Full wwPDB EM Validation Report ⓘ

Mar 13, 2023 – 05:14 PM JST

PDB ID	:	7XKT
EMDB ID	:	EMD-33270
Title	:	Human Cx36/GJD2 (BRIL-fused mutant) gap junction channel in detergents at 2.2 Angstroms resolution
Authors	:	Cho, H.J.; Lee, S.N.; Jeong, H.; Ryu, B.; Lee, H.J.; Woo, J.S.; Lee, H.H.
Deposited on	:	2022-04-20
Resolution	:	2.20 Å(reported)

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

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

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

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

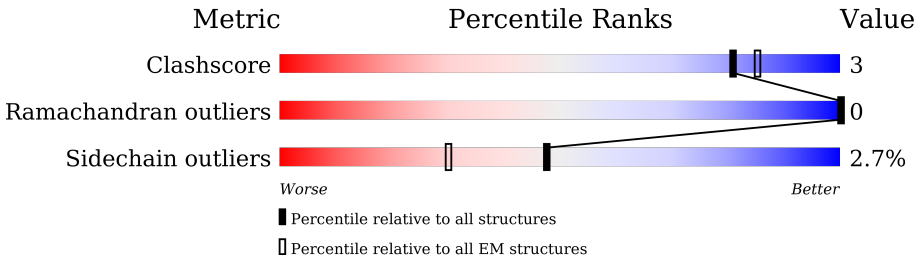
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.1

1 Overall quality at a glance

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

The reported resolution of this entry is 2.20 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	A	358	42% · · 54%
1	B	358	42% · · 54%
1	C	358	42% · · 54%
1	D	358	42% · · 54%
1	E	358	42% · · 54%
1	F	358	42% · · 54%
1	G	358	42% · · 54%
1	H	358	42% · · 54%

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Mol	Chain	Length	Quality of chain
1	I	358	
1	J	358	
1	K	358	
1	L	358	

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 37932 atoms, of which 19452 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 Gap junction delta-2 protein,Soluble cytochrome b562.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	166	Total	C	H	N	O	S	0	0
			2664	876	1334	212	229	13		
1	B	166	Total	C	H	N	O	S	0	0
			2664	876	1334	212	229	13		
1	C	166	Total	C	H	N	O	S	0	0
			2664	876	1334	212	229	13		
1	D	166	Total	C	H	N	O	S	0	0
			2664	876	1334	212	229	13		
1	E	166	Total	C	H	N	O	S	0	0
			2664	876	1334	212	229	13		
1	F	166	Total	C	H	N	O	S	0	0
			2664	876	1334	212	229	13		
1	G	166	Total	C	H	N	O	S	0	0
			2664	876	1334	212	229	13		
1	H	166	Total	C	H	N	O	S	0	0
			2664	876	1334	212	229	13		
1	I	166	Total	C	H	N	O	S	0	0
			2664	876	1334	212	229	13		
1	J	166	Total	C	H	N	O	S	0	0
			2664	876	1334	212	229	13		
1	K	166	Total	C	H	N	O	S	0	0
			2664	876	1334	212	229	13		
1	L	166	Total	C	H	N	O	S	0	0
			2664	876	1334	212	229	13		

There are 156 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	101N	TRP	MET	engineered mutation	UNP P0ABE7
A	105E	ILE	HIS	engineered mutation	UNP P0ABE7
A	105I	LEU	ARG	engineered mutation	UNP P0ABE7
A	322	SER	-	expression tag	UNP Q9UKL4
A	323	ARG	-	expression tag	UNP Q9UKL4
A	324	ASP	-	expression tag	UNP Q9UKL4

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Chain	Residue	Modelled	Actual	Comment	Reference
A	325	TYR	-	expression tag	UNP Q9UKL4
A	326	LYS	-	expression tag	UNP Q9UKL4
A	327	ASP	-	expression tag	UNP Q9UKL4
A	328	ASP	-	expression tag	UNP Q9UKL4
A	329	ASP	-	expression tag	UNP Q9UKL4
A	330	ASP	-	expression tag	UNP Q9UKL4
A	331	LYS	-	expression tag	UNP Q9UKL4
B	101N	TRP	MET	engineered mutation	UNP P0ABE7
B	105E	ILE	HIS	engineered mutation	UNP P0ABE7
B	105I	LEU	ARG	engineered mutation	UNP P0ABE7
B	322	SER	-	expression tag	UNP Q9UKL4
B	323	ARG	-	expression tag	UNP Q9UKL4
B	324	ASP	-	expression tag	UNP Q9UKL4
B	325	TYR	-	expression tag	UNP Q9UKL4
B	326	LYS	-	expression tag	UNP Q9UKL4
B	327	ASP	-	expression tag	UNP Q9UKL4
B	328	ASP	-	expression tag	UNP Q9UKL4
B	329	ASP	-	expression tag	UNP Q9UKL4
B	330	ASP	-	expression tag	UNP Q9UKL4
B	331	LYS	-	expression tag	UNP Q9UKL4
C	101N	TRP	MET	engineered mutation	UNP P0ABE7
C	105E	ILE	HIS	engineered mutation	UNP P0ABE7
C	105I	LEU	ARG	engineered mutation	UNP P0ABE7
C	322	SER	-	expression tag	UNP Q9UKL4
C	323	ARG	-	expression tag	UNP Q9UKL4
C	324	ASP	-	expression tag	UNP Q9UKL4
C	325	TYR	-	expression tag	UNP Q9UKL4
C	326	LYS	-	expression tag	UNP Q9UKL4
C	327	ASP	-	expression tag	UNP Q9UKL4
C	328	ASP	-	expression tag	UNP Q9UKL4
C	329	ASP	-	expression tag	UNP Q9UKL4
C	330	ASP	-	expression tag	UNP Q9UKL4
C	331	LYS	-	expression tag	UNP Q9UKL4
D	101N	TRP	MET	engineered mutation	UNP P0ABE7
D	105E	ILE	HIS	engineered mutation	UNP P0ABE7
D	105I	LEU	ARG	engineered mutation	UNP P0ABE7
D	322	SER	-	expression tag	UNP Q9UKL4
D	323	ARG	-	expression tag	UNP Q9UKL4
D	324	ASP	-	expression tag	UNP Q9UKL4
D	325	TYR	-	expression tag	UNP Q9UKL4
D	326	LYS	-	expression tag	UNP Q9UKL4
D	327	ASP	-	expression tag	UNP Q9UKL4

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Chain	Residue	Modelled	Actual	Comment	Reference
D	328	ASP	-	expression tag	UNP Q9UKL4
D	329	ASP	-	expression tag	UNP Q9UKL4
D	330	ASP	-	expression tag	UNP Q9UKL4
D	331	LYS	-	expression tag	UNP Q9UKL4
E	101N	TRP	MET	engineered mutation	UNP P0ABE7
E	105E	ILE	HIS	engineered mutation	UNP P0ABE7
E	105I	LEU	ARG	engineered mutation	UNP P0ABE7
E	322	SER	-	expression tag	UNP Q9UKL4
E	323	ARG	-	expression tag	UNP Q9UKL4
E	324	ASP	-	expression tag	UNP Q9UKL4
E	325	TYR	-	expression tag	UNP Q9UKL4
E	326	LYS	-	expression tag	UNP Q9UKL4
E	327	ASP	-	expression tag	UNP Q9UKL4
E	328	ASP	-	expression tag	UNP Q9UKL4
E	329	ASP	-	expression tag	UNP Q9UKL4
E	330	ASP	-	expression tag	UNP Q9UKL4
E	331	LYS	-	expression tag	UNP Q9UKL4
F	101N	TRP	MET	engineered mutation	UNP P0ABE7
F	105E	ILE	HIS	engineered mutation	UNP P0ABE7
F	105I	LEU	ARG	engineered mutation	UNP P0ABE7
F	322	SER	-	expression tag	UNP Q9UKL4
F	323	ARG	-	expression tag	UNP Q9UKL4
F	324	ASP	-	expression tag	UNP Q9UKL4
F	325	TYR	-	expression tag	UNP Q9UKL4
F	326	LYS	-	expression tag	UNP Q9UKL4
F	327	ASP	-	expression tag	UNP Q9UKL4
F	328	ASP	-	expression tag	UNP Q9UKL4
F	329	ASP	-	expression tag	UNP Q9UKL4
F	330	ASP	-	expression tag	UNP Q9UKL4
F	331	LYS	-	expression tag	UNP Q9UKL4
G	101N	TRP	MET	engineered mutation	UNP P0ABE7
G	105E	ILE	HIS	engineered mutation	UNP P0ABE7
G	105I	LEU	ARG	engineered mutation	UNP P0ABE7
G	322	SER	-	expression tag	UNP Q9UKL4
G	323	ARG	-	expression tag	UNP Q9UKL4
G	324	ASP	-	expression tag	UNP Q9UKL4
G	325	TYR	-	expression tag	UNP Q9UKL4
G	326	LYS	-	expression tag	UNP Q9UKL4
G	327	ASP	-	expression tag	UNP Q9UKL4
G	328	ASP	-	expression tag	UNP Q9UKL4
G	329	ASP	-	expression tag	UNP Q9UKL4
G	330	ASP	-	expression tag	UNP Q9UKL4

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Chain	Residue	Modelled	Actual	Comment	Reference
G	331	LYS	-	expression tag	UNP Q9UKL4
H	101N	TRP	MET	engineered mutation	UNP P0ABE7
H	105E	ILE	HIS	engineered mutation	UNP P0ABE7
H	105I	LEU	ARG	engineered mutation	UNP P0ABE7
H	322	SER	-	expression tag	UNP Q9UKL4
H	323	ARG	-	expression tag	UNP Q9UKL4
H	324	ASP	-	expression tag	UNP Q9UKL4
H	325	TYR	-	expression tag	UNP Q9UKL4
H	326	LYS	-	expression tag	UNP Q9UKL4
H	327	ASP	-	expression tag	UNP Q9UKL4
H	328	ASP	-	expression tag	UNP Q9UKL4
H	329	ASP	-	expression tag	UNP Q9UKL4
H	330	ASP	-	expression tag	UNP Q9UKL4
H	331	LYS	-	expression tag	UNP Q9UKL4
I	101N	TRP	MET	engineered mutation	UNP P0ABE7
I	105E	ILE	HIS	engineered mutation	UNP P0ABE7
I	105I	LEU	ARG	engineered mutation	UNP P0ABE7
I	322	SER	-	expression tag	UNP Q9UKL4
I	323	ARG	-	expression tag	UNP Q9UKL4
I	324	ASP	-	expression tag	UNP Q9UKL4
I	325	TYR	-	expression tag	UNP Q9UKL4
I	326	LYS	-	expression tag	UNP Q9UKL4
I	327	ASP	-	expression tag	UNP Q9UKL4
I	328	ASP	-	expression tag	UNP Q9UKL4
I	329	ASP	-	expression tag	UNP Q9UKL4
I	330	ASP	-	expression tag	UNP Q9UKL4
I	331	LYS	-	expression tag	UNP Q9UKL4
J	101N	TRP	MET	engineered mutation	UNP P0ABE7
J	105E	ILE	HIS	engineered mutation	UNP P0ABE7
J	105I	LEU	ARG	engineered mutation	UNP P0ABE7
J	322	SER	-	expression tag	UNP Q9UKL4
J	323	ARG	-	expression tag	UNP Q9UKL4
J	324	ASP	-	expression tag	UNP Q9UKL4
J	325	TYR	-	expression tag	UNP Q9UKL4
J	326	LYS	-	expression tag	UNP Q9UKL4
J	327	ASP	-	expression tag	UNP Q9UKL4
J	328	ASP	-	expression tag	UNP Q9UKL4
J	329	ASP	-	expression tag	UNP Q9UKL4
J	330	ASP	-	expression tag	UNP Q9UKL4
J	331	LYS	-	expression tag	UNP Q9UKL4
K	101N	TRP	MET	engineered mutation	UNP P0ABE7
K	105E	ILE	HIS	engineered mutation	UNP P0ABE7

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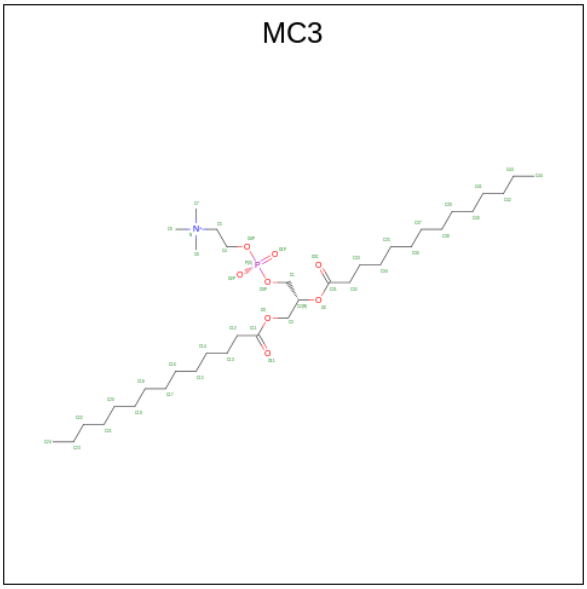
Chain	Residue	Modelled	Actual	Comment	Reference
K	105I	LEU	ARG	engineered mutation	UNP P0ABE7
K	322	SER	-	expression tag	UNP Q9UKL4
K	323	ARG	-	expression tag	UNP Q9UKL4
K	324	ASP	-	expression tag	UNP Q9UKL4
K	325	TYR	-	expression tag	UNP Q9UKL4
K	326	LYS	-	expression tag	UNP Q9UKL4
K	327	ASP	-	expression tag	UNP Q9UKL4
K	328	ASP	-	expression tag	UNP Q9UKL4
K	329	ASP	-	expression tag	UNP Q9UKL4
K	330	ASP	-	expression tag	UNP Q9UKL4
K	331	LYS	-	expression tag	UNP Q9UKL4
L	101N	TRP	MET	engineered mutation	UNP P0ABE7
L	105E	ILE	HIS	engineered mutation	UNP P0ABE7
L	105I	LEU	ARG	engineered mutation	UNP P0ABE7
L	322	SER	-	expression tag	UNP Q9UKL4
L	323	ARG	-	expression tag	UNP Q9UKL4
L	324	ASP	-	expression tag	UNP Q9UKL4
L	325	TYR	-	expression tag	UNP Q9UKL4
L	326	LYS	-	expression tag	UNP Q9UKL4
L	327	ASP	-	expression tag	UNP Q9UKL4
L	328	ASP	-	expression tag	UNP Q9UKL4
L	329	ASP	-	expression tag	UNP Q9UKL4
L	330	ASP	-	expression tag	UNP Q9UKL4
L	331	LYS	-	expression tag	UNP Q9UKL4

- Molecule 2 is 1,2-DIMYRISTOYL-RAC-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: MC3) (formula: $C_{36}H_{72}NO_8P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
2	A	1	Total	C	H	0
			41	14	27	
2	A	1	Total	C	H	0
			27	9	18	
2	A	1	Total	C	H	0
			31	10	21	
2	A	1	Total	C	H	0
			24	8	16	
2	A	1	Total	C	H	0
			37	13	24	
2	A	1	Total	C	H	0
			28	10	18	
2	B	1	Total	C	H	0
			41	14	27	
2	B	1	Total	C	H	0
			27	9	18	
2	B	1	Total	C	H	0
			31	10	21	
2	B	1	Total	C	H	0
			24	8	16	
2	B	1	Total	C	H	0
			37	13	24	
2	B	1	Total	C	H	0
			28	10	18	
2	C	1	Total	C	H	0
			41	14	27	
2	C	1	Total	C	H	0
			27	9	18	
2	C	1	Total	C	H	0
			31	10	21	
2	C	1	Total	C	H	0
			24	8	16	
2	C	1	Total	C	H	0
			37	13	24	
2	C	1	Total	C	H	0
			28	10	18	
2	D	1	Total	C	H	0
			41	14	27	
2	D	1	Total	C	H	0
			27	9	18	
2	D	1	Total	C	H	0
			31	10	21	
2	D	1	Total	C	H	0
			24	8	16	

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Mol	Chain	Residues	Atoms	AltConf
2	D	1	Total C H 37 13 24	0
2	D	1	Total C H 28 10 18	0
2	E	1	Total C H 41 14 27	0
2	E	1	Total C H 27 9 18	0
2	E	1	Total C H 31 10 21	0
2	E	1	Total C H 24 8 16	0
2	E	1	Total C H 37 13 24	0
2	E	1	Total C H 28 10 18	0
2	F	1	Total C H 41 14 27	0
2	F	1	Total C H 27 9 18	0
2	F	1	Total C H 31 10 21	0
2	F	1	Total C H 24 8 16	0
2	F	1	Total C H 37 13 24	0
2	F	1	Total C H 28 10 18	0
2	G	1	Total C H 41 14 27	0
2	G	1	Total C H 27 9 18	0
2	G	1	Total C H 31 10 21	0
2	G	1	Total C H 24 8 16	0
2	G	1	Total C H 37 13 24	0
2	G	1	Total C H 28 10 18	0
2	H	1	Total C H 41 14 27	0

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Mol	Chain	Residues	Atoms	AltConf
2	H	1	Total C H 27 9 18	0
2	H	1	Total C H 31 10 21	0
2	H	1	Total C H 24 8 16	0
2	H	1	Total C H 37 13 24	0
2	H	1	Total C H 28 10 18	0
2	I	1	Total C H 41 14 27	0
2	I	1	Total C H 27 9 18	0
2	I	1	Total C H 31 10 21	0
2	I	1	Total C H 24 8 16	0
2	I	1	Total C H 37 13 24	0
2	I	1	Total C H 28 10 18	0
2	J	1	Total C H 41 14 27	0
2	J	1	Total C H 27 9 18	0
2	J	1	Total C H 31 10 21	0
2	J	1	Total C H 24 8 16	0
2	J	1	Total C H 37 13 24	0
2	J	1	Total C H 28 10 18	0
2	K	1	Total C H 41 14 27	0
2	K	1	Total C H 27 9 18	0
2	K	1	Total C H 31 10 21	0
2	K	1	Total C H 24 8 16	0

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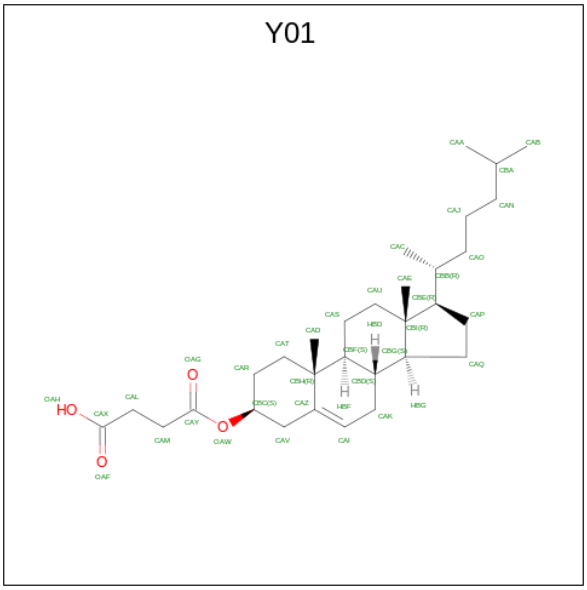
Mol	Chain	Residues	Atoms	AltConf
2	K	1	Total C H 37 13 24	0
2	K	1	Total C H 28 10 18	0
2	L	1	Total C H 41 14 27	0
2	L	1	Total C H 27 9 18	0
2	L	1	Total C H 31 10 21	0
2	L	1	Total C H 24 8 16	0
2	L	1	Total C H 37 13 24	0
2	L	1	Total C H 28 10 18	0

- Molecule 3 is CHOLESTEROL HEMISUCCINATE (three-letter code: Y01) (formula: $C_{31}H_{50}O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
3	A	1	Total C H O 84 31 49 4	0
3	A	1	Total C H O 84 31 49 4	0
3	B	1	Total C H O 84 31 49 4	0

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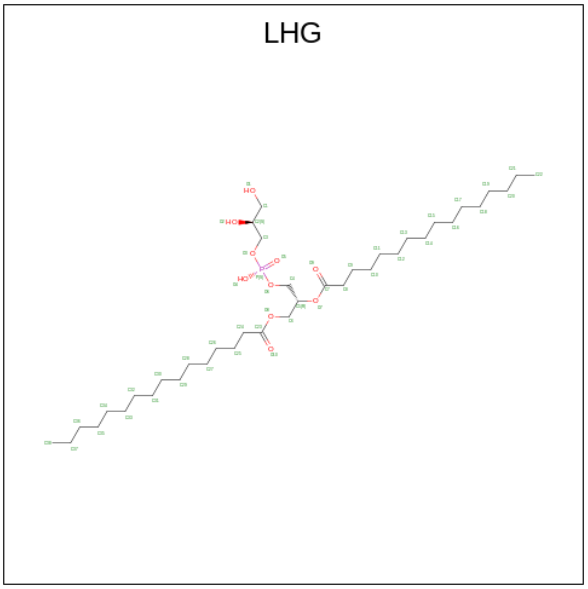
Mol	Chain	Residues	Atoms				AltConf
3	B	1	Total	C	H	O	0
			84	31	49	4	
3	C	1	Total	C	H	O	0
			84	31	49	4	
3	C	1	Total	C	H	O	0
			84	31	49	4	
3	D	1	Total	C	H	O	0
			84	31	49	4	
3	D	1	Total	C	H	O	0
			84	31	49	4	
3	E	1	Total	C	H	O	0
			84	31	49	4	
3	E	1	Total	C	H	O	0
			84	31	49	4	
3	F	1	Total	C	H	O	0
			84	31	49	4	
3	F	1	Total	C	H	O	0
			84	31	49	4	
3	G	1	Total	C	H	O	0
			84	31	49	4	
3	G	1	Total	C	H	O	0
			84	31	49	4	
3	H	1	Total	C	H	O	0
			84	31	49	4	
3	H	1	Total	C	H	O	0
			84	31	49	4	
3	I	1	Total	C	H	O	0
			84	31	49	4	
3	I	1	Total	C	H	O	0
			84	31	49	4	
3	J	1	Total	C	H	O	0
			84	31	49	4	
3	J	1	Total	C	H	O	0
			84	31	49	4	
3	K	1	Total	C	H	O	0
			84	31	49	4	
3	K	1	Total	C	H	O	0
			84	31	49	4	
3	L	1	Total	C	H	O	0
			84	31	49	4	
3	L	1	Total	C	H	O	0
			84	31	49	4	

- Molecule 4 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total	C	H	O	0
			104	35	65	4	
4	B	1	Total	C	H	O	0
			104	35	65	4	
4	C	1	Total	C	H	O	0
			104	35	65	4	
4	D	1	Total	C	H	O	0
			104	35	65	4	
4	E	1	Total	C	H	O	0
			104	35	65	4	
4	F	1	Total	C	H	O	0
			104	35	65	4	
4	G	1	Total	C	H	O	0
			104	35	65	4	
4	H	1	Total	C	H	O	0
			104	35	65	4	
4	I	1	Total	C	H	O	0
			104	35	65	4	
4	J	1	Total	C	H	O	0
			104	35	65	4	
4	K	1	Total	C	H	O	0
			104	35	65	4	
4	L	1	Total	C	H	O	0
			104	35	65	4	

- Molecule 5 is water.

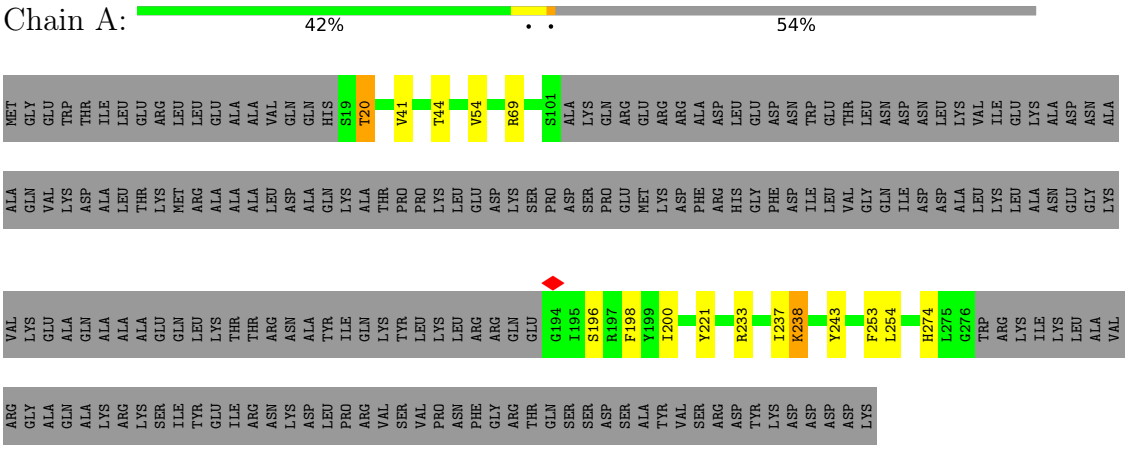
Mol	Chain	Residues	Atoms	AltConf
5	A	37	Total O 37 37	0
5	B	37	Total O 37 37	0
5	C	37	Total O 37 37	0
5	D	37	Total O 37 37	0
5	E	37	Total O 37 37	0
5	F	37	Total O 37 37	0
5	G	37	Total O 37 37	0
5	H	37	Total O 37 37	0
5	I	37	Total O 37 37	0
5	J	37	Total O 37 37	0
5	K	37	Total O 37 37	0
5	L	37	Total O 37 37	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.

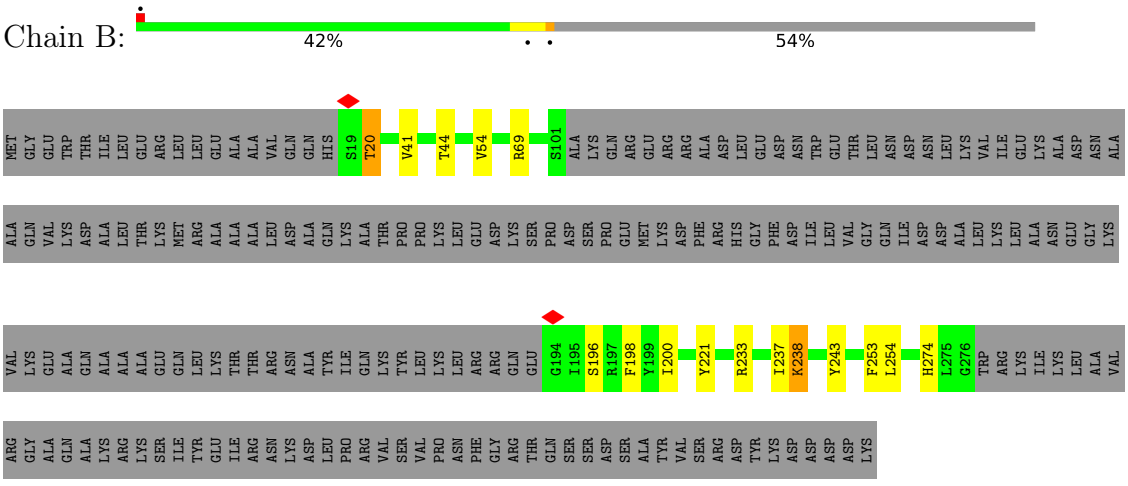
• Molecule 1: Gap junction delta-2 protein,Soluble cytochrome b562

Chain A:



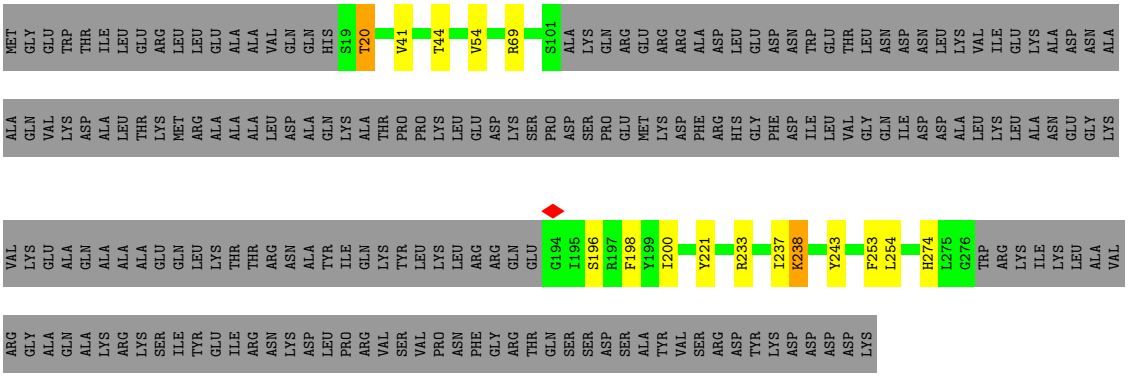
• Molecule 1: Gap junction delta-2 protein,Soluble cytochrome b562

Chain B:



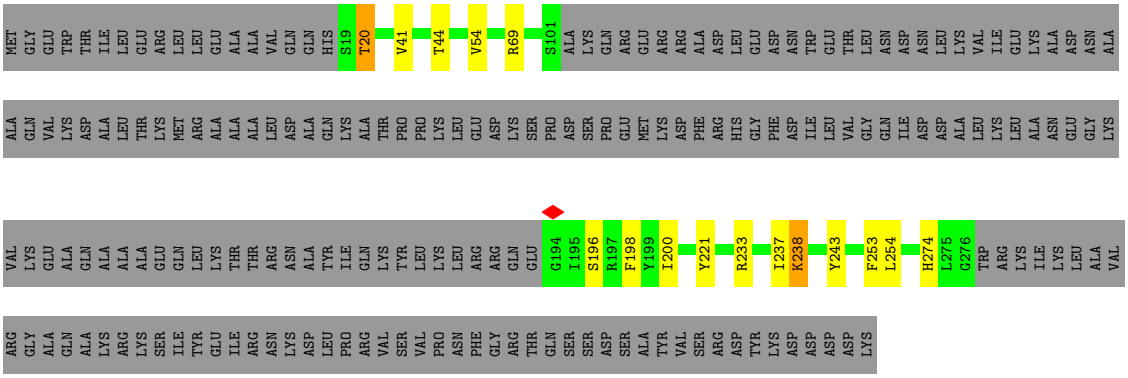
• Molecule 1: Gap junction delta-2 protein,Soluble cytochrome b562

Chain C:



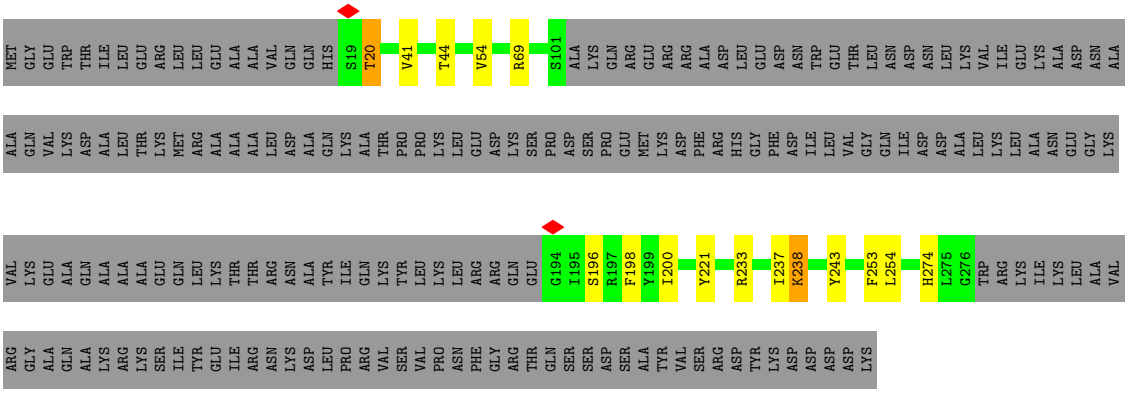
• Molecule 1: Gap junction delta-2 protein,Soluble cytochrome b562

Chain D:



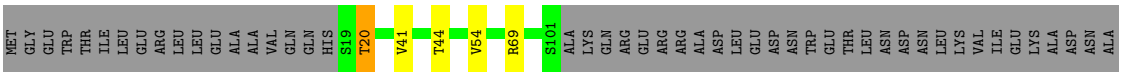
• Molecule 1: Gap junction delta-2 protein,Soluble cytochrome b562

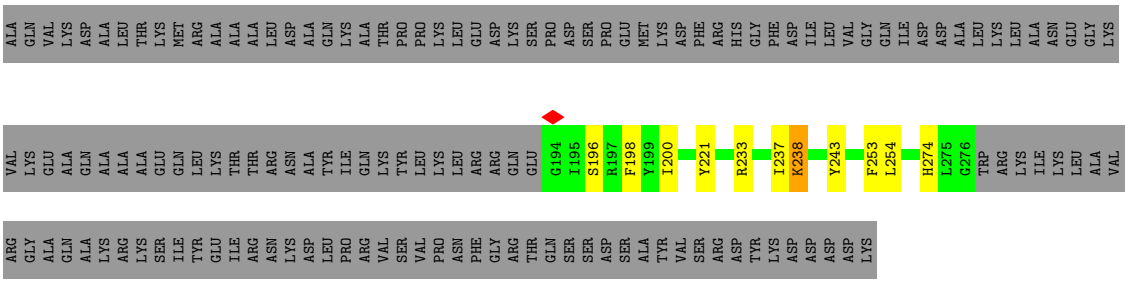
Chain E:



• Molecule 1: Gap junction delta-2 protein,Soluble cytochrome b562

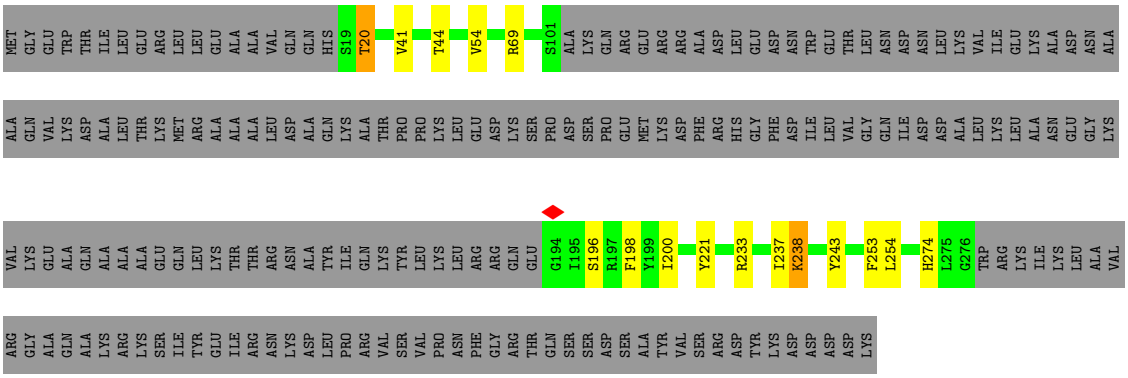
Chain F:





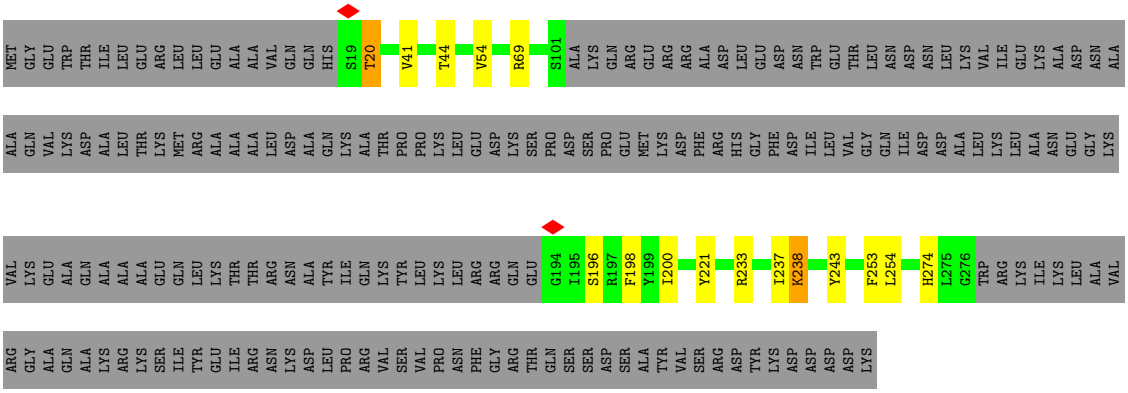
• Molecule 1: Gap junction delta-2 protein,Soluble cytochrome b562

Chain G:



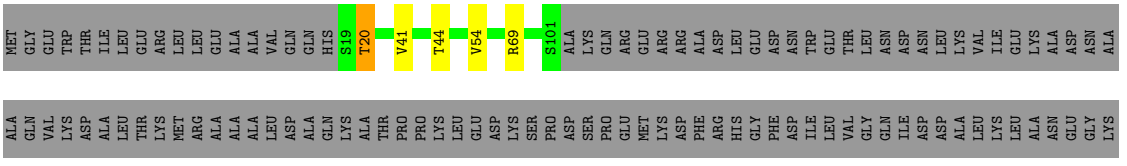
• Molecule 1: Gap junction delta-2 protein,Soluble cytochrome b562

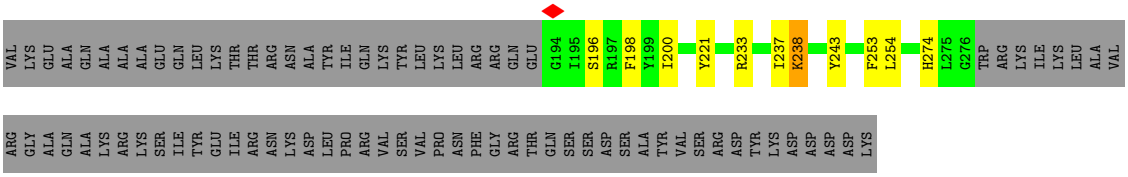
Chain H:



• Molecule 1: Gap junction delta-2 protein,Soluble cytochrome b562

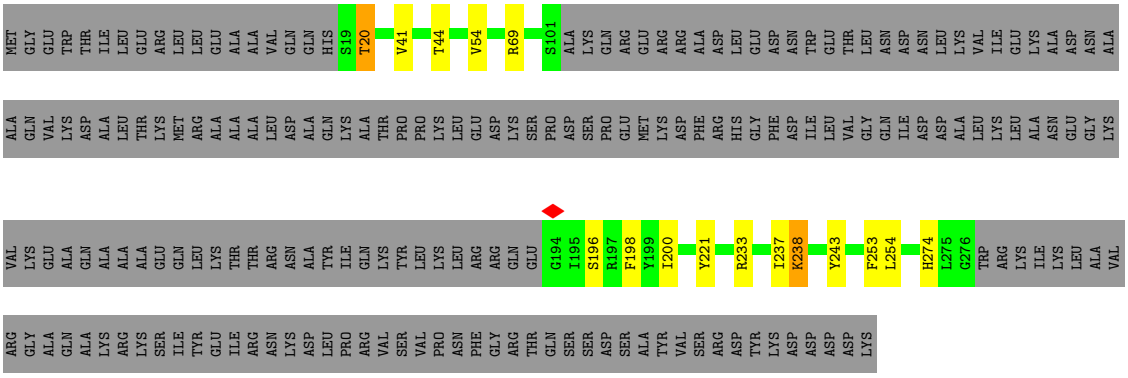
Chain I:





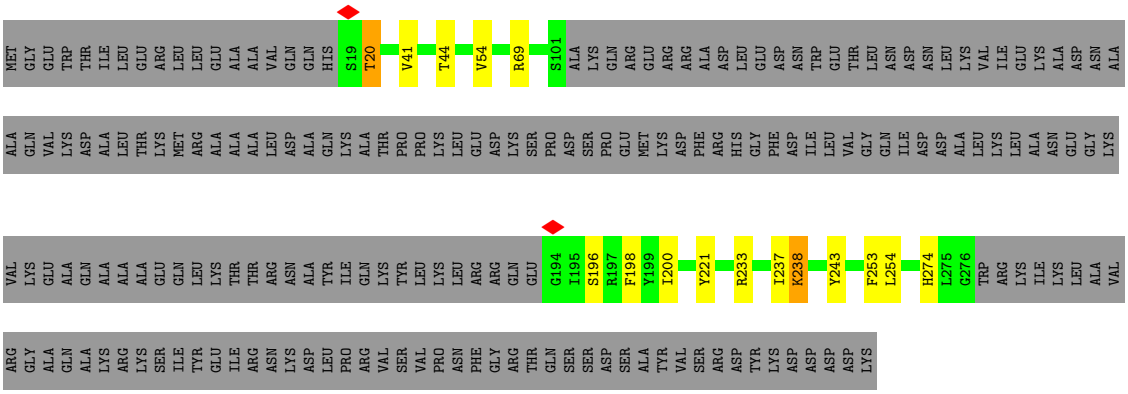
• Molecule 1: Gap junction delta-2 protein,Soluble cytochrome b562

Chain J:



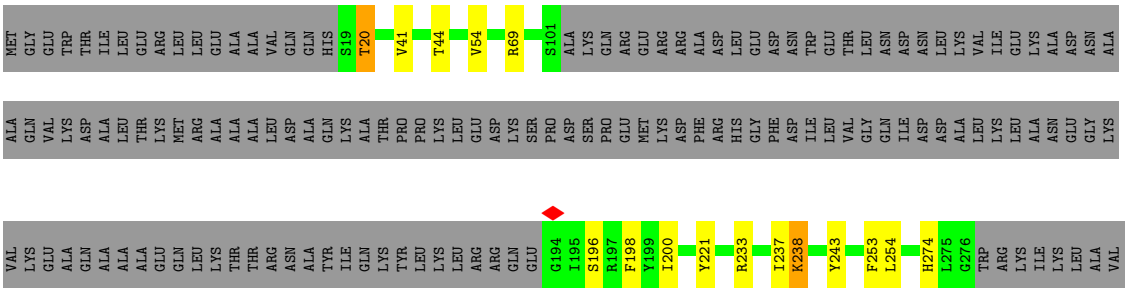
• Molecule 1: Gap junction delta-2 protein,Soluble cytochrome b562

Chain K:



• Molecule 1: Gap junction delta-2 protein,Soluble cytochrome b562

Chain L:



ARG GLY ALA GLN ALA LYS ARG LYS SER ILE TYR GLU ILE ARG ASN LYS ASP LEU PRO ARG VAL SER VAL PRO ASN PHE GLY ARG THR GLN SER SER ASP SER ALA TYR VAL SER ARG ASP TYR LYS ASP ASP ASP ASP LYS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	70095	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	6.331	Depositor
Minimum map value	-3.739	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.155	Depositor
Recommended contour level	0.45	Depositor
Map size (Å)	364.5, 364.5, 364.5	wwPDB
Map dimensions	540, 540, 540	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.675, 0.675, 0.675	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MC3, LHG, Y01

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	A	0.88	3/1362 (0.2%)	0.78	1/1852 (0.1%)
1	B	0.88	3/1362 (0.2%)	0.78	1/1852 (0.1%)
1	C	0.88	3/1362 (0.2%)	0.78	1/1852 (0.1%)
1	D	0.88	3/1362 (0.2%)	0.78	1/1852 (0.1%)
1	E	0.88	3/1362 (0.2%)	0.78	1/1852 (0.1%)
1	F	0.88	3/1362 (0.2%)	0.78	1/1852 (0.1%)
1	G	0.88	3/1362 (0.2%)	0.78	1/1852 (0.1%)
1	H	0.88	3/1362 (0.2%)	0.78	1/1852 (0.1%)
1	I	0.88	3/1362 (0.2%)	0.78	1/1852 (0.1%)
1	J	0.88	3/1362 (0.2%)	0.78	1/1852 (0.1%)
1	K	0.88	3/1362 (0.2%)	0.78	1/1852 (0.1%)
1	L	0.88	3/1362 (0.2%)	0.78	1/1852 (0.1%)
All	All	0.88	36/16344 (0.2%)	0.78	12/22224 (0.1%)

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	54	VAL	CB-CG2	-5.47	1.41	1.52
1	I	54	VAL	CB-CG2	-5.47	1.41	1.52
1	L	54	VAL	CB-CG2	-5.46	1.41	1.52
1	E	54	VAL	CB-CG2	-5.46	1.41	1.52
1	H	54	VAL	CB-CG2	-5.46	1.41	1.52
1	A	54	VAL	CB-CG2	-5.45	1.41	1.52
1	D	54	VAL	CB-CG2	-5.45	1.41	1.52
1	G	54	VAL	CB-CG2	-5.45	1.41	1.52
1	J	54	VAL	CB-CG2	-5.45	1.41	1.52
1	C	54	VAL	CB-CG2	-5.44	1.41	1.52
1	B	54	VAL	CB-CG2	-5.43	1.41	1.52
1	K	54	VAL	CB-CG2	-5.43	1.41	1.52
1	H	243	TYR	CD2-CE2	-5.34	1.31	1.39
1	E	243	TYR	CD2-CE2	-5.34	1.31	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	243	TYR	CD2-CE2	-5.32	1.31	1.39
1	I	243	TYR	CD2-CE2	-5.32	1.31	1.39
1	L	243	TYR	CD2-CE2	-5.32	1.31	1.39
1	A	243	TYR	CD2-CE2	-5.32	1.31	1.39
1	B	243	TYR	CD2-CE2	-5.32	1.31	1.39
1	D	243	TYR	CD2-CE2	-5.32	1.31	1.39
1	G	243	TYR	CD2-CE2	-5.32	1.31	1.39
1	J	243	TYR	CD2-CE2	-5.32	1.31	1.39
1	K	243	TYR	CD2-CE2	-5.32	1.31	1.39
1	F	243	TYR	CD2-CE2	-5.30	1.31	1.39
1	L	221	TYR	CD2-CE2	-5.08	1.31	1.39
1	B	221	TYR	CD2-CE2	-5.06	1.31	1.39
1	E	221	TYR	CD2-CE2	-5.06	1.31	1.39
1	A	221	TYR	CD2-CE2	-5.03	1.31	1.39
1	D	221	TYR	CD2-CE2	-5.03	1.31	1.39
1	G	221	TYR	CD2-CE2	-5.03	1.31	1.39
1	H	221	TYR	CD2-CE2	-5.03	1.31	1.39
1	J	221	TYR	CD2-CE2	-5.03	1.31	1.39
1	K	221	TYR	CD2-CE2	-5.03	1.31	1.39
1	C	221	TYR	CD2-CE2	-5.02	1.31	1.39
1	F	221	TYR	CD2-CE2	-5.02	1.31	1.39
1	I	221	TYR	CD2-CE2	-5.02	1.31	1.39

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	254	LEU	CA-CB-CG	5.88	128.82	115.30
1	C	254	LEU	CA-CB-CG	5.88	128.82	115.30
1	A	254	LEU	CA-CB-CG	5.87	128.80	115.30
1	D	254	LEU	CA-CB-CG	5.87	128.80	115.30
1	G	254	LEU	CA-CB-CG	5.87	128.80	115.30
1	H	254	LEU	CA-CB-CG	5.87	128.80	115.30
1	J	254	LEU	CA-CB-CG	5.87	128.80	115.30
1	F	254	LEU	CA-CB-CG	5.87	128.79	115.30
1	I	254	LEU	CA-CB-CG	5.87	128.79	115.30
1	K	254	LEU	CA-CB-CG	5.86	128.78	115.30
1	L	254	LEU	CA-CB-CG	5.86	128.79	115.30
1	E	254	LEU	CA-CB-CG	5.85	128.76	115.30

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	A	1330	1334	1333	5	0
1	B	1330	1334	1333	5	0
1	C	1330	1334	1333	5	0
1	D	1330	1334	1333	5	0
1	E	1330	1334	1333	5	0
1	F	1330	1334	1333	5	0
1	G	1330	1334	1333	5	0
1	H	1330	1334	1333	5	0
1	I	1330	1334	1333	5	0
1	J	1330	1334	1333	5	0
1	K	1330	1334	1333	5	0
1	L	1330	1334	1333	5	0
2	A	64	124	110	0	0
2	B	64	124	110	0	0
2	C	64	124	110	1	0
2	D	64	124	110	0	0
2	E	64	124	110	0	0
2	F	64	124	110	0	0
2	G	64	124	110	0	0
2	H	64	124	110	0	0
2	I	64	124	110	0	0
2	J	64	124	110	0	0
2	K	64	124	110	0	0
2	L	64	124	110	1	0
3	A	70	98	96	3	0
3	B	70	98	96	3	0
3	C	70	98	96	3	0
3	D	70	98	96	3	0
3	E	70	98	96	3	0
3	F	70	98	96	3	0
3	G	70	98	96	3	0
3	H	70	98	96	3	0
3	I	70	98	96	3	0
3	J	70	98	96	3	0
3	K	70	98	96	3	0
3	L	70	98	96	3	0
4	A	39	65	65	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	39	65	65	0	0
4	C	39	65	65	0	0
4	D	39	65	65	0	0
4	E	39	65	65	0	0
4	F	39	65	65	0	0
4	G	39	65	65	0	0
4	H	39	65	65	0	0
4	I	39	65	65	0	0
4	J	39	65	65	0	0
4	K	39	65	65	0	0
4	L	39	65	65	0	0
5	A	37	0	0	0	0
5	B	37	0	0	0	0
5	C	37	0	0	0	0
5	D	37	0	0	0	0
5	E	37	0	0	0	0
5	F	37	0	0	0	0
5	G	37	0	0	0	0
5	H	37	0	0	0	0
5	I	37	0	0	0	0
5	J	37	0	0	0	0
5	K	37	0	0	0	0
5	L	37	0	0	0	0
All	All	18480	19452	19248	98	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 3.

