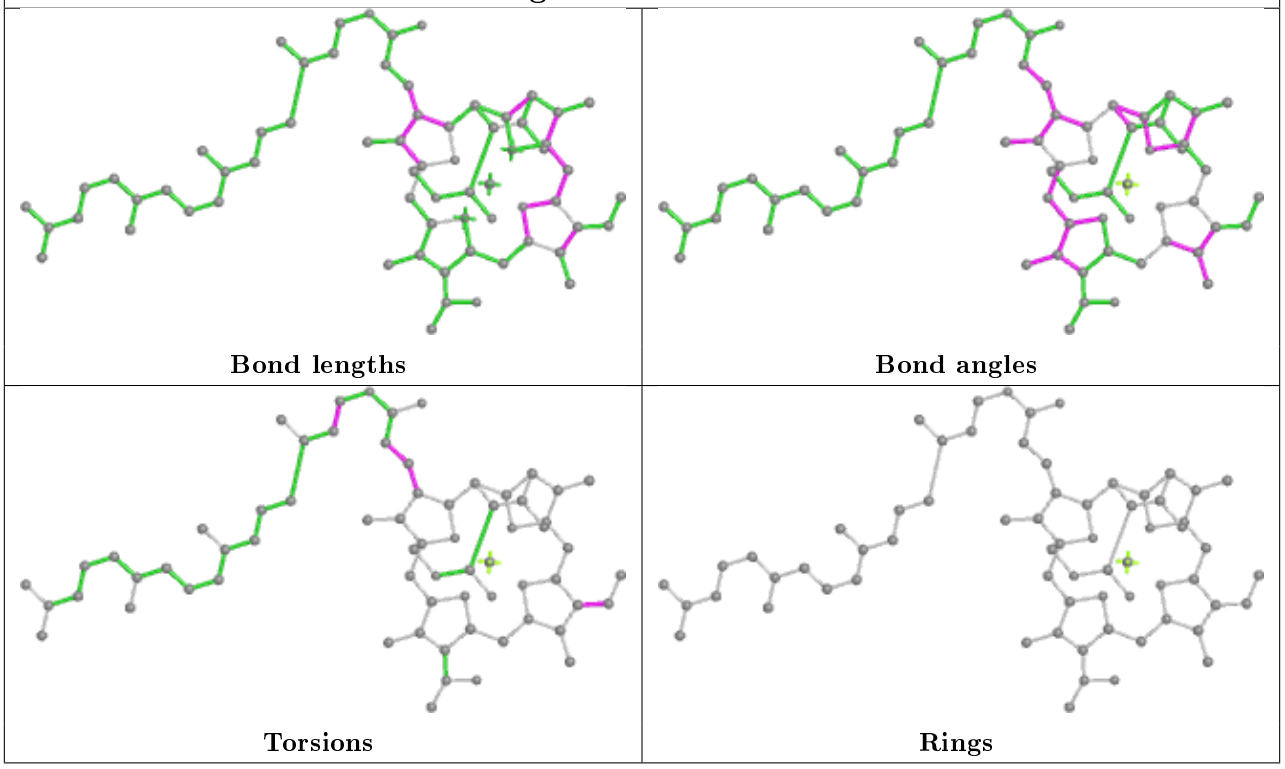


Rings

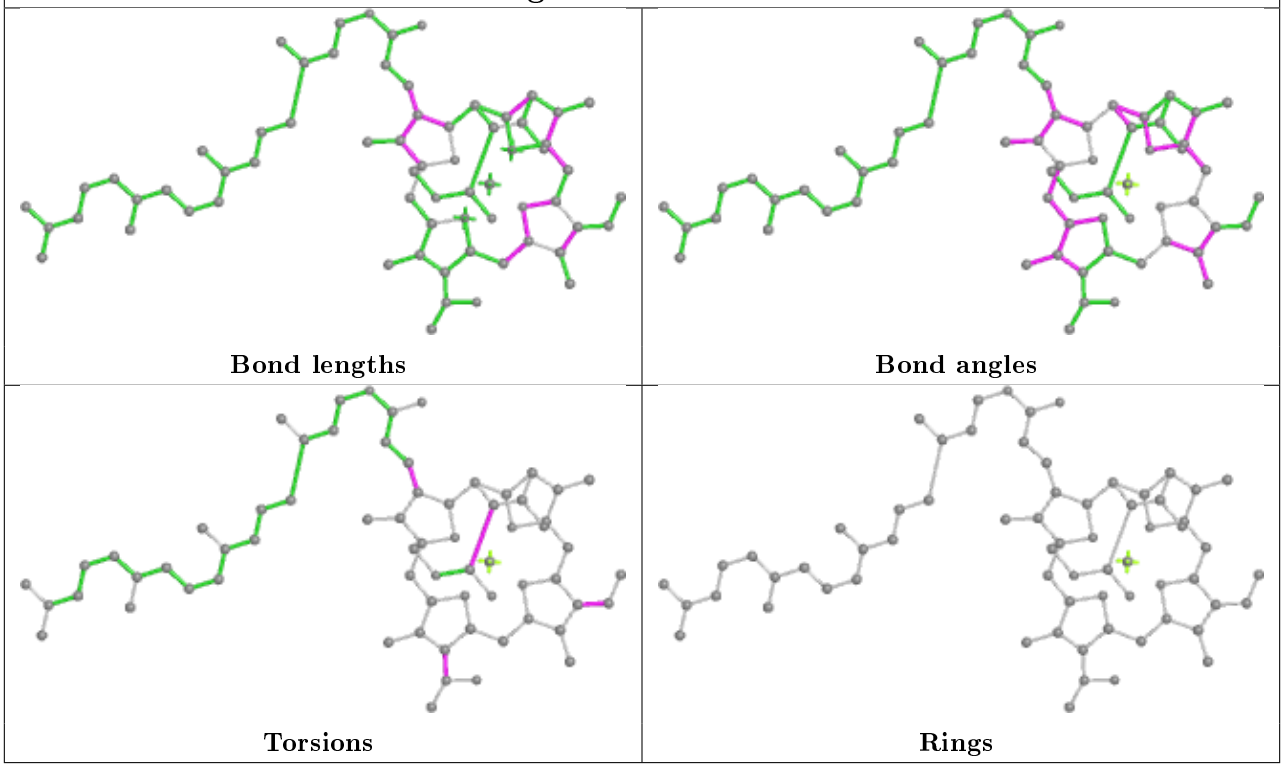
Ligand 07D d 1002



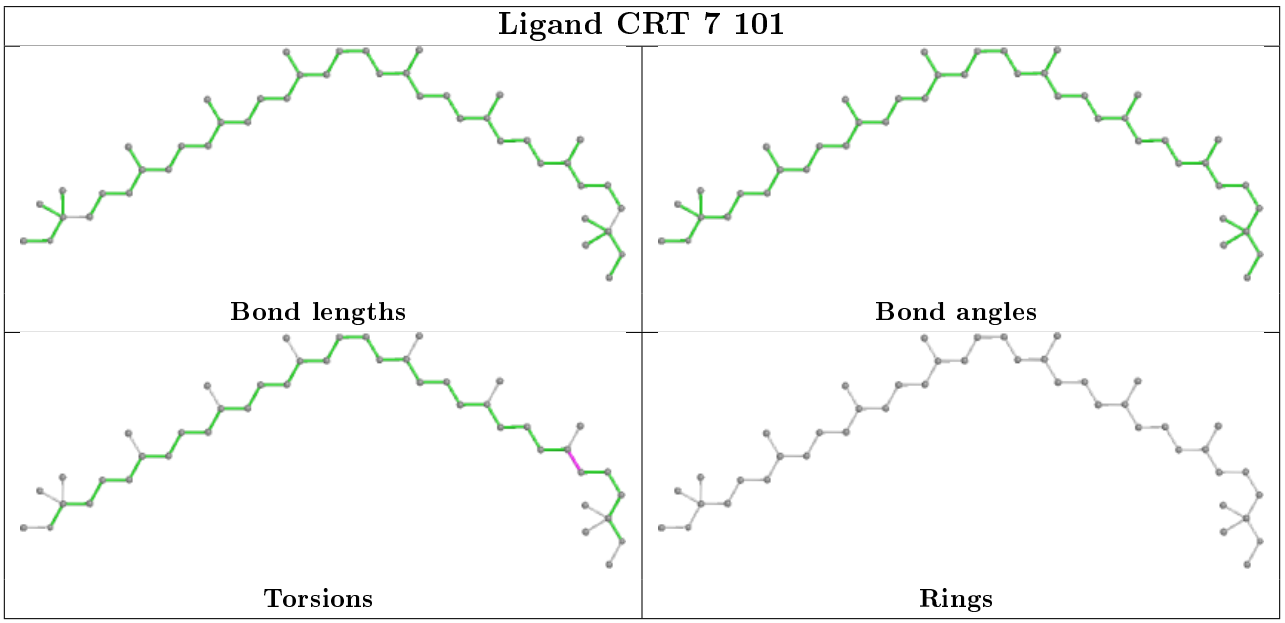
Ligand 07D m 102



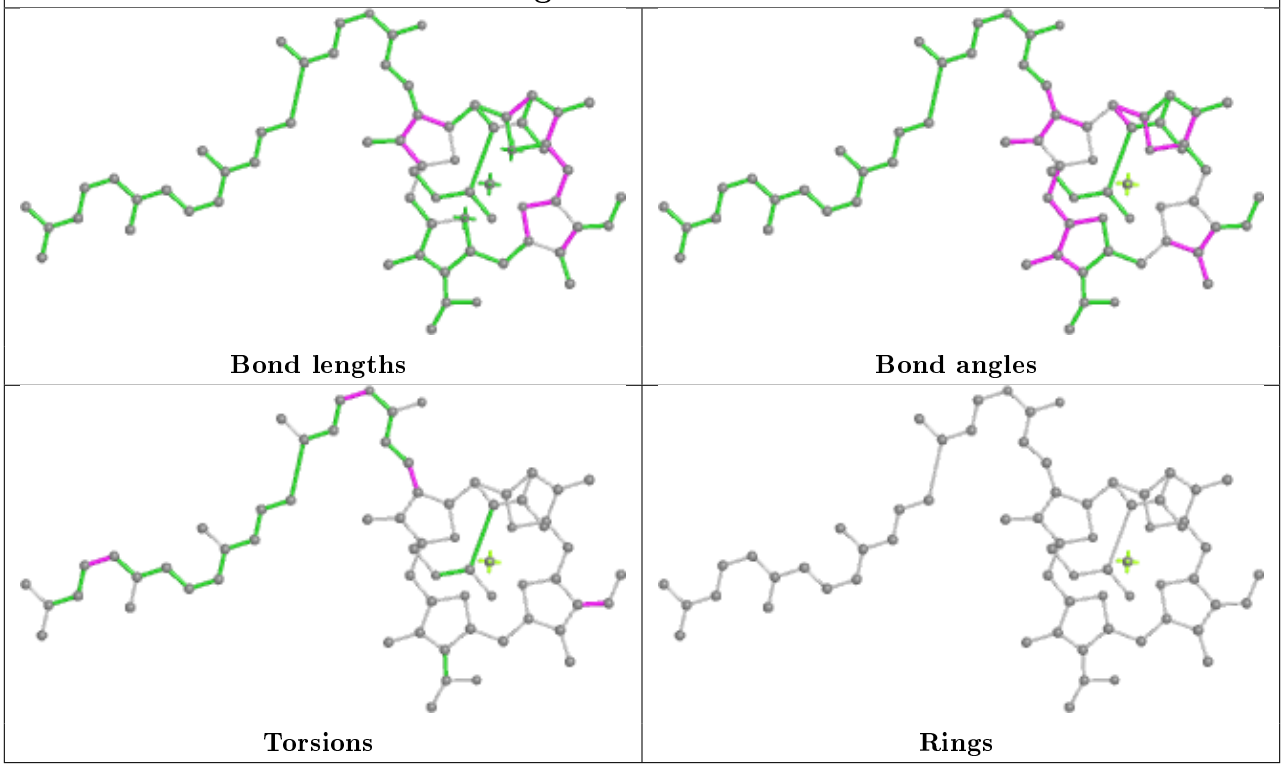
Ligand 07D M 405



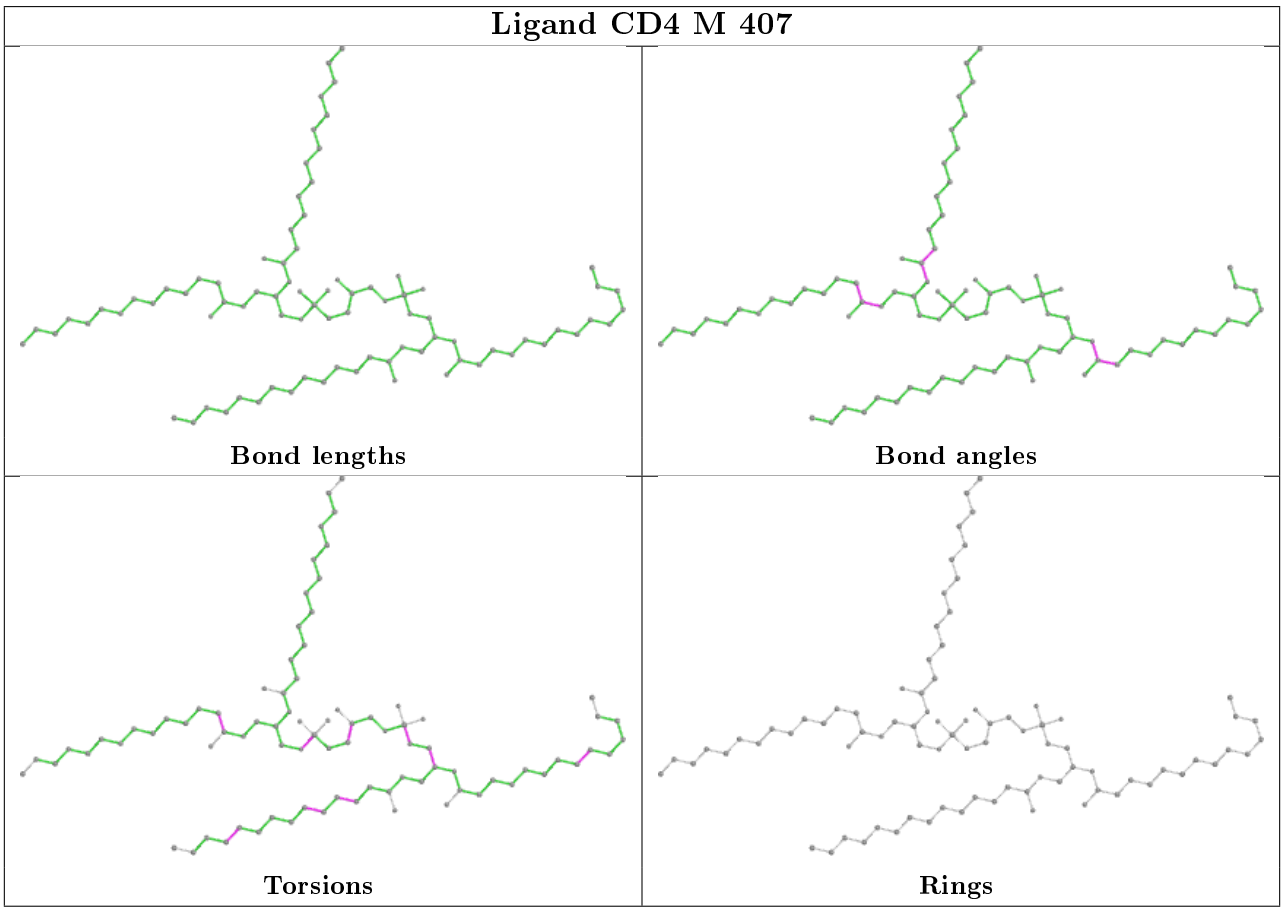
Ligand CRT 7 101



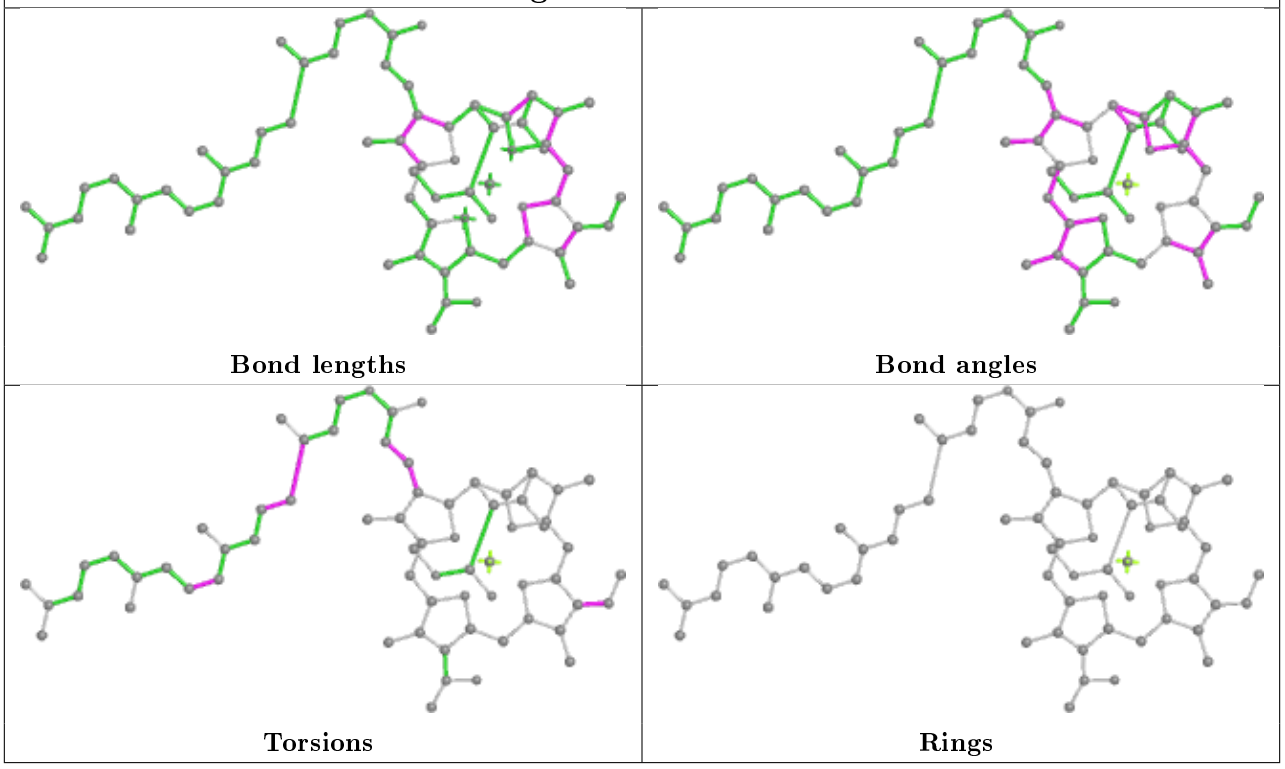
Ligand 07D S 102



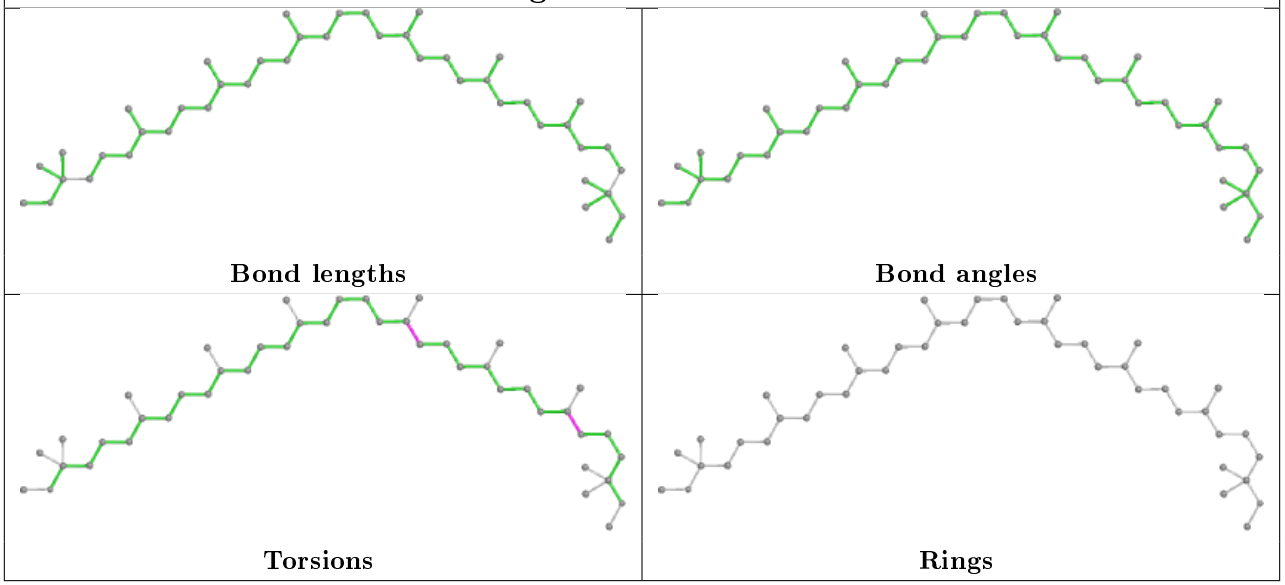
Ligand CD4 M 407



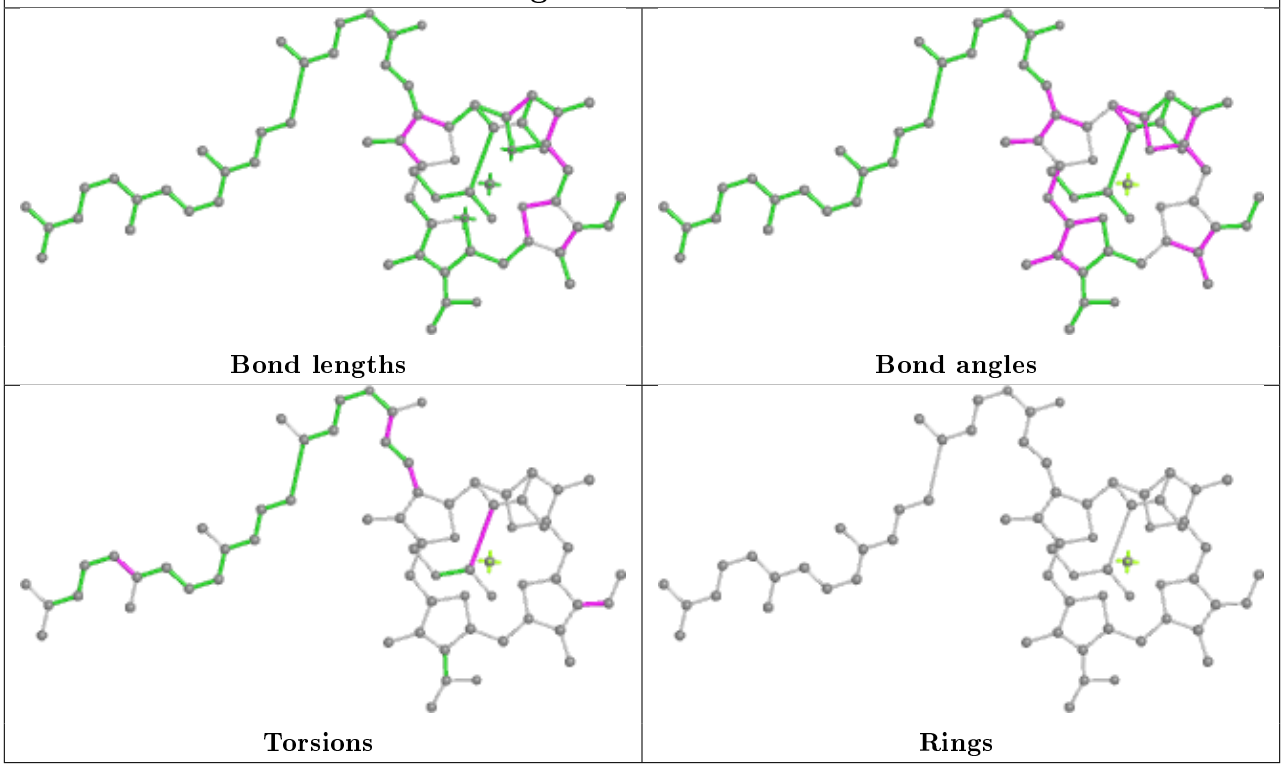