All (98) 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)
3:B:405:Y01:HAU2	3:B:405:Y01:HAC1	1.76	0.67
3:A:405:Y01:HAC1	3:A:405:Y01:HAU2	1.76	0.67
3:J:405:Y01:HAU2	3:J:405:Y01:HAC1	1.76	0.67
3:K:405:Y01:HAC1	3:K:405:Y01:HAU2	1.77	0.67
3:I:405:Y01:HAC1	3:I:405:Y01:HAU2	1.76	0.67
3:G:405:Y01:HAC1	3:G:405:Y01:HAU2	1.76	0.67
3:D:405:Y01:HAC1	3:D:405:Y01:HAU2	1.76	0.67
3:F:405:Y01:HAU2	3:F:405:Y01:HAC1	1.77	0.67
3:E:405:Y01:HAC1	3:E:405:Y01:HAU2	1.76	0.66
3:H:405:Y01:HAC1	3:H:405:Y01:HAU2	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:405:Y01:HAC1	3:C:405:Y01:HAU2	1.76	0.66
3:L:405:Y01:HAC1	3:L:405:Y01:HAU2	1.76	0.65
3:F:405:Y01:HAD1	3:F:405:Y01:OAW	2.06	0.56
3:I:405:Y01:HAD1	3:I:405:Y01:OAW	2.06	0.56
1:B:41:VAL:O	1:B:44:THR:HG22	2.06	0.56
1:K:41:VAL:O	1:K:44:THR:HG22	2.06	0.56
3:C:405:Y01:HAD1	3:C:405:Y01:OAW	2.06	0.55
1:D:41:VAL:O	1:D:44:THR:HG22	2.06	0.55
3:L:405:Y01:HAD1	3:L:405:Y01:OAW	2.06	0.55
1:G:41:VAL:O	1:G:44:THR:HG22	2.06	0.55
3:A:405:Y01:OAW	3:A:405:Y01:HAD1	2.06	0.55
1:I:41:VAL:O	1:I:44:THR:HG22	2.06	0.55
3:J:405:Y01:HAD1	3:J:405:Y01:OAW	2.06	0.55
1:F:41:VAL:O	1:F:44:THR:HG22	2.06	0.55
3:K:405:Y01:HAD1	3:K:405:Y01:OAW	2.06	0.55
1:L:41:VAL:O	1:L:44:THR:HG22	2.06	0.55
3:B:405:Y01:HAD1	3:B:405:Y01:OAW	2.06	0.55
1:C:41:VAL:O	1:C:44:THR:HG22	2.06	0.55
3:G:405:Y01:HAD1	3:G:405:Y01:OAW	2.06	0.55
3:D:405:Y01:OAW	3:D:405:Y01:HAD1	2.06	0.55
1:A:41:VAL:O	1:A:44:THR:HG22	2.06	0.55
1:E:41:VAL:O	1:E:44:THR:HG22	2.06	0.55
1:H:41:VAL:O	1:H:44:THR:HG22	2.06	0.55
1:J:41:VAL:O	1:J:44:THR:HG22	2.06	0.55
3:E:405:Y01:OAW	3:E:405:Y01:HAD1	2.06	0.54
3:H:405:Y01:OAW	3:H:405:Y01:HAD1	2.06	0.54
1:F:69:ARG:HD3	1:F:233:ARG:HH11	1.78	0.49
1:I:69:ARG:HD3	1:I:233:ARG:HH11	1.78	0.49
1:A:69:ARG:HD3	1:A:233:ARG:HH11	1.78	0.48
1:B:69:ARG:HD3	1:B:233:ARG:HH11	1.78	0.48
1:K:69:ARG:HD3	1:K:233:ARG:HH11	1.78	0.48
1:J:69:ARG:HD3	1:J:233:ARG:HH11	1.78	0.48
1:E:69:ARG:HD3	1:E:233:ARG:HH11	1.78	0.48
1:H:69:ARG:HD3	1:H:233:ARG:HH11	1.78	0.48
1:C:69:ARG:HD3	1:C:233:ARG:HH11	1.78	0.47
1:G:69:ARG:HD3	1:G:233:ARG:HH11	1.78	0.47
1:L:69:ARG:HD3	1:L:233:ARG:HH11	1.78	0.47
1:D:69:ARG:HD3	1:D:233:ARG:HH11	1.78	0.47
1:F:237:ILE:HG22	1:F:238:LYS:CE	2.45	0.47
1:I:237:ILE:HG22	1:I:238:LYS:CE	2.45	0.47
1:D:237:ILE:HG22	1:D:238:LYS:CE	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:405:Y01:HAC1	3:F:405:Y01:CAU	2.45	0.47
1:G:237:ILE:HG22	1:G:238:LYS:CE	2.45	0.47
3:I:405:Y01:HAC1	3:I:405:Y01:CAU	2.44	0.47
1:K:237:ILE:HG22	1:K:238:LYS:CE	2.45	0.47
1:L:237:ILE:HG22	1:L:238:LYS:CE	2.45	0.47
1:B:237:ILE:HG22	1:B:238:LYS:CE	2.45	0.46
1:C:237:ILE:HG22	1:C:238:LYS:CE	2.45	0.46
1:A:237:ILE:HG22	1:A:238:LYS:CE	2.45	0.46
1:H:237:ILE:HG22	1:H:238:LYS:CE	2.45	0.46
1:E:237:ILE:HG22	1:E:238:LYS:CE	2.45	0.46
1:J:237:ILE:HG22	1:J:238:LYS:CE	2.45	0.46
1:E:196:SER:O	1:E:200:ILE:HG12	2.17	0.45
1:H:196:SER:O	1:H:200:ILE:HG12	2.17	0.45
1:D:20:THR:HG21	1:D:274:HIS:CG	2.52	0.45
1:G:20:THR:HG21	1:G:274:HIS:CG	2.52	0.45
1:H:20:THR:HG21	1:H:274:HIS:CG	2.51	0.45
1:L:196:SER:O	1:L:200:ILE:HG12	2.16	0.45
1:B:196:SER:O	1:B:200:ILE:HG12	2.16	0.45
1:C:196:SER:O	1:C:200:ILE:HG12	2.16	0.45
1:I:196:SER:O	1:I:200:ILE:HG12	2.17	0.45
3:D:405:Y01:HAC1	3:D:405:Y01:CAU	2.44	0.45
1:E:20:THR:HG21	1:E:274:HIS:CG	2.52	0.45
1:F:196:SER:O	1:F:200:ILE:HG12	2.17	0.45
1:F:20:THR:HG21	1:F:274:HIS:CG	2.52	0.45
1:J:196:SER:O	1:J:200:ILE:HG12	2.16	0.45
1:K:196:SER:O	1:K:200:ILE:HG12	2.16	0.45
1:L:20:THR:HG21	1:L:274:HIS:CG	2.52	0.45
1:A:196:SER:O	1:A:200:ILE:HG12	2.17	0.45
1:C:20:THR:HG21	1:C:274:HIS:CG	2.52	0.45
1:D:196:SER:O	1:D:200:ILE:HG12	2.17	0.45
3:E:405:Y01:HAC1	3:E:405:Y01:CAU	2.44	0.45
3:G:405:Y01:HAC1	3:G:405:Y01:CAU	2.44	0.45
1:I:20:THR:HG21	1:I:274:HIS:CG	2.52	0.45
1:G:196:SER:O	1:G:200:ILE:HG12	2.17	0.45
3:H:405:Y01:HAC1	3:H:405:Y01:CAU	2.44	0.45
3:C:405:Y01:HAC1	3:C:405:Y01:CAU	2.44	0.45
1:A:20:THR:HG21	1:A:274:HIS:CG	2.52	0.45
3:A:405:Y01:HAC1	3:A:405:Y01:CAU	2.44	0.44
1:J:20:THR:HG21	1:J:274:HIS:CG	2.51	0.44
3:J:405:Y01:HAC1	3:J:405:Y01:CAU	2.44	0.44
3:L:405:Y01:HAC1	3:L:405:Y01:CAU	2.44	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:20:THR:HG21	1:K:274:HIS:CG	2.52	0.44
1:B:20:THR:HG21	1:B:274:HIS:CG	2.52	0.44
3:B:405:Y01:HAC1	3:B:405:Y01:CAU	2.44	0.43
3:K:405:Y01:HAC1	3:K:405:Y01:CAU	2.44	0.42
2:C:407:MC3:H391	2:C:407:MC3:H361	1.93	0.41
2:L:407:MC3:H391	2:L:407:MC3:H361	1.93	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	A	162/358 (45%)	160 (99%)	2 (1%)	0	100	100
1	B	162/358 (45%)	160 (99%)	2 (1%)	0	100	100
1	C	162/358 (45%)	160 (99%)	2 (1%)	0	100	100
1	D	162/358 (45%)	160 (99%)	2 (1%)	0	100	100
1	E	162/358 (45%)	160 (99%)	2 (1%)	0	100	100
1	F	162/358 (45%)	160 (99%)	2 (1%)	0	100	100
1	G	162/358 (45%)	160 (99%)	2 (1%)	0	100	100
1	H	162/358 (45%)	160 (99%)	2 (1%)	0	100	100
1	I	162/358 (45%)	160 (99%)	2 (1%)	0	100	100
1	J	162/358 (45%)	160 (99%)	2 (1%)	0	100	100
1	K	162/358 (45%)	160 (99%)	2 (1%)	0	100	100
1	L	162/358 (45%)	160 (99%)	2 (1%)	0	100	100
All	All	1944/4296 (45%)	1920 (99%)	24 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	150/312 (48%)	146 (97%)	4 (3%)	44	57
1	B	150/312 (48%)	146 (97%)	4 (3%)	44	57
1	C	150/312 (48%)	146 (97%)	4 (3%)	44	57
1	D	150/312 (48%)	146 (97%)	4 (3%)	44	57
1	E	150/312 (48%)	146 (97%)	4 (3%)	44	57
1	F	150/312 (48%)	146 (97%)	4 (3%)	44	57
1	G	150/312 (48%)	146 (97%)	4 (3%)	44	57
1	H	150/312 (48%)	146 (97%)	4 (3%)	44	57
1	I	150/312 (48%)	146 (97%)	4 (3%)	44	57
1	J	150/312 (48%)	146 (97%)	4 (3%)	44	57
1	K	150/312 (48%)	146 (97%)	4 (3%)	44	57
1	L	150/312 (48%)	146 (97%)	4 (3%)	44	57
All	All	1800/3744 (48%)	1752 (97%)	48 (3%)	48	57

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	THR
1	A	198	PHE
1	A	238	LYS
1	A	253	PHE
1	B	20	THR
1	B	198	PHE
1	B	238	LYS
1	B	253	PHE
1	C	20	THR
1	C	198	PHE
1	C	238	LYS
1	C	253	PHE
1	D	20	THR
1	D	198	PHE

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Mol	Chain	Res	Type
1	D	238	LYS
1	D	253	PHE
1	E	20	THR
1	E	198	PHE
1	E	238	LYS
1	E	253	PHE
1	F	20	THR
1	F	198	PHE
1	F	238	LYS
1	F	253	PHE
1	G	20	THR
1	G	198	PHE
1	G	238	LYS
1	G	253	PHE
1	H	20	THR
1	H	198	PHE
1	H	238	LYS
1	H	253	PHE
1	I	20	THR
1	I	198	PHE
1	I	238	LYS
1	I	253	PHE
1	J	20	THR
1	J	198	PHE
1	J	238	LYS
1	J	253	PHE
1	K	20	THR
1	K	198	PHE
1	K	238	LYS
1	K	253	PHE
1	L	20	THR
1	L	198	PHE
1	L	238	LYS
1	L	253	PHE

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

Mol	Chain	Res	Type
1	A	100	GLN
1	B	100	GLN
1	C	59	GLN
1	C	100	GLN

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Mol	Chain	Res	Type
1	D	59	GLN
1	D	100	GLN
1	E	100	GLN
1	F	59	GLN
1	F	100	GLN
1	G	100	GLN
1	H	100	GLN
1	I	59	GLN
1	I	100	GLN
1	J	100	GLN
1	K	59	GLN
1	K	100	GLN
1	L	59	GLN
1	L	100	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

108 ligands 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	MC3	K	407	-	12,12,45	0.32	0	11,11,53	0.39	0
2	MC3	C	408	-	9,9,45	0.21	0	8,8,53	0.30	0
4	LHG	H	409	-	38,38,48	0.71	2 (5%)	40,40,54	1.22	5 (12%)
2	MC3	G	408	-	9,9,45	0.21	0	8,8,53	0.30	0
2	MC3	H	404	-	7,7,45	0.32	0	6,6,53	0.21	0
2	MC3	G	403	-	9,9,45	0.25	0	8,8,53	0.41	0
2	MC3	K	404	-	7,7,45	0.32	0	6,6,53	0.22	0
3	Y01	J	406	-	38,38,38	4.74	21 (55%)	57,57,57	2.70	22 (38%)
2	MC3	D	401	-	13,13,45	0.26	0	12,12,53	0.54	0
2	MC3	E	401	-	13,13,45	0.26	0	12,12,53	0.54	0
2	MC3	F	407	-	12,12,45	0.32	0	11,11,53	0.39	0
3	Y01	C	405	-	38,38,38	4.85	22 (57%)	57,57,57	2.47	18 (31%)
2	MC3	B	401	-	13,13,45	0.26	0	12,12,53	0.54	0
2	MC3	G	401	-	13,13,45	0.26	0	12,12,53	0.54	0
3	Y01	D	406	-	38,38,38	4.74	21 (55%)	57,57,57	2.70	22 (38%)
2	MC3	L	408	-	9,9,45	0.21	0	8,8,53	0.30	0
2	MC3	H	401	-	13,13,45	0.26	0	12,12,53	0.54	0
2	MC3	J	407	-	12,12,45	0.32	0	11,11,53	0.39	0
2	MC3	L	402	-	8,8,45	0.28	0	7,7,53	0.35	0
3	Y01	L	405	-	38,38,38	4.85	22 (57%)	57,57,57	2.47	18 (31%)
2	MC3	E	403	-	9,9,45	0.24	0	8,8,53	0.41	0
2	MC3	I	401	-	13,13,45	0.26	0	12,12,53	0.54	0
4	LHG	G	409	-	38,38,48	0.71	2 (5%)	40,40,54	1.22	5 (12%)
2	MC3	C	404	-	7,7,45	0.32	0	6,6,53	0.22	0
3	Y01	I	406	-	38,38,38	4.74	21 (55%)	57,57,57	2.70	21 (36%)
4	LHG	D	409	-	38,38,48	0.71	2 (5%)	40,40,54	1.22	5 (12%)
4	LHG	B	409	-	38,38,48	0.71	2 (5%)	40,40,54	1.21	5 (12%)
2	MC3	E	402	-	8,8,45	0.28	0	7,7,53	0.34	0
2	MC3	K	408	-	9,9,45	0.21	0	8,8,53	0.30	0
2	MC3	J	401	-	13,13,45	0.26	0	12,12,53	0.54	0
2	MC3	K	403	-	9,9,45	0.24	0	8,8,53	0.41	0
2	MC3	H	402	-	8,8,45	0.28	0	7,7,53	0.35	0
2	MC3	K	402	-	8,8,45	0.28	0	7,7,53	0.35	0
4	LHG	L	409	-	38,38,48	0.70	2 (5%)	40,40,54	1.22	5 (12%)
3	Y01	G	406	-	38,38,38	4.74	21 (55%)	57,57,57	2.70	22 (38%)
3	Y01	E	405	-	38,38,38	4.85	22 (57%)	57,57,57	2.48	18 (31%)
2	MC3	L	401	-	13,13,45	0.26	0	12,12,53	0.54	0
4	LHG	I	409	-	38,38,48	0.71	2 (5%)	40,40,54	1.21	5 (12%)
2	MC3	H	407	-	12,12,45	0.32	0	11,11,53	0.39	0
2	MC3	K	401	-	13,13,45	0.26	0	12,12,53	0.54	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	MC3	F	402	-	8,8,45	0.28	0	7,7,53	0.35	0
2	MC3	I	402	-	8,8,45	0.28	0	7,7,53	0.35	0
2	MC3	J	404	-	7,7,45	0.32	0	6,6,53	0.21	0
2	MC3	D	402	-	8,8,45	0.28	0	7,7,53	0.35	0
3	Y01	A	406	-	38,38,38	4.74	21 (55%)	57,57,57	2.70	22 (38%)
2	MC3	I	403	-	9,9,45	0.25	0	8,8,53	0.41	0
2	MC3	G	402	-	8,8,45	0.28	0	7,7,53	0.35	0
2	MC3	J	403	-	9,9,45	0.25	0	8,8,53	0.41	0
2	MC3	J	402	-	8,8,45	0.28	0	7,7,53	0.35	0
2	MC3	E	408	-	9,9,45	0.21	0	8,8,53	0.30	0
2	MC3	G	404	-	7,7,45	0.32	0	6,6,53	0.22	0
2	MC3	C	402	-	8,8,45	0.27	0	7,7,53	0.34	0
3	Y01	K	405	-	38,38,38	4.84	22 (57%)	57,57,57	2.48	18 (31%)
2	MC3	F	404	-	7,7,45	0.32	0	6,6,53	0.22	0
4	LHG	A	409	-	38,38,48	0.71	2 (5%)	40,40,54	1.22	5 (12%)
2	MC3	H	408	-	9,9,45	0.21	0	8,8,53	0.30	0
2	MC3	A	402	-	8,8,45	0.28	0	7,7,53	0.35	0
3	Y01	D	405	-	38,38,38	4.85	22 (57%)	57,57,57	2.48	18 (31%)
2	MC3	B	407	-	12,12,45	0.32	0	11,11,53	0.39	0
2	MC3	L	407	-	12,12,45	0.32	0	11,11,53	0.39	0
2	MC3	C	407	-	12,12,45	0.32	0	11,11,53	0.39	0
3	Y01	F	405	-	38,38,38	4.84	22 (57%)	57,57,57	2.47	18 (31%)
2	MC3	B	404	-	7,7,45	0.32	0	6,6,53	0.21	0
2	MC3	I	408	-	9,9,45	0.21	0	8,8,53	0.30	0
2	MC3	F	403	-	9,9,45	0.24	0	8,8,53	0.41	0
4	LHG	E	409	-	38,38,48	0.70	2 (5%)	40,40,54	1.22	5 (12%)
2	MC3	A	401	-	13,13,45	0.26	0	12,12,53	0.54	0
3	Y01	A	405	-	38,38,38	4.85	22 (57%)	57,57,57	2.48	18 (31%)
3	Y01	B	405	-	38,38,38	4.84	22 (57%)	57,57,57	2.48	18 (31%)
2	MC3	H	403	-	9,9,45	0.24	0	8,8,53	0.41	0
3	Y01	H	405	-	38,38,38	4.84	22 (57%)	57,57,57	2.48	18 (31%)
3	Y01	L	406	-	38,38,38	4.74	21 (55%)	57,57,57	2.70	21 (36%)
2	MC3	I	404	-	7,7,45	0.32	0	6,6,53	0.22	0
2	MC3	G	407	-	12,12,45	0.32	0	11,11,53	0.39	0
2	MC3	I	407	-	12,12,45	0.32	0	11,11,53	0.39	0
4	LHG	K	409	-	38,38,48	0.71	2 (5%)	40,40,54	1.21	5 (12%)
2	MC3	D	404	-	7,7,45	0.32	0	6,6,53	0.22	0
2	MC3	F	408	-	9,9,45	0.21	0	8,8,53	0.30	0
2	MC3	D	408	-	9,9,45	0.22	0	8,8,53	0.30	0
2	MC3	B	408	-	9,9,45	0.21	0	8,8,53	0.30	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	Y01	C	406	-	38,38,38	4.74	21 (55%)	57,57,57	2.70	22 (38%)
2	MC3	D	403	-	9,9,45	0.25	0	8,8,53	0.41	0
2	MC3	B	403	-	9,9,45	0.24	0	8,8,53	0.41	0
2	MC3	L	403	-	9,9,45	0.25	0	8,8,53	0.41	0
2	MC3	D	407	-	12,12,45	0.32	0	11,11,53	0.39	0
4	LHG	F	409	-	38,38,48	0.71	2 (5%)	40,40,54	1.21	5 (12%)
2	MC3	C	401	-	13,13,45	0.26	0	12,12,53	0.54	0
3	Y01	E	406	-	38,38,38	4.74	21 (55%)	57,57,57	2.70	21 (36%)
3	Y01	F	406	-	38,38,38	4.74	21 (55%)	57,57,57	2.70	22 (38%)
3	Y01	B	406	-	38,38,38	4.74	21 (55%)	57,57,57	2.71	22 (38%)
2	MC3	J	408	-	9,9,45	0.21	0	8,8,53	0.30	0
2	MC3	A	408	-	9,9,45	0.21	0	8,8,53	0.30	0
2	MC3	F	401	-	13,13,45	0.26	0	12,12,53	0.54	0
3	Y01	I	405	-	38,38,38	4.84	22 (57%)	57,57,57	2.47	18 (31%)
2	MC3	E	407	-	12,12,45	0.32	0	11,11,53	0.39	0
3	Y01	H	406	-	38,38,38	4.74	21 (55%)	57,57,57	2.70	21 (36%)
2	MC3	L	404	-	7,7,45	0.32	0	6,6,53	0.22	0
2	MC3	A	404	-	7,7,45	0.32	0	6,6,53	0.22	0
3	Y01	J	405	-	38,38,38	4.85	22 (57%)	57,57,57	2.47	18 (31%)
3	Y01	K	406	-	38,38,38	4.75	21 (55%)	57,57,57	2.71	22 (38%)
2	MC3	C	403	-	9,9,45	0.25	0	8,8,53	0.41	0
2	MC3	B	402	-	8,8,45	0.28	0	7,7,53	0.34	0
4	LHG	J	409	-	38,38,48	0.71	2 (5%)	40,40,54	1.22	5 (12%)
4	LHG	C	409	-	38,38,48	0.70	2 (5%)	40,40,54	1.21	5 (12%)
2	MC3	A	403	-	9,9,45	0.25	0	8,8,53	0.41	0
2	MC3	A	407	-	12,12,45	0.32	0	11,11,53	0.39	0
3	Y01	G	405	-	38,38,38	4.85	22 (57%)	57,57,57	2.48	18 (31%)
2	MC3	E	404	-	7,7,45	0.32	0	6,6,53	0.21	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	MC3	K	407	-	-	5/10/10/49	-
2	MC3	C	408	-	-	4/7/7/49	-
4	LHG	H	409	-	-	23/39/39/53	-
2	MC3	G	408	-	-	4/7/7/49	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MC3	H	404	-	-	4/5/5/49	-
2	MC3	G	403	-	-	3/7/7/49	-
2	MC3	K	404	-	-	4/5/5/49	-
3	Y01	J	406	-	-	9/19/77/77	0/4/4/4
2	MC3	D	401	-	-	5/11/11/49	-
2	MC3	E	401	-	-	5/11/11/49	-
2	MC3	F	407	-	-	5/10/10/49	-
3	Y01	C	405	-	-	4/19/77/77	0/4/4/4
2	MC3	B	401	-	-	5/11/11/49	-
2	MC3	G	401	-	-	5/11/11/49	-
3	Y01	D	406	-	-	9/19/77/77	0/4/4/4
2	MC3	L	408	-	-	4/7/7/49	-
2	MC3	H	401	-	-	5/11/11/49	-
2	MC3	J	407	-	-	5/10/10/49	-
2	MC3	L	402	-	-	2/6/6/49	-
3	Y01	L	405	-	-	4/19/77/77	0/4/4/4
2	MC3	E	403	-	-	3/7/7/49	-
2	MC3	I	401	-	-	5/11/11/49	-
4	LHG	G	409	-	-	23/39/39/53	-
2	MC3	C	404	-	-	4/5/5/49	-
3	Y01	I	406	-	-	9/19/77/77	0/4/4/4
4	LHG	D	409	-	-	23/39/39/53	-
4	LHG	B	409	-	-	23/39/39/53	-
2	MC3	E	402	-	-	2/6/6/49	-
2	MC3	K	408	-	-	4/7/7/49	-
2	MC3	J	401	-	-	5/11/11/49	-
2	MC3	K	403	-	-	3/7/7/49	-
2	MC3	H	402	-	-	2/6/6/49	-
2	MC3	K	402	-	-	2/6/6/49	-
4	LHG	L	409	-	-	23/39/39/53	-
3	Y01	G	406	-	-	9/19/77/77	0/4/4/4
3	Y01	E	405	-	-	4/19/77/77	0/4/4/4
2	MC3	L	401	-	-	5/11/11/49	-
4	LHG	I	409	-	-	23/39/39/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MC3	H	407	-	-	5/10/10/49	-
2	MC3	K	401	-	-	5/11/11/49	-
2	MC3	F	402	-	-	2/6/6/49	-
2	MC3	I	402	-	-	2/6/6/49	-
2	MC3	J	404	-	-	4/5/5/49	-
2	MC3	D	402	-	-	2/6/6/49	-
3	Y01	A	406	-	-	9/19/77/77	0/4/4/4
2	MC3	I	403	-	-	3/7/7/49	-
2	MC3	G	402	-	-	2/6/6/49	-
2	MC3	J	403	-	-	3/7/7/49	-
2	MC3	J	402	-	-	2/6/6/49	-
2	MC3	E	408	-	-	4/7/7/49	-
2	MC3	G	404	-	-	4/5/5/49	-
2	MC3	C	402	-	-	2/6/6/49	-
3	Y01	K	405	-	-	4/19/77/77	0/4/4/4
2	MC3	F	404	-	-	4/5/5/49	-
4	LHG	A	409	-	-	23/39/39/53	-
2	MC3	H	408	-	-	4/7/7/49	-
2	MC3	A	402	-	-	2/6/6/49	-
3	Y01	D	405	-	-	4/19/77/77	0/4/4/4
2	MC3	B	407	-	-	5/10/10/49	-
2	MC3	L	407	-	-	5/10/10/49	-
2	MC3	C	407	-	-	5/10/10/49	-
3	Y01	F	405	-	-	4/19/77/77	0/4/4/4
2	MC3	B	404	-	-	4/5/5/49	-
2	MC3	I	408	-	-	4/7/7/49	-
2	MC3	F	403	-	-	3/7/7/49	-
4	LHG	E	409	-	-	23/39/39/53	-
2	MC3	A	401	-	-	5/11/11/49	-
3	Y01	A	405	-	-	4/19/77/77	0/4/4/4
3	Y01	B	405	-	-	4/19/77/77	0/4/4/4
2	MC3	H	403	-	-	3/7/7/49	-
3	Y01	H	405	-	-	4/19/77/77	0/4/4/4
3	Y01	L	406	-	-	9/19/77/77	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MC3	I	404	-	-	4/5/5/49	-
2	MC3	G	407	-	-	5/10/10/49	-
2	MC3	I	407	-	-	5/10/10/49	-
4	LHG	K	409	-	-	23/39/39/53	-
2	MC3	D	404	-	-	4/5/5/49	-
2	MC3	F	408	-	-	4/7/7/49	-
2	MC3	D	408	-	-	4/7/7/49	-
2	MC3	B	408	-	-	4/7/7/49	-
3	Y01	C	406	-	-	9/19/77/77	0/4/4/4
2	MC3	D	403	-	-	3/7/7/49	-
2	MC3	B	403	-	-	3/7/7/49	-
2	MC3	L	403	-	-	3/7/7/49	-
2	MC3	D	407	-	-	5/10/10/49	-
4	LHG	F	409	-	-	23/39/39/53	-
2	MC3	C	401	-	-	5/11/11/49	-
3	Y01	E	406	-	-	9/19/77/77	0/4/4/4
3	Y01	F	406	-	-	9/19/77/77	0/4/4/4
3	Y01	B	406	-	-	9/19/77/77	0/4/4/4
2	MC3	J	408	-	-	4/7/7/49	-
2	MC3	A	408	-	-	4/7/7/49	-
2	MC3	F	401	-	-	5/11/11/49	-
3	Y01	I	405	-	-	4/19/77/77	0/4/4/4
2	MC3	E	407	-	-	5/10/10/49	-
3	Y01	H	406	-	-	9/19/77/77	0/4/4/4
2	MC3	L	404	-	-	4/5/5/49	-
2	MC3	A	404	-	-	4/5/5/49	-
3	Y01	J	405	-	-	4/19/77/77	0/4/4/4
3	Y01	K	406	-	-	9/19/77/77	0/4/4/4
2	MC3	C	403	-	-	3/7/7/49	-
2	MC3	B	402	-	-	2/6/6/49	-
4	LHG	J	409	-	-	23/39/39/53	-
4	LHG	C	409	-	-	23/39/39/53	-
2	MC3	A	403	-	-	3/7/7/49	-
2	MC3	A	407	-	-	5/10/10/49	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	Y01	G	405	-	-	4/19/77/77	0/4/4/4
2	MC3	E	404	-	-	4/5/5/49	-