Ligand 07D Y 102



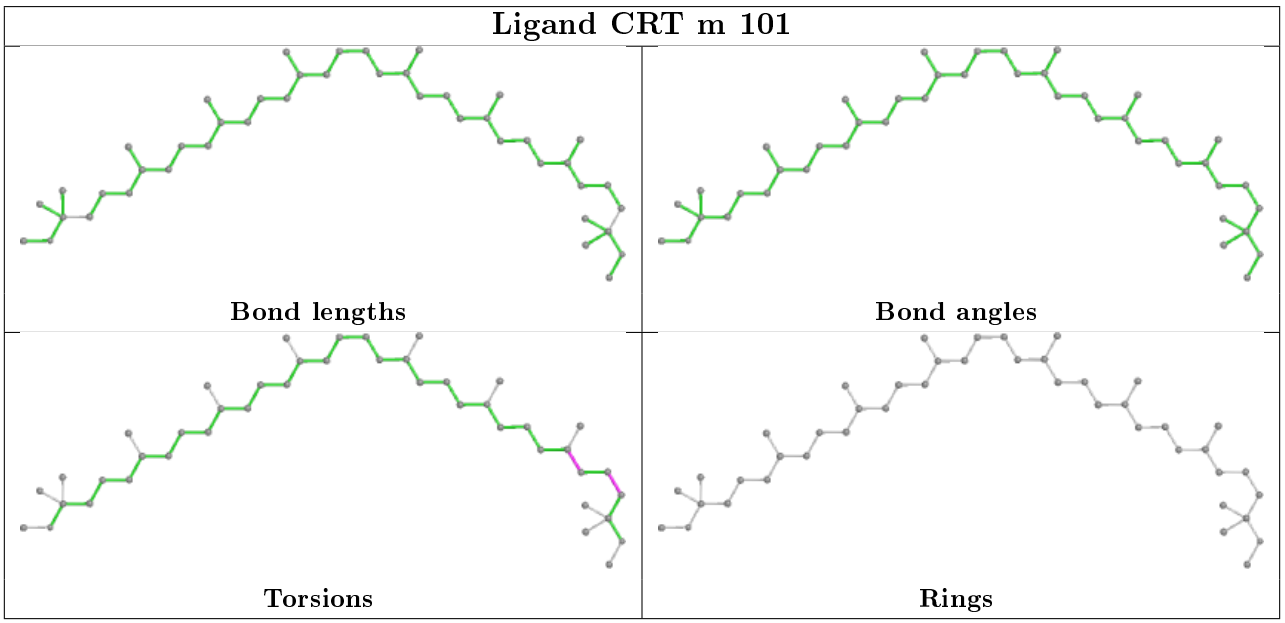
Ligand CRT 5 101



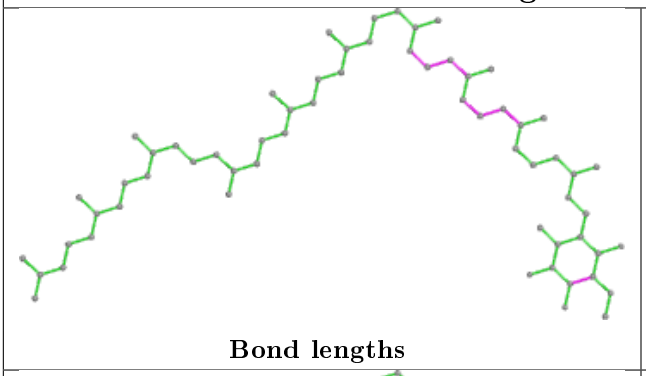
Ligand 07D A 101



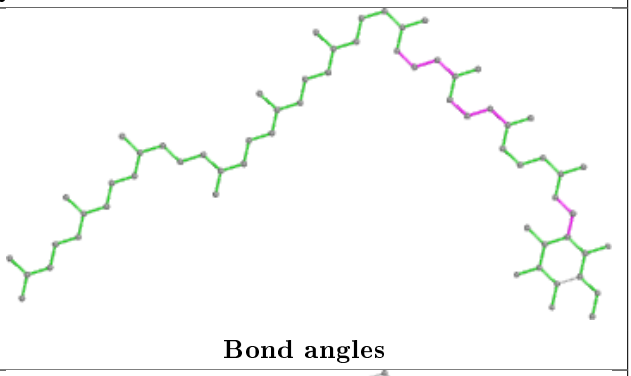
Ligand CRT m 101



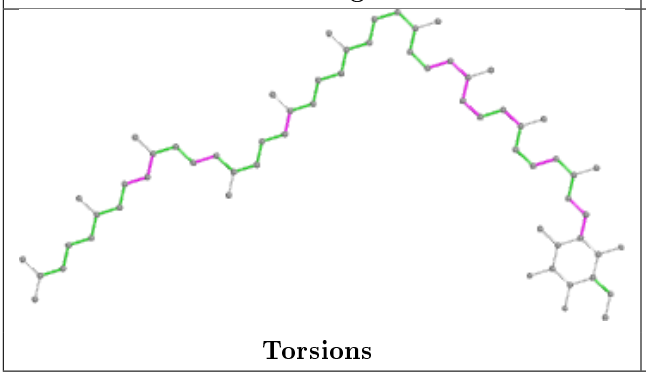
Ligand RQ0 L 1002



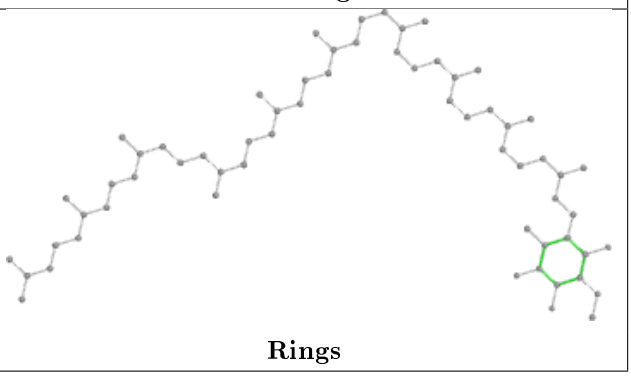
Bond lengths



Bond angles

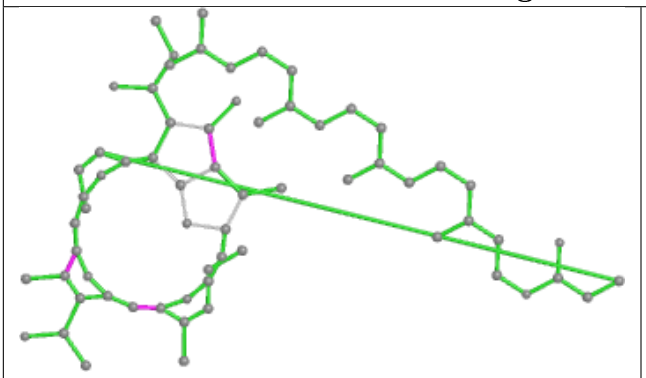


Torsions

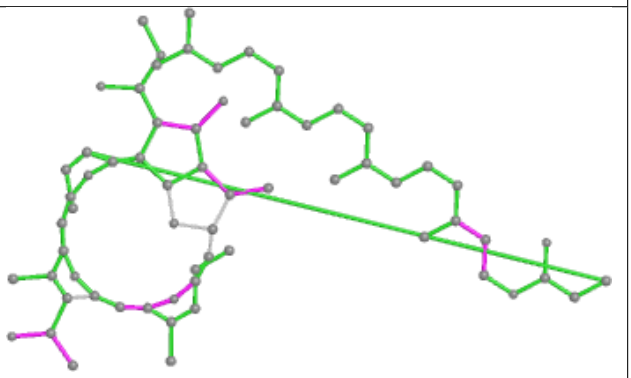