All (540) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	405	Y01	CAI-CAZ	-13.19	1.03	1.33
3	C	405	Y01	CAI-CAZ	-13.18	1.03	1.33
3	L	405	Y01	CAI-CAZ	-13.18	1.03	1.33
3	J	405	Y01	CAI-CAZ	-13.17	1.03	1.33
3	A	405	Y01	CAI-CAZ	-13.16	1.03	1.33
3	D	405	Y01	CAI-CAZ	-13.16	1.03	1.33
3	G	405	Y01	CAI-CAZ	-13.16	1.03	1.33
3	H	405	Y01	CAI-CAZ	-13.15	1.03	1.33
3	B	405	Y01	CAI-CAZ	-13.14	1.04	1.33
3	F	405	Y01	CAI-CAZ	-13.14	1.04	1.33
3	I	405	Y01	CAI-CAZ	-13.14	1.04	1.33
3	K	405	Y01	CAI-CAZ	-13.14	1.04	1.33
3	K	406	Y01	CAI-CAZ	-12.53	1.05	1.33
3	H	406	Y01	CAI-CAZ	-12.52	1.05	1.33
3	A	406	Y01	CAI-CAZ	-12.51	1.05	1.33
3	D	406	Y01	CAI-CAZ	-12.51	1.05	1.33
3	G	406	Y01	CAI-CAZ	-12.51	1.05	1.33
3	J	406	Y01	CAI-CAZ	-12.51	1.05	1.33
3	C	406	Y01	CAI-CAZ	-12.51	1.05	1.33
3	F	406	Y01	CAI-CAZ	-12.51	1.05	1.33
3	I	406	Y01	CAI-CAZ	-12.51	1.05	1.33
3	L	406	Y01	CAI-CAZ	-12.51	1.05	1.33
3	B	406	Y01	CAI-CAZ	-12.50	1.05	1.33
3	E	406	Y01	CAI-CAZ	-12.49	1.05	1.33
3	B	405	Y01	CBD-CBG	-9.97	1.34	1.53
3	E	405	Y01	CBD-CBG	-9.97	1.34	1.53
3	K	405	Y01	CBD-CBG	-9.97	1.34	1.53
3	A	405	Y01	CBD-CBG	-9.96	1.34	1.53
3	D	405	Y01	CBD-CBG	-9.96	1.34	1.53
3	G	405	Y01	CBD-CBG	-9.96	1.34	1.53
3	J	405	Y01	CBD-CBG	-9.96	1.34	1.53
3	I	405	Y01	CBD-CBG	-9.95	1.34	1.53
3	C	405	Y01	CBD-CBG	-9.95	1.34	1.53
3	F	405	Y01	CBD-CBG	-9.95	1.34	1.53
3	L	405	Y01	CBD-CBG	-9.95	1.34	1.53
3	H	405	Y01	CBD-CBG	-9.95	1.34	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	405	Y01	CAK-CAI	-9.31	1.30	1.50
3	H	405	Y01	CAK-CAI	-9.31	1.30	1.50
3	B	405	Y01	CAK-CAI	-9.29	1.30	1.50
3	K	405	Y01	CAK-CAI	-9.29	1.30	1.50
3	A	405	Y01	CAK-CAI	-9.29	1.30	1.50
3	D	405	Y01	CAK-CAI	-9.29	1.30	1.50
3	G	405	Y01	CAK-CAI	-9.29	1.30	1.50
3	J	405	Y01	CAK-CAI	-9.29	1.30	1.50
3	F	405	Y01	CAK-CAI	-9.29	1.30	1.50
3	I	405	Y01	CAK-CAI	-9.29	1.30	1.50
3	L	405	Y01	CAK-CAI	-9.29	1.30	1.50
3	C	405	Y01	CAK-CAI	-9.26	1.30	1.50
3	B	406	Y01	CBD-CBG	-9.07	1.36	1.53
3	K	406	Y01	CBD-CBG	-9.07	1.36	1.53
3	C	406	Y01	CBD-CBG	-9.06	1.36	1.53
3	F	406	Y01	CBD-CBG	-9.06	1.36	1.53
3	I	406	Y01	CBD-CBG	-9.06	1.36	1.53
3	L	406	Y01	CBD-CBG	-9.06	1.36	1.53
3	A	406	Y01	CBD-CBG	-9.05	1.36	1.53
3	D	406	Y01	CBD-CBG	-9.05	1.36	1.53
3	G	406	Y01	CBD-CBG	-9.05	1.36	1.53
3	J	406	Y01	CBD-CBG	-9.05	1.36	1.53
3	E	406	Y01	CBD-CBG	-9.03	1.36	1.53
3	H	406	Y01	CBD-CBG	-9.03	1.36	1.53
3	B	405	Y01	CBD-CBF	8.76	1.70	1.53
3	E	405	Y01	CBD-CBF	8.76	1.70	1.53
3	K	405	Y01	CBD-CBF	8.76	1.70	1.53
3	A	405	Y01	CBD-CBF	8.75	1.70	1.53
3	D	405	Y01	CBD-CBF	8.75	1.70	1.53
3	G	405	Y01	CBD-CBF	8.75	1.70	1.53
3	C	405	Y01	CBD-CBF	8.73	1.70	1.53
3	I	405	Y01	CBD-CBF	8.73	1.70	1.53
3	F	405	Y01	CBD-CBF	8.72	1.70	1.53
3	L	405	Y01	CBD-CBF	8.72	1.70	1.53
3	H	405	Y01	CBD-CBF	8.71	1.70	1.53
3	J	405	Y01	CBD-CBF	8.70	1.70	1.53
3	K	406	Y01	CBD-CBF	8.68	1.70	1.53
3	B	406	Y01	CBD-CBF	8.67	1.70	1.53
3	E	406	Y01	CBD-CBF	8.67	1.70	1.53
3	H	406	Y01	CBD-CBF	8.67	1.70	1.53
3	A	406	Y01	CBD-CBF	8.67	1.70	1.53
3	D	406	Y01	CBD-CBF	8.67	1.70	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	406	Y01	CBD-CBF	8.67	1.70	1.53
3	J	406	Y01	CBD-CBF	8.67	1.70	1.53
3	C	406	Y01	CBD-CBF	8.67	1.70	1.53
3	F	406	Y01	CBD-CBF	8.67	1.70	1.53
3	I	406	Y01	CBD-CBF	8.67	1.70	1.53
3	L	406	Y01	CBD-CBF	8.67	1.70	1.53
3	E	406	Y01	CAU-CAS	8.64	1.71	1.53
3	H	406	Y01	CAU-CAS	8.64	1.71	1.53
3	A	406	Y01	CAU-CAS	8.62	1.71	1.53
3	D	406	Y01	CAU-CAS	8.62	1.71	1.53
3	G	406	Y01	CAU-CAS	8.62	1.71	1.53
3	J	406	Y01	CAU-CAS	8.62	1.71	1.53
3	B	406	Y01	CAU-CAS	8.62	1.71	1.53
3	K	406	Y01	CAU-CAS	8.62	1.71	1.53
3	C	406	Y01	CAU-CAS	8.61	1.71	1.53
3	F	406	Y01	CAU-CAS	8.61	1.71	1.53
3	I	406	Y01	CAU-CAS	8.61	1.71	1.53
3	L	406	Y01	CAU-CAS	8.61	1.71	1.53
3	F	405	Y01	CAU-CAS	8.45	1.71	1.53
3	L	405	Y01	CAU-CAS	8.45	1.71	1.53
3	C	405	Y01	CAU-CAS	8.45	1.71	1.53
3	I	405	Y01	CAU-CAS	8.45	1.71	1.53
3	B	405	Y01	CAU-CAS	8.43	1.71	1.53
3	E	405	Y01	CAU-CAS	8.43	1.71	1.53
3	H	405	Y01	CAU-CAS	8.43	1.71	1.53
3	A	405	Y01	CAU-CAS	8.43	1.71	1.53
3	D	405	Y01	CAU-CAS	8.43	1.71	1.53
3	G	405	Y01	CAU-CAS	8.43	1.71	1.53
3	J	405	Y01	CAU-CAS	8.43	1.71	1.53
3	K	405	Y01	CAU-CAS	8.40	1.71	1.53
3	A	406	Y01	CAK-CAI	-8.33	1.32	1.50
3	D	406	Y01	CAK-CAI	-8.33	1.32	1.50
3	G	406	Y01	CAK-CAI	-8.33	1.32	1.50
3	J	406	Y01	CAK-CAI	-8.33	1.32	1.50
3	B	406	Y01	CAK-CAI	-8.32	1.32	1.50
3	H	406	Y01	CAK-CAI	-8.32	1.32	1.50
3	K	406	Y01	CAK-CAI	-8.32	1.32	1.50
3	C	406	Y01	CAK-CAI	-8.32	1.32	1.50
3	F	406	Y01	CAK-CAI	-8.32	1.32	1.50
3	I	406	Y01	CAK-CAI	-8.32	1.32	1.50
3	L	406	Y01	CAK-CAI	-8.32	1.32	1.50
3	E	406	Y01	CAK-CAI	-8.31	1.32	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	406	Y01	CAT-CBH	7.94	1.69	1.54
3	E	406	Y01	CAT-CBH	7.94	1.69	1.54
3	H	406	Y01	CAT-CBH	7.94	1.69	1.54
3	K	406	Y01	CAT-CBH	7.94	1.69	1.54
3	C	406	Y01	CAT-CBH	7.94	1.69	1.54
3	I	406	Y01	CAT-CBH	7.94	1.69	1.54
3	L	406	Y01	CAT-CBH	7.94	1.69	1.54
3	A	406	Y01	CAT-CBH	7.94	1.69	1.54
3	D	406	Y01	CAT-CBH	7.94	1.69	1.54
3	G	406	Y01	CAT-CBH	7.94	1.69	1.54
3	F	406	Y01	CAT-CBH	7.92	1.69	1.54
3	J	406	Y01	CAT-CBH	7.89	1.69	1.54
3	J	405	Y01	CAU-CBI	-7.85	1.40	1.54
3	B	406	Y01	CBH-CAZ	-7.85	1.37	1.52
3	E	406	Y01	CBH-CAZ	-7.84	1.37	1.52
3	H	406	Y01	CBH-CAZ	-7.84	1.37	1.52
3	K	406	Y01	CBH-CAZ	-7.84	1.37	1.52
3	A	406	Y01	CBH-CAZ	-7.82	1.37	1.52
3	D	406	Y01	CBH-CAZ	-7.82	1.37	1.52
3	G	406	Y01	CBH-CAZ	-7.82	1.37	1.52
3	C	405	Y01	CAU-CBI	-7.81	1.40	1.54
3	I	405	Y01	CAU-CBI	-7.81	1.40	1.54
3	H	405	Y01	CAU-CBI	-7.81	1.40	1.54
3	B	405	Y01	CAU-CBI	-7.80	1.40	1.54
3	E	405	Y01	CAU-CBI	-7.80	1.40	1.54
3	A	405	Y01	CAU-CBI	-7.80	1.40	1.54
3	D	405	Y01	CAU-CBI	-7.80	1.40	1.54
3	G	405	Y01	CAU-CBI	-7.80	1.40	1.54
3	F	405	Y01	CAU-CBI	-7.80	1.40	1.54
3	L	405	Y01	CAU-CBI	-7.80	1.40	1.54
3	C	406	Y01	CBH-CAZ	-7.79	1.37	1.52
3	F	406	Y01	CBH-CAZ	-7.79	1.37	1.52
3	I	406	Y01	CBH-CAZ	-7.79	1.37	1.52
3	L	406	Y01	CBH-CAZ	-7.79	1.37	1.52
3	J	406	Y01	CBH-CAZ	-7.78	1.37	1.52
3	K	405	Y01	CAU-CBI	-7.75	1.40	1.54
3	B	406	Y01	CAU-CBI	-7.65	1.40	1.54
3	E	406	Y01	CAU-CBI	-7.65	1.40	1.54
3	H	406	Y01	CAU-CBI	-7.65	1.40	1.54
3	A	406	Y01	CAU-CBI	-7.64	1.40	1.54
3	D	406	Y01	CAU-CBI	-7.64	1.40	1.54
3	G	406	Y01	CAU-CBI	-7.64	1.40	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	406	Y01	CAU-CBI	-7.64	1.40	1.54
3	C	406	Y01	CAU-CBI	-7.63	1.40	1.54
3	F	406	Y01	CAU-CBI	-7.63	1.40	1.54
3	I	406	Y01	CAU-CBI	-7.63	1.40	1.54
3	L	406	Y01	CAU-CBI	-7.63	1.40	1.54
3	K	406	Y01	CAU-CBI	-7.63	1.40	1.54
3	F	405	Y01	CAT-CBH	7.62	1.68	1.54
3	I	405	Y01	CAT-CBH	7.62	1.68	1.54
3	L	405	Y01	CAT-CBH	7.62	1.68	1.54
3	J	405	Y01	CAT-CBH	7.62	1.68	1.54
3	C	405	Y01	CAT-CBH	7.62	1.68	1.54
3	A	405	Y01	CAT-CBH	7.59	1.68	1.54
3	D	405	Y01	CAT-CBH	7.59	1.68	1.54
3	G	405	Y01	CAT-CBH	7.59	1.68	1.54
3	E	405	Y01	CAT-CBH	7.59	1.68	1.54
3	H	405	Y01	CAT-CBH	7.59	1.68	1.54
3	B	405	Y01	CAT-CBH	7.59	1.68	1.54
3	K	405	Y01	CAT-CBH	7.59	1.68	1.54
3	E	405	Y01	CBH-CAZ	-7.16	1.38	1.52
3	A	405	Y01	CBH-CAZ	-7.14	1.38	1.52
3	B	405	Y01	CBH-CAZ	-7.14	1.38	1.52
3	D	405	Y01	CBH-CAZ	-7.14	1.38	1.52
3	G	405	Y01	CBH-CAZ	-7.14	1.38	1.52
3	H	405	Y01	CBH-CAZ	-7.14	1.38	1.52
3	J	405	Y01	CBH-CAZ	-7.14	1.38	1.52
3	K	405	Y01	CBH-CAZ	-7.14	1.38	1.52
3	C	405	Y01	CBH-CAZ	-7.13	1.38	1.52
3	F	405	Y01	CBH-CAZ	-7.13	1.38	1.52
3	I	405	Y01	CBH-CAZ	-7.13	1.38	1.52
3	L	405	Y01	CBH-CAZ	-7.13	1.38	1.52
3	C	406	Y01	CBH-CBF	-6.70	1.44	1.56
3	F	406	Y01	CBH-CBF	-6.70	1.44	1.56
3	I	406	Y01	CBH-CBF	-6.70	1.44	1.56
3	L	406	Y01	CBH-CBF	-6.70	1.44	1.56
3	K	406	Y01	CBH-CBF	-6.69	1.44	1.56
3	E	405	Y01	CBH-CBF	-6.69	1.44	1.56
3	E	406	Y01	CBH-CBF	-6.68	1.44	1.56
3	H	406	Y01	CBH-CBF	-6.68	1.44	1.56
3	C	405	Y01	CBH-CBF	-6.68	1.44	1.56
3	F	405	Y01	CBH-CBF	-6.68	1.44	1.56
3	I	405	Y01	CBH-CBF	-6.68	1.44	1.56
3	L	405	Y01	CBH-CBF	-6.68	1.44	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	405	Y01	CBH-CBF	-6.68	1.44	1.56
3	D	405	Y01	CBH-CBF	-6.68	1.44	1.56
3	G	405	Y01	CBH-CBF	-6.68	1.44	1.56
3	J	405	Y01	CBH-CBF	-6.68	1.44	1.56
3	A	406	Y01	CBH-CBF	-6.68	1.44	1.56
3	D	406	Y01	CBH-CBF	-6.68	1.44	1.56
3	G	406	Y01	CBH-CBF	-6.68	1.44	1.56
3	J	406	Y01	CBH-CBF	-6.68	1.44	1.56
3	B	405	Y01	CBH-CBF	-6.67	1.44	1.56
3	H	405	Y01	CBH-CBF	-6.67	1.44	1.56
3	K	405	Y01	CBH-CBF	-6.67	1.44	1.56
3	B	406	Y01	CBH-CBF	-6.63	1.44	1.56
3	H	405	Y01	CAS-CBF	6.35	1.64	1.53
3	E	405	Y01	CAS-CBF	6.33	1.64	1.53
3	A	405	Y01	CAS-CBF	6.32	1.64	1.53
3	D	405	Y01	CAS-CBF	6.32	1.64	1.53
3	G	405	Y01	CAS-CBF	6.32	1.64	1.53
3	J	405	Y01	CAS-CBF	6.32	1.64	1.53
3	C	405	Y01	CAS-CBF	6.32	1.64	1.53
3	F	405	Y01	CAS-CBF	6.32	1.64	1.53
3	I	405	Y01	CAS-CBF	6.32	1.64	1.53
3	L	405	Y01	CAS-CBF	6.32	1.64	1.53
3	B	405	Y01	CAS-CBF	6.31	1.64	1.53
3	K	405	Y01	CAS-CBF	6.29	1.64	1.53
3	K	406	Y01	CAS-CBF	5.79	1.63	1.53
3	C	406	Y01	CAS-CBF	5.77	1.63	1.53
3	F	406	Y01	CAS-CBF	5.77	1.63	1.53
3	I	406	Y01	CAS-CBF	5.77	1.63	1.53
3	L	406	Y01	CAS-CBF	5.77	1.63	1.53
3	A	406	Y01	CAS-CBF	5.74	1.63	1.53
3	D	406	Y01	CAS-CBF	5.74	1.63	1.53
3	G	406	Y01	CAS-CBF	5.74	1.63	1.53
3	J	406	Y01	CAS-CBF	5.73	1.63	1.53
3	B	406	Y01	CAS-CBF	5.72	1.63	1.53
3	E	406	Y01	CAS-CBF	5.72	1.63	1.53
3	H	406	Y01	CAS-CBF	5.72	1.63	1.53
3	E	405	Y01	CAQ-CBG	4.48	1.63	1.54
3	K	405	Y01	CAQ-CBG	4.48	1.63	1.54
3	A	405	Y01	CAQ-CBG	4.45	1.63	1.54
3	D	405	Y01	CAQ-CBG	4.45	1.63	1.54
3	G	405	Y01	CAQ-CBG	4.45	1.63	1.54
3	J	405	Y01	CAQ-CBG	4.45	1.63	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	405	Y01	CAQ-CBG	4.44	1.63	1.54
3	F	405	Y01	CAQ-CBG	4.44	1.63	1.54
3	I	405	Y01	CAQ-CBG	4.44	1.63	1.54
3	L	405	Y01	CAQ-CBG	4.44	1.63	1.54
3	B	405	Y01	CAQ-CBG	4.44	1.63	1.54
3	H	405	Y01	CAQ-CBG	4.44	1.63	1.54
3	B	406	Y01	CAQ-CAP	4.42	1.66	1.54
3	K	406	Y01	CAQ-CAP	4.40	1.66	1.54
3	E	406	Y01	CAQ-CAP	4.40	1.66	1.54
3	H	406	Y01	CAQ-CAP	4.40	1.66	1.54
3	A	406	Y01	CAQ-CAP	4.40	1.66	1.54
3	D	406	Y01	CAQ-CAP	4.40	1.66	1.54
3	G	406	Y01	CAQ-CAP	4.40	1.66	1.54
3	J	406	Y01	CAQ-CAP	4.40	1.66	1.54
3	C	406	Y01	CAQ-CAP	4.40	1.66	1.54
3	F	406	Y01	CAQ-CAP	4.40	1.66	1.54
3	I	406	Y01	CAQ-CAP	4.40	1.66	1.54
3	L	406	Y01	CAQ-CAP	4.40	1.66	1.54
3	B	406	Y01	CAQ-CBG	4.33	1.63	1.54
3	E	406	Y01	CAQ-CBG	4.33	1.63	1.54
3	H	406	Y01	CAQ-CBG	4.33	1.63	1.54
3	K	406	Y01	CAQ-CBG	4.33	1.63	1.54
3	A	406	Y01	CAQ-CBG	4.33	1.63	1.54
3	D	406	Y01	CAQ-CBG	4.33	1.63	1.54
3	G	406	Y01	CAQ-CBG	4.33	1.63	1.54
3	J	406	Y01	CAQ-CBG	4.33	1.63	1.54
3	C	406	Y01	CAQ-CBG	4.32	1.63	1.54
3	F	406	Y01	CAQ-CBG	4.32	1.63	1.54
3	I	406	Y01	CAQ-CBG	4.32	1.63	1.54
3	L	406	Y01	CAQ-CBG	4.32	1.63	1.54
3	E	405	Y01	CAQ-CAP	4.32	1.65	1.54
3	H	405	Y01	CAQ-CAP	4.32	1.65	1.54
3	C	405	Y01	CAQ-CAP	4.31	1.65	1.54
3	B	405	Y01	CAQ-CAP	4.31	1.65	1.54
3	K	405	Y01	CAQ-CAP	4.31	1.65	1.54
3	A	405	Y01	CAQ-CAP	4.30	1.65	1.54
3	D	405	Y01	CAQ-CAP	4.30	1.65	1.54
3	G	405	Y01	CAQ-CAP	4.30	1.65	1.54
3	J	405	Y01	CAQ-CAP	4.30	1.65	1.54
3	B	406	Y01	OAW-CAY	4.30	1.46	1.34
3	K	406	Y01	OAW-CAY	4.30	1.46	1.34
3	F	405	Y01	CAQ-CAP	4.30	1.65	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	405	Y01	CAQ-CAP	4.30	1.65	1.54
3	L	405	Y01	CAQ-CAP	4.30	1.65	1.54
3	A	406	Y01	OAW-CAY	4.28	1.46	1.34
3	D	406	Y01	OAW-CAY	4.28	1.46	1.34
3	G	406	Y01	OAW-CAY	4.28	1.46	1.34
3	J	406	Y01	OAW-CAY	4.28	1.46	1.34
3	F	406	Y01	OAW-CAY	4.28	1.46	1.34
3	C	406	Y01	OAW-CAY	4.27	1.46	1.34
3	I	406	Y01	OAW-CAY	4.27	1.46	1.34
3	L	406	Y01	OAW-CAY	4.27	1.46	1.34
3	E	406	Y01	OAW-CAY	4.27	1.46	1.34
3	H	406	Y01	OAW-CAY	4.27	1.46	1.34
3	C	406	Y01	CAK-CBD	4.21	1.60	1.53
3	F	406	Y01	CAK-CBD	4.21	1.60	1.53
3	I	406	Y01	CAK-CBD	4.21	1.60	1.53
3	L	406	Y01	CAK-CBD	4.21	1.60	1.53
3	J	406	Y01	CAK-CBD	4.21	1.60	1.53
3	B	406	Y01	CAK-CBD	4.17	1.60	1.53
3	E	406	Y01	CAK-CBD	4.17	1.60	1.53
3	H	406	Y01	CAK-CBD	4.17	1.60	1.53
3	K	406	Y01	CAK-CBD	4.17	1.60	1.53
3	A	406	Y01	CAK-CBD	4.17	1.60	1.53
3	D	406	Y01	CAK-CBD	4.17	1.60	1.53
3	G	406	Y01	CAK-CBD	4.17	1.60	1.53
3	C	405	Y01	OAW-CAY	4.09	1.45	1.34
3	A	405	Y01	OAW-CAY	4.09	1.45	1.34
3	D	405	Y01	OAW-CAY	4.09	1.45	1.34
3	F	405	Y01	OAW-CAY	4.09	1.45	1.34
3	G	405	Y01	OAW-CAY	4.09	1.45	1.34
3	I	405	Y01	OAW-CAY	4.09	1.45	1.34
3	J	405	Y01	OAW-CAY	4.09	1.45	1.34
3	L	405	Y01	OAW-CAY	4.09	1.45	1.34
3	B	405	Y01	OAW-CAY	4.09	1.45	1.34
3	E	405	Y01	OAW-CAY	4.09	1.45	1.34
3	H	405	Y01	OAW-CAY	4.09	1.45	1.34
3	K	405	Y01	OAW-CAY	4.09	1.45	1.34
3	K	406	Y01	CBI-CBE	3.62	1.61	1.55
3	F	406	Y01	CBI-CBE	3.62	1.61	1.55
3	A	406	Y01	CBI-CBE	3.60	1.61	1.55
3	B	406	Y01	CBI-CBE	3.60	1.61	1.55
3	D	406	Y01	CBI-CBE	3.60	1.61	1.55
3	G	406	Y01	CBI-CBE	3.60	1.61	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	406	Y01	CBI-CBE	3.60	1.61	1.55
3	L	405	Y01	CAK-CBD	3.58	1.59	1.53
3	I	406	Y01	CBI-CBE	3.58	1.61	1.55
3	L	406	Y01	CBI-CBE	3.58	1.61	1.55
3	C	405	Y01	CAK-CBD	3.58	1.59	1.53
3	F	405	Y01	CAK-CBD	3.58	1.59	1.53
3	B	405	Y01	CAK-CBD	3.58	1.59	1.53
3	K	405	Y01	CAK-CBD	3.58	1.59	1.53
3	E	406	Y01	CBI-CBE	3.58	1.61	1.55
3	H	406	Y01	CBI-CBE	3.58	1.61	1.55
3	A	405	Y01	CAK-CBD	3.57	1.59	1.53
3	D	405	Y01	CAK-CBD	3.57	1.59	1.53
3	G	405	Y01	CAK-CBD	3.57	1.59	1.53
3	J	405	Y01	CAK-CBD	3.57	1.59	1.53
3	E	405	Y01	CAK-CBD	3.56	1.59	1.53
3	H	405	Y01	CAK-CBD	3.56	1.59	1.53
3	C	406	Y01	CBI-CBE	3.56	1.61	1.55
3	I	405	Y01	CAK-CBD	3.53	1.59	1.53
3	C	405	Y01	CBI-CBE	2.98	1.60	1.55
3	I	405	Y01	CBI-CBE	2.98	1.60	1.55
3	H	405	Y01	CBI-CBE	2.97	1.60	1.55
3	A	405	Y01	CBI-CBE	2.97	1.60	1.55
3	D	405	Y01	CBI-CBE	2.97	1.60	1.55
3	G	405	Y01	CBI-CBE	2.97	1.60	1.55
3	J	405	Y01	CBI-CBE	2.97	1.60	1.55
3	B	405	Y01	CBI-CBE	2.97	1.60	1.55
3	E	405	Y01	CBI-CBE	2.97	1.60	1.55
3	K	405	Y01	CBI-CBE	2.97	1.60	1.55
3	F	405	Y01	CBI-CBE	2.96	1.60	1.55
3	L	405	Y01	CBI-CBE	2.96	1.60	1.55
4	F	409	LHG	O7-C5	-2.77	1.42	1.47
4	I	409	LHG	O7-C5	-2.77	1.42	1.47
4	B	409	LHG	O7-C5	-2.76	1.42	1.47
4	H	409	LHG	O7-C5	-2.76	1.42	1.47
4	K	409	LHG	O7-C5	-2.76	1.42	1.47
4	J	409	LHG	O7-C5	-2.75	1.42	1.47
4	A	409	LHG	O7-C5	-2.74	1.42	1.47
4	D	409	LHG	O7-C5	-2.74	1.42	1.47
4	G	409	LHG	O7-C5	-2.74	1.42	1.47
4	C	409	LHG	O7-C5	-2.72	1.42	1.47
4	L	409	LHG	O7-C5	-2.72	1.42	1.47
4	E	409	LHG	O7-C5	-2.72	1.42	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	405	Y01	OAW-CBC	-2.67	1.39	1.46
3	C	405	Y01	OAW-CBC	-2.67	1.39	1.46
3	F	405	Y01	OAW-CBC	-2.67	1.39	1.46
3	I	405	Y01	OAW-CBC	-2.67	1.39	1.46
3	L	405	Y01	OAW-CBC	-2.67	1.39	1.46
3	A	405	Y01	OAW-CBC	-2.67	1.39	1.46
3	D	405	Y01	OAW-CBC	-2.67	1.39	1.46
3	G	405	Y01	OAW-CBC	-2.67	1.39	1.46
3	J	405	Y01	OAW-CBC	-2.67	1.39	1.46
3	E	405	Y01	OAW-CBC	-2.65	1.40	1.46
3	H	405	Y01	OAW-CBC	-2.65	1.40	1.46
3	K	405	Y01	OAW-CBC	-2.65	1.40	1.46
3	L	406	Y01	CAO-CBB	2.64	1.61	1.54
3	A	406	Y01	CAO-CBB	2.63	1.61	1.54
3	D	406	Y01	CAO-CBB	2.63	1.61	1.54
3	G	406	Y01	CAO-CBB	2.63	1.61	1.54
3	J	406	Y01	CAO-CBB	2.63	1.61	1.54
3	B	406	Y01	CAO-CBB	2.62	1.61	1.54
3	E	406	Y01	CAO-CBB	2.62	1.61	1.54
3	C	406	Y01	CAO-CBB	2.62	1.61	1.54
3	F	406	Y01	CAO-CBB	2.62	1.61	1.54
3	I	406	Y01	CAO-CBB	2.61	1.61	1.54
3	H	406	Y01	CAO-CBB	2.59	1.61	1.54
3	K	406	Y01	CAO-CBB	2.59	1.61	1.54
3	K	405	Y01	CBI-CBG	-2.57	1.50	1.55
3	F	405	Y01	CBI-CBG	-2.55	1.50	1.55
3	I	405	Y01	CBI-CBG	-2.55	1.50	1.55
3	L	405	Y01	CBI-CBG	-2.55	1.50	1.55
3	A	405	Y01	CBI-CBG	-2.55	1.50	1.55
3	D	405	Y01	CBI-CBG	-2.55	1.50	1.55
3	G	405	Y01	CBI-CBG	-2.55	1.50	1.55
3	J	405	Y01	CBI-CBG	-2.55	1.50	1.55
3	B	405	Y01	CBI-CBG	-2.55	1.50	1.55
3	H	405	Y01	CBI-CBG	-2.55	1.50	1.55
3	E	405	Y01	CBI-CBG	-2.52	1.50	1.55
3	C	405	Y01	CBI-CBG	-2.51	1.50	1.55
3	A	406	Y01	CAV-CAZ	2.40	1.56	1.51
3	D	406	Y01	CAV-CAZ	2.40	1.56	1.51
3	G	406	Y01	CAV-CAZ	2.40	1.56	1.51
3	J	406	Y01	CAV-CAZ	2.40	1.56	1.51
3	K	406	Y01	CAV-CAZ	2.40	1.56	1.51
3	C	406	Y01	CAV-CAZ	2.40	1.56	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	406	Y01	CAV-CAZ	2.40	1.56	1.51
3	F	406	Y01	CAV-CAZ	2.40	1.56	1.51
3	H	406	Y01	CAV-CAZ	2.40	1.56	1.51
3	L	406	Y01	CAV-CAZ	2.40	1.56	1.51
3	L	405	Y01	CAO-CBB	2.39	1.60	1.54
3	B	406	Y01	CAV-CAZ	2.39	1.56	1.51
3	B	405	Y01	CAO-CBB	2.39	1.60	1.54
3	H	405	Y01	CAO-CBB	2.39	1.60	1.54
3	A	405	Y01	CAO-CBB	2.37	1.60	1.54
3	D	405	Y01	CAO-CBB	2.37	1.60	1.54
3	G	405	Y01	CAO-CBB	2.37	1.60	1.54
3	J	405	Y01	CAO-CBB	2.37	1.60	1.54
3	I	406	Y01	CAV-CAZ	2.37	1.56	1.51
3	F	405	Y01	CAO-CBB	2.37	1.60	1.54
3	I	405	Y01	CAO-CBB	2.37	1.60	1.54
3	E	405	Y01	CAO-CBB	2.36	1.60	1.54
3	K	405	Y01	CAO-CBB	2.36	1.60	1.54
3	C	405	Y01	CAO-CBB	2.35	1.60	1.54
3	H	405	Y01	CAJ-CAO	2.30	1.62	1.52
3	E	405	Y01	CAJ-CAO	2.30	1.62	1.52
3	F	405	Y01	CAJ-CAO	2.29	1.62	1.52
3	C	405	Y01	CAV-CAZ	2.29	1.56	1.51
3	E	405	Y01	CAV-CAZ	2.28	1.56	1.51
3	A	405	Y01	CAJ-CAO	2.28	1.61	1.52
3	D	405	Y01	CAJ-CAO	2.28	1.61	1.52
3	G	405	Y01	CAJ-CAO	2.28	1.61	1.52
3	J	405	Y01	CAJ-CAO	2.28	1.61	1.52
3	I	405	Y01	CAJ-CAO	2.28	1.61	1.52
3	L	405	Y01	CAJ-CAO	2.28	1.61	1.52
3	F	405	Y01	CAV-CAZ	2.28	1.56	1.51
3	B	405	Y01	CAJ-CAO	2.28	1.61	1.52
3	K	405	Y01	CAJ-CAO	2.28	1.61	1.52
3	A	405	Y01	CAV-CAZ	2.27	1.56	1.51
3	D	405	Y01	CAV-CAZ	2.27	1.56	1.51
3	G	405	Y01	CAV-CAZ	2.27	1.56	1.51
3	J	405	Y01	CAV-CAZ	2.27	1.56	1.51
3	C	405	Y01	CAJ-CAO	2.27	1.61	1.52
3	E	406	Y01	CAJ-CAO	2.26	1.61	1.52
3	K	406	Y01	CAJ-CAO	2.26	1.61	1.52
3	I	406	Y01	CAJ-CAO	2.26	1.61	1.52
3	A	406	Y01	CAJ-CAO	2.26	1.61	1.52
3	D	406	Y01	CAJ-CAO	2.26	1.61	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	406	Y01	CAJ-CAO	2.26	1.61	1.52
3	J	406	Y01	CAJ-CAO	2.26	1.61	1.52
3	I	406	Y01	OAW-CBC	-2.25	1.41	1.46
3	B	406	Y01	OAW-CBC	-2.25	1.41	1.46
3	I	405	Y01	CAV-CAZ	2.25	1.56	1.51
3	B	405	Y01	CAV-CAZ	2.25	1.56	1.51
3	H	405	Y01	CAV-CAZ	2.25	1.56	1.51
3	K	405	Y01	CAV-CAZ	2.25	1.56	1.51
3	C	406	Y01	CAJ-CAO	2.24	1.61	1.52
3	L	406	Y01	CAJ-CAO	2.24	1.61	1.52
3	B	406	Y01	CAJ-CAO	2.24	1.61	1.52
3	H	406	Y01	CAJ-CAO	2.24	1.61	1.52
3	L	405	Y01	CAV-CAZ	2.24	1.56	1.51
3	F	406	Y01	CAJ-CAO	2.24	1.61	1.52
3	C	406	Y01	OAW-CBC	-2.23	1.41	1.46
3	F	406	Y01	OAW-CBC	-2.23	1.41	1.46
3	L	406	Y01	OAW-CBC	-2.23	1.41	1.46
3	K	406	Y01	OAW-CBC	-2.22	1.41	1.46
3	A	406	Y01	OAW-CBC	-2.22	1.41	1.46
3	D	406	Y01	OAW-CBC	-2.22	1.41	1.46
3	G	406	Y01	OAW-CBC	-2.22	1.41	1.46
3	J	406	Y01	OAW-CBC	-2.22	1.41	1.46
3	E	406	Y01	OAW-CBC	-2.20	1.41	1.46
3	H	406	Y01	OAW-CBC	-2.20	1.41	1.46
3	E	406	Y01	CAM-CAY	2.17	1.57	1.50
3	H	406	Y01	CAM-CAY	2.17	1.57	1.50
3	E	405	Y01	CBB-CBE	-2.16	1.50	1.54
3	H	405	Y01	CBB-CBE	-2.16	1.50	1.54
3	A	406	Y01	CAM-CAY	2.16	1.57	1.50
3	D	406	Y01	CAM-CAY	2.16	1.57	1.50
3	G	406	Y01	CAM-CAY	2.16	1.57	1.50
3	J	406	Y01	CAM-CAY	2.16	1.57	1.50
3	C	406	Y01	CAM-CAY	2.16	1.57	1.50
3	I	406	Y01	CAM-CAY	2.16	1.57	1.50
3	L	406	Y01	CAM-CAY	2.16	1.57	1.50
3	B	406	Y01	CAM-CAY	2.16	1.57	1.50
3	K	406	Y01	CAM-CAY	2.16	1.57	1.50
3	L	405	Y01	CBB-CBE	-2.16	1.50	1.54
3	F	406	Y01	CAM-CAY	2.15	1.57	1.50
3	B	405	Y01	CBB-CBE	-2.13	1.50	1.54
3	K	405	Y01	CBB-CBE	-2.13	1.50	1.54
3	C	405	Y01	CBB-CBE	-2.13	1.50	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	405	Y01	CBB-CBE	-2.13	1.50	1.54
3	A	405	Y01	CBB-CBE	-2.13	1.50	1.54
3	D	405	Y01	CBB-CBE	-2.13	1.50	1.54
3	G	405	Y01	CBB-CBE	-2.13	1.50	1.54
3	J	405	Y01	CBB-CBE	-2.13	1.50	1.54
4	I	409	LHG	O8-C6	-2.12	1.40	1.45
4	F	409	LHG	O8-C6	-2.12	1.40	1.45
4	H	409	LHG	O8-C6	-2.10	1.40	1.45
4	B	409	LHG	O8-C6	-2.10	1.40	1.45
4	K	409	LHG	O8-C6	-2.10	1.40	1.45
3	C	405	Y01	CAM-CAY	2.09	1.56	1.50
3	F	405	Y01	CAM-CAY	2.09	1.56	1.50
3	I	405	Y01	CAM-CAY	2.09	1.56	1.50
3	L	405	Y01	CAM-CAY	2.09	1.56	1.50
4	D	409	LHG	O8-C6	-2.09	1.40	1.45
3	I	405	Y01	CBB-CBE	-2.09	1.50	1.54
4	A	409	LHG	O8-C6	-2.09	1.40	1.45
4	G	409	LHG	O8-C6	-2.09	1.40	1.45
3	A	405	Y01	CAM-CAY	2.08	1.56	1.50
3	D	405	Y01	CAM-CAY	2.08	1.56	1.50
3	G	405	Y01	CAM-CAY	2.08	1.56	1.50
3	J	405	Y01	CAM-CAY	2.08	1.56	1.50
4	C	409	LHG	O8-C6	-2.08	1.40	1.45
3	B	405	Y01	CAM-CAY	2.08	1.56	1.50
3	K	405	Y01	CAM-CAY	2.08	1.56	1.50
4	J	409	LHG	O8-C6	-2.08	1.40	1.45
3	E	406	Y01	CAR-CBC	2.07	1.56	1.51
3	H	406	Y01	CAR-CBC	2.07	1.56	1.51
3	K	406	Y01	CAR-CBC	2.07	1.56	1.51
4	E	409	LHG	O8-C6	-2.07	1.40	1.45
4	L	409	LHG	O8-C6	-2.07	1.40	1.45
3	A	406	Y01	CAR-CBC	2.07	1.56	1.51
3	D	406	Y01	CAR-CBC	2.07	1.56	1.51
3	G	406	Y01	CAR-CBC	2.07	1.56	1.51
3	C	406	Y01	CAR-CBC	2.06	1.56	1.51
3	F	406	Y01	CAR-CBC	2.06	1.56	1.51
3	I	406	Y01	CAR-CBC	2.06	1.56	1.51
3	L	406	Y01	CAR-CBC	2.06	1.56	1.51
3	B	406	Y01	CAR-CBC	2.06	1.56	1.51
3	E	405	Y01	CAM-CAY	2.05	1.56	1.50
3	H	405	Y01	CAM-CAY	2.05	1.56	1.50
3	J	406	Y01	CAR-CBC	2.05	1.56	1.51