Rings

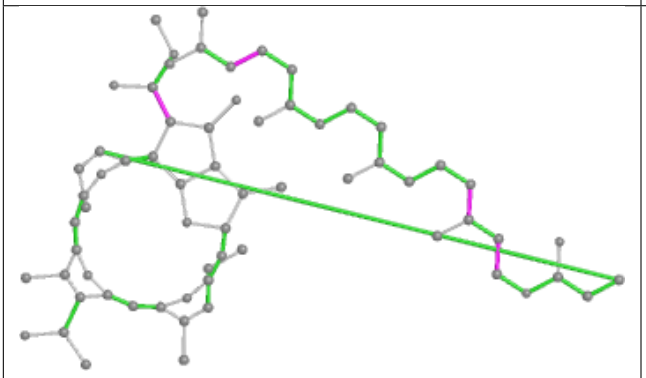
Ligand BPH L 1001



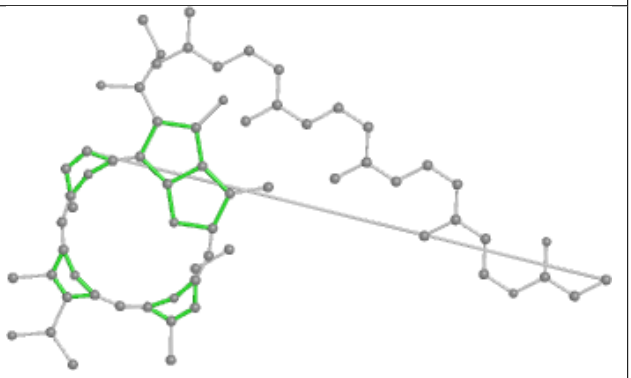
Bond lengths



Bond angles

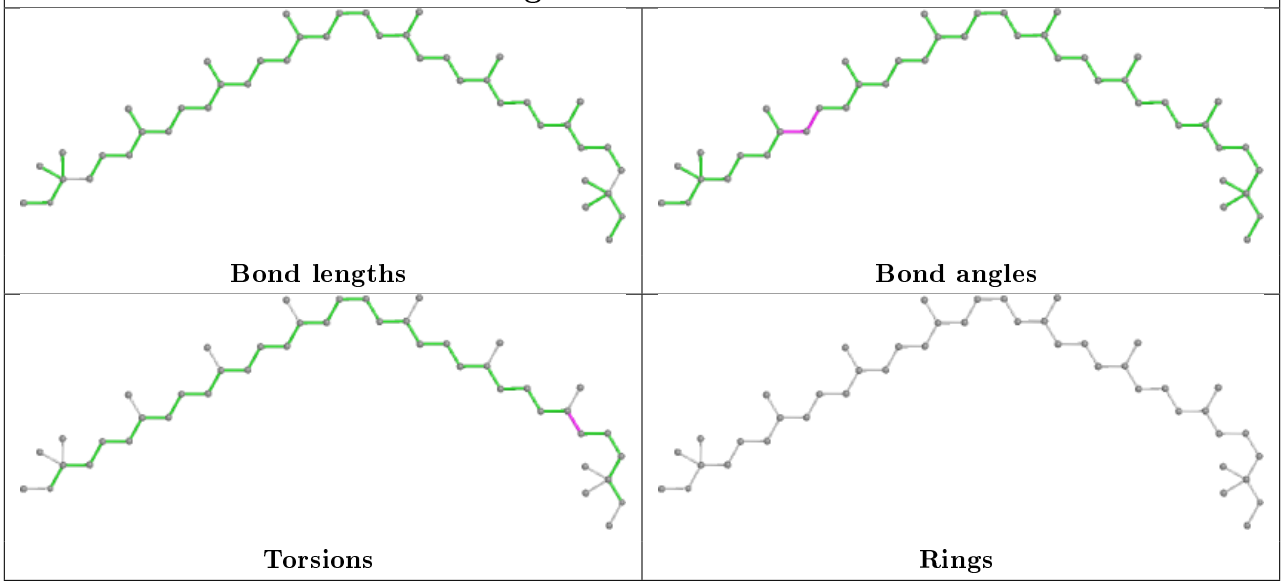


Torsions

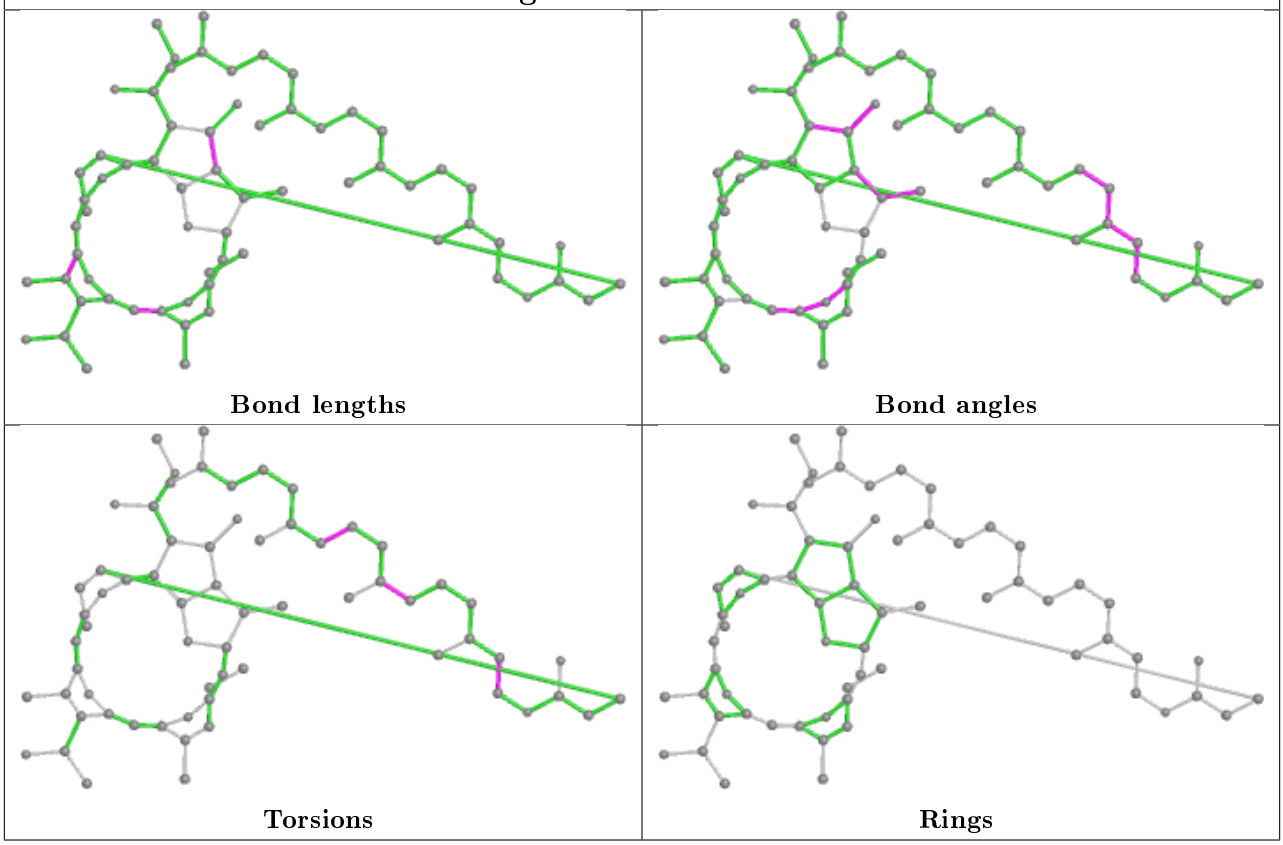


Rings

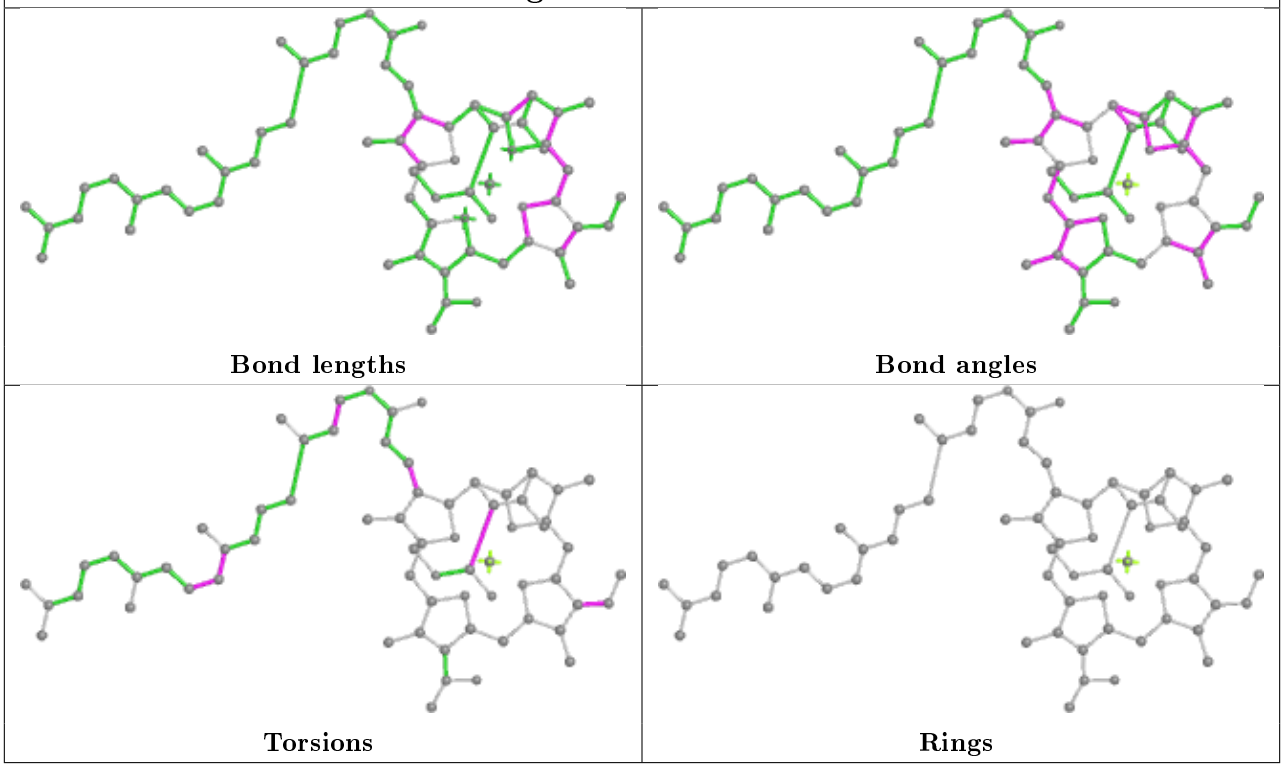
Ligand CRT Y 101



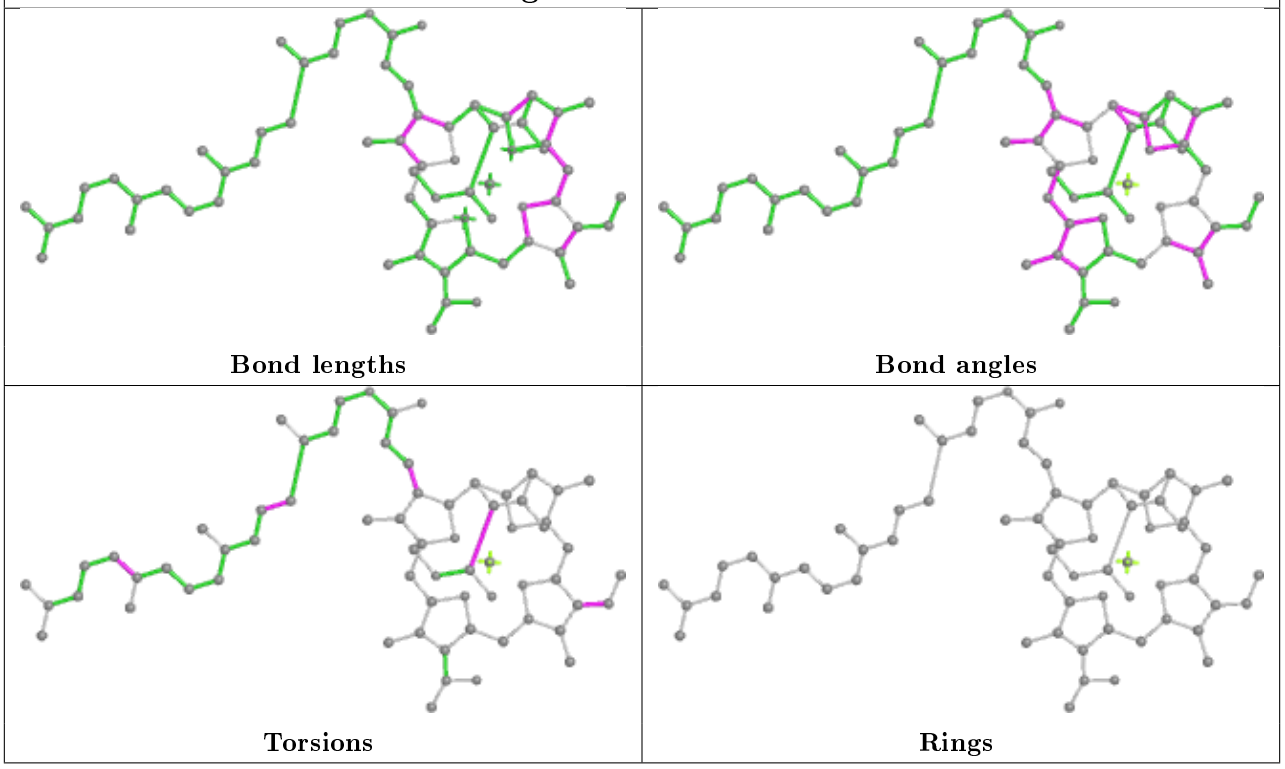
Ligand BPH M 402



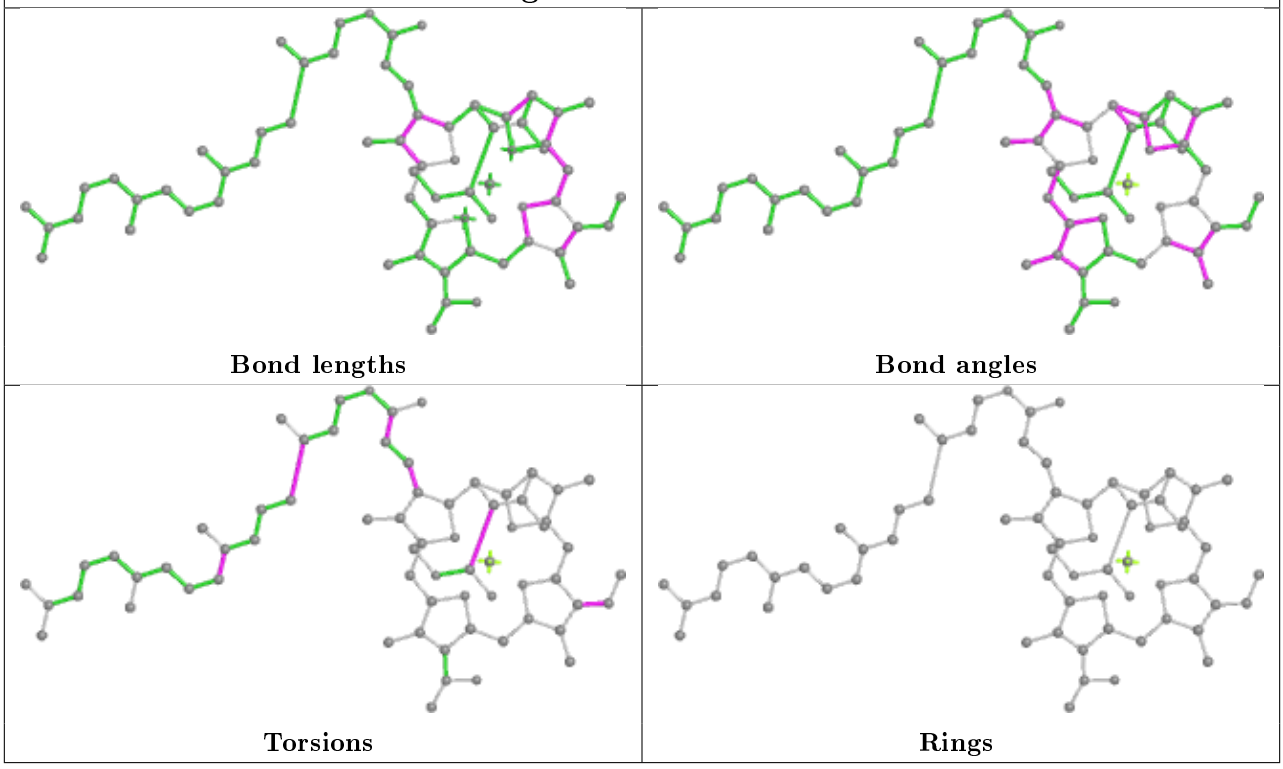
Ligand 07D 8 1001



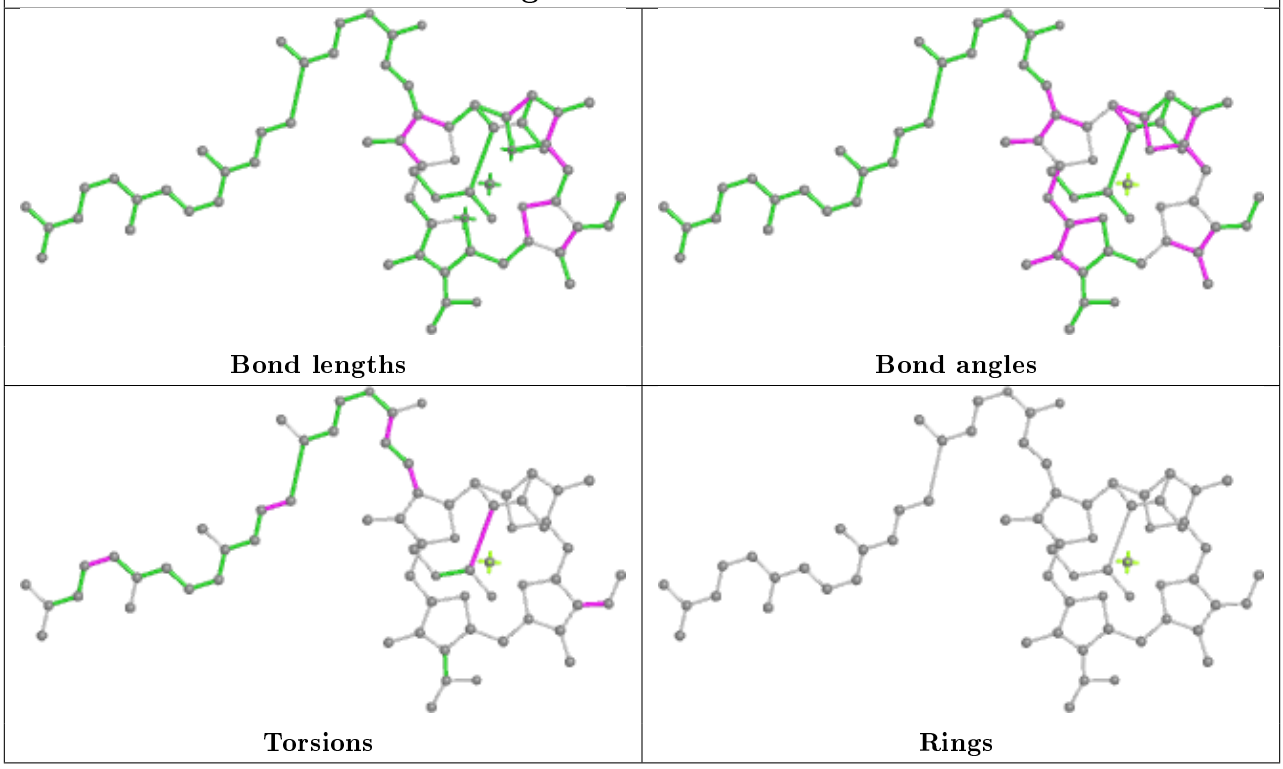
Ligand 07D G 1001



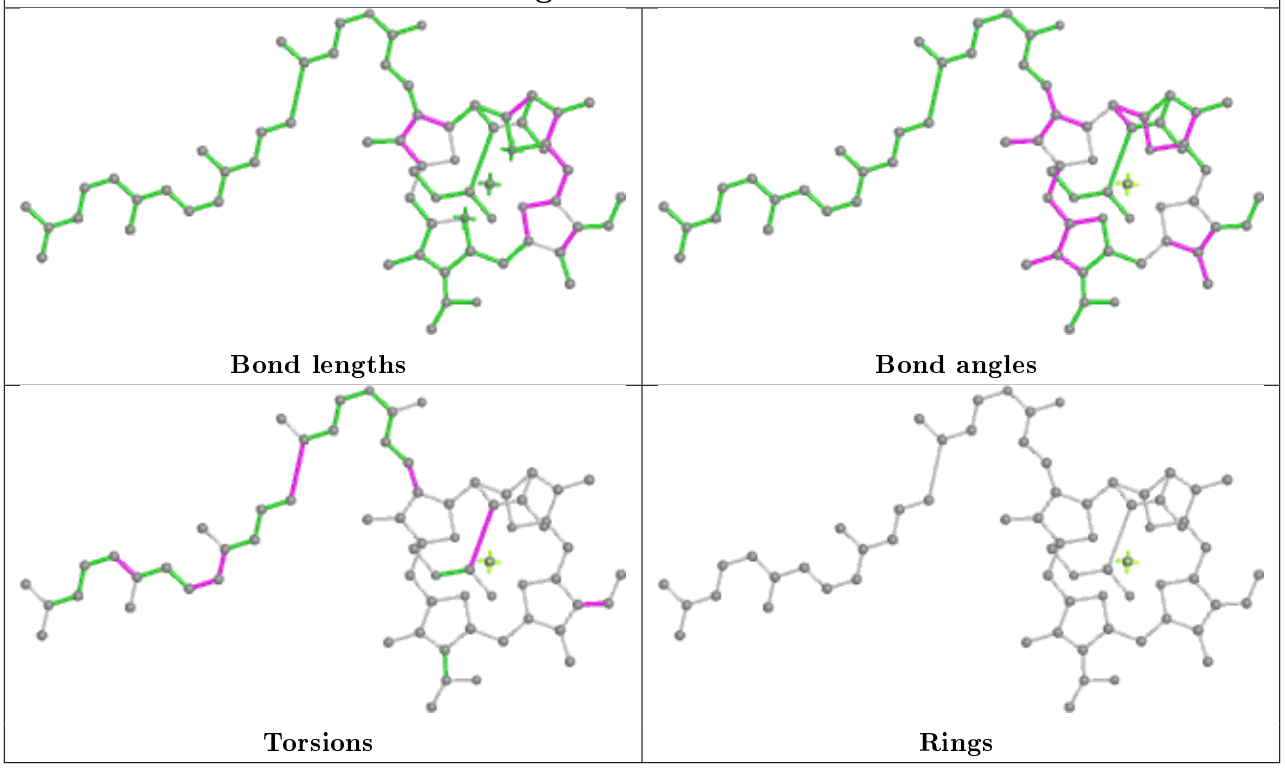
Ligand 07D V 1001



Ligand 07D D 1001



Ligand 07D 5 102



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

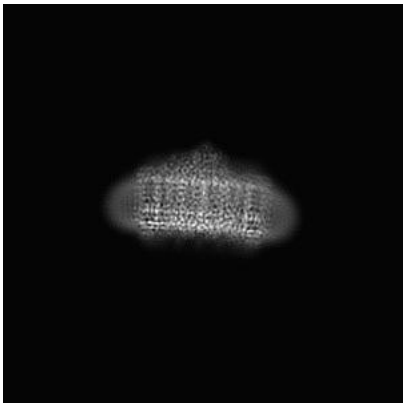
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-13110. These allow visual inspection of the internal detail of the map and identification of artifacts.

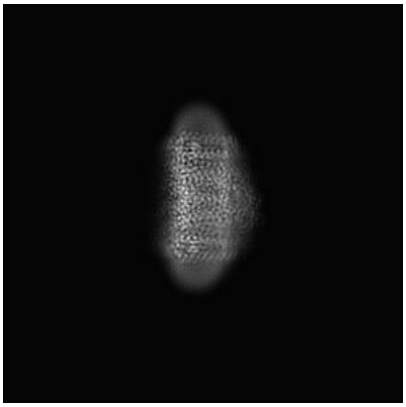