All (536) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	405	Y01	CAK-CBD-CBF	-7.85	100.20	109.71
3	K	405	Y01	CAK-CBD-CBF	-7.85	100.20	109.71
3	L	405	Y01	CAK-CBD-CBF	-7.85	100.20	109.71
3	H	405	Y01	CAK-CBD-CBF	-7.84	100.21	109.71
3	A	405	Y01	CAK-CBD-CBF	-7.84	100.22	109.71
3	D	405	Y01	CAK-CBD-CBF	-7.84	100.22	109.71
3	G	405	Y01	CAK-CBD-CBF	-7.84	100.22	109.71
3	E	405	Y01	CAK-CBD-CBF	-7.84	100.22	109.71
3	J	405	Y01	CAK-CBD-CBF	-7.83	100.22	109.71
3	F	405	Y01	CAK-CBD-CBF	-7.82	100.23	109.71
3	I	405	Y01	CAK-CBD-CBF	-7.80	100.26	109.71
3	C	405	Y01	CAK-CBD-CBF	-7.80	100.26	109.71
3	C	406	Y01	CAK-CBD-CBF	-7.45	100.69	109.71
3	F	406	Y01	CAK-CBD-CBF	-7.45	100.69	109.71
3	I	406	Y01	CAK-CBD-CBF	-7.45	100.69	109.71
3	L	406	Y01	CAK-CBD-CBF	-7.45	100.69	109.71
3	K	406	Y01	CAK-CBD-CBF	-7.44	100.70	109.71
3	B	406	Y01	CAK-CBD-CBF	-7.43	100.71	109.71
3	E	406	Y01	CAK-CBD-CBF	-7.43	100.71	109.71
3	H	406	Y01	CAK-CBD-CBF	-7.43	100.71	109.71
3	A	406	Y01	CAK-CBD-CBF	-7.43	100.71	109.71
3	D	406	Y01	CAK-CBD-CBF	-7.43	100.71	109.71
3	G	406	Y01	CAK-CBD-CBF	-7.43	100.71	109.71
3	J	406	Y01	CAK-CBD-CBF	-7.42	100.72	109.71
3	C	405	Y01	CAV-CAZ-CAI	-6.87	110.70	120.61
3	E	405	Y01	CAV-CAZ-CAI	-6.87	110.70	120.61
3	A	405	Y01	CAV-CAZ-CAI	-6.87	110.71	120.61
3	D	405	Y01	CAV-CAZ-CAI	-6.87	110.71	120.61
3	G	405	Y01	CAV-CAZ-CAI	-6.87	110.71	120.61
3	H	405	Y01	CAV-CAZ-CAI	-6.87	110.71	120.61
3	I	405	Y01	CAV-CAZ-CAI	-6.86	110.72	120.61
3	J	405	Y01	CAV-CAZ-CAI	-6.86	110.73	120.61
3	L	405	Y01	CAV-CAZ-CAI	-6.85	110.74	120.61
3	F	405	Y01	CAV-CAZ-CAI	-6.85	110.74	120.61
3	B	405	Y01	CAV-CAZ-CAI	-6.84	110.75	120.61
3	K	405	Y01	CAV-CAZ-CAI	-6.84	110.75	120.61
3	J	406	Y01	CBC-CAV-CAZ	-6.79	100.97	111.52
3	E	406	Y01	CBC-CAV-CAZ	-6.78	100.98	111.52
3	H	406	Y01	CBC-CAV-CAZ	-6.78	100.98	111.52
3	B	406	Y01	CBC-CAV-CAZ	-6.78	100.99	111.52
3	A	406	Y01	CBC-CAV-CAZ	-6.77	101.01	111.52
3	D	406	Y01	CBC-CAV-CAZ	-6.77	101.01	111.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	G	406	Y01	CBC-CAV-CAZ	-6.77	101.01	111.52
3	I	406	Y01	CBC-CAV-CAZ	-6.76	101.01	111.52
3	K	406	Y01	CBC-CAV-CAZ	-6.76	101.02	111.52
3	C	406	Y01	CBC-CAV-CAZ	-6.76	101.02	111.52
3	F	406	Y01	CBC-CAV-CAZ	-6.76	101.02	111.52
3	L	406	Y01	CBC-CAV-CAZ	-6.76	101.02	111.52
3	B	406	Y01	CBH-CBF-CBD	-6.09	103.60	112.73
3	K	406	Y01	CBH-CBF-CBD	-6.07	103.63	112.73
3	A	406	Y01	CBH-CBF-CBD	-6.07	103.63	112.73
3	D	406	Y01	CBH-CBF-CBD	-6.07	103.63	112.73
3	G	406	Y01	CBH-CBF-CBD	-6.07	103.63	112.73
3	J	406	Y01	CBH-CBF-CBD	-6.07	103.63	112.73
3	E	406	Y01	CBH-CBF-CBD	-6.06	103.64	112.73
3	H	406	Y01	CBH-CBF-CBD	-6.06	103.64	112.73
3	C	406	Y01	CBH-CBF-CBD	-6.05	103.66	112.73
3	F	406	Y01	CBH-CBF-CBD	-6.05	103.66	112.73
3	I	406	Y01	CBH-CBF-CBD	-6.05	103.66	112.73
3	L	406	Y01	CBH-CBF-CBD	-6.05	103.66	112.73
3	B	405	Y01	CAQ-CBG-CBD	-5.83	109.47	119.08
3	E	405	Y01	CAQ-CBG-CBD	-5.83	109.48	119.08
3	K	405	Y01	CAQ-CBG-CBD	-5.83	109.48	119.08
3	A	405	Y01	CAQ-CBG-CBD	-5.82	109.49	119.08
3	D	405	Y01	CAQ-CBG-CBD	-5.82	109.49	119.08
3	G	405	Y01	CAQ-CBG-CBD	-5.82	109.49	119.08
3	J	405	Y01	CAQ-CBG-CBD	-5.82	109.49	119.08
3	I	405	Y01	CAQ-CBG-CBD	-5.82	109.50	119.08
3	C	405	Y01	CAQ-CBG-CBD	-5.81	109.51	119.08
3	F	405	Y01	CAQ-CBG-CBD	-5.81	109.51	119.08
3	H	405	Y01	CAQ-CBG-CBD	-5.81	109.51	119.08
3	L	405	Y01	CAQ-CBG-CBD	-5.81	109.51	119.08
3	C	406	Y01	OAW-CAY-CAM	5.61	123.59	111.50
3	I	406	Y01	OAW-CAY-CAM	5.61	123.59	111.50
3	L	406	Y01	OAW-CAY-CAM	5.61	123.59	111.50
3	B	406	Y01	OAW-CAY-CAM	5.61	123.59	111.50
3	K	406	Y01	OAW-CAY-CAM	5.61	123.59	111.50
3	A	406	Y01	OAW-CAY-CAM	5.60	123.56	111.50
3	D	406	Y01	OAW-CAY-CAM	5.60	123.56	111.50
3	G	406	Y01	OAW-CAY-CAM	5.60	123.56	111.50
3	J	406	Y01	OAW-CAY-CAM	5.60	123.56	111.50
3	E	406	Y01	OAW-CAY-CAM	5.58	123.54	111.50
3	H	406	Y01	OAW-CAY-CAM	5.58	123.54	111.50
3	F	406	Y01	OAW-CAY-CAM	5.58	123.53	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	405	Y01	CBH-CBF-CBD	-5.26	104.84	112.73
3	C	405	Y01	CBH-CBF-CBD	-5.26	104.85	112.73
3	F	405	Y01	CBH-CBF-CBD	-5.26	104.85	112.73
3	I	405	Y01	CBH-CBF-CBD	-5.26	104.85	112.73
3	L	405	Y01	CBH-CBF-CBD	-5.26	104.85	112.73
3	A	405	Y01	CBH-CBF-CBD	-5.25	104.86	112.73
3	D	405	Y01	CBH-CBF-CBD	-5.25	104.86	112.73
3	G	405	Y01	CBH-CBF-CBD	-5.25	104.86	112.73
3	H	405	Y01	CBH-CBF-CBD	-5.24	104.87	112.73
3	B	405	Y01	CBH-CBF-CBD	-5.24	104.88	112.73
3	K	405	Y01	CBH-CBF-CBD	-5.24	104.88	112.73
3	J	405	Y01	CBH-CBF-CBD	-5.23	104.89	112.73
3	K	406	Y01	CAK-CBD-CBG	5.08	118.28	110.91
3	A	406	Y01	CAK-CBD-CBG	5.06	118.25	110.91
3	D	406	Y01	CAK-CBD-CBG	5.06	118.25	110.91
3	G	406	Y01	CAK-CBD-CBG	5.06	118.25	110.91
3	B	406	Y01	CAK-CBD-CBG	5.06	118.23	110.91
3	E	406	Y01	CAK-CBD-CBG	5.06	118.23	110.91
3	H	406	Y01	CAK-CBD-CBG	5.06	118.23	110.91
3	J	406	Y01	CAK-CBD-CBG	5.05	118.22	110.91
3	C	406	Y01	CAK-CBD-CBG	5.04	118.21	110.91
3	F	406	Y01	CAK-CBD-CBG	5.04	118.21	110.91
3	I	406	Y01	CAK-CBD-CBG	5.04	118.21	110.91
3	L	406	Y01	CAK-CBD-CBG	5.04	118.21	110.91
3	E	406	Y01	CAQ-CBG-CBD	-4.88	111.05	119.08
3	H	406	Y01	CAQ-CBG-CBD	-4.88	111.05	119.08
3	K	406	Y01	CAQ-CBG-CBD	-4.87	111.07	119.08
3	A	406	Y01	CAQ-CBG-CBD	-4.86	111.07	119.08
3	D	406	Y01	CAQ-CBG-CBD	-4.86	111.07	119.08
3	G	406	Y01	CAQ-CBG-CBD	-4.86	111.07	119.08
3	J	406	Y01	CAQ-CBG-CBD	-4.86	111.07	119.08
3	B	406	Y01	CAQ-CBG-CBD	-4.85	111.09	119.08
3	C	406	Y01	CAQ-CBG-CBD	-4.84	111.11	119.08
3	F	406	Y01	CAQ-CBG-CBD	-4.84	111.11	119.08
3	I	406	Y01	CAQ-CBG-CBD	-4.84	111.11	119.08
3	L	406	Y01	CAQ-CBG-CBD	-4.84	111.11	119.08
3	E	405	Y01	CAS-CBF-CBH	4.57	119.09	113.08
3	K	405	Y01	CAS-CBF-CBH	4.55	119.07	113.08
3	A	405	Y01	CAS-CBF-CBH	4.53	119.05	113.08
3	B	405	Y01	CAS-CBF-CBH	4.53	119.05	113.08
3	C	405	Y01	CAS-CBF-CBH	4.53	119.05	113.08
3	D	405	Y01	CAS-CBF-CBH	4.53	119.05	113.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	405	Y01	CAS-CBF-CBH	4.53	119.05	113.08
3	G	405	Y01	CAS-CBF-CBH	4.53	119.05	113.08
3	I	405	Y01	CAS-CBF-CBH	4.53	119.05	113.08
3	J	405	Y01	CAS-CBF-CBH	4.53	119.05	113.08
3	L	405	Y01	CAS-CBF-CBH	4.53	119.05	113.08
3	H	405	Y01	CAS-CBF-CBH	4.53	119.04	113.08
3	K	406	Y01	CAS-CBF-CBH	4.31	118.76	113.08
3	J	406	Y01	CAS-CBF-CBH	4.29	118.73	113.08
3	B	406	Y01	CAS-CBF-CBH	4.29	118.73	113.08
3	A	406	Y01	CAS-CBF-CBH	4.29	118.73	113.08
3	D	406	Y01	CAS-CBF-CBH	4.29	118.73	113.08
3	G	406	Y01	CAS-CBF-CBH	4.29	118.73	113.08
3	E	406	Y01	CAS-CBF-CBH	4.29	118.73	113.08
3	H	406	Y01	CAS-CBF-CBH	4.29	118.73	113.08
3	C	406	Y01	CAS-CBF-CBH	4.29	118.72	113.08
3	F	406	Y01	CAS-CBF-CBH	4.29	118.72	113.08
3	I	406	Y01	CAS-CBF-CBH	4.29	118.72	113.08
3	L	406	Y01	CAS-CBF-CBH	4.29	118.72	113.08
3	K	406	Y01	CBG-CBI-CBE	4.14	104.98	100.07
3	B	406	Y01	CBG-CBI-CBE	4.14	104.98	100.07
3	C	406	Y01	CBG-CBI-CBE	4.14	104.98	100.07
3	J	406	Y01	CBG-CBI-CBE	4.14	104.97	100.07
3	I	406	Y01	CBG-CBI-CBE	4.14	104.97	100.07
3	L	406	Y01	CBG-CBI-CBE	4.14	104.97	100.07
3	F	406	Y01	CBG-CBI-CBE	4.12	104.96	100.07
3	A	406	Y01	CBG-CBI-CBE	4.12	104.96	100.07
3	D	406	Y01	CBG-CBI-CBE	4.12	104.96	100.07
3	G	406	Y01	CBG-CBI-CBE	4.12	104.96	100.07
3	E	406	Y01	CBG-CBI-CBE	4.11	104.94	100.07
3	H	406	Y01	CBG-CBI-CBE	4.11	104.94	100.07
3	F	406	Y01	CAC-CBB-CBE	-3.94	106.89	112.92
3	B	406	Y01	CAC-CBB-CBE	-3.94	106.89	112.92
3	K	406	Y01	CAC-CBB-CBE	-3.94	106.89	112.92
3	A	406	Y01	CAC-CBB-CBE	-3.93	106.91	112.92
3	D	406	Y01	CAC-CBB-CBE	-3.93	106.91	112.92
3	G	406	Y01	CAC-CBB-CBE	-3.93	106.91	112.92
3	J	406	Y01	CAC-CBB-CBE	-3.93	106.91	112.92
3	C	406	Y01	CAC-CBB-CBE	-3.92	106.92	112.92
3	I	406	Y01	CAC-CBB-CBE	-3.92	106.92	112.92
3	H	406	Y01	CAC-CBB-CBE	-3.92	106.92	112.92
3	E	405	Y01	OAW-CAY-CAM	3.92	119.95	111.50
3	H	405	Y01	OAW-CAY-CAM	3.92	119.95	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	405	Y01	OAW-CAY-CAM	3.91	119.94	111.50
3	B	405	Y01	CAK-CAI-CAZ	3.91	132.28	125.06
3	K	405	Y01	CAK-CAI-CAZ	3.91	132.28	125.06
3	B	405	Y01	OAW-CAY-CAM	3.91	119.93	111.50
3	K	405	Y01	OAW-CAY-CAM	3.91	119.93	111.50
3	E	406	Y01	CAC-CBB-CBE	-3.91	106.94	112.92
4	E	409	LHG	C5-O7-C7	-3.91	112.85	117.88
3	A	405	Y01	OAW-CAY-CAM	3.91	119.92	111.50
3	D	405	Y01	OAW-CAY-CAM	3.91	119.92	111.50
3	G	405	Y01	OAW-CAY-CAM	3.91	119.92	111.50
3	J	405	Y01	OAW-CAY-CAM	3.91	119.92	111.50
3	L	406	Y01	CAC-CBB-CBE	-3.90	106.94	112.92
3	C	405	Y01	CAK-CAI-CAZ	3.90	132.26	125.06
4	L	409	LHG	C5-O7-C7	-3.90	112.86	117.88
3	J	405	Y01	CAK-CAI-CAZ	3.90	132.25	125.06
4	J	409	LHG	C5-O7-C7	-3.90	112.87	117.88
3	F	405	Y01	OAW-CAY-CAM	3.89	119.89	111.50
3	I	405	Y01	OAW-CAY-CAM	3.89	119.89	111.50
3	L	405	Y01	OAW-CAY-CAM	3.89	119.89	111.50
3	E	405	Y01	CAK-CAI-CAZ	3.89	132.23	125.06
4	C	409	LHG	C5-O7-C7	-3.89	112.88	117.88
3	A	405	Y01	CAK-CAI-CAZ	3.89	132.23	125.06
3	D	405	Y01	CAK-CAI-CAZ	3.89	132.23	125.06
3	G	405	Y01	CAK-CAI-CAZ	3.89	132.23	125.06
3	F	405	Y01	CAK-CAI-CAZ	3.88	132.22	125.06
3	I	405	Y01	CAK-CAI-CAZ	3.88	132.22	125.06
4	A	409	LHG	C5-O7-C7	-3.88	112.88	117.88
4	D	409	LHG	C5-O7-C7	-3.88	112.88	117.88
4	G	409	LHG	C5-O7-C7	-3.88	112.88	117.88
3	L	405	Y01	CAK-CAI-CAZ	3.88	132.21	125.06
4	K	409	LHG	C5-O7-C7	-3.87	112.90	117.88
4	F	409	LHG	C5-O7-C7	-3.86	112.91	117.88
4	I	409	LHG	C5-O7-C7	-3.86	112.91	117.88
3	H	405	Y01	CAK-CAI-CAZ	3.86	132.18	125.06
3	C	406	Y01	CAO-CBB-CBE	3.85	118.24	110.28
4	B	409	LHG	C5-O7-C7	-3.85	112.92	117.88
4	H	409	LHG	C5-O7-C7	-3.85	112.92	117.88
3	E	406	Y01	CAO-CBB-CBE	3.85	118.23	110.28
3	F	406	Y01	CAO-CBB-CBE	3.84	118.21	110.28
3	I	406	Y01	CAO-CBB-CBE	3.84	118.21	110.28
3	B	406	Y01	CAO-CBB-CBE	3.83	118.21	110.28
3	H	406	Y01	CAO-CBB-CBE	3.83	118.21	110.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	K	406	Y01	CAO-CBB-CBE	3.83	118.20	110.28
3	A	406	Y01	CAO-CBB-CBE	3.83	118.20	110.28
3	D	406	Y01	CAO-CBB-CBE	3.83	118.20	110.28
3	G	406	Y01	CAO-CBB-CBE	3.83	118.20	110.28
3	J	406	Y01	CAO-CBB-CBE	3.83	118.20	110.28
3	E	405	Y01	CBH-CAZ-CAI	3.82	128.75	122.90
3	L	406	Y01	CAO-CBB-CBE	3.82	118.17	110.28
3	H	405	Y01	CBH-CAZ-CAI	3.81	128.73	122.90
3	A	405	Y01	CBH-CAZ-CAI	3.80	128.72	122.90
3	D	405	Y01	CBH-CAZ-CAI	3.80	128.72	122.90
3	G	405	Y01	CBH-CAZ-CAI	3.80	128.72	122.90
3	C	405	Y01	CBH-CAZ-CAI	3.80	128.72	122.90
3	L	405	Y01	CBH-CAZ-CAI	3.80	128.72	122.90
3	F	405	Y01	CBH-CAZ-CAI	3.79	128.71	122.90
3	I	405	Y01	CBH-CAZ-CAI	3.79	128.71	122.90
3	J	405	Y01	CBH-CAZ-CAI	3.79	128.70	122.90
3	B	405	Y01	CBH-CAZ-CAI	3.78	128.68	122.90
3	K	405	Y01	CBH-CAZ-CAI	3.78	128.68	122.90
3	C	406	Y01	CAE-CBI-CAU	-3.44	105.16	110.59
3	F	406	Y01	CAE-CBI-CAU	-3.44	105.16	110.59
3	I	406	Y01	CAE-CBI-CAU	-3.44	105.16	110.59
3	K	406	Y01	CAE-CBI-CAU	-3.43	105.18	110.59
3	L	406	Y01	CAE-CBI-CAU	-3.43	105.18	110.59
3	A	406	Y01	CAE-CBI-CAU	-3.42	105.19	110.59
3	D	406	Y01	CAE-CBI-CAU	-3.42	105.19	110.59
3	G	406	Y01	CAE-CBI-CAU	-3.42	105.19	110.59
3	J	406	Y01	CAE-CBI-CAU	-3.42	105.19	110.59
3	B	406	Y01	CAE-CBI-CAU	-3.41	105.21	110.59
3	E	406	Y01	CAE-CBI-CAU	-3.39	105.24	110.59
3	H	406	Y01	CAE-CBI-CAU	-3.39	105.24	110.59
3	B	406	Y01	CAK-CAI-CAZ	3.37	131.28	125.06
3	K	406	Y01	CAK-CAI-CAZ	3.36	131.26	125.06
3	H	406	Y01	CAK-CAI-CAZ	3.36	131.25	125.06
3	C	406	Y01	CAK-CAI-CAZ	3.35	131.25	125.06
3	F	406	Y01	CAK-CAI-CAZ	3.35	131.25	125.06
3	I	406	Y01	CAK-CAI-CAZ	3.35	131.25	125.06
3	L	406	Y01	CAK-CAI-CAZ	3.35	131.25	125.06
3	A	406	Y01	CAK-CAI-CAZ	3.35	131.25	125.06
3	D	406	Y01	CAK-CAI-CAZ	3.35	131.25	125.06
3	G	406	Y01	CAK-CAI-CAZ	3.35	131.25	125.06
3	J	406	Y01	CAK-CAI-CAZ	3.35	131.25	125.06
3	E	406	Y01	CAK-CAI-CAZ	3.31	131.17	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	405	Y01	CAV-CAZ-CBH	3.13	120.57	116.42
3	A	405	Y01	CAV-CAZ-CBH	3.12	120.57	116.42
3	D	405	Y01	CAV-CAZ-CBH	3.12	120.57	116.42
3	G	405	Y01	CAV-CAZ-CBH	3.12	120.57	116.42
3	I	405	Y01	CAV-CAZ-CBH	3.12	120.57	116.42
3	J	405	Y01	CAV-CAZ-CBH	3.12	120.57	116.42
3	B	405	Y01	CAV-CAZ-CBH	3.12	120.56	116.42
3	H	405	Y01	CAV-CAZ-CBH	3.12	120.56	116.42
3	K	405	Y01	CAV-CAZ-CBH	3.12	120.56	116.42
3	F	405	Y01	CAV-CAZ-CBH	3.11	120.55	116.42
3	E	405	Y01	CAV-CAZ-CBH	3.10	120.54	116.42
3	L	405	Y01	CAV-CAZ-CBH	3.10	120.54	116.42
3	C	406	Y01	OAW-CBC-CAV	3.05	114.36	108.12
3	F	406	Y01	OAW-CBC-CAV	3.05	114.36	108.12
3	L	406	Y01	OAW-CBC-CAV	3.05	114.36	108.12
3	I	406	Y01	OAW-CBC-CAV	3.04	114.35	108.12
3	E	406	Y01	OAW-CBC-CAV	3.04	114.34	108.12
3	H	406	Y01	OAW-CBC-CAV	3.04	114.34	108.12
3	A	406	Y01	OAW-CBC-CAV	3.04	114.34	108.12
3	D	406	Y01	OAW-CBC-CAV	3.04	114.34	108.12
3	G	406	Y01	OAW-CBC-CAV	3.04	114.34	108.12
3	K	406	Y01	OAW-CBC-CAV	3.04	114.34	108.12
3	B	406	Y01	OAW-CBC-CAV	3.02	114.31	108.12
3	J	406	Y01	OAW-CBC-CAV	3.02	114.30	108.12
3	E	405	Y01	CAS-CBF-CBD	-3.01	107.41	111.75
3	F	405	Y01	CAS-CBF-CBD	-3.00	107.43	111.75
3	L	405	Y01	CAS-CBF-CBD	-3.00	107.43	111.75
3	A	405	Y01	CAS-CBF-CBD	-3.00	107.43	111.75
3	D	405	Y01	CAS-CBF-CBD	-3.00	107.43	111.75
3	G	405	Y01	CAS-CBF-CBD	-3.00	107.43	111.75
3	J	405	Y01	CAS-CBF-CBD	-3.00	107.43	111.75
3	K	405	Y01	CAS-CBF-CBD	-3.00	107.43	111.75
3	H	405	Y01	CAS-CBF-CBD	-3.00	107.44	111.75
3	C	405	Y01	CAS-CBF-CBD	-2.98	107.45	111.75
3	I	405	Y01	CAS-CBF-CBD	-2.98	107.45	111.75
3	B	405	Y01	CAS-CBF-CBD	-2.98	107.46	111.75
3	L	406	Y01	CAC-CBB-CAO	-2.93	105.77	110.36
3	C	406	Y01	CAC-CBB-CAO	-2.93	105.78	110.36
3	A	406	Y01	CAC-CBB-CAO	-2.92	105.78	110.36
3	D	406	Y01	CAC-CBB-CAO	-2.92	105.78	110.36
3	G	406	Y01	CAC-CBB-CAO	-2.92	105.78	110.36
3	J	406	Y01	CAC-CBB-CAO	-2.92	105.78	110.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	H	406	Y01	CAC-CBB-CAO	-2.92	105.78	110.36
3	H	405	Y01	CAU-CBI-CBG	2.92	111.80	107.27
3	E	406	Y01	CAC-CBB-CAO	-2.91	105.80	110.36
3	F	406	Y01	CAC-CBB-CAO	-2.91	105.80	110.36
3	B	406	Y01	CAC-CBB-CAO	-2.91	105.80	110.36
3	K	406	Y01	CAC-CBB-CAO	-2.91	105.80	110.36
3	I	406	Y01	CAC-CBB-CAO	-2.91	105.81	110.36
3	J	405	Y01	CAU-CBI-CBG	2.90	111.77	107.27
3	F	405	Y01	CAU-CBI-CBG	2.90	111.77	107.27
3	L	405	Y01	CAU-CBI-CBG	2.90	111.77	107.27
3	B	405	Y01	CAU-CBI-CBG	2.90	111.76	107.27
3	A	405	Y01	CAU-CBI-CBG	2.89	111.76	107.27
3	D	405	Y01	CAU-CBI-CBG	2.89	111.76	107.27
3	G	405	Y01	CAU-CBI-CBG	2.89	111.76	107.27
3	C	405	Y01	CAU-CBI-CBG	2.88	111.73	107.27
3	I	405	Y01	CAU-CBI-CBG	2.88	111.73	107.27
3	K	405	Y01	CAU-CBI-CBG	2.87	111.73	107.27
3	E	405	Y01	CAU-CBI-CBG	2.86	111.71	107.27
3	I	406	Y01	CAJ-CAO-CBB	-2.74	107.16	115.03
3	E	406	Y01	CAJ-CAO-CBB	-2.73	107.18	115.03
3	K	406	Y01	CAJ-CAO-CBB	-2.73	107.18	115.03
3	A	406	Y01	CAJ-CAO-CBB	-2.73	107.19	115.03
3	D	406	Y01	CAJ-CAO-CBB	-2.73	107.19	115.03
3	G	406	Y01	CAJ-CAO-CBB	-2.73	107.19	115.03
3	J	406	Y01	CAJ-CAO-CBB	-2.73	107.19	115.03
3	F	406	Y01	CAJ-CAO-CBB	-2.73	107.19	115.03
3	B	406	Y01	CAJ-CAO-CBB	-2.73	107.19	115.03
3	H	406	Y01	CAJ-CAO-CBB	-2.73	107.19	115.03
3	L	406	Y01	CAJ-CAO-CBB	-2.72	107.20	115.03
3	C	406	Y01	CAJ-CAO-CBB	-2.72	107.22	115.03
3	L	406	Y01	CAD-CBH-CBF	2.59	114.77	111.68
3	B	406	Y01	CAD-CBH-CBF	2.59	114.77	111.68
3	K	406	Y01	CAD-CBH-CBF	2.58	114.76	111.68
3	F	405	Y01	CAE-CBI-CAU	-2.57	106.53	110.59
3	L	405	Y01	CAE-CBI-CAU	-2.57	106.53	110.59
3	A	406	Y01	CAD-CBH-CBF	2.57	114.75	111.68
3	D	406	Y01	CAD-CBH-CBF	2.57	114.75	111.68
3	G	406	Y01	CAD-CBH-CBF	2.57	114.75	111.68
3	C	406	Y01	CAD-CBH-CBF	2.57	114.74	111.68
3	F	406	Y01	CAD-CBH-CBF	2.57	114.74	111.68
3	I	406	Y01	CAD-CBH-CBF	2.57	114.74	111.68
3	K	405	Y01	CAE-CBI-CAU	-2.57	106.53	110.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	J	405	Y01	CAE-CBI-CAU	-2.56	106.54	110.59
3	E	406	Y01	CAD-CBH-CBF	2.56	114.73	111.68
3	H	406	Y01	CAD-CBH-CBF	2.56	114.73	111.68
3	J	406	Y01	CAD-CBH-CBF	2.55	114.73	111.68
3	E	405	Y01	CAE-CBI-CAU	-2.55	106.56	110.59
3	H	405	Y01	CAE-CBI-CAU	-2.55	106.56	110.59
3	A	405	Y01	CAE-CBI-CAU	-2.55	106.57	110.59
3	D	405	Y01	CAE-CBI-CAU	-2.55	106.57	110.59
3	G	405	Y01	CAE-CBI-CAU	-2.55	106.57	110.59
3	B	405	Y01	CAE-CBI-CAU	-2.54	106.58	110.59
3	C	405	Y01	CAE-CBI-CAU	-2.53	106.59	110.59
3	I	405	Y01	CAE-CBI-CAU	-2.53	106.59	110.59
3	C	405	Y01	CAP-CAQ-CBG	-2.53	100.12	105.13
3	B	405	Y01	CAP-CAQ-CBG	-2.53	100.12	105.13
3	K	405	Y01	CAP-CAQ-CBG	-2.53	100.12	105.13
3	H	405	Y01	CAP-CAQ-CBG	-2.53	100.12	105.13
3	E	405	Y01	CAP-CAQ-CBG	-2.53	100.13	105.13
3	A	405	Y01	CAP-CAQ-CBG	-2.53	100.13	105.13
3	D	405	Y01	CAP-CAQ-CBG	-2.53	100.13	105.13
3	G	405	Y01	CAP-CAQ-CBG	-2.53	100.13	105.13
3	J	405	Y01	CAP-CAQ-CBG	-2.53	100.13	105.13
3	F	405	Y01	CAP-CAQ-CBG	-2.52	100.13	105.13
3	I	405	Y01	CAP-CAQ-CBG	-2.52	100.13	105.13
3	L	405	Y01	CAP-CAQ-CBG	-2.52	100.13	105.13
4	E	409	LHG	C27-C26-C25	-2.52	101.61	114.42
4	I	409	LHG	C27-C26-C25	-2.52	101.62	114.42
4	F	409	LHG	C27-C26-C25	-2.52	101.63	114.42
4	H	409	LHG	C27-C26-C25	-2.52	101.64	114.42
4	L	409	LHG	C27-C26-C25	-2.52	101.65	114.42
4	A	409	LHG	C27-C26-C25	-2.52	101.66	114.42
4	G	409	LHG	C27-C26-C25	-2.52	101.66	114.42
4	B	409	LHG	C27-C26-C25	-2.51	101.67	114.42
4	K	409	LHG	C27-C26-C25	-2.51	101.67	114.42
4	D	409	LHG	C27-C26-C25	-2.51	101.68	114.42
4	J	409	LHG	C27-C26-C25	-2.51	101.68	114.42
4	C	409	LHG	C27-C26-C25	-2.50	101.71	114.42
3	B	405	Y01	CBC-CAV-CAZ	2.40	115.25	111.52
3	L	405	Y01	CBC-CAV-CAZ	2.40	115.24	111.52
3	K	405	Y01	CBC-CAV-CAZ	2.38	115.22	111.52
3	H	405	Y01	CBC-CAV-CAZ	2.38	115.21	111.52
3	C	405	Y01	CBC-CAV-CAZ	2.38	115.21	111.52
3	E	405	Y01	CBC-CAV-CAZ	2.37	115.20	111.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	405	Y01	CBC-CAV-CAZ	2.37	115.20	111.52
3	A	405	Y01	CBC-CAV-CAZ	2.37	115.20	111.52
3	D	405	Y01	CBC-CAV-CAZ	2.37	115.20	111.52
3	G	405	Y01	CBC-CAV-CAZ	2.37	115.20	111.52
3	I	405	Y01	CBC-CAV-CAZ	2.37	115.20	111.52
3	J	405	Y01	CBC-CAV-CAZ	2.37	115.20	111.52
3	I	405	Y01	CAC-CBB-CBE	-2.33	109.35	112.92
3	E	405	Y01	CAC-CBB-CBE	-2.32	109.36	112.92
3	H	405	Y01	CAC-CBB-CBE	-2.32	109.36	112.92
3	C	405	Y01	CAC-CBB-CBE	-2.32	109.36	112.92
3	F	405	Y01	CAC-CBB-CBE	-2.32	109.36	112.92
3	A	405	Y01	CAC-CBB-CBE	-2.31	109.38	112.92
3	D	405	Y01	CAC-CBB-CBE	-2.31	109.38	112.92
3	G	405	Y01	CAC-CBB-CBE	-2.31	109.38	112.92
3	J	405	Y01	CAC-CBB-CBE	-2.31	109.38	112.92
3	K	405	Y01	CAC-CBB-CBE	-2.31	109.39	112.92
3	L	405	Y01	CAC-CBB-CBE	-2.30	109.40	112.92
3	B	405	Y01	CAC-CBB-CBE	-2.30	109.40	112.92
3	E	405	Y01	CAT-CBH-CBF	-2.27	105.56	108.73
3	F	405	Y01	CAT-CBH-CBF	-2.26	105.57	108.73
3	I	405	Y01	CAT-CBH-CBF	-2.26	105.57	108.73
3	L	405	Y01	CAT-CBH-CBF	-2.26	105.57	108.73
3	H	405	Y01	CAT-CBH-CBF	-2.25	105.59	108.73
3	A	405	Y01	CAT-CBH-CBF	-2.24	105.60	108.73
3	C	405	Y01	CAT-CBH-CBF	-2.24	105.60	108.73
3	D	405	Y01	CAT-CBH-CBF	-2.24	105.60	108.73
3	G	405	Y01	CAT-CBH-CBF	-2.24	105.60	108.73
3	J	405	Y01	CAT-CBH-CBF	-2.23	105.61	108.73
3	B	405	Y01	CAT-CBH-CBF	-2.22	105.62	108.73
3	K	405	Y01	CAT-CBH-CBF	-2.22	105.62	108.73
4	D	409	LHG	O8-C23-C24	2.21	118.84	111.91
4	B	409	LHG	O8-C23-C24	2.21	118.83	111.91
4	H	409	LHG	O8-C23-C24	2.20	118.83	111.91
4	E	409	LHG	O8-C23-C24	2.20	118.81	111.91
4	C	409	LHG	O8-C23-C24	2.20	118.81	111.91
4	A	409	LHG	O8-C23-C24	2.20	118.81	111.91
4	G	409	LHG	O8-C23-C24	2.20	118.81	111.91
4	J	409	LHG	O8-C23-C24	2.20	118.81	111.91
4	L	409	LHG	O8-C23-C24	2.20	118.80	111.91
3	J	406	Y01	CBF-CBH-CAZ	-2.19	106.21	109.65
4	F	409	LHG	O8-C23-C24	2.19	118.79	111.91
4	I	409	LHG	O8-C23-C24	2.19	118.79	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	K	409	LHG	O8-C23-C24	2.19	118.78	111.91
3	C	406	Y01	CBF-CBH-CAZ	-2.18	106.23	109.65
3	F	406	Y01	CBF-CBH-CAZ	-2.18	106.23	109.65
3	I	406	Y01	CBF-CBH-CAZ	-2.18	106.23	109.65
3	L	406	Y01	CBF-CBH-CAZ	-2.18	106.23	109.65
3	E	406	Y01	CBF-CBH-CAZ	-2.18	106.23	109.65
3	H	406	Y01	CBF-CBH-CAZ	-2.18	106.23	109.65
3	J	406	Y01	CAS-CBF-CBD	-2.18	108.62	111.75
3	A	406	Y01	CBF-CBH-CAZ	-2.18	106.24	109.65
3	D	406	Y01	CBF-CBH-CAZ	-2.18	106.24	109.65
3	G	406	Y01	CBF-CBH-CAZ	-2.18	106.24	109.65
3	K	406	Y01	CBF-CBH-CAZ	-2.18	106.24	109.65
3	C	406	Y01	CAS-CBF-CBD	-2.18	108.62	111.75
3	F	406	Y01	CAS-CBF-CBD	-2.18	108.62	111.75
3	I	406	Y01	CAS-CBF-CBD	-2.18	108.62	111.75
3	L	406	Y01	CAS-CBF-CBD	-2.18	108.62	111.75
3	B	406	Y01	CBF-CBH-CAZ	-2.18	106.24	109.65
3	K	406	Y01	CAS-CBF-CBD	-2.17	108.62	111.75
3	A	406	Y01	CAS-CBF-CBD	-2.16	108.65	111.75
3	D	406	Y01	CAS-CBF-CBD	-2.16	108.65	111.75
3	G	406	Y01	CAS-CBF-CBD	-2.16	108.65	111.75
3	B	406	Y01	CAS-CBF-CBD	-2.15	108.65	111.75
3	E	406	Y01	CAS-CBF-CBD	-2.15	108.65	111.75
3	H	406	Y01	CAS-CBF-CBD	-2.15	108.65	111.75
4	E	409	LHG	C11-C10-C9	-2.15	103.49	114.42
4	J	409	LHG	C11-C10-C9	-2.15	103.49	114.42
4	H	409	LHG	C11-C10-C9	-2.15	103.51	114.42
4	B	409	LHG	C11-C10-C9	-2.15	103.52	114.42
4	A	409	LHG	C11-C10-C9	-2.15	103.52	114.42
4	D	409	LHG	C11-C10-C9	-2.15	103.52	114.42
4	G	409	LHG	C11-C10-C9	-2.15	103.52	114.42
4	C	409	LHG	C11-C10-C9	-2.15	103.53	114.42
4	F	409	LHG	C11-C10-C9	-2.15	103.53	114.42
4	I	409	LHG	C11-C10-C9	-2.15	103.53	114.42
4	K	409	LHG	C11-C10-C9	-2.14	103.54	114.42
3	E	406	Y01	CAM-CAL-CAX	-2.14	108.99	113.60
3	H	406	Y01	CAM-CAL-CAX	-2.14	108.99	113.60
4	L	409	LHG	C11-C10-C9	-2.14	103.56	114.42
3	F	406	Y01	CAM-CAL-CAX	-2.13	109.01	113.60
3	E	406	Y01	CBH-CAZ-CAI	2.13	126.16	122.90
3	C	406	Y01	CAM-CAL-CAX	-2.12	109.03	113.60
3	L	406	Y01	CAM-CAL-CAX	-2.12	109.03	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	406	Y01	CAM-CAL-CAX	-2.12	109.04	113.60
3	D	406	Y01	CAM-CAL-CAX	-2.12	109.04	113.60
3	G	406	Y01	CAM-CAL-CAX	-2.12	109.04	113.60
3	J	406	Y01	CAM-CAL-CAX	-2.12	109.04	113.60
3	I	406	Y01	CAM-CAL-CAX	-2.12	109.05	113.60
3	B	405	Y01	CAQ-CBG-CBI	2.12	106.39	103.84
3	H	405	Y01	CAQ-CBG-CBI	2.12	106.39	103.84
3	B	406	Y01	CAM-CAL-CAX	-2.12	109.05	113.60
3	K	406	Y01	CAM-CAL-CAX	-2.12	109.05	113.60
3	A	405	Y01	CAQ-CBG-CBI	2.10	106.38	103.84
3	C	405	Y01	CAQ-CBG-CBI	2.10	106.38	103.84
3	D	405	Y01	CAQ-CBG-CBI	2.10	106.38	103.84
3	G	405	Y01	CAQ-CBG-CBI	2.10	106.38	103.84
3	J	405	Y01	CAQ-CBG-CBI	2.10	106.38	103.84
3	F	405	Y01	CAQ-CBG-CBI	2.10	106.37	103.84
3	I	405	Y01	CAQ-CBG-CBI	2.10	106.37	103.84
3	L	405	Y01	CAQ-CBG-CBI	2.10	106.37	103.84
4	H	409	LHG	C20-C19-C18	-2.10	103.77	114.42
3	H	406	Y01	CBH-CAZ-CAI	2.10	126.12	122.90
4	E	409	LHG	C20-C19-C18	-2.10	103.77	114.42
3	J	406	Y01	CBH-CAZ-CAI	2.10	126.11	122.90
4	C	409	LHG	C20-C19-C18	-2.09	103.80	114.42
3	K	406	Y01	CBH-CAZ-CAI	2.09	126.11	122.90
4	A	409	LHG	C20-C19-C18	-2.09	103.80	114.42
4	D	409	LHG	C20-C19-C18	-2.09	103.80	114.42
4	G	409	LHG	C20-C19-C18	-2.09	103.80	114.42
4	J	409	LHG	C20-C19-C18	-2.09	103.80	114.42
4	F	409	LHG	C20-C19-C18	-2.09	103.80	114.42
4	L	409	LHG	C20-C19-C18	-2.09	103.80	114.42
3	C	405	Y01	CAP-CBE-CBB	-2.09	108.91	112.15
4	B	409	LHG	C20-C19-C18	-2.09	103.81	114.42
3	K	405	Y01	CAQ-CBG-CBI	2.09	106.36	103.84
4	K	409	LHG	C20-C19-C18	-2.09	103.82	114.42
3	A	406	Y01	CBH-CAZ-CAI	2.09	126.10	122.90
3	D	406	Y01	CBH-CAZ-CAI	2.09	126.10	122.90
3	G	406	Y01	CBH-CAZ-CAI	2.09	126.10	122.90
4	I	409	LHG	C20-C19-C18	-2.09	103.83	114.42
3	E	405	Y01	CAP-CBE-CBB	-2.08	108.92	112.15
3	H	405	Y01	CAP-CBE-CBB	-2.08	108.92	112.15
3	I	405	Y01	CAP-CBE-CBB	-2.08	108.92	112.15
3	C	406	Y01	CBH-CAZ-CAI	2.08	126.09	122.90
3	F	406	Y01	CBH-CAZ-CAI	2.08	126.09	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	I	406	Y01	CBH-CAZ-CAI	2.08	126.09	122.90
3	L	406	Y01	CBH-CAZ-CAI	2.08	126.09	122.90
3	A	405	Y01	CAP-CBE-CBB	-2.08	108.93	112.15
3	D	405	Y01	CAP-CBE-CBB	-2.08	108.93	112.15
3	G	405	Y01	CAP-CBE-CBB	-2.08	108.93	112.15
3	J	405	Y01	CAP-CBE-CBB	-2.08	108.93	112.15
3	F	405	Y01	CAP-CBE-CBB	-2.08	108.93	112.15
3	E	405	Y01	CAQ-CBG-CBI	2.08	106.35	103.84
3	B	405	Y01	CAP-CBE-CBB	-2.08	108.93	112.15
3	K	405	Y01	CAP-CBE-CBB	-2.08	108.93	112.15
3	J	406	Y01	CAT-CBH-CAZ	2.07	112.55	108.75
3	E	406	Y01	CAT-CBH-CAZ	2.07	112.54	108.75
3	H	406	Y01	CAT-CBH-CAZ	2.07	112.54	108.75
3	K	406	Y01	CAT-CBH-CAZ	2.07	112.54	108.75
3	A	406	Y01	CAT-CBH-CAZ	2.06	112.53	108.75
3	D	406	Y01	CAT-CBH-CAZ	2.06	112.53	108.75
3	G	406	Y01	CAT-CBH-CAZ	2.06	112.53	108.75
3	B	406	Y01	CBH-CAZ-CAI	2.06	126.06	122.90
3	L	405	Y01	CAP-CBE-CBB	-2.06	108.96	112.15
3	C	406	Y01	CAT-CBH-CAZ	2.05	112.51	108.75
3	I	406	Y01	CAT-CBH-CAZ	2.05	112.51	108.75
3	L	406	Y01	CAT-CBH-CAZ	2.05	112.51	108.75
3	B	406	Y01	CAT-CBH-CAZ	2.05	112.50	108.75
3	F	406	Y01	CAT-CBH-CAZ	2.05	112.50	108.75
3	B	406	Y01	CAU-CBI-CBE	-2.03	113.54	116.57
3	C	406	Y01	CAU-CBI-CBE	-2.02	113.55	116.57
3	K	406	Y01	CAU-CBI-CBE	-2.01	113.56	116.57
3	A	406	Y01	CAU-CBI-CBE	-2.01	113.57	116.57
3	D	406	Y01	CAU-CBI-CBE	-2.01	113.57	116.57
3	G	406	Y01	CAU-CBI-CBE	-2.01	113.57	116.57
3	J	406	Y01	CAU-CBI-CBE	-2.01	113.57	116.57
3	F	406	Y01	CAU-CBI-CBE	-2.00	113.58	116.57

There are no chirality outliers.

All (708) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	409	LHG	C24-C23-O8-C6
4	B	409	LHG	C24-C23-O8-C6
4	C	409	LHG	C24-C23-O8-C6
4	D	409	LHG	C24-C23-O8-C6
4	E	409	LHG	C24-C23-O8-C6

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Mol	Chain	Res	Type	Atoms
4	F	409	LHG	C24-C23-O8-C6
4	G	409	LHG	C24-C23-O8-C6
4	H	409	LHG	C24-C23-O8-C6
4	I	409	LHG	C24-C23-O8-C6
4	J	409	LHG	C24-C23-O8-C6
4	K	409	LHG	C24-C23-O8-C6
4	L	409	LHG	C24-C23-O8-C6
2	A	407	MC3	C36-C37-C38-C39
2	B	407	MC3	C36-C37-C38-C39
2	C	407	MC3	C36-C37-C38-C39
2	D	407	MC3	C36-C37-C38-C39
2	E	407	MC3	C36-C37-C38-C39
2	F	407	MC3	C36-C37-C38-C39
2	G	407	MC3	C36-C37-C38-C39
2	H	407	MC3	C36-C37-C38-C39
2	I	407	MC3	C36-C37-C38-C39
2	J	407	MC3	C36-C37-C38-C39
2	K	407	MC3	C36-C37-C38-C39
2	L	407	MC3	C36-C37-C38-C39
2	A	408	MC3	C35-C36-C37-C38
2	B	408	MC3	C35-C36-C37-C38
2	C	408	MC3	C35-C36-C37-C38
2	D	408	MC3	C35-C36-C37-C38
2	E	408	MC3	C35-C36-C37-C38
2	F	408	MC3	C35-C36-C37-C38
2	G	408	MC3	C35-C36-C37-C38
2	H	408	MC3	C35-C36-C37-C38
2	I	408	MC3	C35-C36-C37-C38
2	J	408	MC3	C35-C36-C37-C38
2	K	408	MC3	C35-C36-C37-C38
2	L	408	MC3	C35-C36-C37-C38
4	A	409	LHG	C23-C24-C25-C26
4	B	409	LHG	C23-C24-C25-C26
4	C	409	LHG	C23-C24-C25-C26
4	D	409	LHG	C23-C24-C25-C26
4	E	409	LHG	C23-C24-C25-C26
4	F	409	LHG	C23-C24-C25-C26
4	G	409	LHG	C23-C24-C25-C26
4	H	409	LHG	C23-C24-C25-C26
4	I	409	LHG	C23-C24-C25-C26
4	J	409	LHG	C23-C24-C25-C26
4	K	409	LHG	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
4	L	409	LHG	C23-C24-C25-C26
4	A	409	LHG	O10-C23-O8-C6
4	B	409	LHG	O10-C23-O8-C6
4	C	409	LHG	O10-C23-O8-C6
4	D	409	LHG	O10-C23-O8-C6
4	E	409	LHG	O10-C23-O8-C6
4	F	409	LHG	O10-C23-O8-C6
4	G	409	LHG	O10-C23-O8-C6
4	H	409	LHG	O10-C23-O8-C6
4	I	409	LHG	O10-C23-O8-C6
4	J	409	LHG	O10-C23-O8-C6
4	K	409	LHG	O10-C23-O8-C6
4	L	409	LHG	O10-C23-O8-C6
4	A	409	LHG	C7-C8-C9-C10
4	B	409	LHG	C7-C8-C9-C10
4	C	409	LHG	C7-C8-C9-C10
4	D	409	LHG	C7-C8-C9-C10
4	E	409	LHG	C7-C8-C9-C10
4	F	409	LHG	C7-C8-C9-C10
4	G	409	LHG	C7-C8-C9-C10
4	H	409	LHG	C7-C8-C9-C10
4	I	409	LHG	C7-C8-C9-C10
4	J	409	LHG	C7-C8-C9-C10
4	K	409	LHG	C7-C8-C9-C10
4	L	409	LHG	C7-C8-C9-C10
2	A	402	MC3	C36-C37-C38-C39
2	B	402	MC3	C36-C37-C38-C39
2	C	402	MC3	C36-C37-C38-C39
2	D	402	MC3	C36-C37-C38-C39
2	E	402	MC3	C36-C37-C38-C39
2	F	402	MC3	C36-C37-C38-C39
2	G	402	MC3	C36-C37-C38-C39
2	H	402	MC3	C36-C37-C38-C39
2	I	402	MC3	C36-C37-C38-C39
2	J	402	MC3	C36-C37-C38-C39
2	K	402	MC3	C36-C37-C38-C39
2	L	402	MC3	C36-C37-C38-C39
4	A	409	LHG	C18-C19-C20-C21
4	B	409	LHG	C18-C19-C20-C21
4	D	409	LHG	C18-C19-C20-C21
4	E	409	LHG	C18-C19-C20-C21
4	G	409	LHG	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
4	J	409	LHG	C18-C19-C20-C21
4	K	409	LHG	C18-C19-C20-C21
4	C	409	LHG	C18-C19-C20-C21
4	F	409	LHG	C18-C19-C20-C21
4	H	409	LHG	C18-C19-C20-C21
4	I	409	LHG	C18-C19-C20-C21
4	L	409	LHG	C18-C19-C20-C21
2	A	407	MC3	C39-C40-C41-C42
2	B	407	MC3	C39-C40-C41-C42
2	C	407	MC3	C39-C40-C41-C42
2	D	407	MC3	C39-C40-C41-C42
2	E	407	MC3	C39-C40-C41-C42
2	G	407	MC3	C39-C40-C41-C42
2	H	407	MC3	C39-C40-C41-C42
2	J	407	MC3	C39-C40-C41-C42
2	K	407	MC3	C39-C40-C41-C42
2	L	407	MC3	C39-C40-C41-C42
2	A	401	MC3	C35-C36-C37-C38
2	B	401	MC3	C35-C36-C37-C38
2	C	401	MC3	C35-C36-C37-C38
2	D	401	MC3	C35-C36-C37-C38
2	E	401	MC3	C35-C36-C37-C38
2	F	401	MC3	C35-C36-C37-C38
2	F	407	MC3	C39-C40-C41-C42
2	G	401	MC3	C35-C36-C37-C38
2	H	401	MC3	C35-C36-C37-C38
2	I	401	MC3	C35-C36-C37-C38
2	I	407	MC3	C39-C40-C41-C42
2	J	401	MC3	C35-C36-C37-C38
2	K	401	MC3	C35-C36-C37-C38
2	L	401	MC3	C35-C36-C37-C38
3	A	406	Y01	CAC-CBB-CBE-CAP
3	B	406	Y01	CAC-CBB-CBE-CAP
3	C	406	Y01	CAC-CBB-CBE-CAP
3	D	406	Y01	CAC-CBB-CBE-CAP
3	E	406	Y01	CAC-CBB-CBE-CAP
3	F	406	Y01	CAC-CBB-CBE-CAP
3	G	406	Y01	CAC-CBB-CBE-CAP
3	H	406	Y01	CAC-CBB-CBE-CAP
3	I	406	Y01	CAC-CBB-CBE-CAP
3	J	406	Y01	CAC-CBB-CBE-CAP
3	K	406	Y01	CAC-CBB-CBE-CAP