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

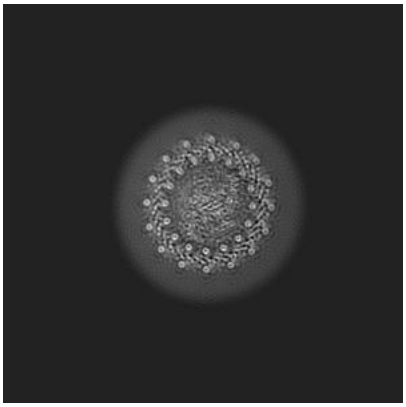
6.1.1 Primary map



X



Y

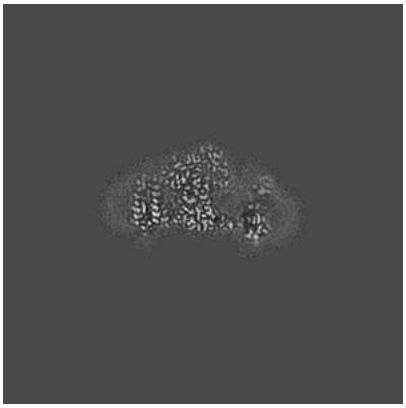


Z

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

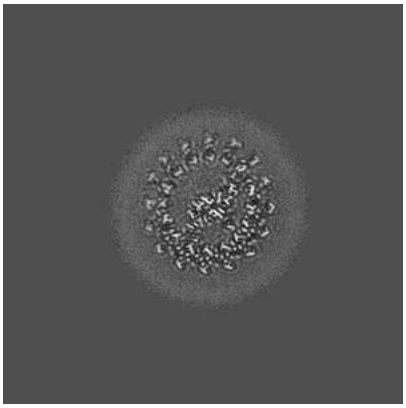
6.2 Central slices

6.2.1 Primary map



X Index: 128

Y Index: 128

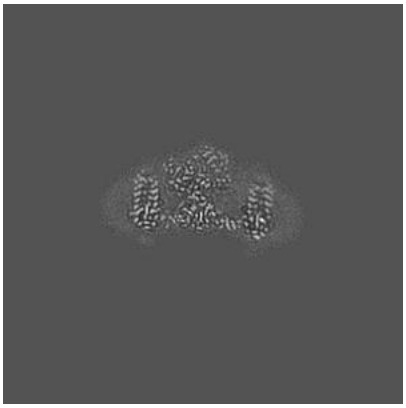


Z Index: 128

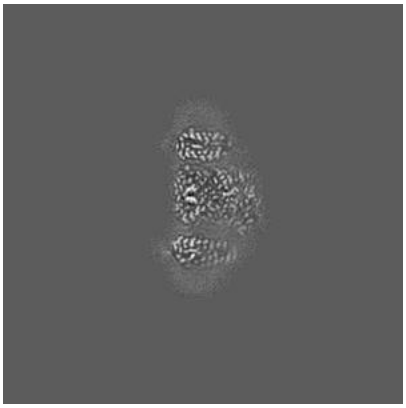
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

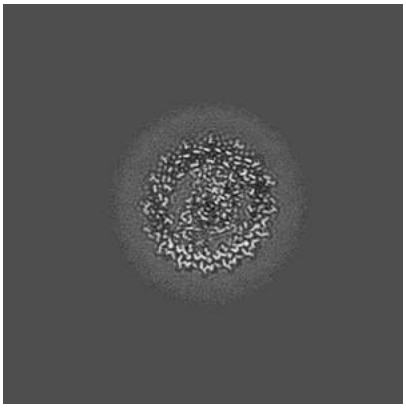
6.3.1 Primary map



X Index: 131



Y Index: 126

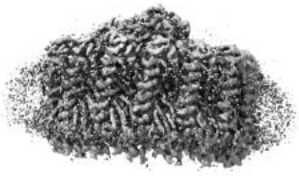


Z Index: 115

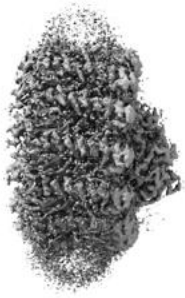
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

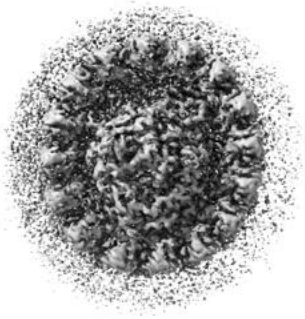
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0165. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