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Mol	Chain	Res	Type	Atoms
3	L	406	Y01	CAC-CBB-CBE-CAP
2	A	401	MC3	C40-C41-C42-C43
2	B	401	MC3	C40-C41-C42-C43
2	C	401	MC3	C40-C41-C42-C43
2	D	401	MC3	C40-C41-C42-C43
2	E	401	MC3	C40-C41-C42-C43
2	F	401	MC3	C40-C41-C42-C43
2	G	401	MC3	C40-C41-C42-C43
2	H	401	MC3	C40-C41-C42-C43
2	I	401	MC3	C40-C41-C42-C43
2	J	401	MC3	C40-C41-C42-C43
2	K	401	MC3	C40-C41-C42-C43
2	L	401	MC3	C40-C41-C42-C43
3	A	405	Y01	CAJ-CAO-CBB-CAC
3	B	405	Y01	CAJ-CAO-CBB-CAC
3	C	405	Y01	CAJ-CAO-CBB-CAC
3	D	405	Y01	CAJ-CAO-CBB-CAC
3	E	405	Y01	CAJ-CAO-CBB-CAC
3	F	405	Y01	CAJ-CAO-CBB-CAC
3	G	405	Y01	CAJ-CAO-CBB-CAC
3	H	405	Y01	CAJ-CAO-CBB-CAC
3	I	405	Y01	CAJ-CAO-CBB-CAC
3	J	405	Y01	CAJ-CAO-CBB-CAC
3	K	405	Y01	CAJ-CAO-CBB-CAC
3	L	405	Y01	CAJ-CAO-CBB-CAC
4	A	409	LHG	C32-C33-C34-C35
4	B	409	LHG	C32-C33-C34-C35
4	C	409	LHG	C32-C33-C34-C35
4	D	409	LHG	C32-C33-C34-C35
4	E	409	LHG	C32-C33-C34-C35
4	F	409	LHG	C32-C33-C34-C35
4	G	409	LHG	C32-C33-C34-C35
4	H	409	LHG	C32-C33-C34-C35
4	I	409	LHG	C32-C33-C34-C35
4	J	409	LHG	C32-C33-C34-C35
4	K	409	LHG	C32-C33-C34-C35
4	L	409	LHG	C32-C33-C34-C35
4	A	409	LHG	C30-C31-C32-C33
4	B	409	LHG	C30-C31-C32-C33
4	C	409	LHG	C30-C31-C32-C33
4	D	409	LHG	C30-C31-C32-C33
4	E	409	LHG	C30-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
4	F	409	LHG	C30-C31-C32-C33
4	G	409	LHG	C30-C31-C32-C33
4	H	409	LHG	C30-C31-C32-C33
4	I	409	LHG	C30-C31-C32-C33
4	J	409	LHG	C30-C31-C32-C33
4	K	409	LHG	C30-C31-C32-C33
4	L	409	LHG	C30-C31-C32-C33
4	A	409	LHG	C10-C11-C12-C13
4	B	409	LHG	C10-C11-C12-C13
4	C	409	LHG	C10-C11-C12-C13
4	D	409	LHG	C10-C11-C12-C13
4	E	409	LHG	C10-C11-C12-C13
4	F	409	LHG	C10-C11-C12-C13
4	G	409	LHG	C10-C11-C12-C13
4	H	409	LHG	C10-C11-C12-C13
4	I	409	LHG	C10-C11-C12-C13
4	J	409	LHG	C10-C11-C12-C13
4	K	409	LHG	C10-C11-C12-C13
4	L	409	LHG	C10-C11-C12-C13
4	A	409	LHG	C27-C28-C29-C30
4	B	409	LHG	C27-C28-C29-C30
4	C	409	LHG	C27-C28-C29-C30
4	E	409	LHG	C27-C28-C29-C30
4	F	409	LHG	C27-C28-C29-C30
4	G	409	LHG	C27-C28-C29-C30
4	I	409	LHG	C27-C28-C29-C30
4	J	409	LHG	C27-C28-C29-C30
4	K	409	LHG	C27-C28-C29-C30
4	L	409	LHG	C27-C28-C29-C30
4	D	409	LHG	C27-C28-C29-C30
4	H	409	LHG	C27-C28-C29-C30
4	A	409	LHG	C28-C29-C30-C31
4	B	409	LHG	C28-C29-C30-C31
4	C	409	LHG	C28-C29-C30-C31
4	D	409	LHG	C28-C29-C30-C31
4	E	409	LHG	C28-C29-C30-C31
4	F	409	LHG	C28-C29-C30-C31
4	G	409	LHG	C28-C29-C30-C31
4	H	409	LHG	C28-C29-C30-C31
4	I	409	LHG	C28-C29-C30-C31
4	J	409	LHG	C28-C29-C30-C31
4	K	409	LHG	C28-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
4	L	409	LHG	C28-C29-C30-C31
3	A	406	Y01	CAC-CBB-CBE-CBI
3	B	406	Y01	CAC-CBB-CBE-CBI
3	C	406	Y01	CAC-CBB-CBE-CBI
3	D	406	Y01	CAC-CBB-CBE-CBI
3	E	406	Y01	CAC-CBB-CBE-CBI
3	F	406	Y01	CAC-CBB-CBE-CBI
3	G	406	Y01	CAC-CBB-CBE-CBI
3	H	406	Y01	CAC-CBB-CBE-CBI
3	I	406	Y01	CAC-CBB-CBE-CBI
3	J	406	Y01	CAC-CBB-CBE-CBI
3	K	406	Y01	CAC-CBB-CBE-CBI
3	L	406	Y01	CAC-CBB-CBE-CBI
4	A	409	LHG	C13-C14-C15-C16
4	B	409	LHG	C13-C14-C15-C16
4	C	409	LHG	C13-C14-C15-C16
4	D	409	LHG	C13-C14-C15-C16
4	E	409	LHG	C13-C14-C15-C16
4	F	409	LHG	C13-C14-C15-C16
4	G	409	LHG	C13-C14-C15-C16
4	H	409	LHG	C13-C14-C15-C16
4	I	409	LHG	C13-C14-C15-C16
4	J	409	LHG	C13-C14-C15-C16
4	K	409	LHG	C13-C14-C15-C16
4	L	409	LHG	C13-C14-C15-C16
2	A	402	MC3	C34-C35-C36-C37
2	B	402	MC3	C34-C35-C36-C37
2	C	402	MC3	C34-C35-C36-C37
2	D	402	MC3	C34-C35-C36-C37
2	F	402	MC3	C34-C35-C36-C37
2	G	402	MC3	C34-C35-C36-C37
2	H	402	MC3	C34-C35-C36-C37
2	I	402	MC3	C34-C35-C36-C37
2	K	402	MC3	C34-C35-C36-C37
2	E	402	MC3	C34-C35-C36-C37
2	J	402	MC3	C34-C35-C36-C37
2	L	402	MC3	C34-C35-C36-C37
4	E	409	LHG	C16-C17-C18-C19
4	A	409	LHG	C16-C17-C18-C19
4	D	409	LHG	C16-C17-C18-C19
4	G	409	LHG	C16-C17-C18-C19
4	H	409	LHG	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
4	I	409	LHG	C16-C17-C18-C19
4	J	409	LHG	C16-C17-C18-C19
4	K	409	LHG	C16-C17-C18-C19
4	B	409	LHG	C16-C17-C18-C19
4	C	409	LHG	C16-C17-C18-C19
4	F	409	LHG	C16-C17-C18-C19
4	L	409	LHG	C16-C17-C18-C19
4	A	409	LHG	C14-C15-C16-C17
4	B	409	LHG	C14-C15-C16-C17
4	C	409	LHG	C14-C15-C16-C17
4	D	409	LHG	C14-C15-C16-C17
4	E	409	LHG	C14-C15-C16-C17
4	F	409	LHG	C14-C15-C16-C17
4	G	409	LHG	C14-C15-C16-C17
4	H	409	LHG	C14-C15-C16-C17
4	I	409	LHG	C14-C15-C16-C17
4	J	409	LHG	C14-C15-C16-C17
4	K	409	LHG	C14-C15-C16-C17
4	L	409	LHG	C14-C15-C16-C17
2	E	407	MC3	C32-C33-C34-C35
2	F	407	MC3	C32-C33-C34-C35
2	J	407	MC3	C32-C33-C34-C35
2	A	407	MC3	C32-C33-C34-C35
2	B	407	MC3	C32-C33-C34-C35
2	C	407	MC3	C32-C33-C34-C35
2	D	407	MC3	C32-C33-C34-C35
2	G	407	MC3	C32-C33-C34-C35
2	H	407	MC3	C32-C33-C34-C35
2	I	407	MC3	C32-C33-C34-C35
2	K	407	MC3	C32-C33-C34-C35
2	L	407	MC3	C32-C33-C34-C35
4	A	409	LHG	C26-C27-C28-C29
4	D	409	LHG	C26-C27-C28-C29
4	F	409	LHG	C26-C27-C28-C29
4	G	409	LHG	C26-C27-C28-C29
4	H	409	LHG	C26-C27-C28-C29
4	I	409	LHG	C26-C27-C28-C29
4	J	409	LHG	C26-C27-C28-C29
4	K	409	LHG	C26-C27-C28-C29
4	L	409	LHG	C26-C27-C28-C29
4	B	409	LHG	C26-C27-C28-C29
4	C	409	LHG	C26-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
4	E	409	LHG	C26-C27-C28-C29
2	B	404	MC3	C36-C37-C38-C39
2	C	404	MC3	C36-C37-C38-C39
2	A	404	MC3	C36-C37-C38-C39
2	D	404	MC3	C36-C37-C38-C39
2	E	404	MC3	C36-C37-C38-C39
2	F	404	MC3	C36-C37-C38-C39
2	G	404	MC3	C36-C37-C38-C39
2	H	404	MC3	C36-C37-C38-C39
2	I	404	MC3	C36-C37-C38-C39
2	J	404	MC3	C36-C37-C38-C39
2	K	404	MC3	C36-C37-C38-C39
2	L	404	MC3	C36-C37-C38-C39
2	A	404	MC3	C35-C36-C37-C38
2	B	404	MC3	C35-C36-C37-C38
2	C	404	MC3	C35-C36-C37-C38
2	D	404	MC3	C35-C36-C37-C38
2	E	404	MC3	C35-C36-C37-C38
2	F	404	MC3	C35-C36-C37-C38
2	G	404	MC3	C35-C36-C37-C38
2	H	404	MC3	C35-C36-C37-C38
2	I	404	MC3	C35-C36-C37-C38
2	J	404	MC3	C35-C36-C37-C38
2	K	404	MC3	C35-C36-C37-C38
2	L	404	MC3	C35-C36-C37-C38
3	A	406	Y01	CAO-CBB-CBE-CAP
3	B	406	Y01	CAO-CBB-CBE-CAP
3	C	406	Y01	CAO-CBB-CBE-CAP
3	D	406	Y01	CAO-CBB-CBE-CAP
3	E	406	Y01	CAO-CBB-CBE-CAP
3	F	406	Y01	CAO-CBB-CBE-CAP
3	G	406	Y01	CAO-CBB-CBE-CAP
3	H	406	Y01	CAO-CBB-CBE-CAP
3	I	406	Y01	CAO-CBB-CBE-CAP
3	J	406	Y01	CAO-CBB-CBE-CAP
3	K	406	Y01	CAO-CBB-CBE-CAP
3	L	406	Y01	CAO-CBB-CBE-CAP
2	A	408	MC3	C31-C32-C33-C34
2	B	408	MC3	C31-C32-C33-C34
2	C	408	MC3	C31-C32-C33-C34
2	D	408	MC3	C31-C32-C33-C34
2	E	408	MC3	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
2	F	408	MC3	C31-C32-C33-C34
2	G	408	MC3	C31-C32-C33-C34
2	I	408	MC3	C31-C32-C33-C34
2	L	408	MC3	C31-C32-C33-C34
2	H	408	MC3	C31-C32-C33-C34
2	J	408	MC3	C31-C32-C33-C34
2	K	408	MC3	C31-C32-C33-C34
4	A	409	LHG	C15-C16-C17-C18
4	B	409	LHG	C15-C16-C17-C18
4	G	409	LHG	C15-C16-C17-C18
4	I	409	LHG	C15-C16-C17-C18
4	L	409	LHG	C15-C16-C17-C18
4	C	409	LHG	C15-C16-C17-C18
4	D	409	LHG	C15-C16-C17-C18
4	E	409	LHG	C15-C16-C17-C18
4	F	409	LHG	C15-C16-C17-C18
4	H	409	LHG	C15-C16-C17-C18
4	J	409	LHG	C15-C16-C17-C18
4	K	409	LHG	C15-C16-C17-C18
2	E	407	MC3	C40-C41-C42-C43
2	A	407	MC3	C40-C41-C42-C43
2	B	407	MC3	C40-C41-C42-C43
2	C	407	MC3	C40-C41-C42-C43
2	D	407	MC3	C40-C41-C42-C43
2	F	407	MC3	C40-C41-C42-C43
2	G	407	MC3	C40-C41-C42-C43
2	H	407	MC3	C40-C41-C42-C43
2	I	407	MC3	C40-C41-C42-C43
2	J	407	MC3	C40-C41-C42-C43
2	K	407	MC3	C40-C41-C42-C43
2	L	407	MC3	C40-C41-C42-C43
3	A	406	Y01	CAO-CBB-CBE-CBI
3	B	406	Y01	CAO-CBB-CBE-CBI
3	C	406	Y01	CAO-CBB-CBE-CBI
3	D	406	Y01	CAO-CBB-CBE-CBI
3	E	406	Y01	CAO-CBB-CBE-CBI
3	F	406	Y01	CAO-CBB-CBE-CBI
3	G	406	Y01	CAO-CBB-CBE-CBI
3	H	406	Y01	CAO-CBB-CBE-CBI
3	I	406	Y01	CAO-CBB-CBE-CBI
3	J	406	Y01	CAO-CBB-CBE-CBI
3	K	406	Y01	CAO-CBB-CBE-CBI

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Mol	Chain	Res	Type	Atoms
3	L	406	Y01	CAO-CBB-CBE-CBI
2	A	403	MC3	C40-C41-C42-C43
2	C	403	MC3	C40-C41-C42-C43
2	D	403	MC3	C40-C41-C42-C43
2	E	403	MC3	C40-C41-C42-C43
2	G	403	MC3	C40-C41-C42-C43
2	H	403	MC3	C40-C41-C42-C43
2	J	403	MC3	C40-C41-C42-C43
2	L	403	MC3	C40-C41-C42-C43
2	F	403	MC3	C40-C41-C42-C43
2	I	403	MC3	C40-C41-C42-C43
2	K	403	MC3	C40-C41-C42-C43
2	B	403	MC3	C40-C41-C42-C43
3	A	406	Y01	CAO-CAJ-CAN-CBA
3	C	406	Y01	CAO-CAJ-CAN-CBA
3	D	406	Y01	CAO-CAJ-CAN-CBA
3	E	406	Y01	CAO-CAJ-CAN-CBA
3	F	406	Y01	CAO-CAJ-CAN-CBA
3	G	406	Y01	CAO-CAJ-CAN-CBA
3	H	406	Y01	CAO-CAJ-CAN-CBA
3	I	406	Y01	CAO-CAJ-CAN-CBA
3	J	406	Y01	CAO-CAJ-CAN-CBA
3	L	406	Y01	CAO-CAJ-CAN-CBA
3	B	406	Y01	CAO-CAJ-CAN-CBA
3	K	406	Y01	CAO-CAJ-CAN-CBA
2	A	407	MC3	C31-C32-C33-C34
2	B	407	MC3	C31-C32-C33-C34
2	C	407	MC3	C31-C32-C33-C34
2	D	407	MC3	C31-C32-C33-C34
2	E	407	MC3	C31-C32-C33-C34
2	F	407	MC3	C31-C32-C33-C34
2	G	407	MC3	C31-C32-C33-C34
2	I	407	MC3	C31-C32-C33-C34
2	J	407	MC3	C31-C32-C33-C34
2	K	407	MC3	C31-C32-C33-C34
2	L	407	MC3	C31-C32-C33-C34
2	H	407	MC3	C31-C32-C33-C34
4	A	409	LHG	C12-C13-C14-C15
4	E	409	LHG	C12-C13-C14-C15
4	G	409	LHG	C12-C13-C14-C15
4	H	409	LHG	C12-C13-C14-C15
4	I	409	LHG	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
4	L	409	LHG	C12-C13-C14-C15
4	B	409	LHG	C12-C13-C14-C15
4	C	409	LHG	C12-C13-C14-C15
4	D	409	LHG	C12-C13-C14-C15
4	F	409	LHG	C12-C13-C14-C15
4	J	409	LHG	C12-C13-C14-C15
4	K	409	LHG	C12-C13-C14-C15
3	L	406	Y01	CAN-CAJ-CAO-CBB
2	A	408	MC3	C37-C38-C39-C40
2	B	408	MC3	C37-C38-C39-C40
2	C	408	MC3	C37-C38-C39-C40
2	D	408	MC3	C37-C38-C39-C40
2	E	408	MC3	C37-C38-C39-C40
2	F	408	MC3	C37-C38-C39-C40
2	G	408	MC3	C37-C38-C39-C40
2	H	408	MC3	C37-C38-C39-C40
2	K	408	MC3	C37-C38-C39-C40
2	L	408	MC3	C37-C38-C39-C40
2	I	408	MC3	C37-C38-C39-C40
2	J	408	MC3	C37-C38-C39-C40
3	A	406	Y01	CAN-CAJ-CAO-CBB
3	C	406	Y01	CAN-CAJ-CAO-CBB
3	D	406	Y01	CAN-CAJ-CAO-CBB
3	E	406	Y01	CAN-CAJ-CAO-CBB
3	F	406	Y01	CAN-CAJ-CAO-CBB
3	G	406	Y01	CAN-CAJ-CAO-CBB
3	H	406	Y01	CAN-CAJ-CAO-CBB
3	I	406	Y01	CAN-CAJ-CAO-CBB
3	J	406	Y01	CAN-CAJ-CAO-CBB
3	B	406	Y01	CAN-CAJ-CAO-CBB
3	K	406	Y01	CAN-CAJ-CAO-CBB
4	A	409	LHG	C8-C7-O7-C5
4	B	409	LHG	C8-C7-O7-C5
4	C	409	LHG	C8-C7-O7-C5
4	D	409	LHG	C8-C7-O7-C5
4	E	409	LHG	C8-C7-O7-C5
4	G	409	LHG	C8-C7-O7-C5
4	H	409	LHG	C8-C7-O7-C5
4	K	409	LHG	C8-C7-O7-C5
4	L	409	LHG	C8-C7-O7-C5
4	K	409	LHG	C33-C34-C35-C36
4	A	409	LHG	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
4	D	409	LHG	C33-C34-C35-C36
4	E	409	LHG	C33-C34-C35-C36
4	G	409	LHG	C33-C34-C35-C36
4	H	409	LHG	C33-C34-C35-C36
4	J	409	LHG	C33-C34-C35-C36
4	L	409	LHG	C33-C34-C35-C36
4	B	409	LHG	C33-C34-C35-C36
4	C	409	LHG	C33-C34-C35-C36
4	F	409	LHG	C33-C34-C35-C36
4	I	409	LHG	C33-C34-C35-C36
4	F	409	LHG	C8-C7-O7-C5
4	I	409	LHG	C8-C7-O7-C5
4	J	409	LHG	C8-C7-O7-C5
4	E	409	LHG	C29-C30-C31-C32
4	A	409	LHG	C29-C30-C31-C32
4	G	409	LHG	C29-C30-C31-C32
4	B	409	LHG	C29-C30-C31-C32
4	C	409	LHG	C29-C30-C31-C32
4	D	409	LHG	C29-C30-C31-C32
4	F	409	LHG	C29-C30-C31-C32
4	H	409	LHG	C29-C30-C31-C32
4	I	409	LHG	C29-C30-C31-C32
4	J	409	LHG	C29-C30-C31-C32
4	K	409	LHG	C29-C30-C31-C32
4	L	409	LHG	C29-C30-C31-C32
3	A	406	Y01	CAJ-CAN-CBA-CAA
3	C	406	Y01	CAJ-CAN-CBA-CAA
3	D	406	Y01	CAJ-CAN-CBA-CAA
3	G	406	Y01	CAJ-CAN-CBA-CAA
3	H	406	Y01	CAJ-CAN-CBA-CAA
3	J	406	Y01	CAJ-CAN-CBA-CAA
3	K	406	Y01	CAJ-CAN-CBA-CAA
3	B	406	Y01	CAJ-CAN-CBA-CAA
3	E	406	Y01	CAJ-CAN-CBA-CAA
3	F	406	Y01	CAJ-CAN-CBA-CAA
3	I	406	Y01	CAJ-CAN-CBA-CAA
3	L	406	Y01	CAJ-CAN-CBA-CAA
3	F	406	Y01	CAM-CAL-CAX-OAH
3	A	406	Y01	CAM-CAL-CAX-OAH
3	B	406	Y01	CAM-CAL-CAX-OAH
3	C	406	Y01	CAM-CAL-CAX-OAH
3	D	406	Y01	CAM-CAL-CAX-OAH

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Mol	Chain	Res	Type	Atoms
3	E	406	Y01	CAM-CAL-CAX-OAH
3	G	406	Y01	CAM-CAL-CAX-OAH
3	H	406	Y01	CAM-CAL-CAX-OAH
3	I	406	Y01	CAM-CAL-CAX-OAH
3	J	406	Y01	CAM-CAL-CAX-OAH
3	K	406	Y01	CAM-CAL-CAX-OAH
3	L	406	Y01	CAM-CAL-CAX-OAH
4	C	409	LHG	C11-C10-C9-C8
4	E	409	LHG	C11-C10-C9-C8
4	F	409	LHG	C11-C10-C9-C8
4	I	409	LHG	C11-C10-C9-C8
4	J	409	LHG	C11-C10-C9-C8
4	A	409	LHG	C11-C10-C9-C8
4	B	409	LHG	C11-C10-C9-C8
4	D	409	LHG	C11-C10-C9-C8
4	G	409	LHG	C11-C10-C9-C8
4	K	409	LHG	C11-C10-C9-C8
4	H	409	LHG	C11-C10-C9-C8
4	L	409	LHG	C11-C10-C9-C8
2	C	401	MC3	C33-C34-C35-C36
2	E	401	MC3	C33-C34-C35-C36
2	A	401	MC3	C33-C34-C35-C36
2	B	401	MC3	C33-C34-C35-C36
2	D	401	MC3	C33-C34-C35-C36
2	F	401	MC3	C33-C34-C35-C36
2	G	401	MC3	C33-C34-C35-C36
2	H	401	MC3	C33-C34-C35-C36
2	I	401	MC3	C33-C34-C35-C36
2	J	401	MC3	C33-C34-C35-C36
2	L	401	MC3	C33-C34-C35-C36
2	B	404	MC3	C39-C40-C41-C42
2	C	404	MC3	C39-C40-C41-C42
2	E	404	MC3	C39-C40-C41-C42
2	F	404	MC3	C39-C40-C41-C42
2	H	404	MC3	C39-C40-C41-C42
2	I	404	MC3	C39-C40-C41-C42
2	K	401	MC3	C33-C34-C35-C36
2	A	404	MC3	C39-C40-C41-C42
2	D	404	MC3	C39-C40-C41-C42
2	G	404	MC3	C39-C40-C41-C42
2	J	404	MC3	C39-C40-C41-C42
2	K	404	MC3	C39-C40-C41-C42

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Mol	Chain	Res	Type	Atoms
2	L	404	MC3	C39-C40-C41-C42
4	E	409	LHG	O9-C7-O7-C5
4	K	409	LHG	O9-C7-O7-C5
4	L	409	LHG	O9-C7-O7-C5
3	L	406	Y01	CAM-CAL-CAX-OAF
3	A	406	Y01	CAM-CAL-CAX-OAF
3	B	406	Y01	CAM-CAL-CAX-OAF
3	C	406	Y01	CAM-CAL-CAX-OAF
3	D	406	Y01	CAM-CAL-CAX-OAF
3	E	406	Y01	CAM-CAL-CAX-OAF
3	F	406	Y01	CAM-CAL-CAX-OAF
3	G	406	Y01	CAM-CAL-CAX-OAF
3	H	406	Y01	CAM-CAL-CAX-OAF
3	I	406	Y01	CAM-CAL-CAX-OAF
3	J	406	Y01	CAM-CAL-CAX-OAF
3	K	406	Y01	CAM-CAL-CAX-OAF
4	B	409	LHG	C9-C10-C11-C12
4	K	409	LHG	C9-C10-C11-C12
4	L	409	LHG	C9-C10-C11-C12
4	A	409	LHG	C9-C10-C11-C12
4	D	409	LHG	C9-C10-C11-C12
4	G	409	LHG	C9-C10-C11-C12
4	H	409	LHG	C9-C10-C11-C12
4	J	409	LHG	C9-C10-C11-C12
4	E	409	LHG	C9-C10-C11-C12
4	F	409	LHG	C9-C10-C11-C12
4	I	409	LHG	C9-C10-C11-C12
4	C	409	LHG	C9-C10-C11-C12
4	A	409	LHG	O9-C7-O7-C5
4	B	409	LHG	O9-C7-O7-C5
4	C	409	LHG	O9-C7-O7-C5
4	D	409	LHG	O9-C7-O7-C5
4	F	409	LHG	O9-C7-O7-C5
4	G	409	LHG	O9-C7-O7-C5
4	J	409	LHG	O9-C7-O7-C5
4	I	409	LHG	O9-C7-O7-C5
2	C	403	MC3	C38-C39-C40-C41
2	J	403	MC3	C38-C39-C40-C41
3	B	405	Y01	CAM-CAL-CAX-OAH
3	C	405	Y01	CAM-CAL-CAX-OAH
3	G	405	Y01	CAM-CAL-CAX-OAH
3	I	405	Y01	CAM-CAL-CAX-OAH

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Mol	Chain	Res	Type	Atoms
3	K	405	Y01	CAM-CAL-CAX-OAH
2	A	403	MC3	C38-C39-C40-C41
2	B	403	MC3	C38-C39-C40-C41
2	D	403	MC3	C38-C39-C40-C41
2	E	403	MC3	C38-C39-C40-C41
2	G	403	MC3	C38-C39-C40-C41
2	H	403	MC3	C38-C39-C40-C41
2	K	403	MC3	C38-C39-C40-C41
2	I	403	MC3	C38-C39-C40-C41
2	L	403	MC3	C38-C39-C40-C41
4	H	409	LHG	O9-C7-O7-C5
2	F	403	MC3	C38-C39-C40-C41
3	A	405	Y01	CAM-CAL-CAX-OAH
3	D	405	Y01	CAM-CAL-CAX-OAH
3	F	405	Y01	CAM-CAL-CAX-OAH
3	H	405	Y01	CAM-CAL-CAX-OAH
3	L	405	Y01	CAM-CAL-CAX-OAH
3	J	405	Y01	CAM-CAL-CAX-OAH
4	E	409	LHG	C25-C26-C27-C28
4	A	409	LHG	C25-C26-C27-C28
4	B	409	LHG	C25-C26-C27-C28
4	D	409	LHG	C25-C26-C27-C28
4	G	409	LHG	C25-C26-C27-C28
4	J	409	LHG	C25-C26-C27-C28
4	K	409	LHG	C25-C26-C27-C28
4	H	409	LHG	C25-C26-C27-C28
4	L	409	LHG	C25-C26-C27-C28
3	E	405	Y01	CAM-CAL-CAX-OAH
4	C	409	LHG	C25-C26-C27-C28
4	F	409	LHG	C25-C26-C27-C28
4	I	409	LHG	C25-C26-C27-C28
2	E	403	MC3	C41-C42-C43-C44
2	F	403	MC3	C41-C42-C43-C44
2	H	403	MC3	C41-C42-C43-C44
2	I	403	MC3	C41-C42-C43-C44
2	J	403	MC3	C41-C42-C43-C44
2	A	403	MC3	C41-C42-C43-C44
2	D	403	MC3	C41-C42-C43-C44
2	G	403	MC3	C41-C42-C43-C44
2	B	403	MC3	C41-C42-C43-C44
2	K	403	MC3	C41-C42-C43-C44
2	C	403	MC3	C41-C42-C43-C44

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Mol	Chain	Res	Type	Atoms
2	L	403	MC3	C41-C42-C43-C44
3	E	405	Y01	CAM-CAL-CAX-OAF
3	H	405	Y01	CAM-CAL-CAX-OAF
3	J	405	Y01	CAM-CAL-CAX-OAF
3	A	405	Y01	CAM-CAL-CAX-OAF
3	B	405	Y01	CAM-CAL-CAX-OAF
3	C	405	Y01	CAM-CAL-CAX-OAF
3	D	405	Y01	CAM-CAL-CAX-OAF
3	F	405	Y01	CAM-CAL-CAX-OAF
3	G	405	Y01	CAM-CAL-CAX-OAF
3	I	405	Y01	CAM-CAL-CAX-OAF
3	K	405	Y01	CAM-CAL-CAX-OAF
3	L	405	Y01	CAM-CAL-CAX-OAF
2	C	401	MC3	C37-C38-C39-C40
2	H	401	MC3	C32-C33-C34-C35
2	A	401	MC3	C32-C33-C34-C35
2	B	401	MC3	C32-C33-C34-C35
2	D	401	MC3	C32-C33-C34-C35
2	E	401	MC3	C32-C33-C34-C35
2	E	401	MC3	C37-C38-C39-C40
2	G	401	MC3	C32-C33-C34-C35
2	J	401	MC3	C32-C33-C34-C35
2	L	401	MC3	C32-C33-C34-C35
2	A	401	MC3	C37-C38-C39-C40
2	D	401	MC3	C37-C38-C39-C40
2	G	401	MC3	C37-C38-C39-C40
2	H	401	MC3	C37-C38-C39-C40
2	K	401	MC3	C32-C33-C34-C35
2	L	401	MC3	C37-C38-C39-C40
2	F	401	MC3	C32-C33-C34-C35
2	F	401	MC3	C37-C38-C39-C40
2	I	401	MC3	C32-C33-C34-C35
2	I	401	MC3	C37-C38-C39-C40
2	J	401	MC3	C37-C38-C39-C40
2	B	401	MC3	C37-C38-C39-C40
2	C	401	MC3	C32-C33-C34-C35
2	E	404	MC3	C38-C39-C40-C41
2	H	404	MC3	C38-C39-C40-C41
2	J	404	MC3	C38-C39-C40-C41
2	K	401	MC3	C37-C38-C39-C40
2	L	404	MC3	C38-C39-C40-C41
2	A	404	MC3	C38-C39-C40-C41

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Mol	Chain	Res	Type	Atoms
2	B	404	MC3	C38-C39-C40-C41
2	C	404	MC3	C38-C39-C40-C41
2	D	404	MC3	C38-C39-C40-C41
2	F	404	MC3	C38-C39-C40-C41
2	G	404	MC3	C38-C39-C40-C41
2	I	404	MC3	C38-C39-C40-C41
2	K	404	MC3	C38-C39-C40-C41
2	F	408	MC3	C33-C34-C35-C36
2	I	408	MC3	C33-C34-C35-C36
2	B	408	MC3	C33-C34-C35-C36
2	E	408	MC3	C33-C34-C35-C36
2	K	408	MC3	C33-C34-C35-C36
2	A	408	MC3	C33-C34-C35-C36
2	C	408	MC3	C33-C34-C35-C36
2	D	408	MC3	C33-C34-C35-C36
2	G	408	MC3	C33-C34-C35-C36
2	J	408	MC3	C33-C34-C35-C36
2	L	408	MC3	C33-C34-C35-C36
2	H	408	MC3	C33-C34-C35-C36
3	A	405	Y01	CAN-CAJ-CAO-CBB
3	B	405	Y01	CAN-CAJ-CAO-CBB
3	C	405	Y01	CAN-CAJ-CAO-CBB
3	D	405	Y01	CAN-CAJ-CAO-CBB
3	E	405	Y01	CAN-CAJ-CAO-CBB
3	F	405	Y01	CAN-CAJ-CAO-CBB
3	G	405	Y01	CAN-CAJ-CAO-CBB
3	H	405	Y01	CAN-CAJ-CAO-CBB
3	I	405	Y01	CAN-CAJ-CAO-CBB
3	J	405	Y01	CAN-CAJ-CAO-CBB
3	K	405	Y01	CAN-CAJ-CAO-CBB
3	L	405	Y01	CAN-CAJ-CAO-CBB

There are no ring outliers.

14 monomers are involved in 38 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	405	Y01	3	0
3	L	405	Y01	3	0
3	E	405	Y01	3	0
3	K	405	Y01	3	0
3	D	405	Y01	3	0
2	L	407	MC3	1	0

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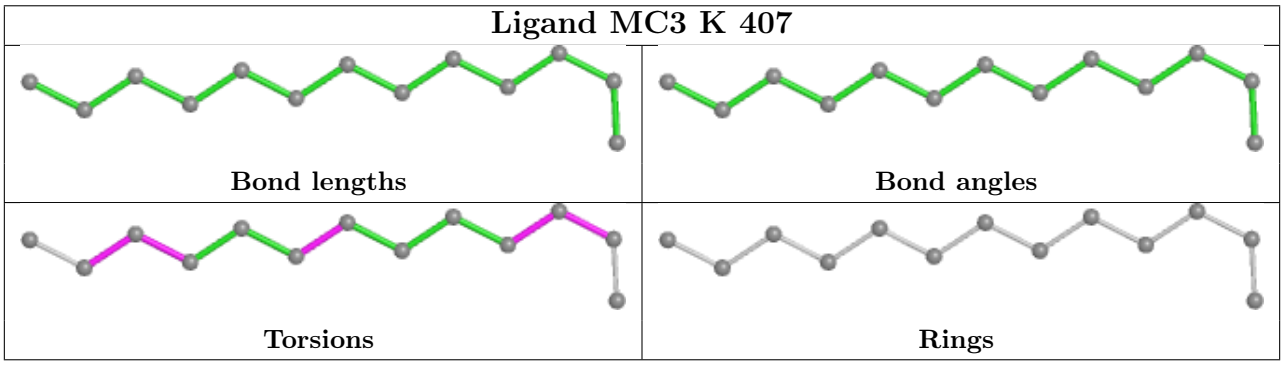
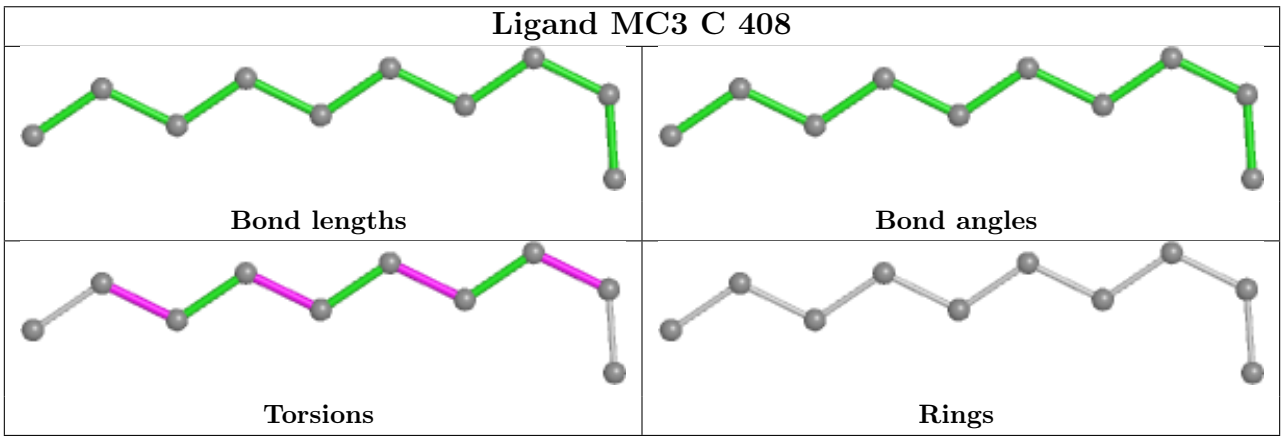
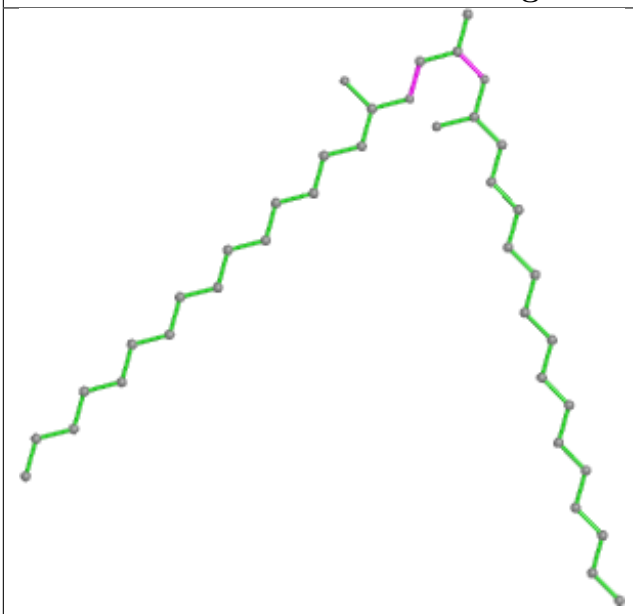
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	407	MC3	1	0
3	F	405	Y01	3	0
3	A	405	Y01	3	0
3	B	405	Y01	3	0
3	H	405	Y01	3	0
3	I	405	Y01	3	0
3	J	405	Y01	3	0
3	G	405	Y01	3	0

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.

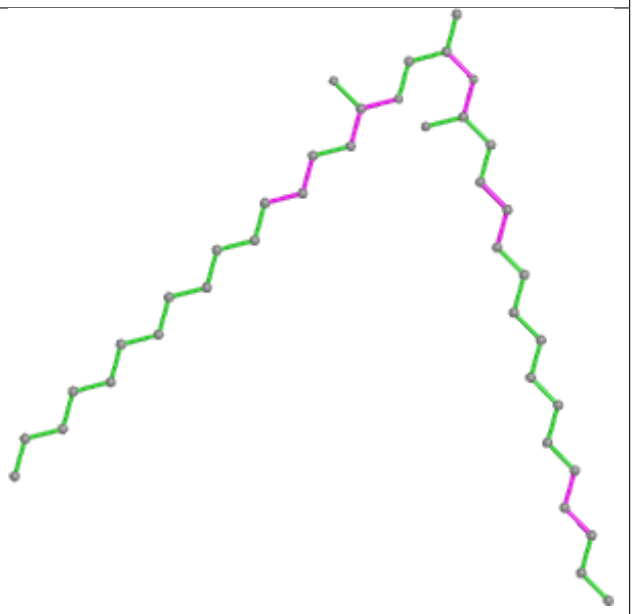




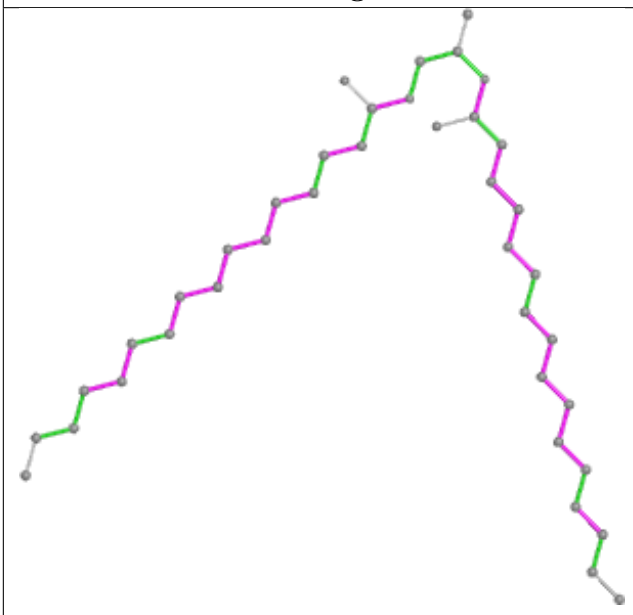
Ligand LHG H 409



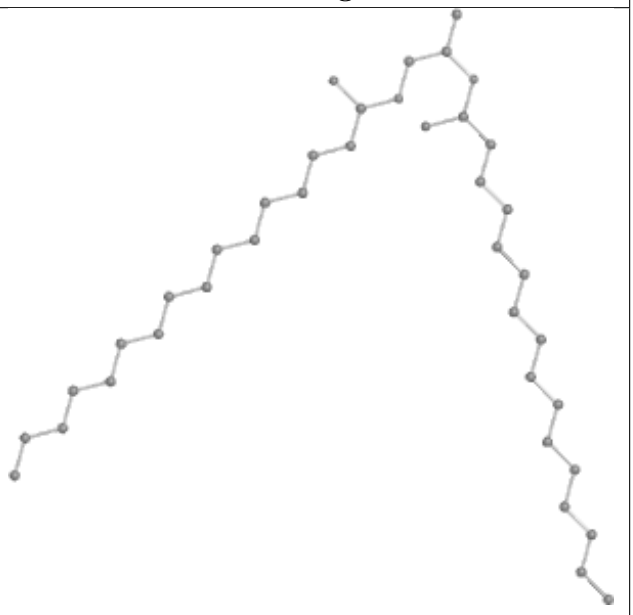
Bond lengths



Bond angles

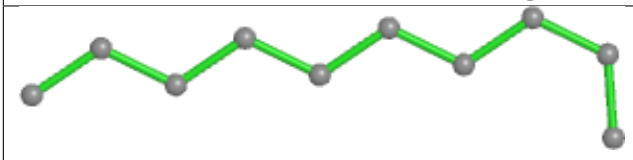


Torsions

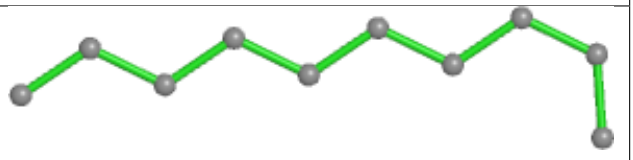


Rings

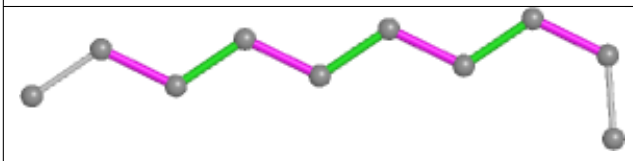
Ligand MC3 G 408



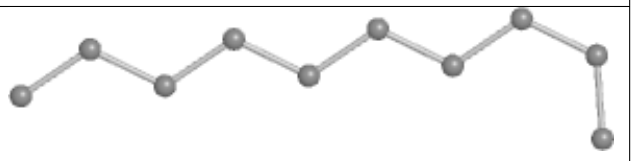
Bond lengths



Bond angles

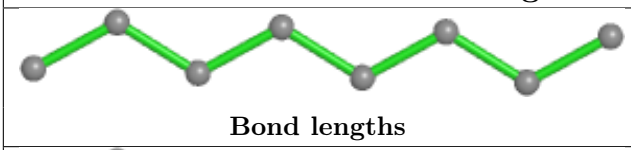


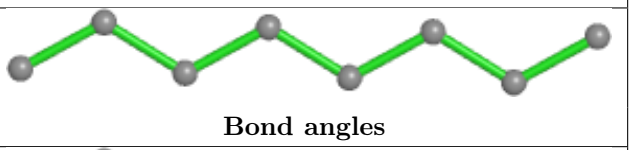
Torsions

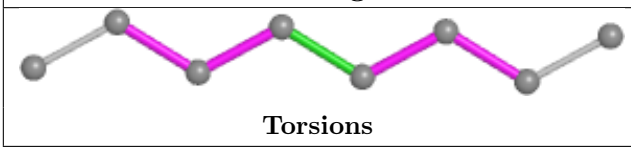


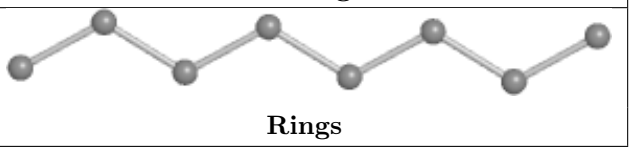
Rings

Ligand MC3 H 404

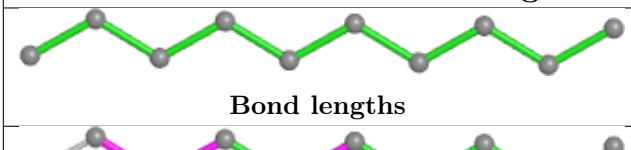

Bond lengths

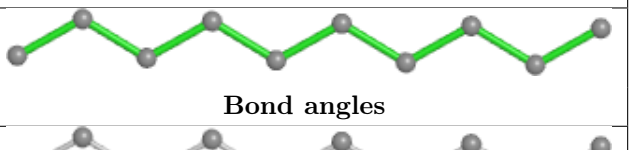

Bond angles

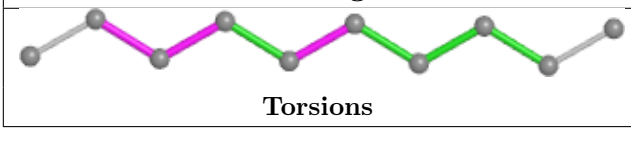

Torsions

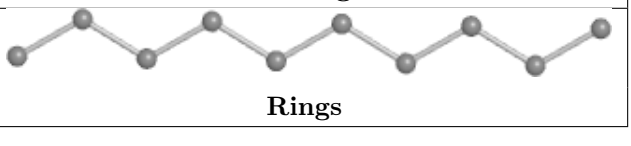

Rings

Ligand MC3 G 403

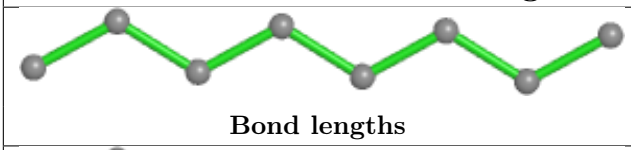

Bond lengths

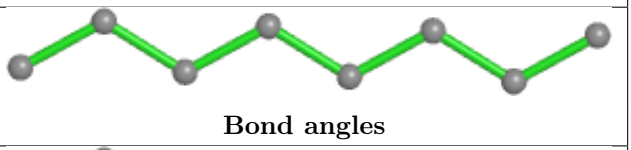

Bond angles


Torsions


Rings

Ligand MC3 K 404


Bond lengths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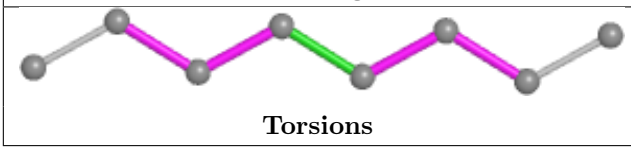
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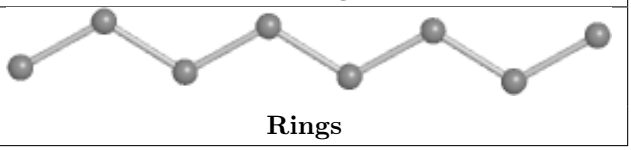
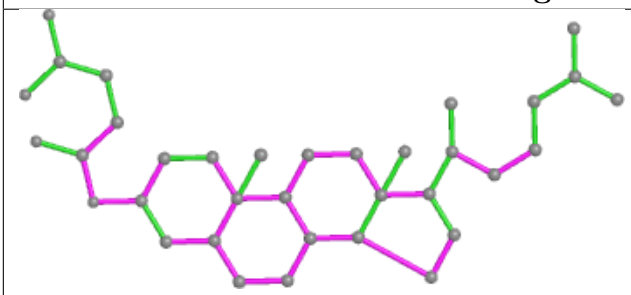
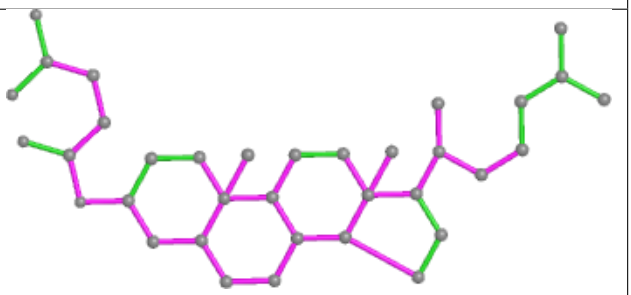
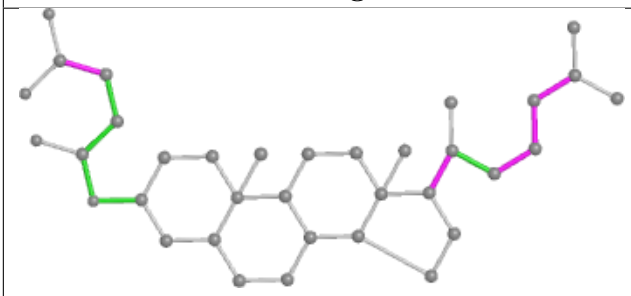
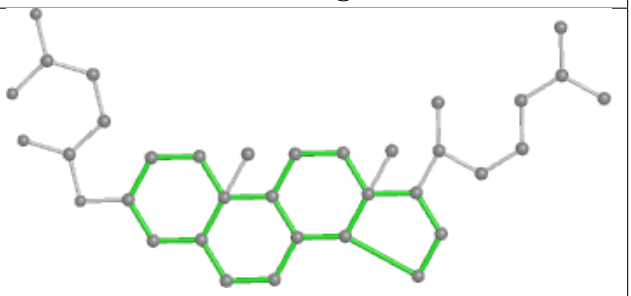