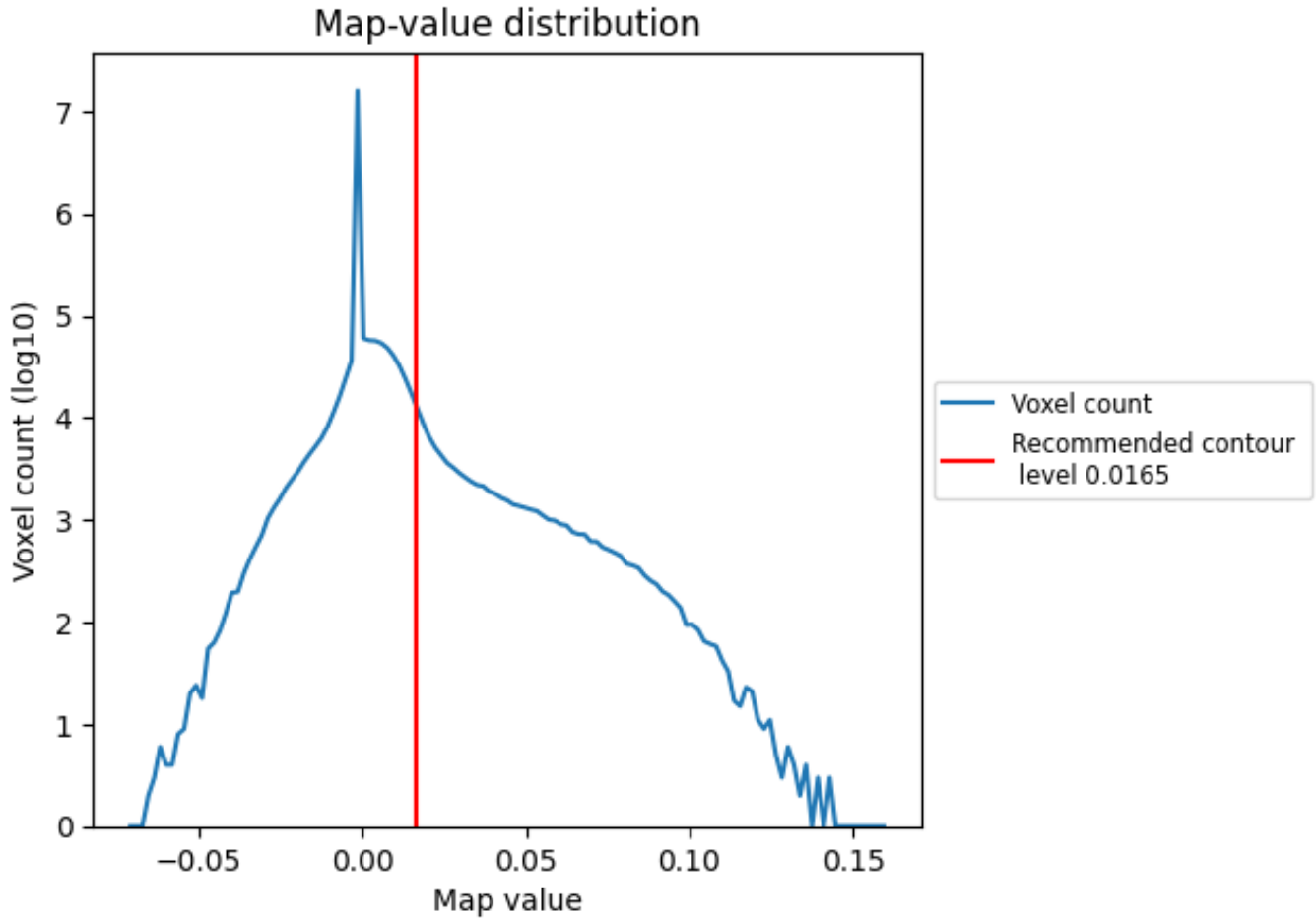
6.5 Mask visualisation (i)

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

7 Map analysis

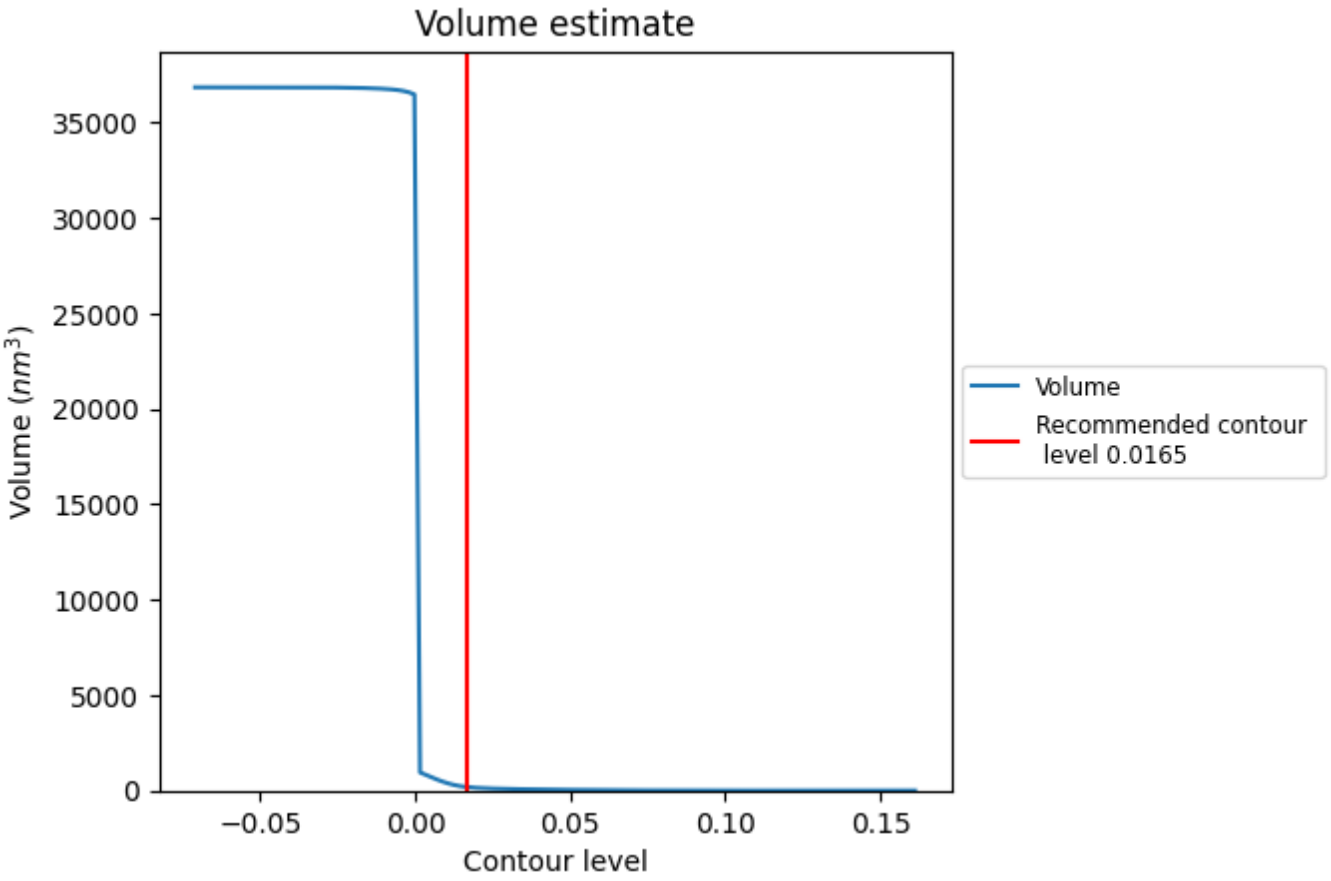
This section contains the results of statistical analysis of the map.

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.

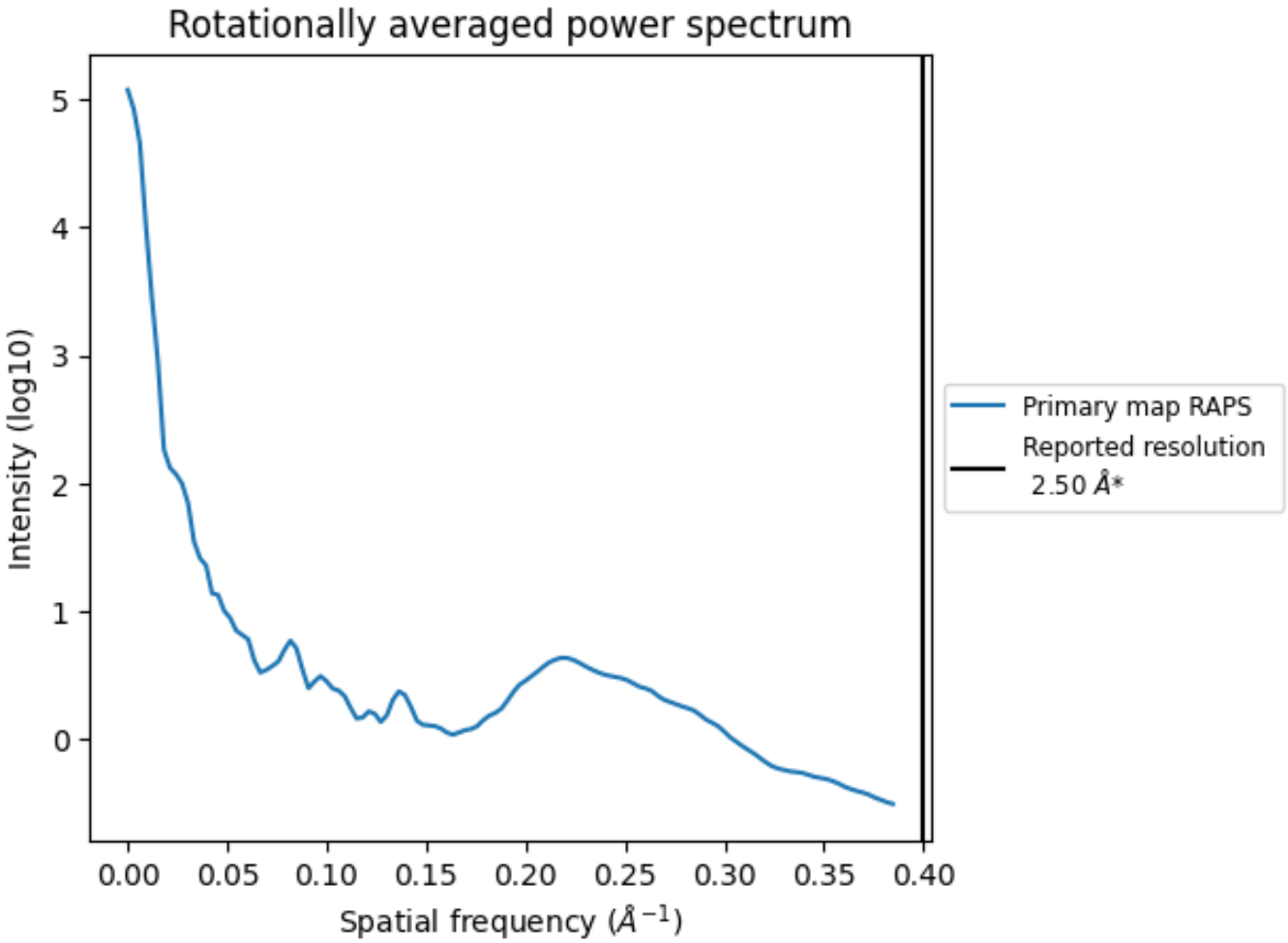
7.2 Volume estimate



The volume at the recommended contour level is 189 nm^3; this corresponds to an approximate mass of 171 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)

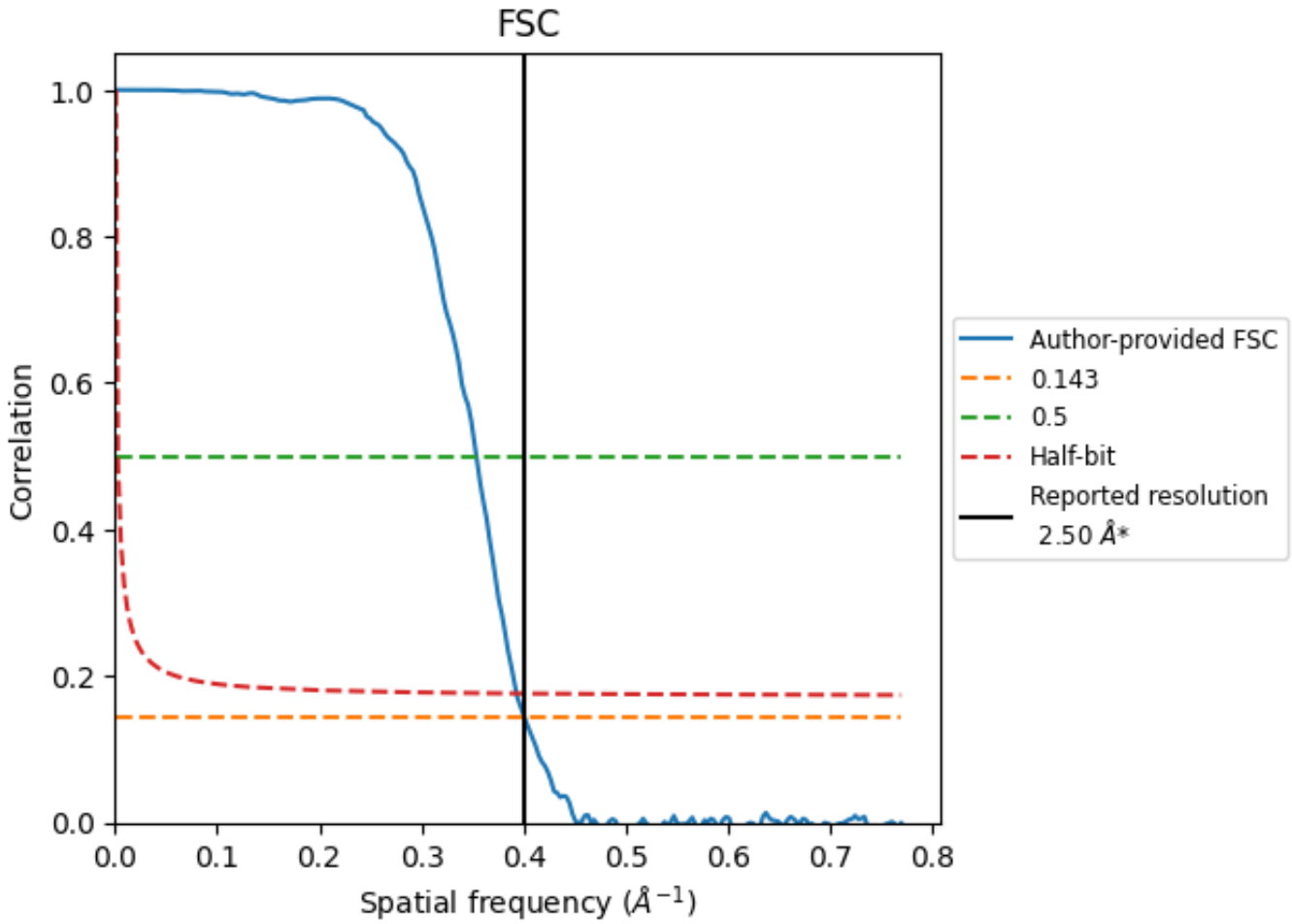


*Reported resolution corresponds to spatial frequency of 0.400 Å^{-1}

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 0.400 Å^{-1}

8.2 Resolution estimates (i)

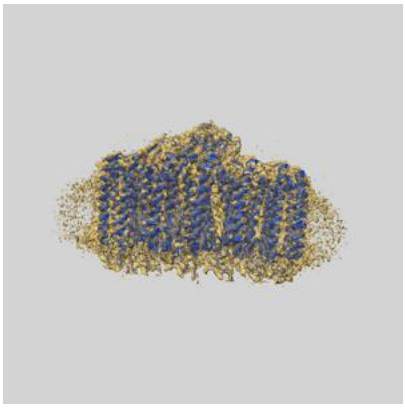
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.50	-	-
Author-provided FSC curve	2.49	2.83	2.55
Unmasked-calculated*	-	-	-

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

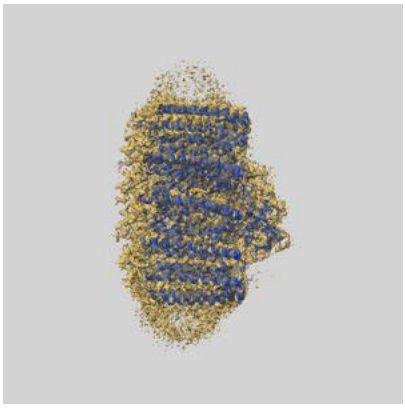
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-13110 and PDB model 7OY8. Per-residue inclusion information can be found in section 3 on page 19.

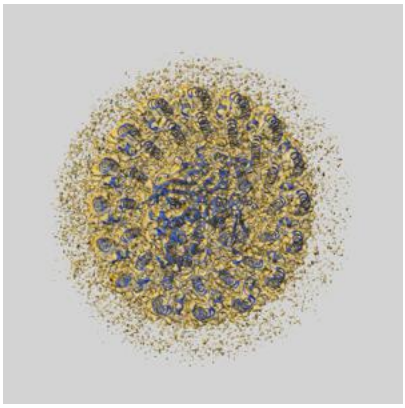
9.1 Map-model overlay



X



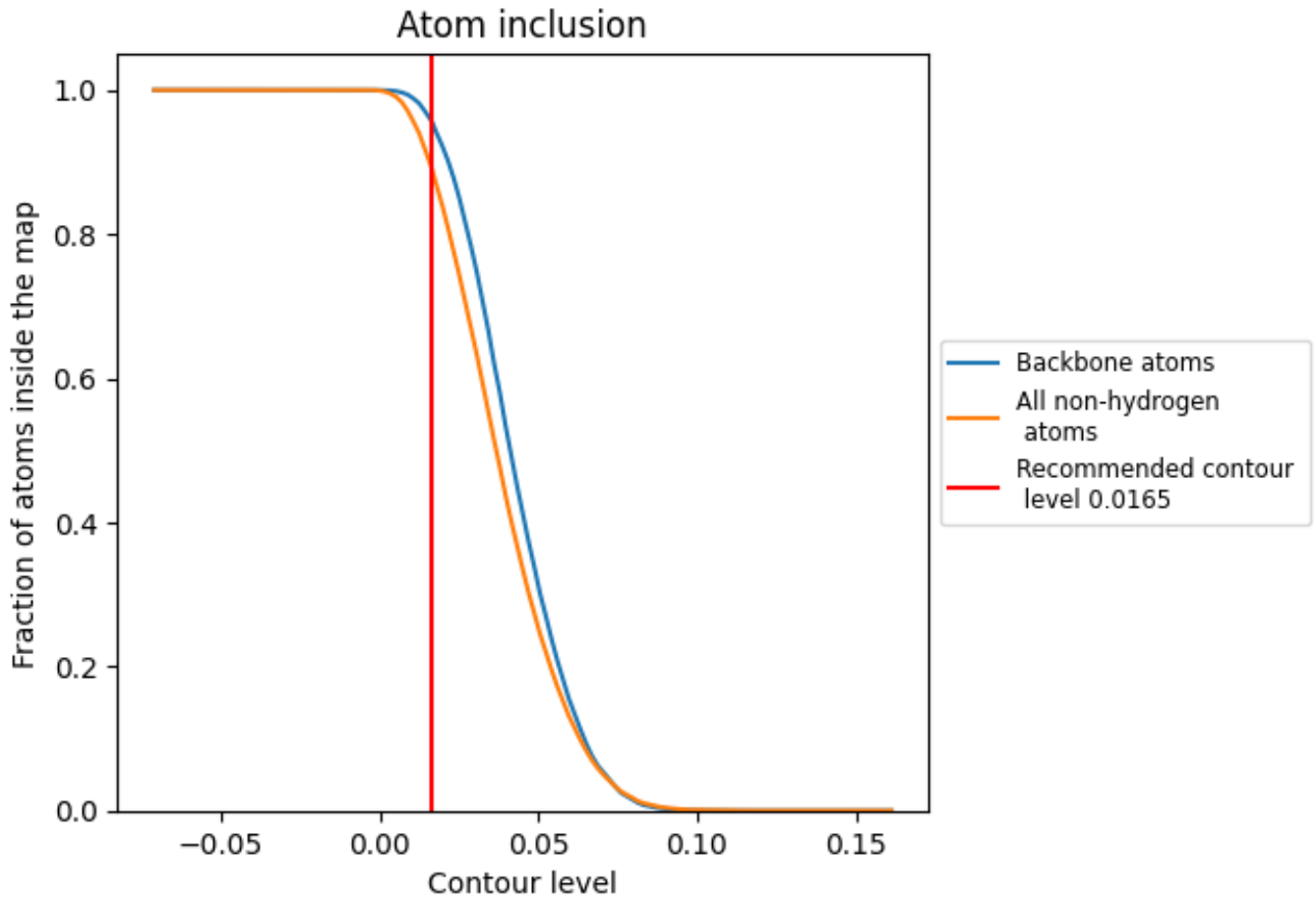
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0165 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 Atom inclusion (i)



At the recommended contour level, 96% of all backbone atoms, 89% of all non-hydrogen atoms, are inside the map.