Rings

Ligand Y01 J 406

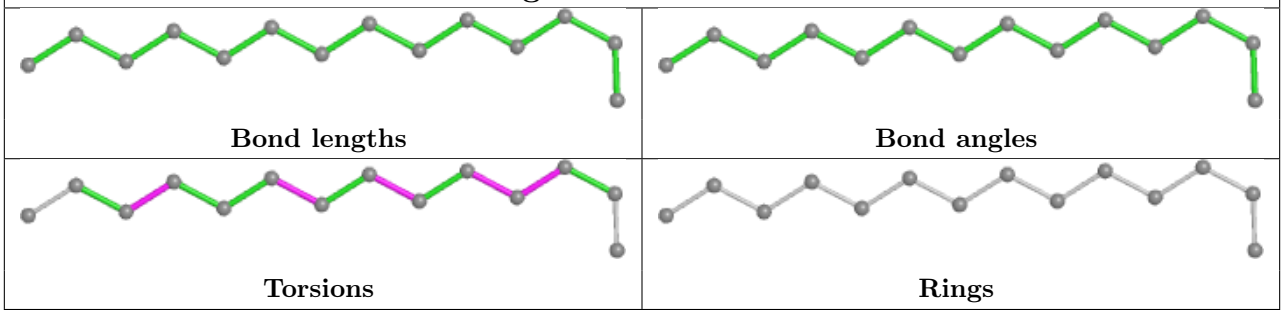

Bond lengths


Bond angles

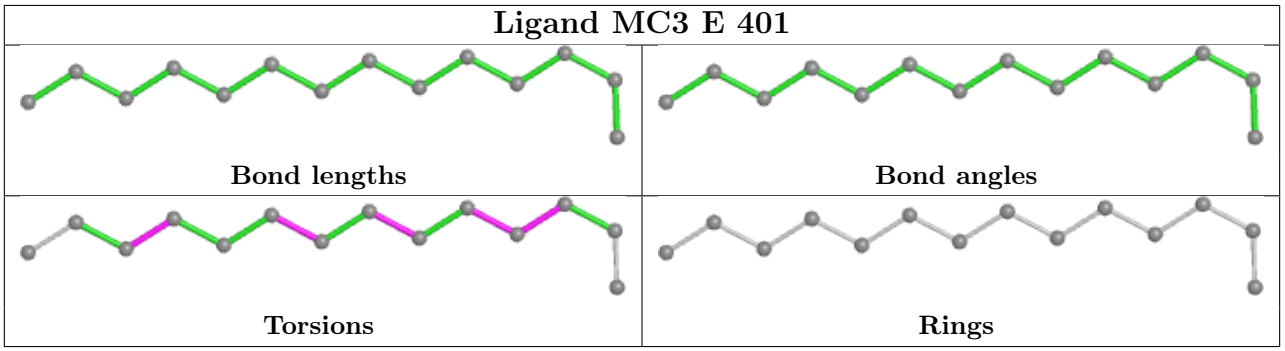

Torsions


Rings

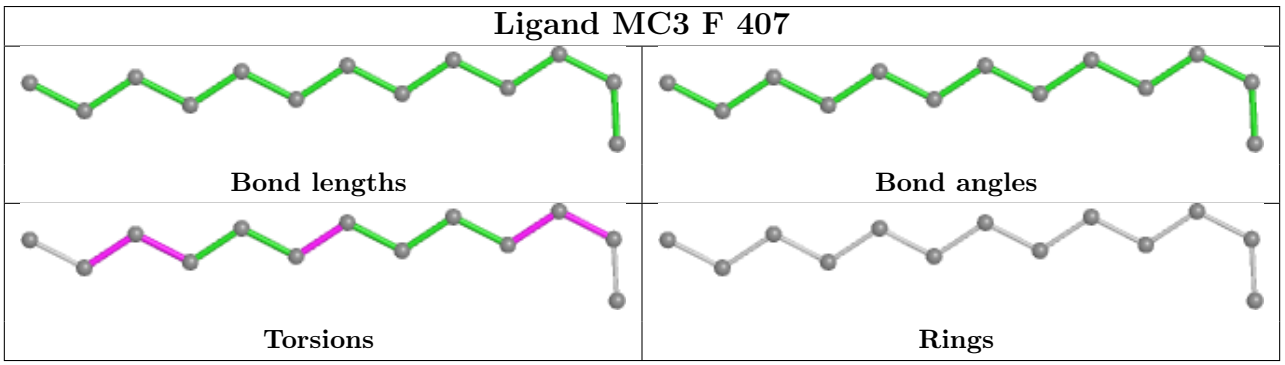
Ligand MC3 D 401



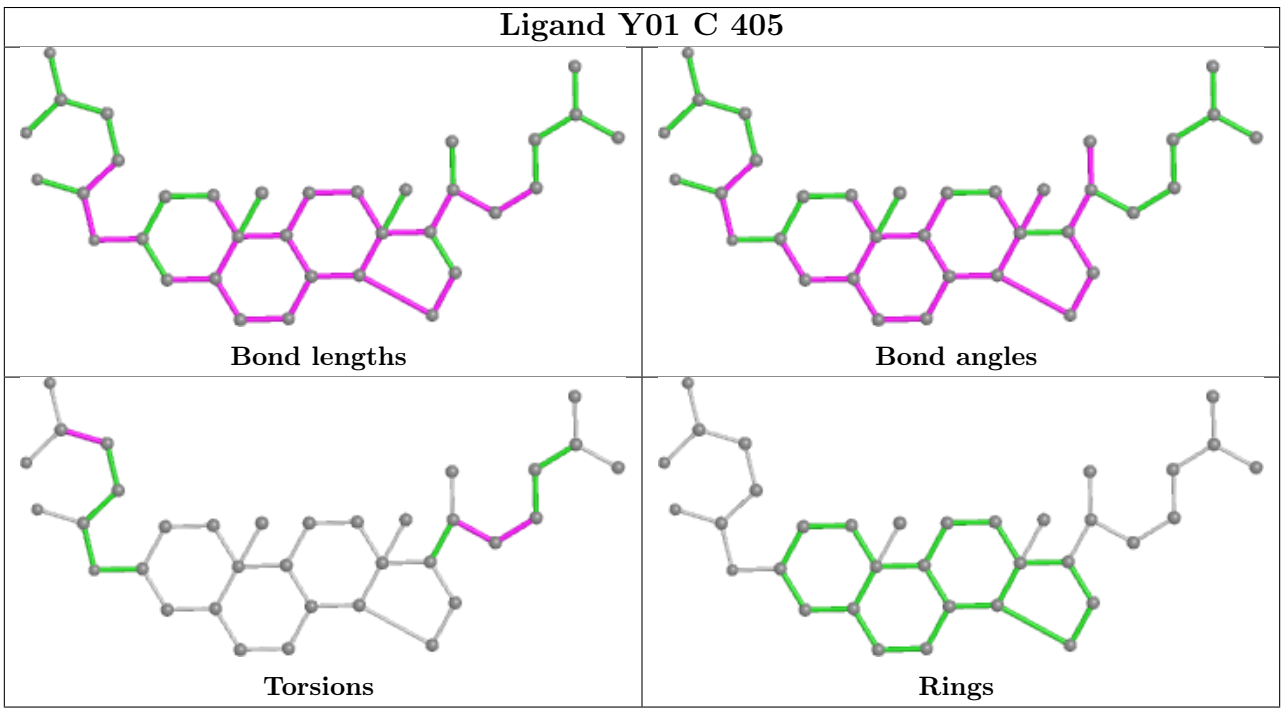
Ligand MC3 E 401



Ligand MC3 F 407



Ligand Y01 C 405



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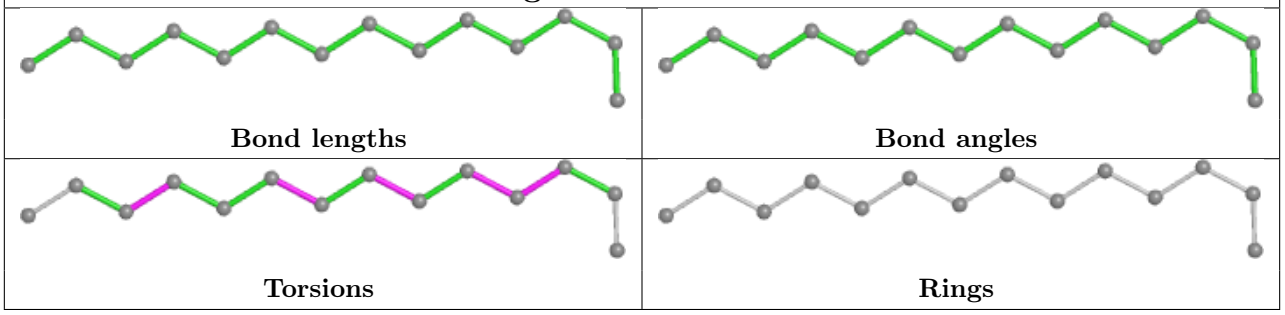
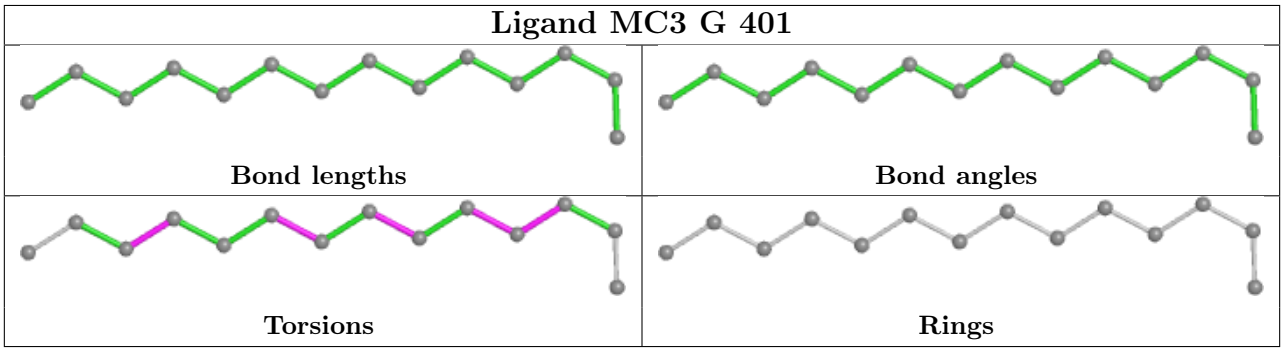
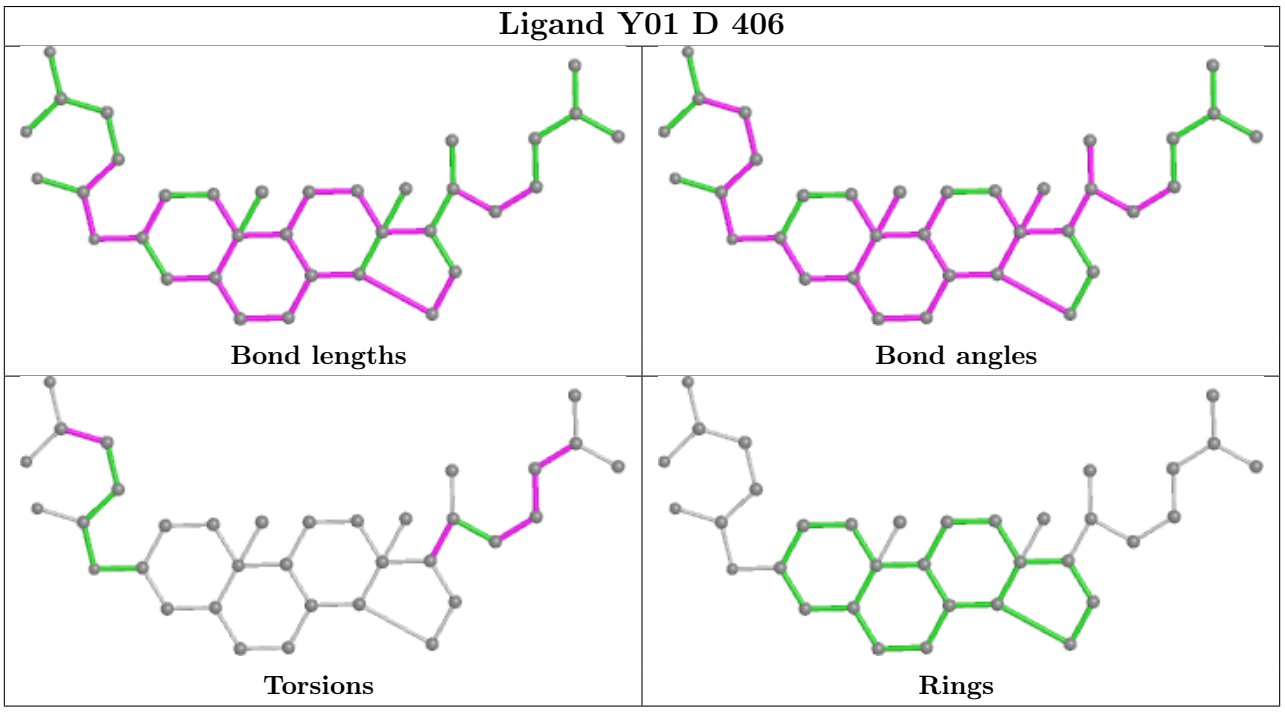


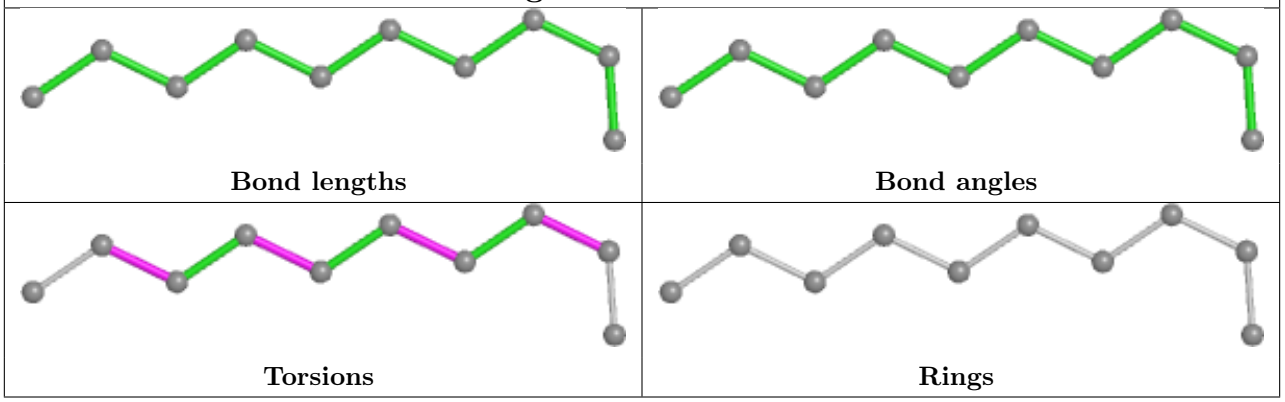
Ligand MC3 G 401



Ligand Y01 D 406



Ligand MC3 L 408



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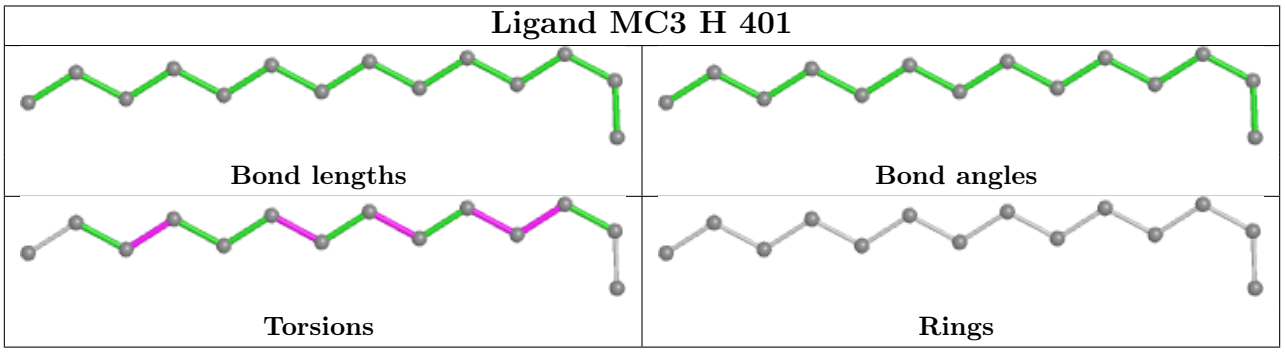

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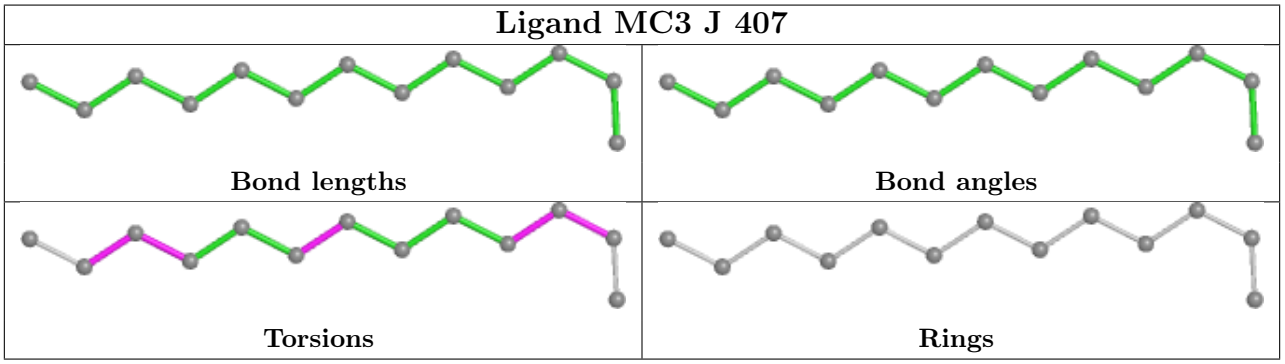

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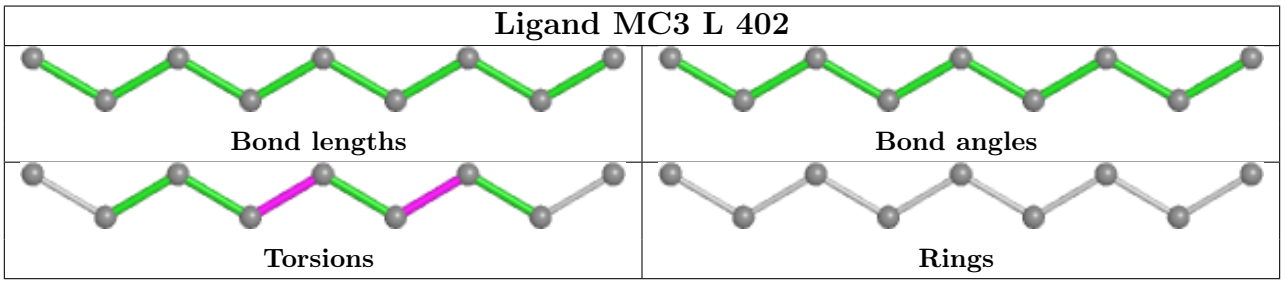

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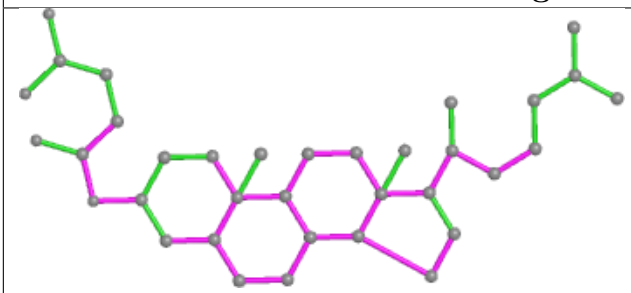
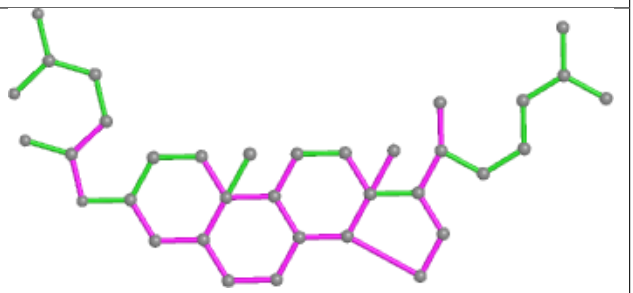
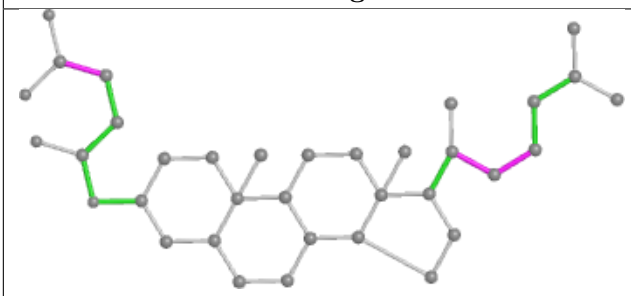


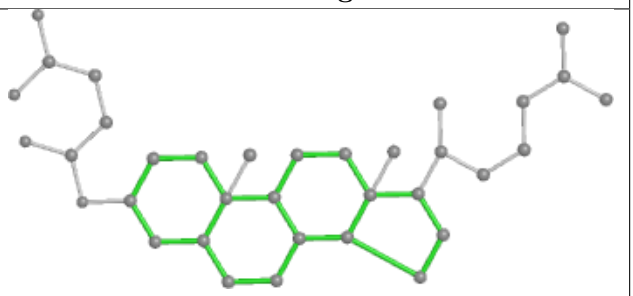
Bond lengths



Bond angles



Torsions

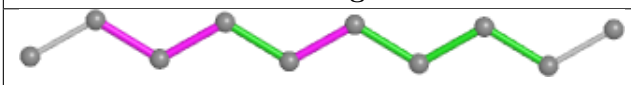


Rings

Ligand MC3 E 403

Bond lengths

Bond angles



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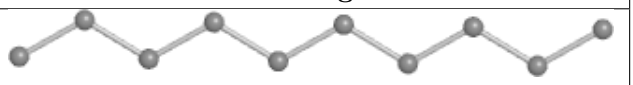
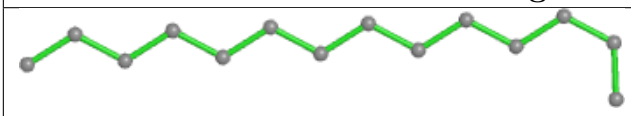


Rings

Ligand MC3 I 401



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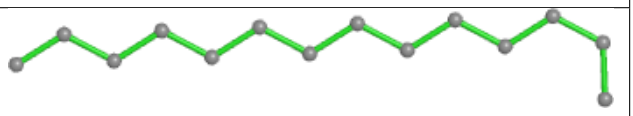

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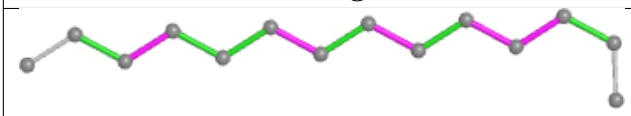

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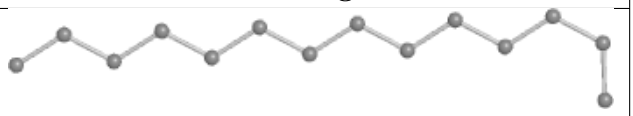
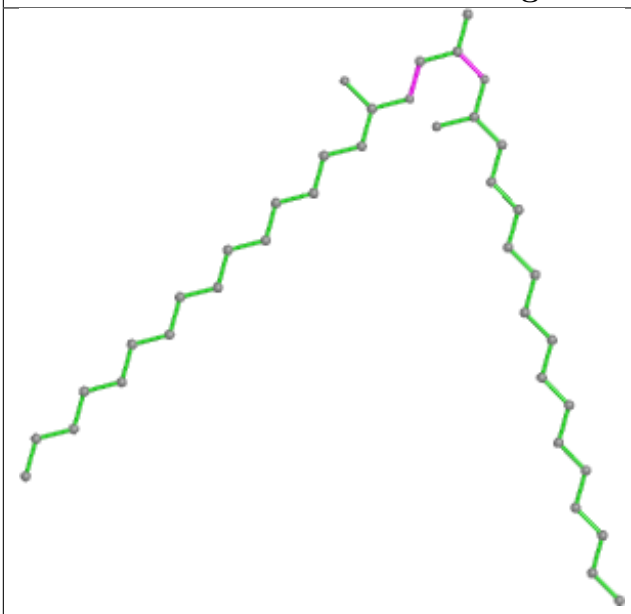


Rings

Ligand LHG G 409



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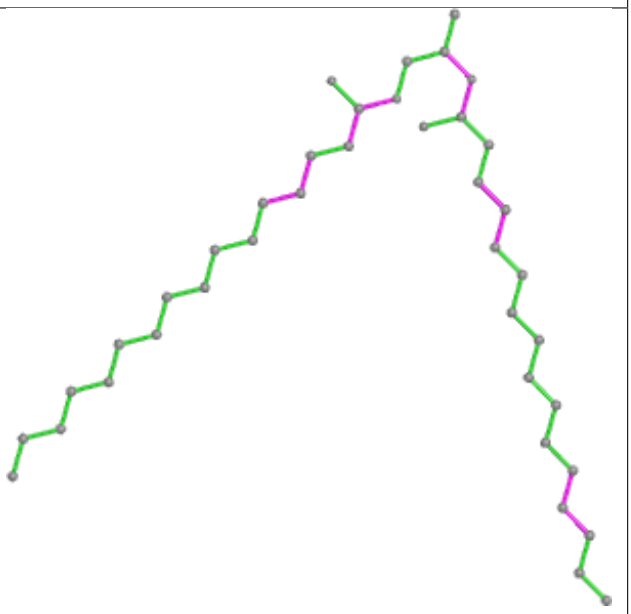

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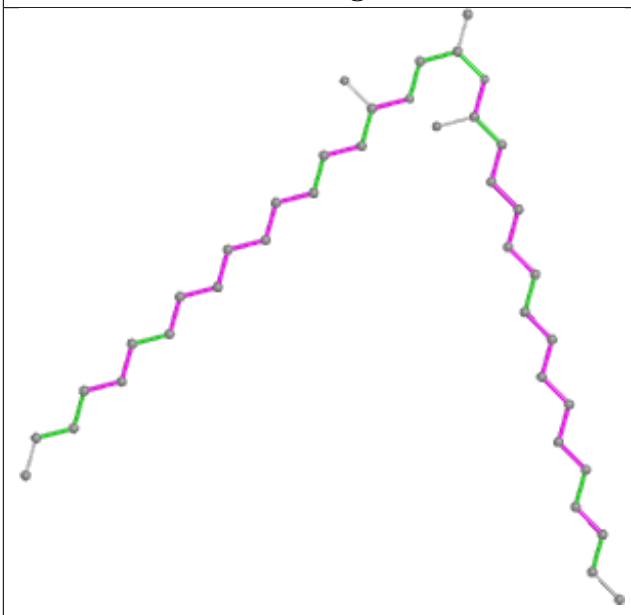

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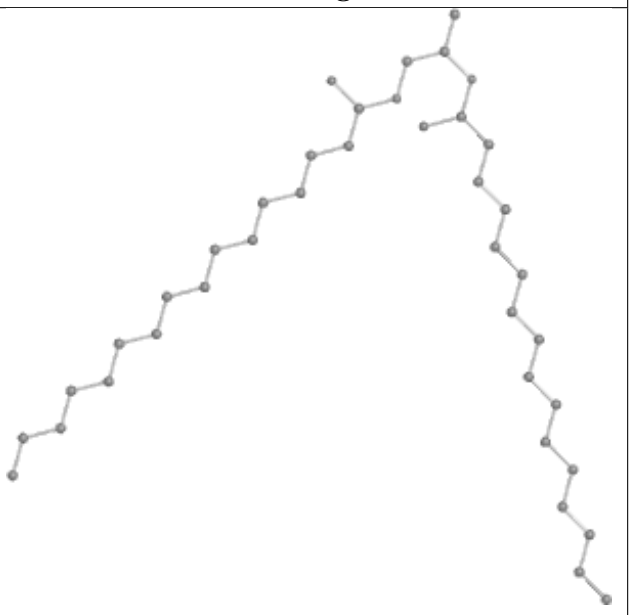
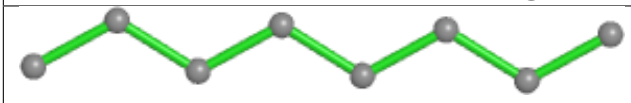


Rings

Ligand MC3 C 404



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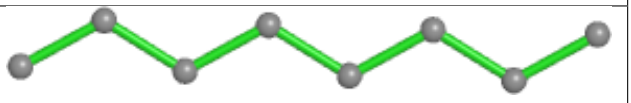

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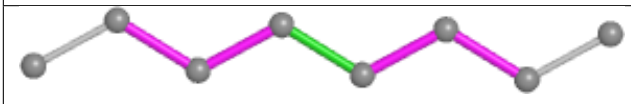

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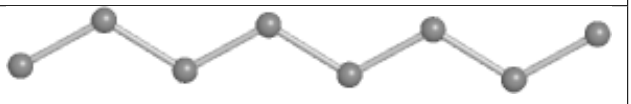
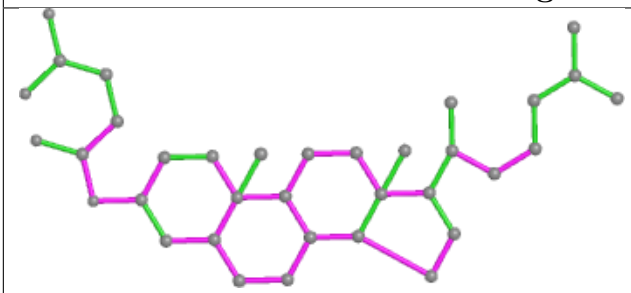


Rings

Ligand Y01 I 406



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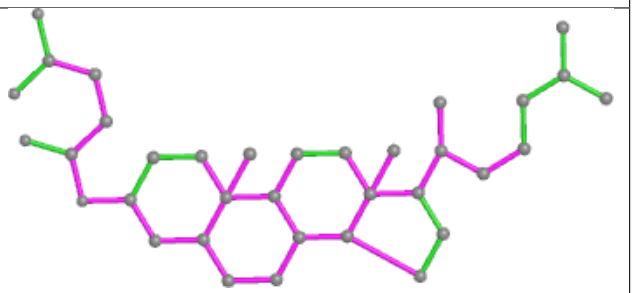

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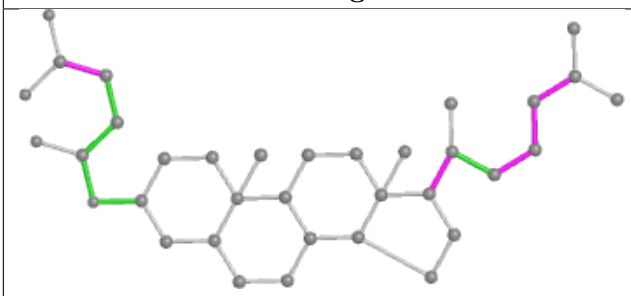

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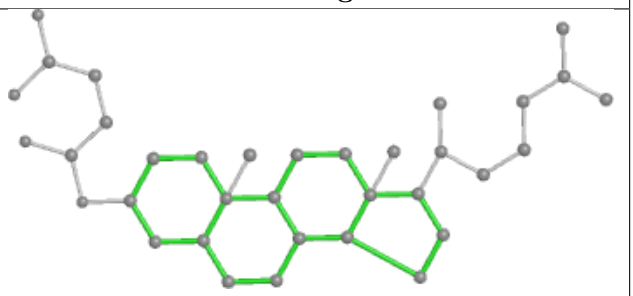
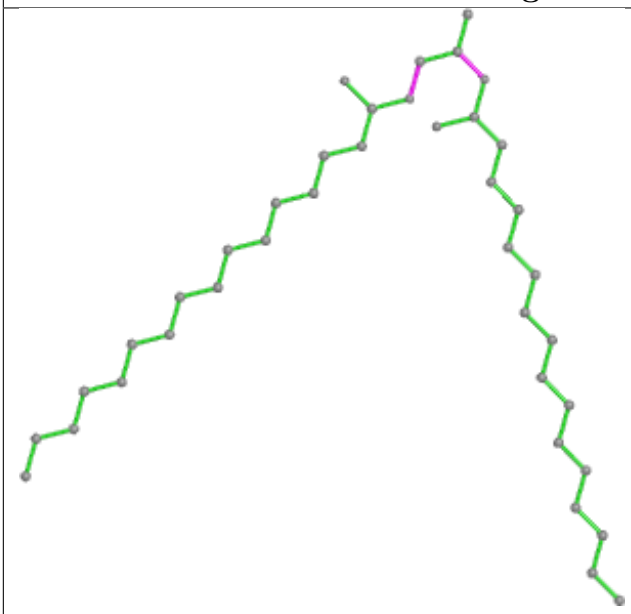


Rings

Ligand LHG D 409



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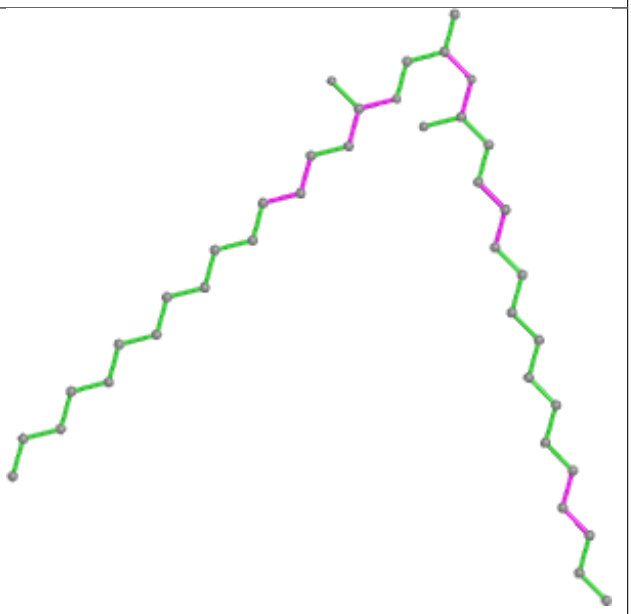

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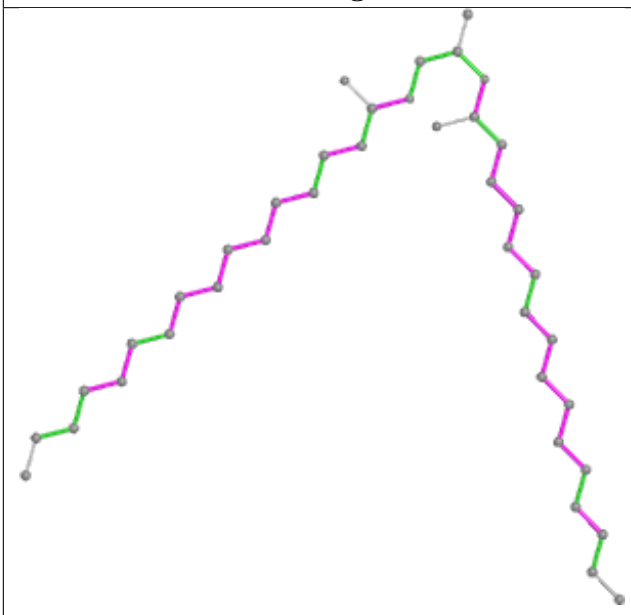

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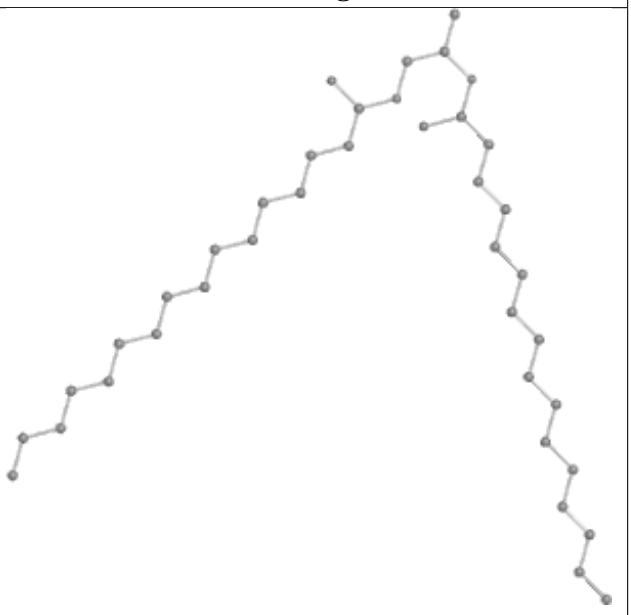
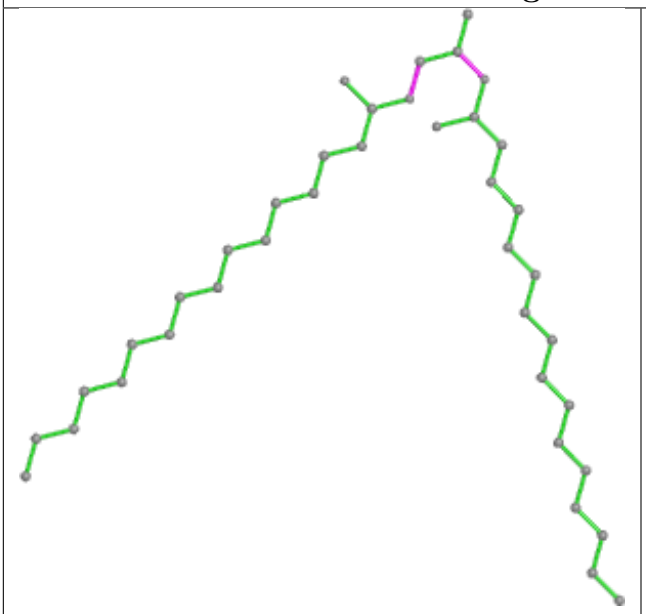


Rings

Ligand LHG B 409



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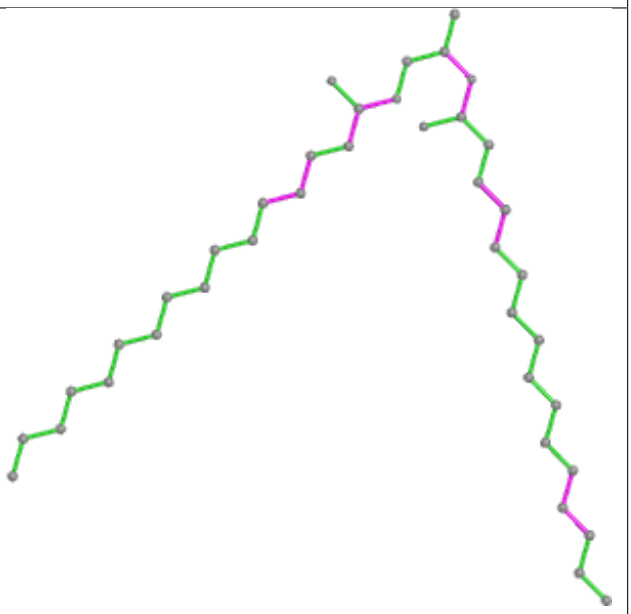

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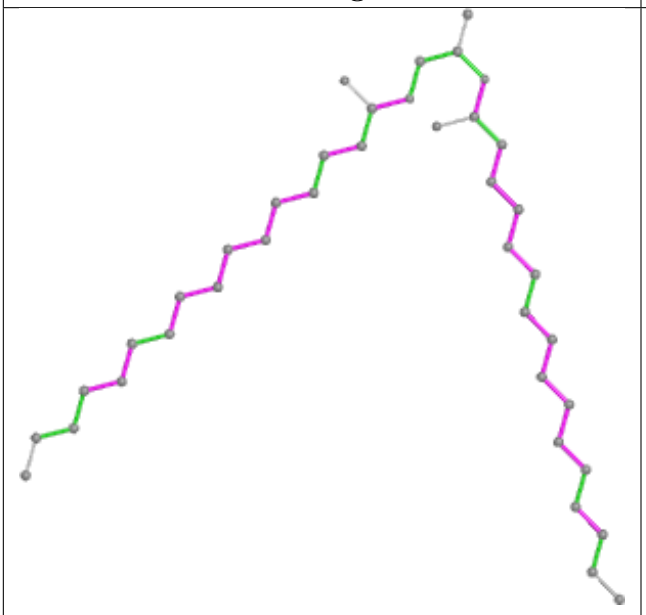

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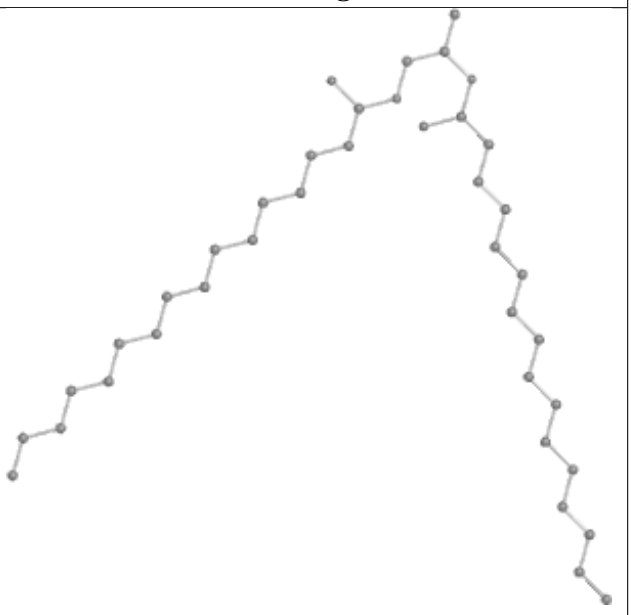
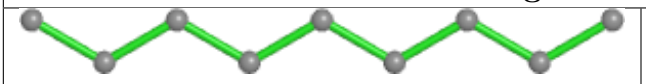


Rings

Ligand MC3 E 402



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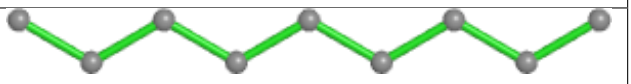

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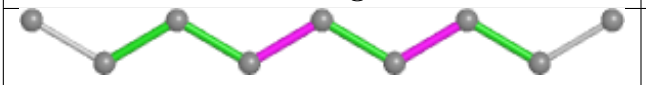
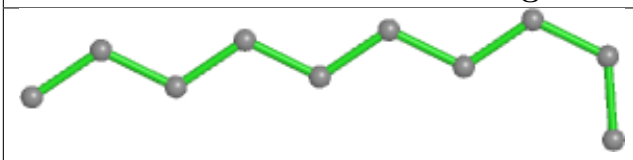
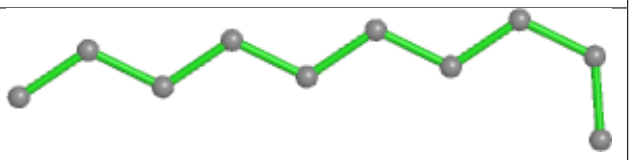
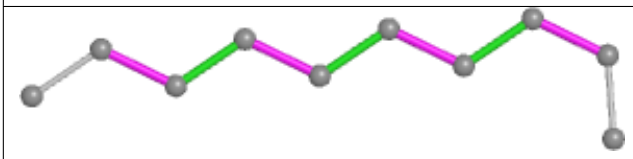
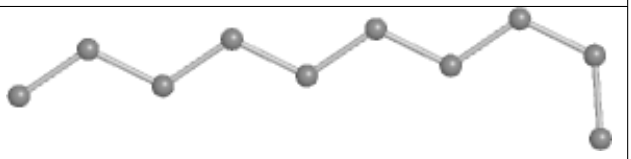
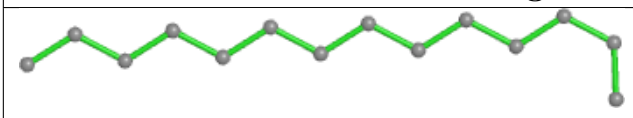
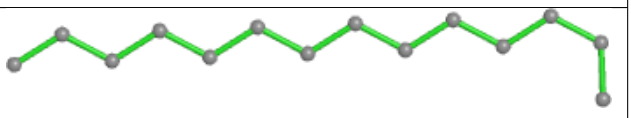
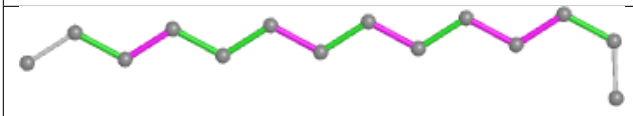
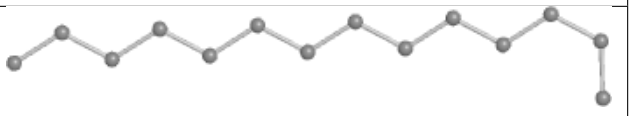


Torsions

Rings

Ligand MC3 K 408	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand MC3 J 401	
 Bond lengths	 Bond angles
 Torsions	 Rings

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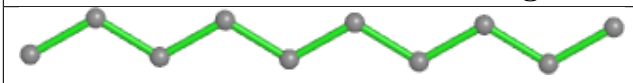
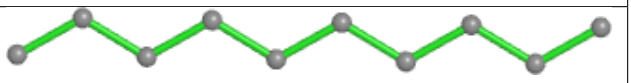
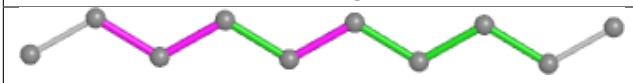
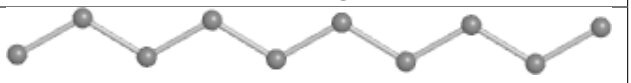
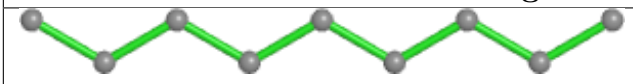
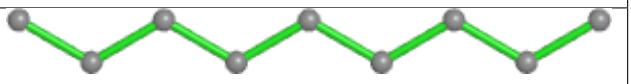
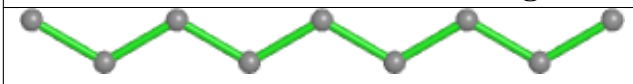
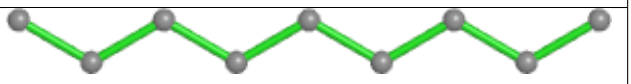
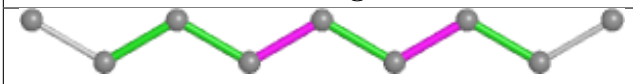
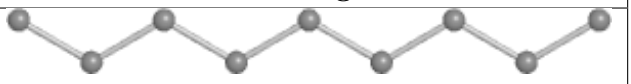
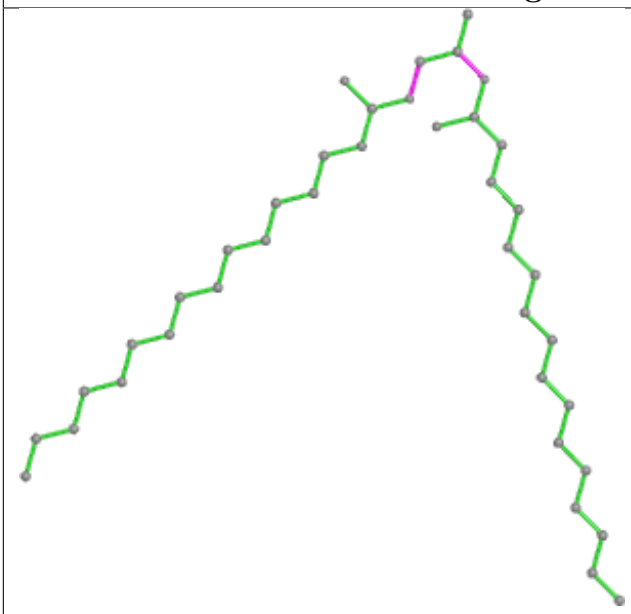
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand MC3 H 402	
 Bond lengths	 Bond angles
Torsions	Rings

Ligand MC3 K 402	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LHG L 409



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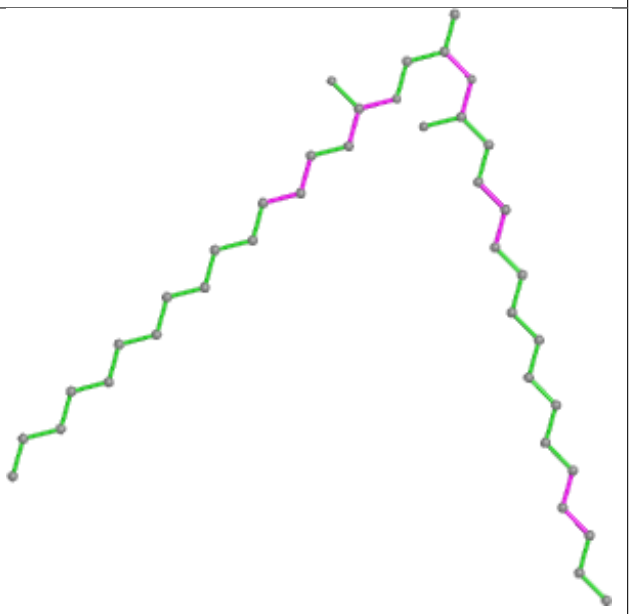
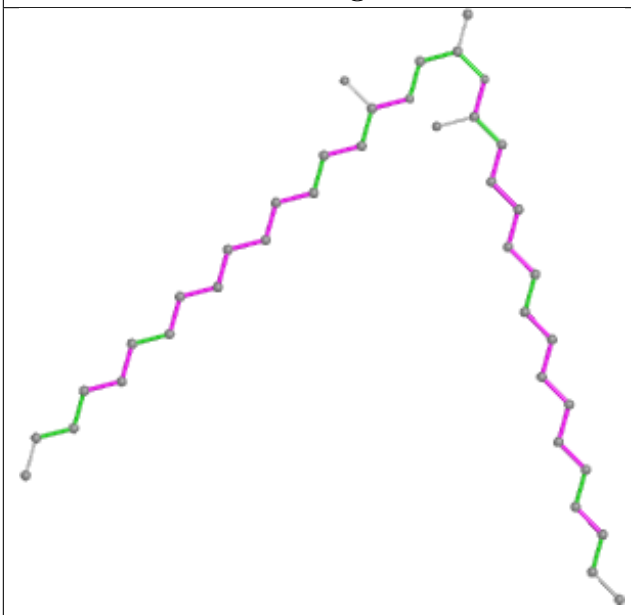
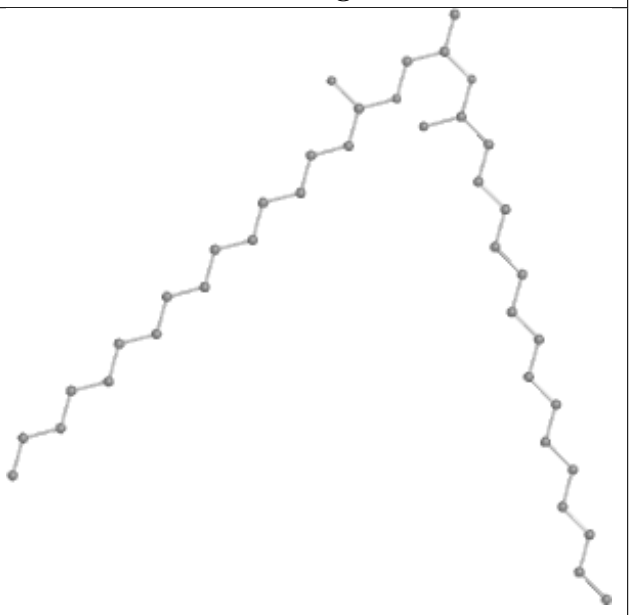


Bond angles

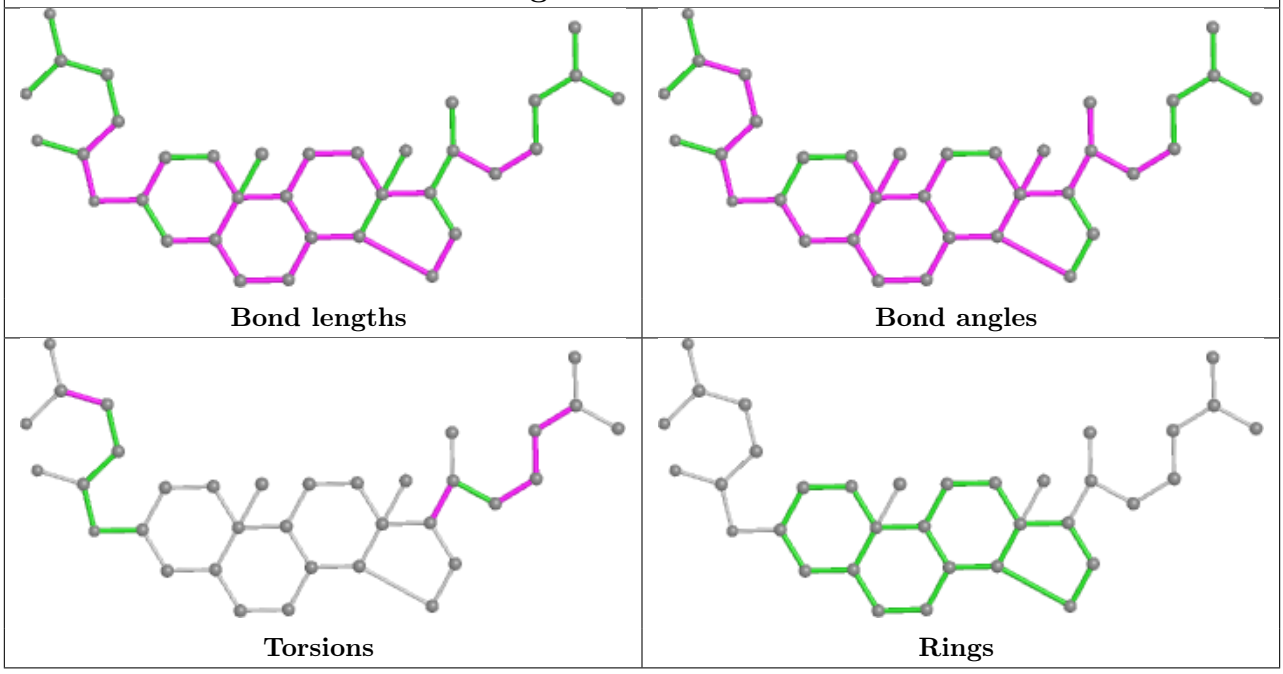


Torsions

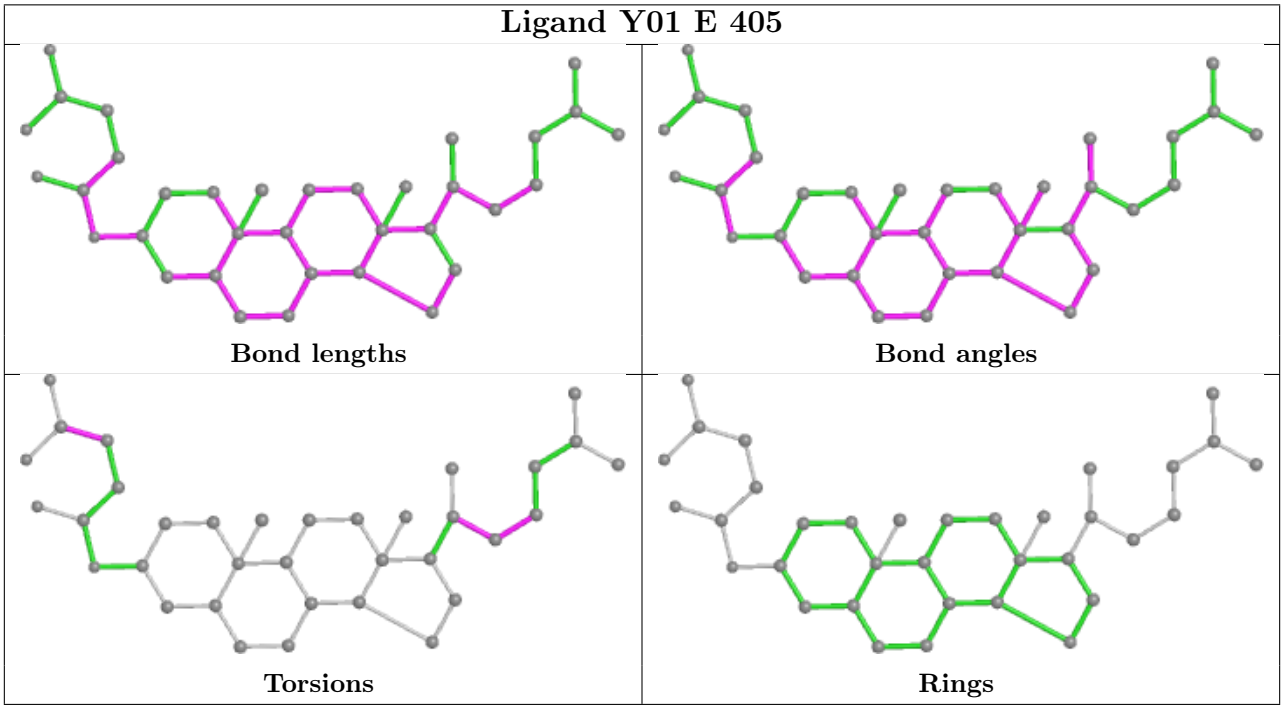


Rings

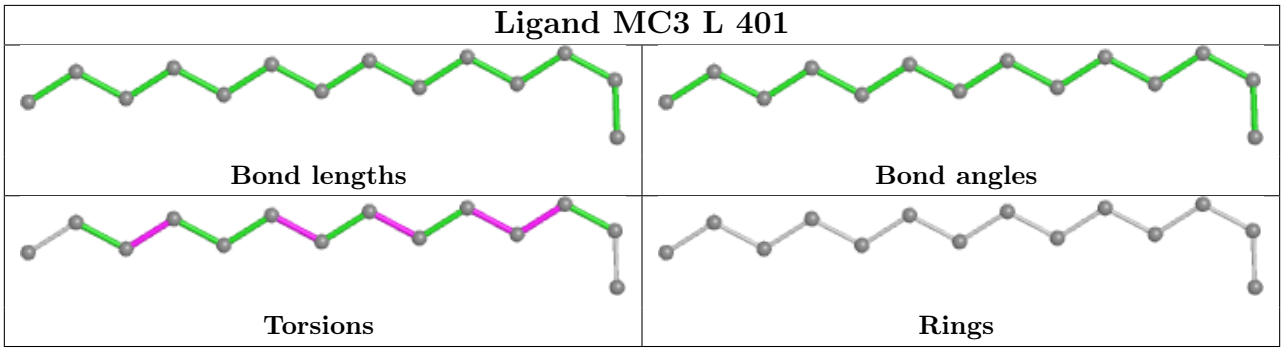
Ligand Y01 G 406



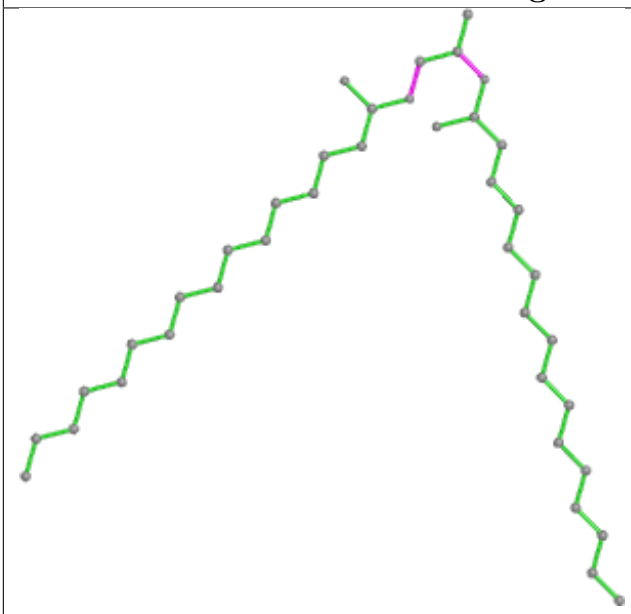
Ligand Y01 E 405



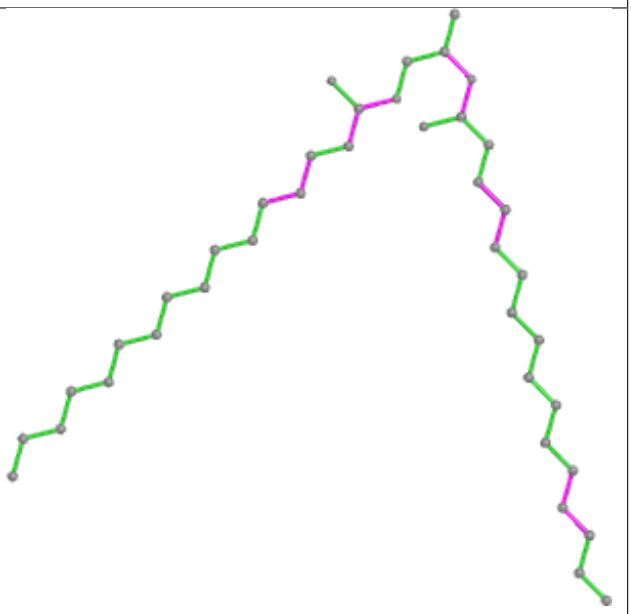
Ligand MC3 L 401



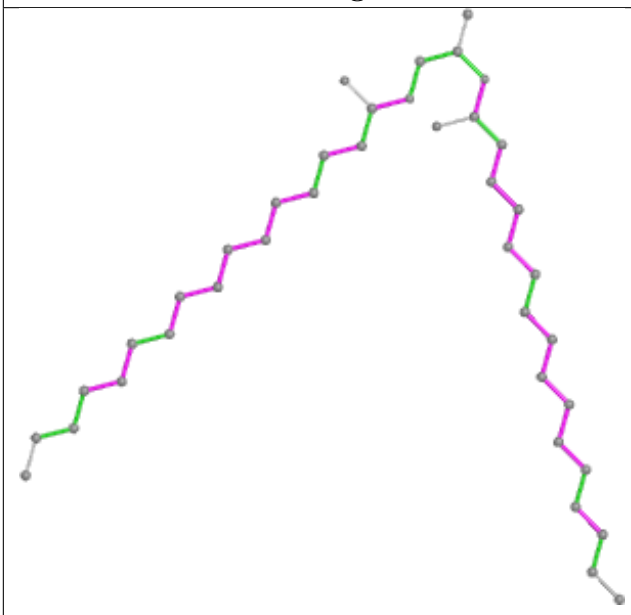
Ligand LHG I 409



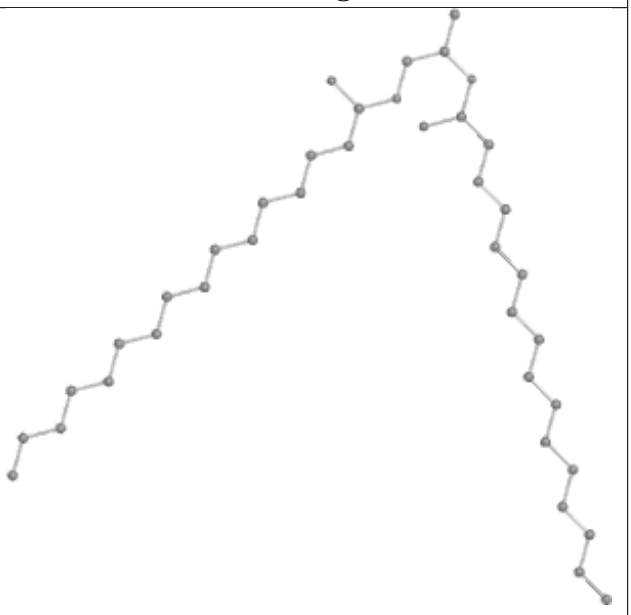
Bond lengths



Bond angles

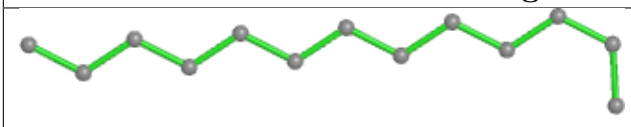


Torsions

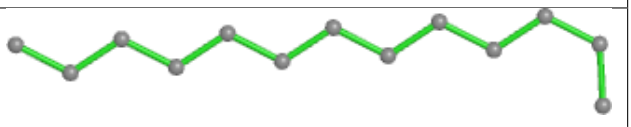


Rings

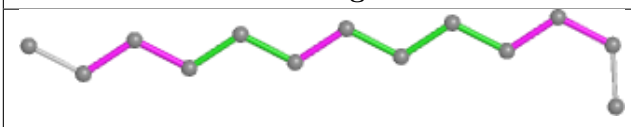
Ligand MC3 H 407



Bond lengths



Bond angles



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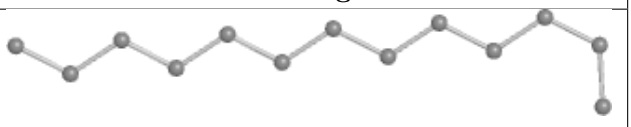
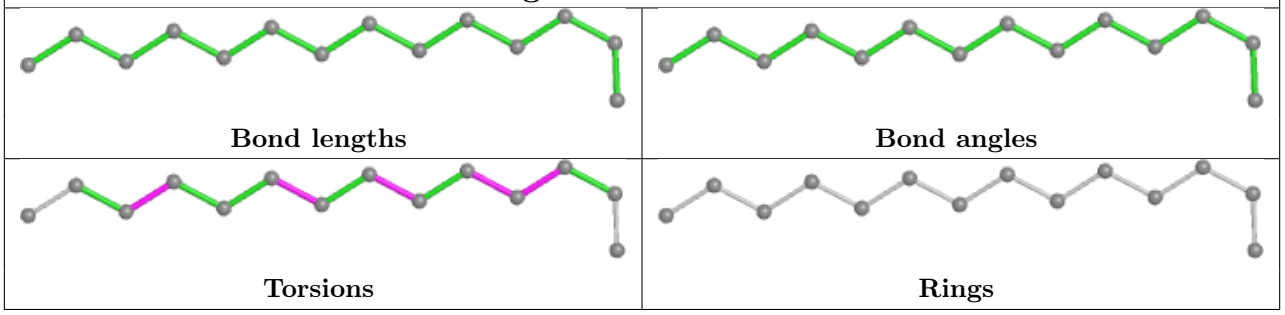
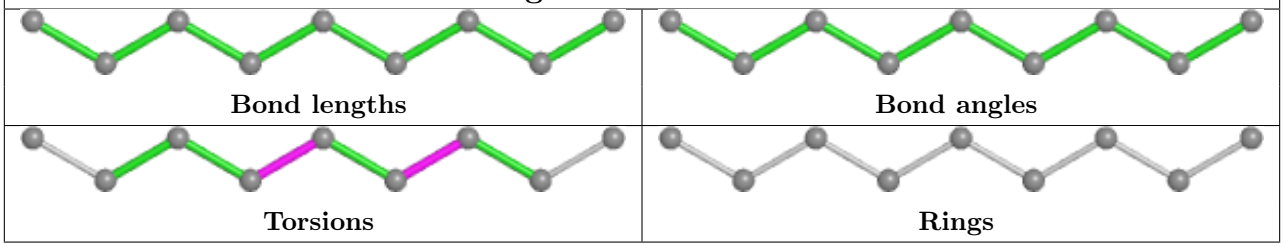


Rings

Ligand MC3 K 401



Ligand MC3 F 402



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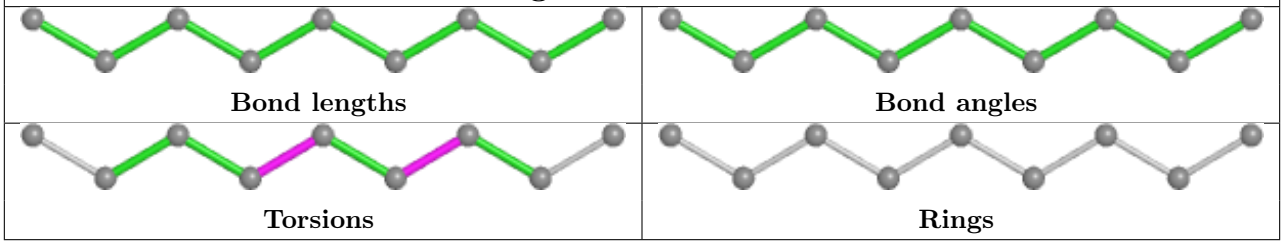
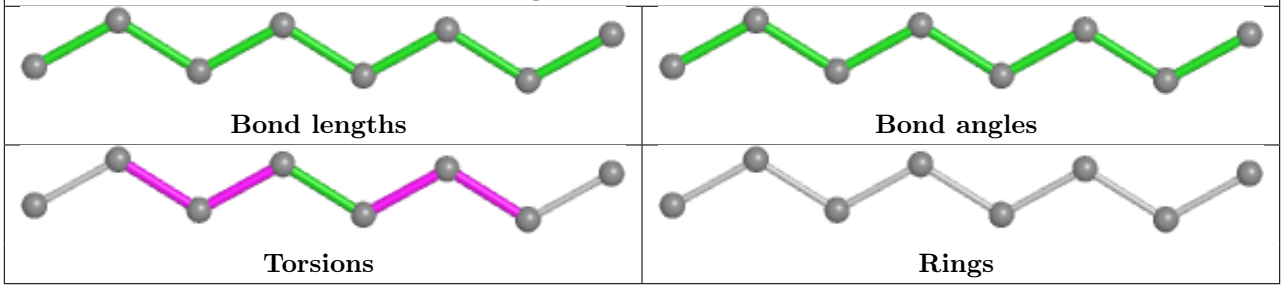
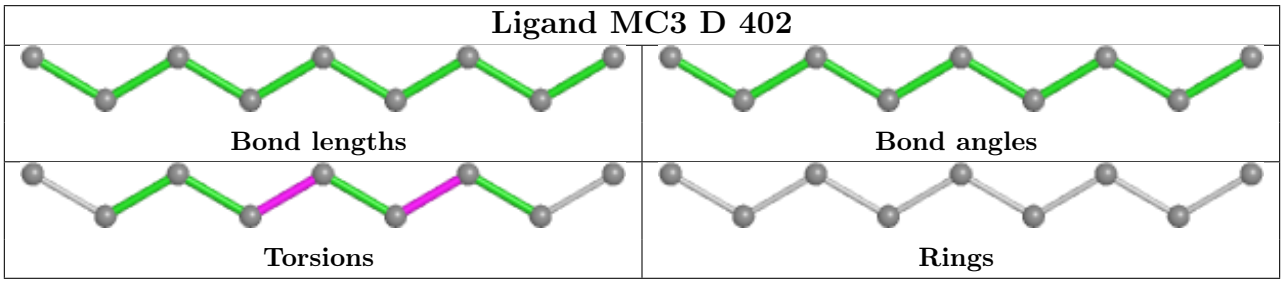


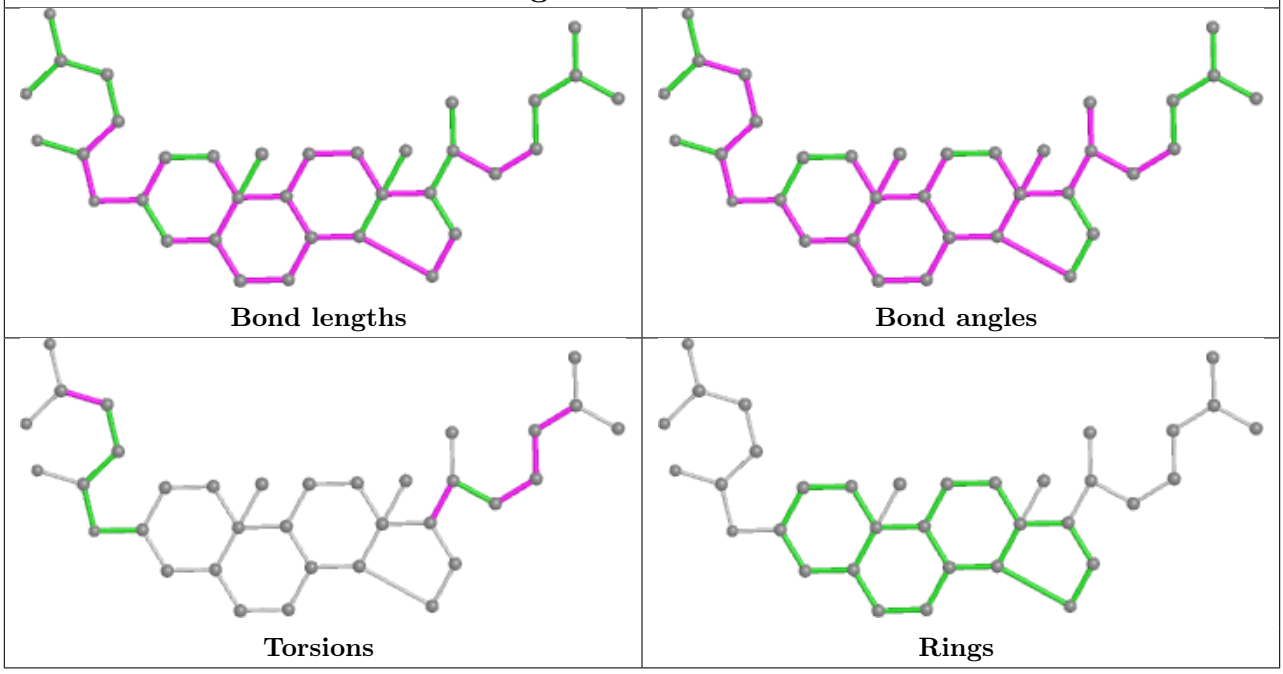
Ligand MC3 J 404



Ligand MC3 D 402



Ligand Y01 A 406



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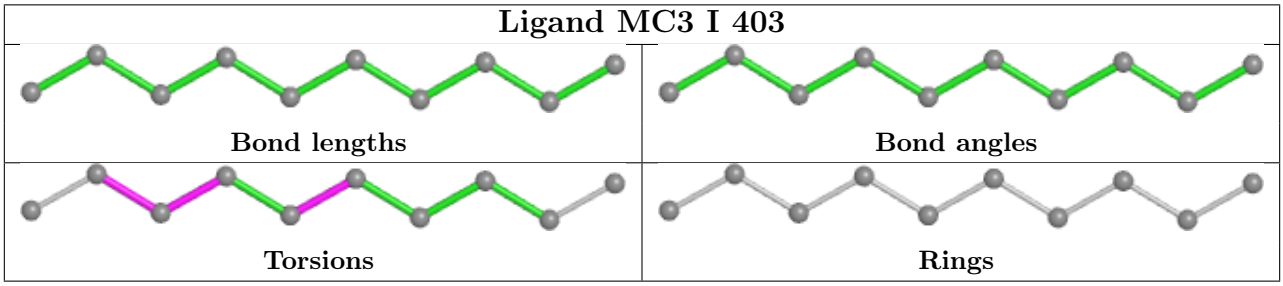
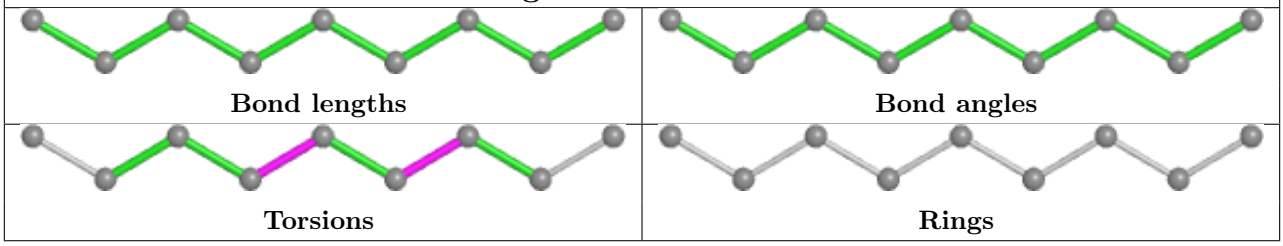
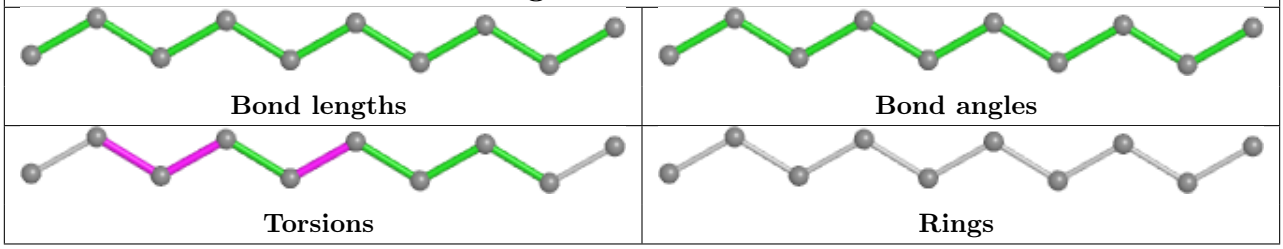


Ligand MC3 G 402



Ligand MC3 J 403



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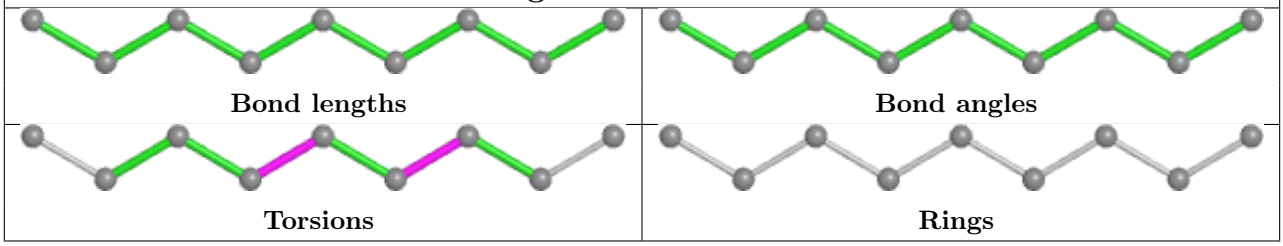
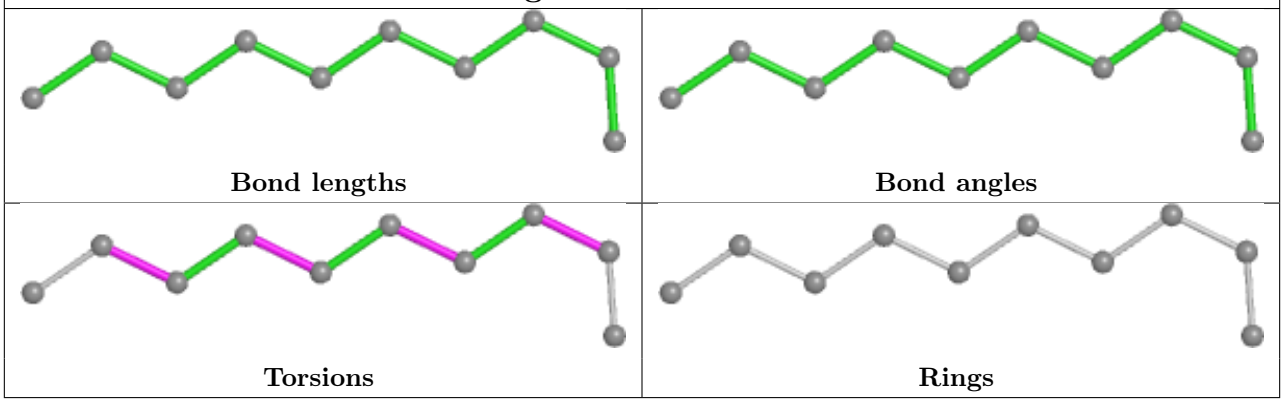


Ligand MC3 E 408



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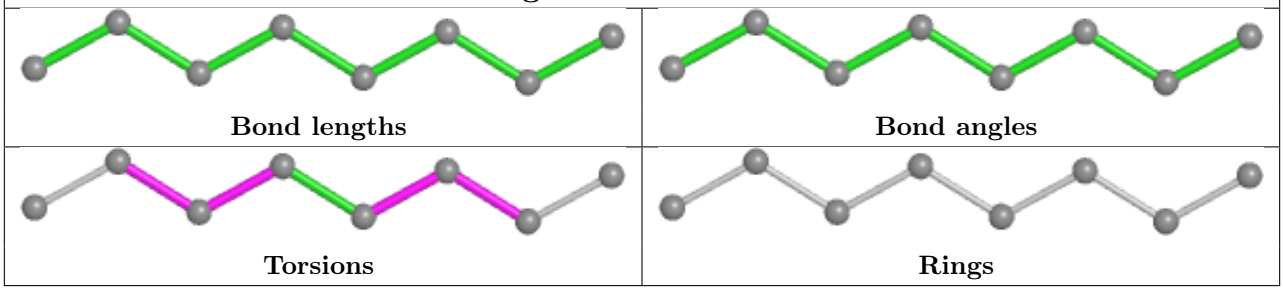
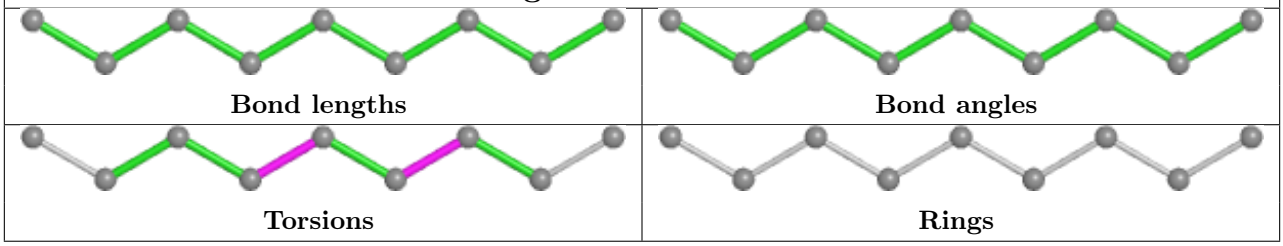
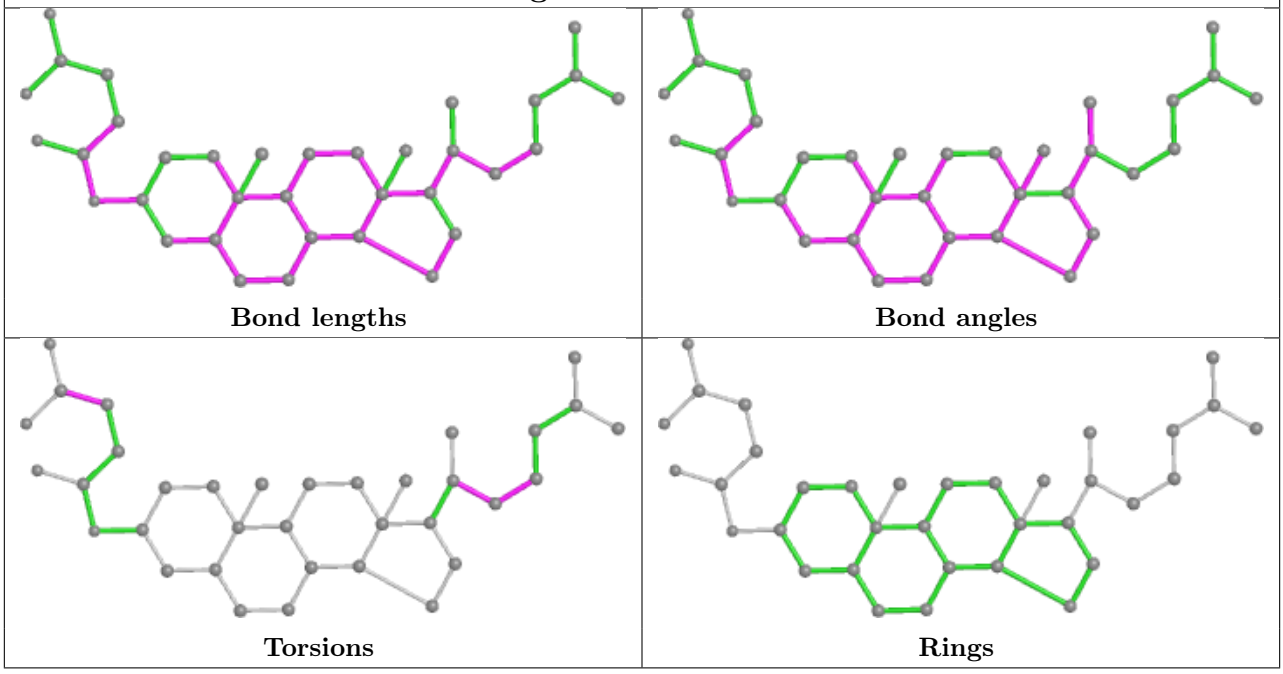


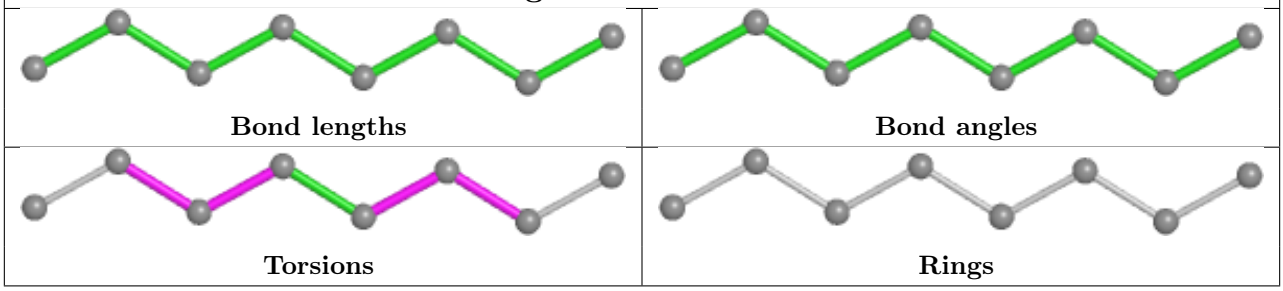
Ligand MC3 C 402



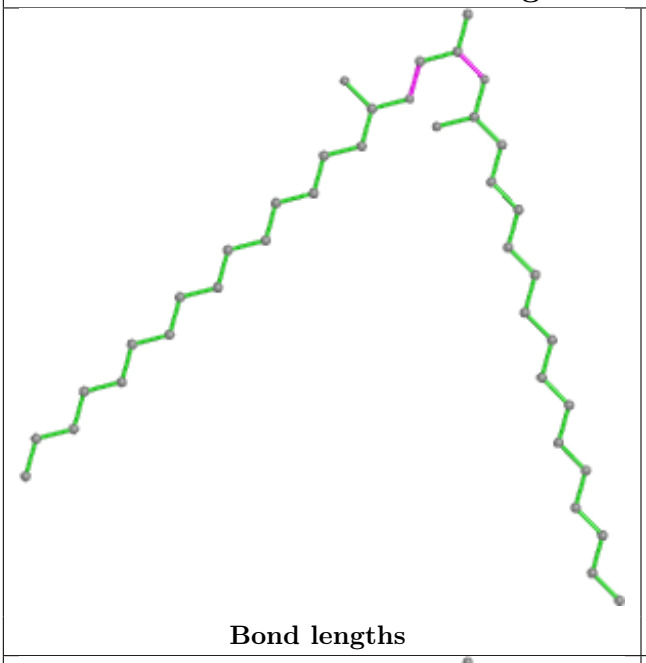
Ligand Y01 K 405



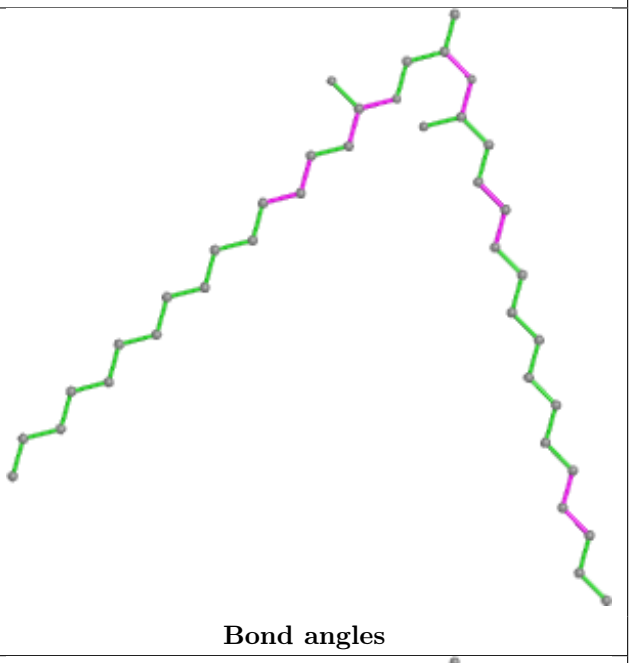
Ligand MC3 F 404



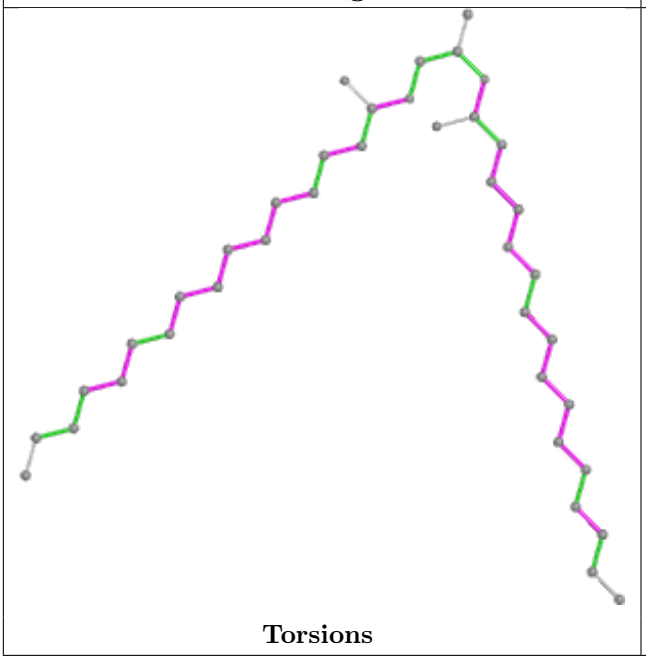
Ligand LHG A 409



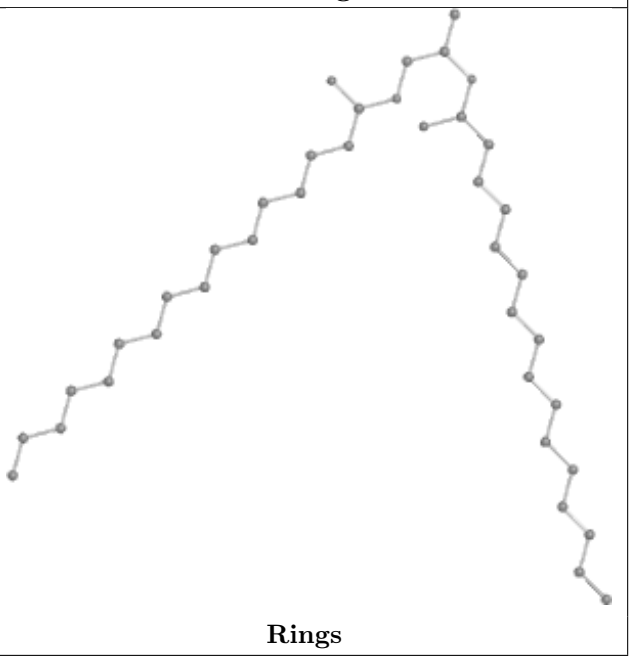
Bond lengths



Bond angles

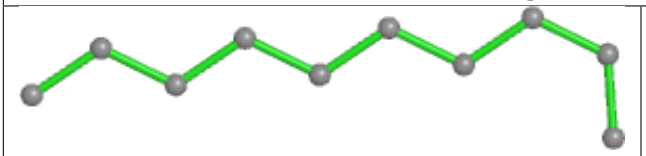


Torsions

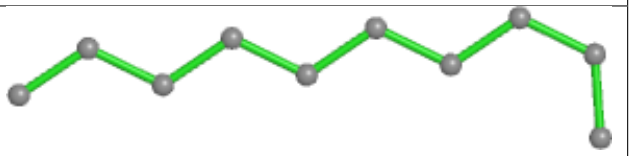


Rings

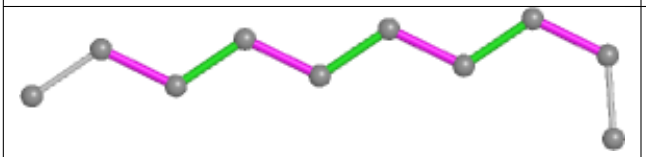
Ligand MC3 H 408



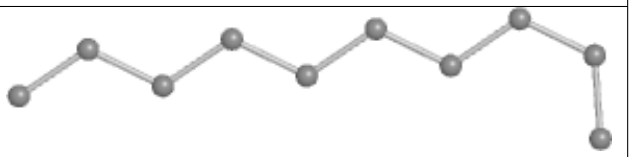
Bond lengths



Bond angles

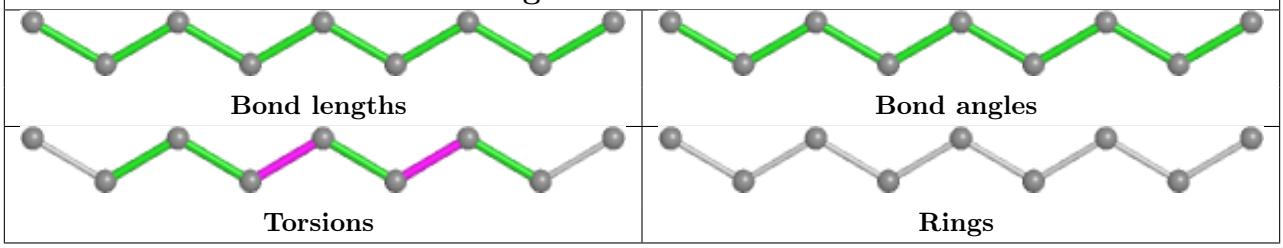


Torsions

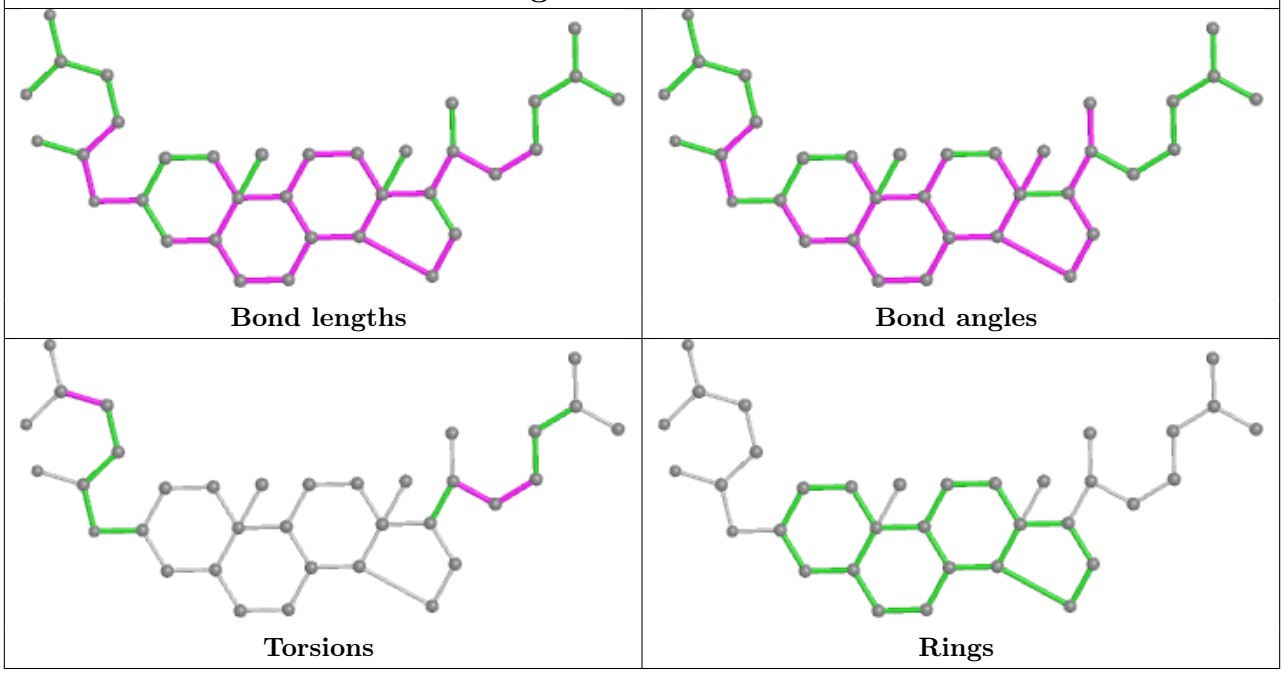


Rings

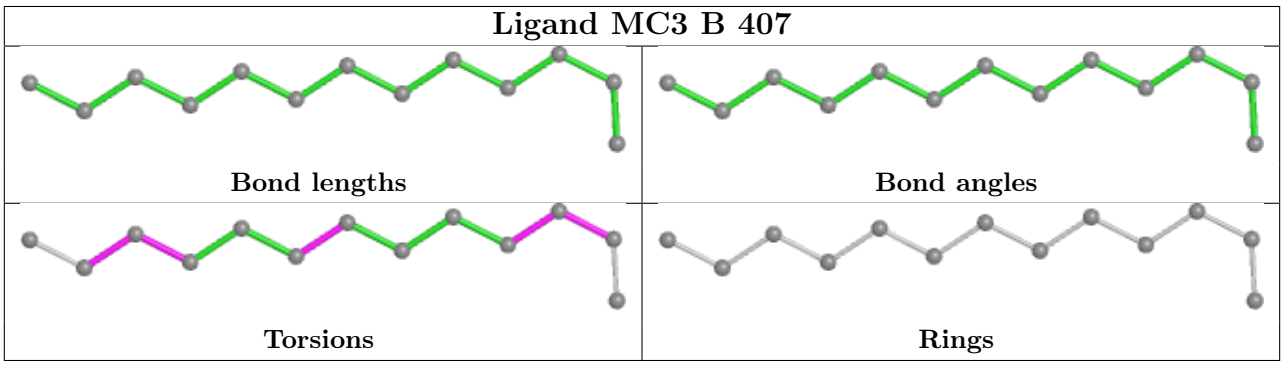
Ligand MC3 A 402



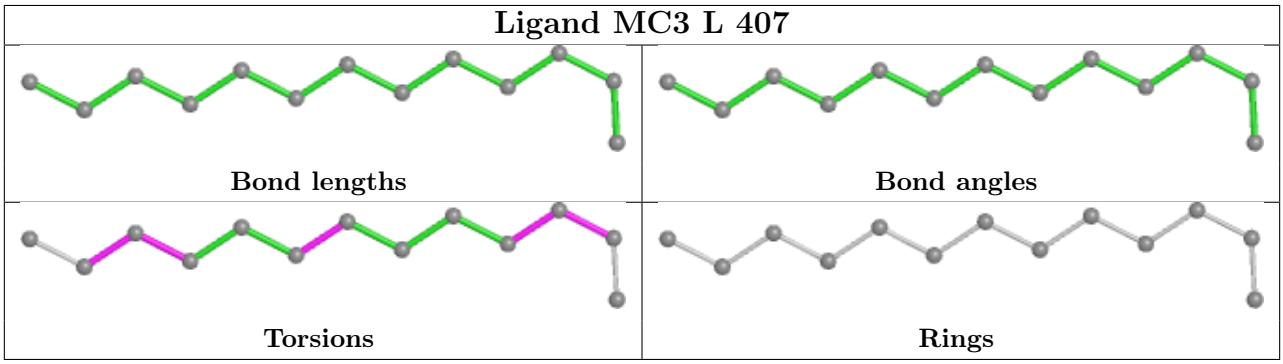
Ligand Y01 D 405



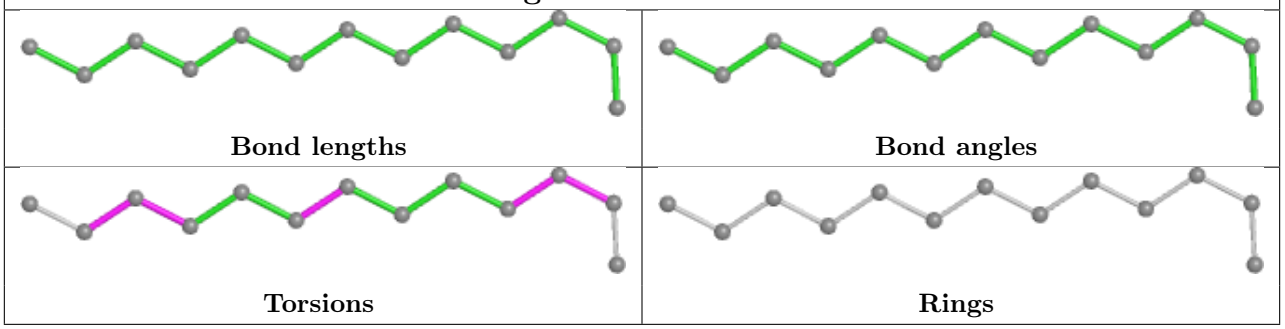
Ligand MC3 B 407



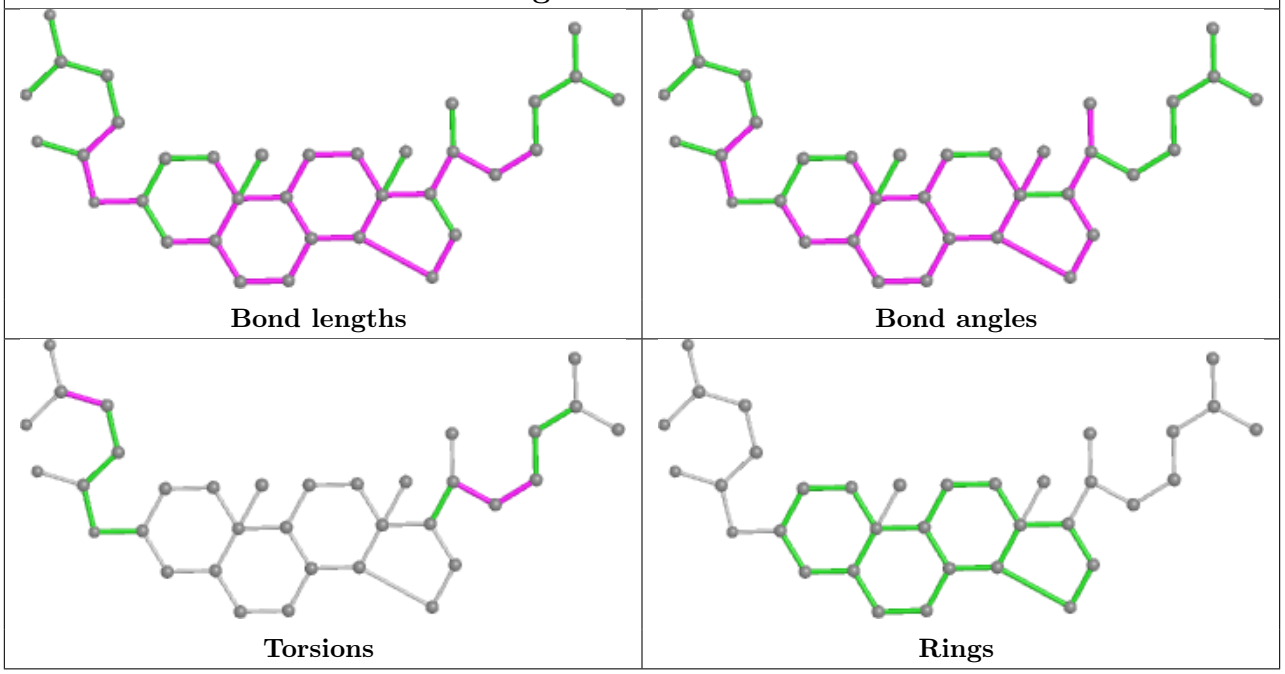
Ligand MC3 L 407



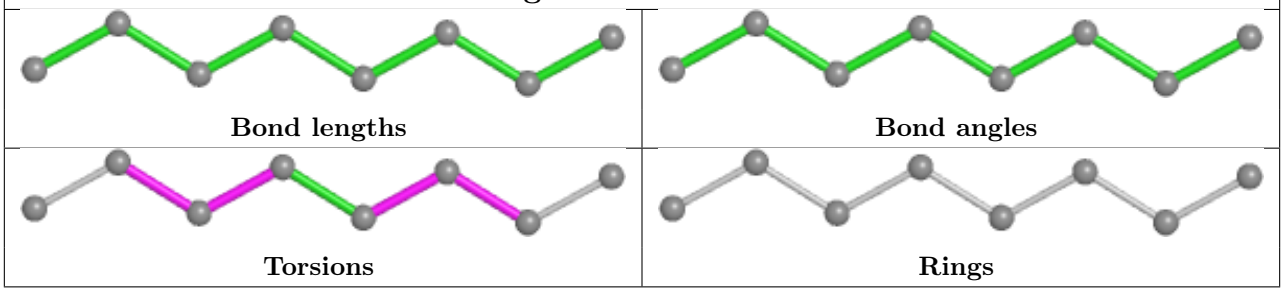
Ligand MC3 C 407

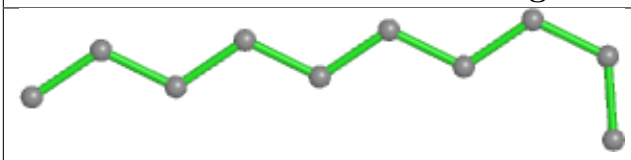
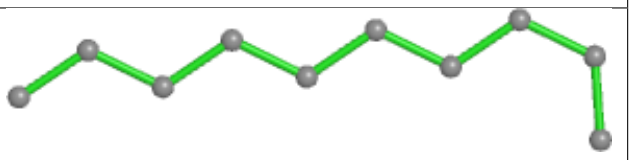
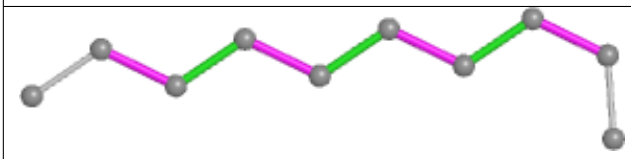
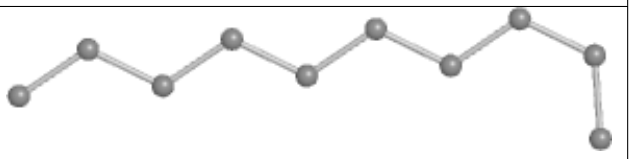


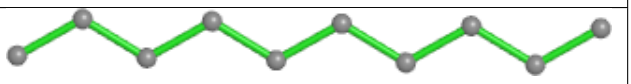
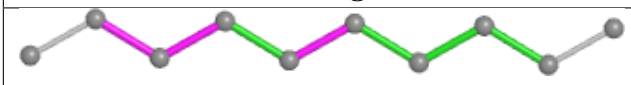
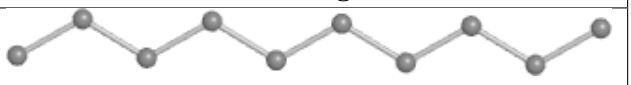
Ligand Y01 F 405



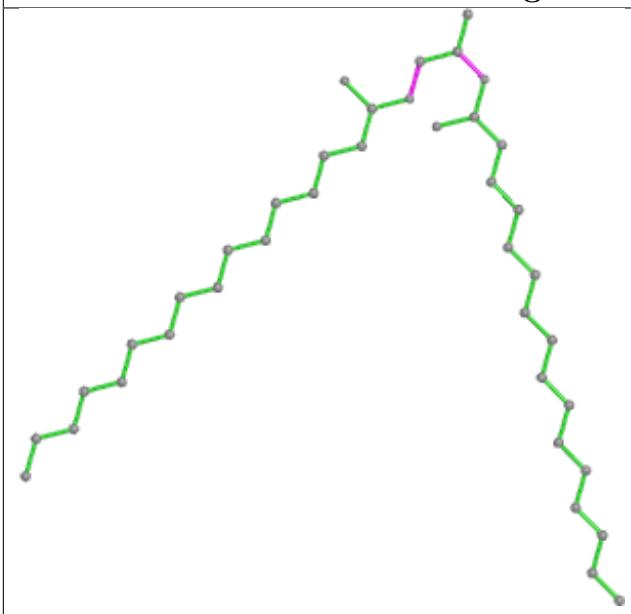
Ligand MC3 B 404



Ligand MC3 I 408	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand MC3 F 403	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LHG E 409



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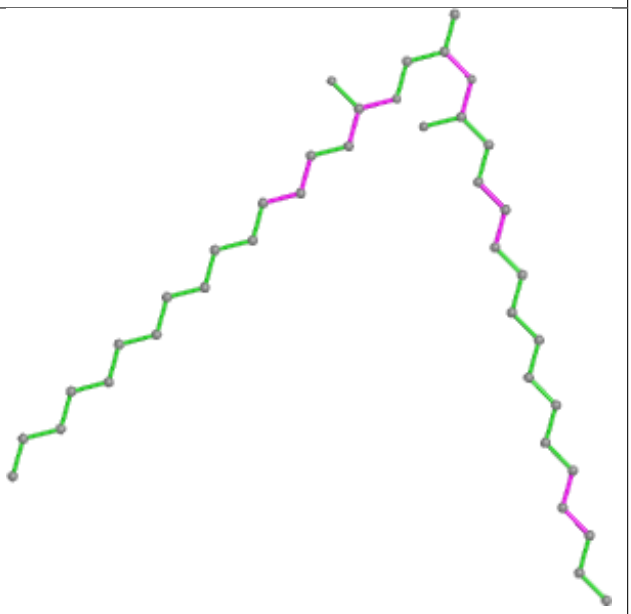

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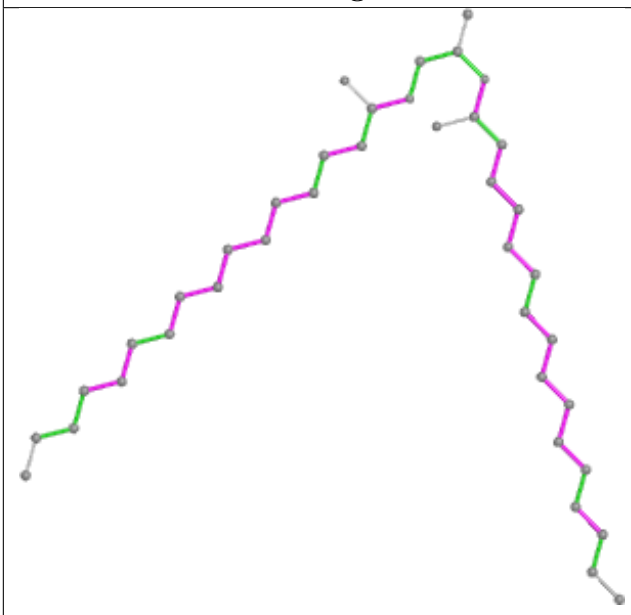

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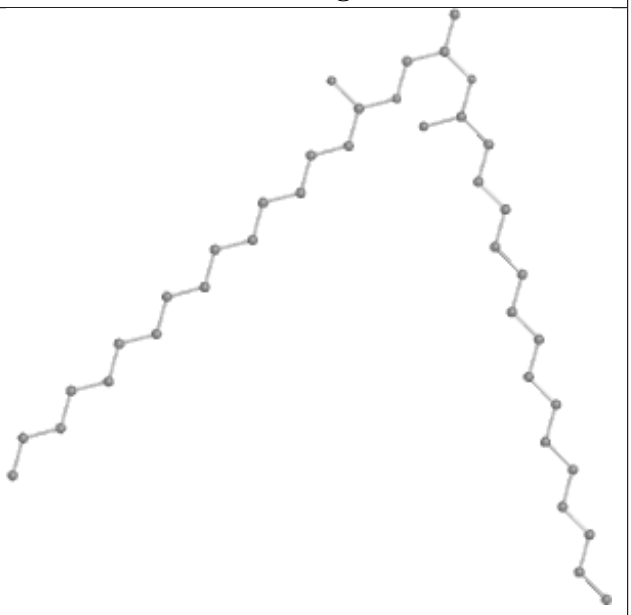
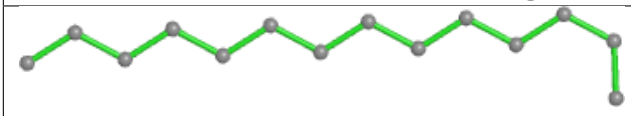


Rings

Ligand MC3 A 401



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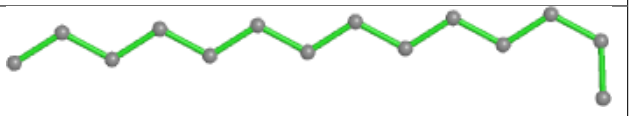

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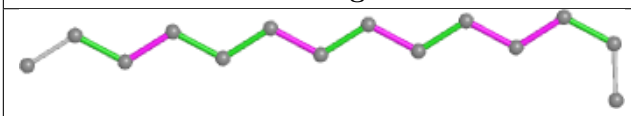

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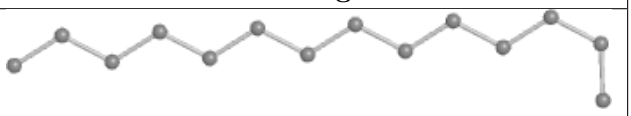

Rings

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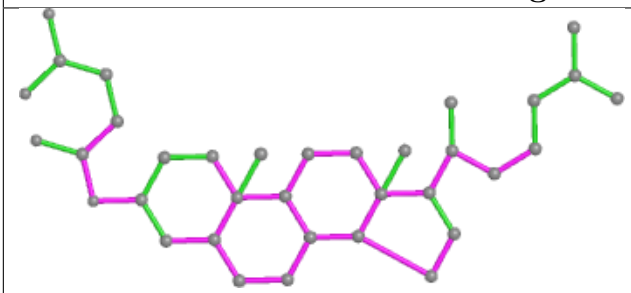

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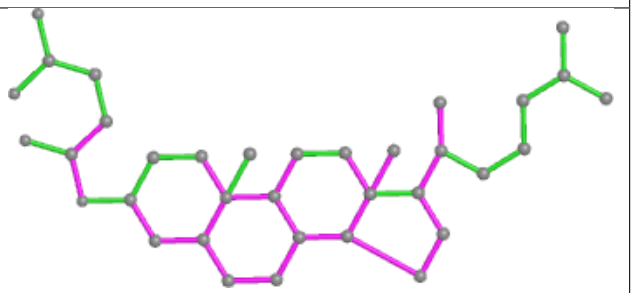

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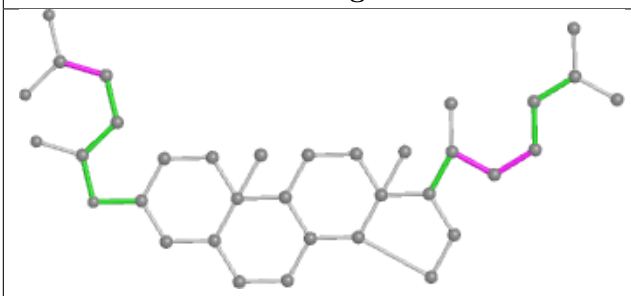

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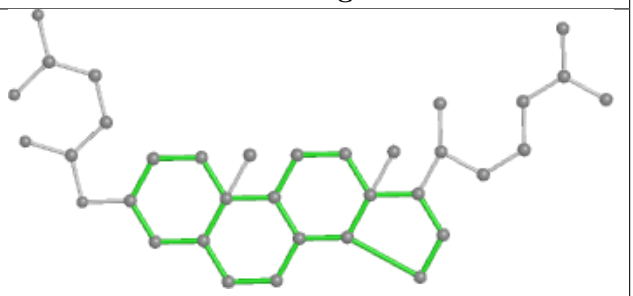
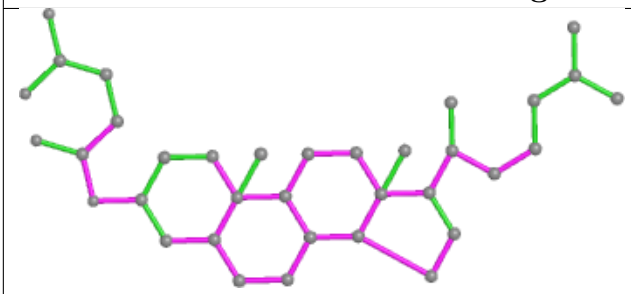


Rings

Ligand Y01 B 405



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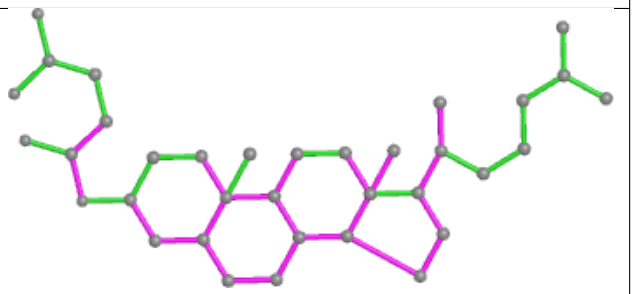

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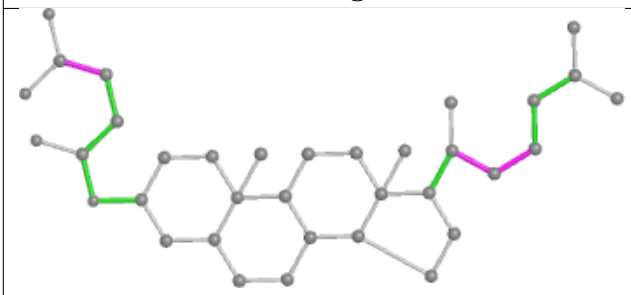

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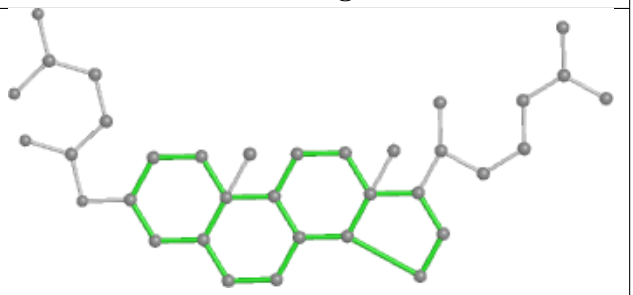


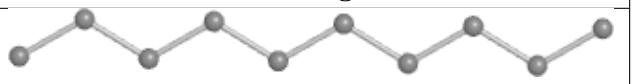
Rings

Ligand MC3 H 403

Bond lengths

Bond angles

Torsions



Rings

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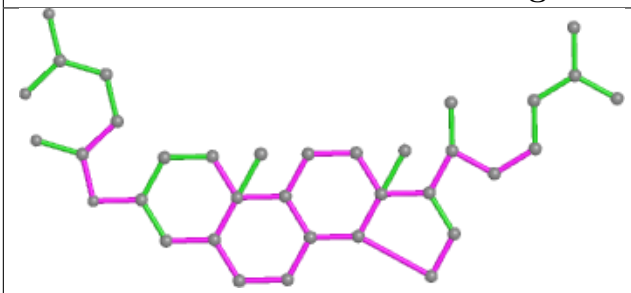

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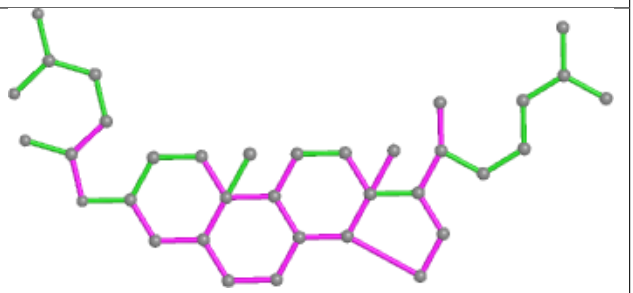

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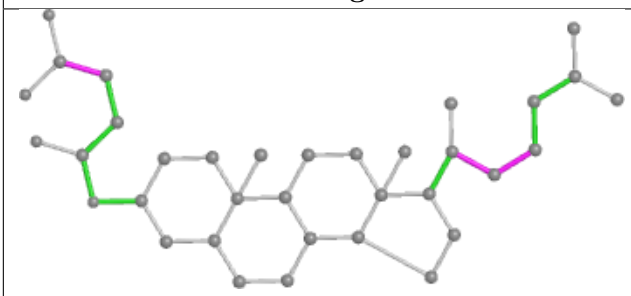

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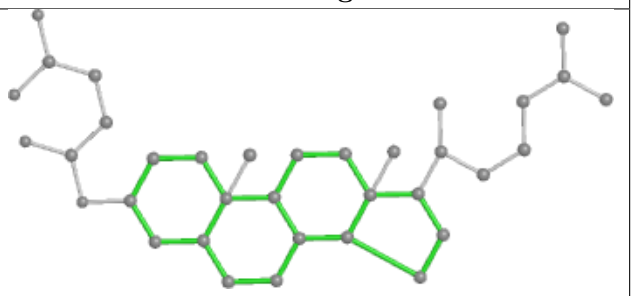
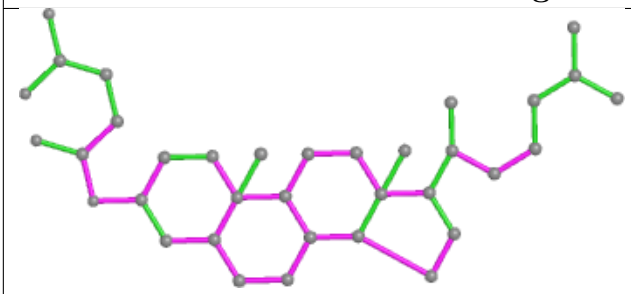


Rings

Ligand Y01 L 406



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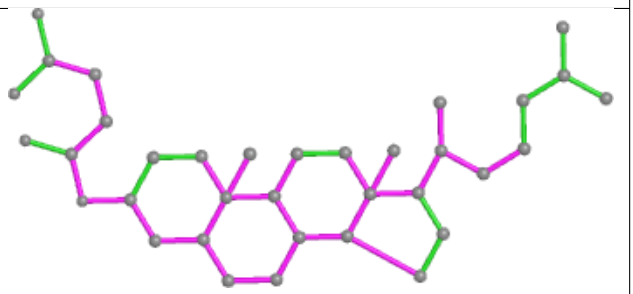

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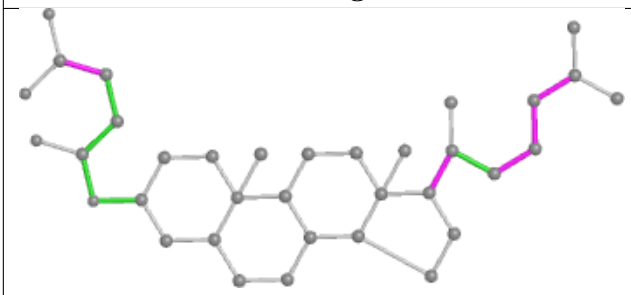

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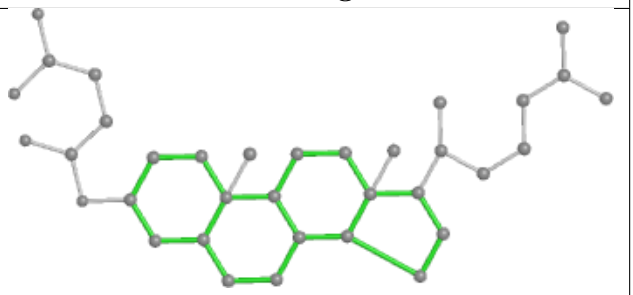
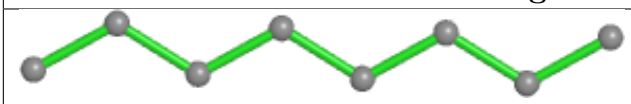


Rings

Ligand MC3 I 404



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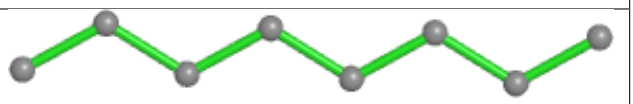

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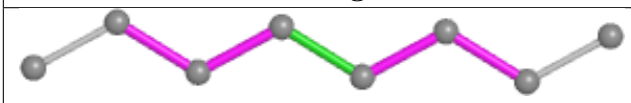

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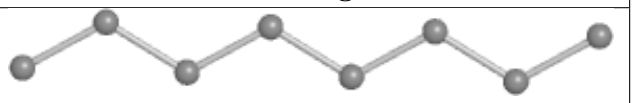
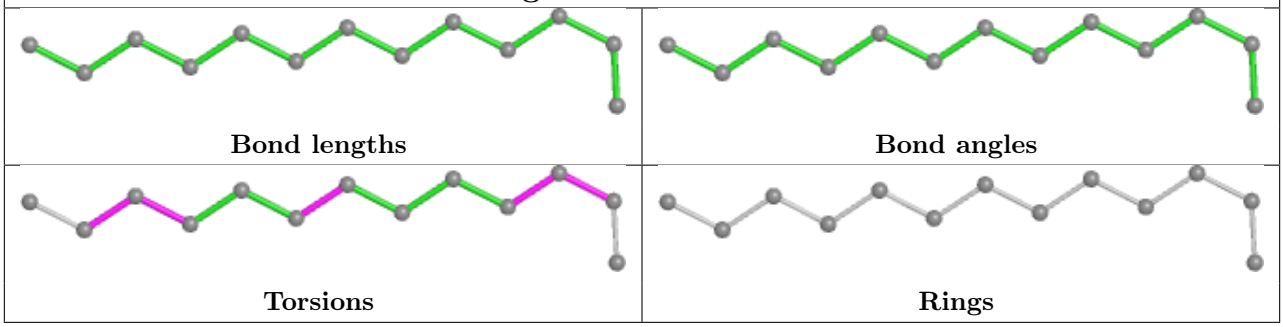


Rings

Ligand MC3 G 407



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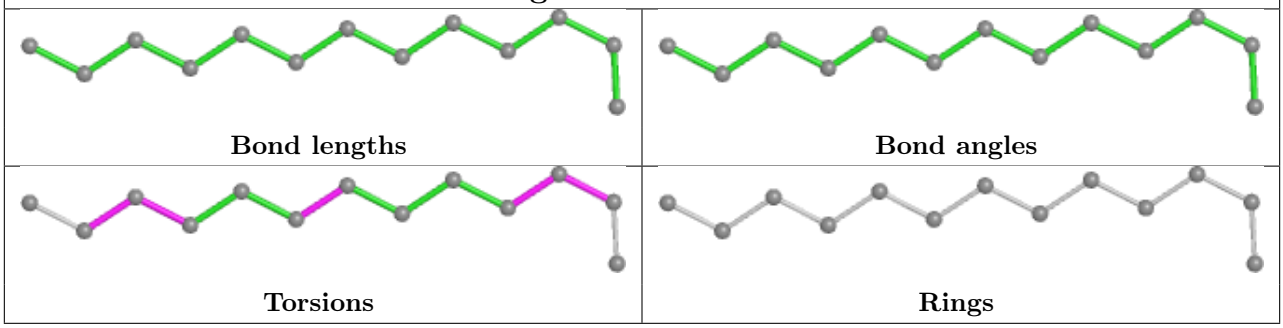
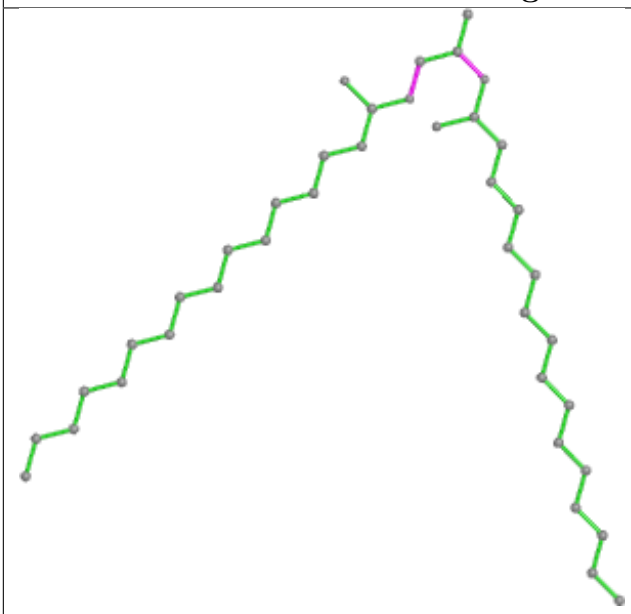


Ligand LHG K 409



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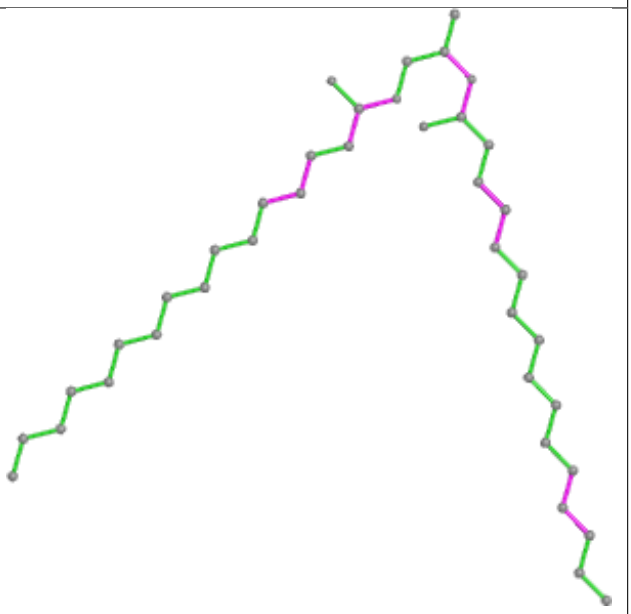

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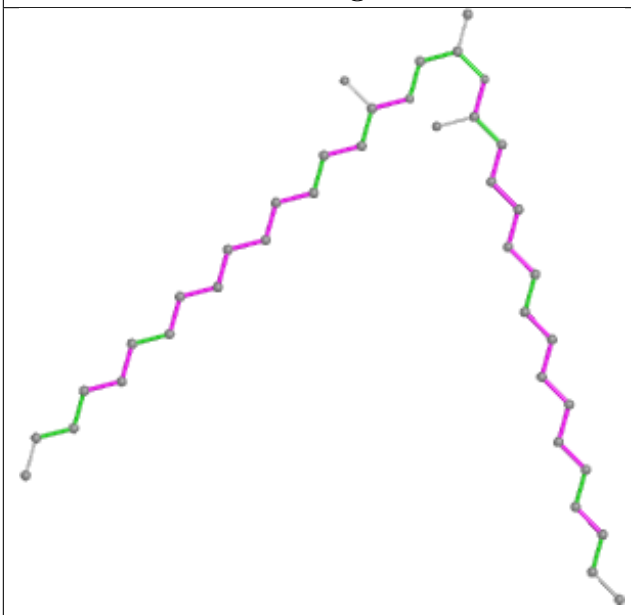

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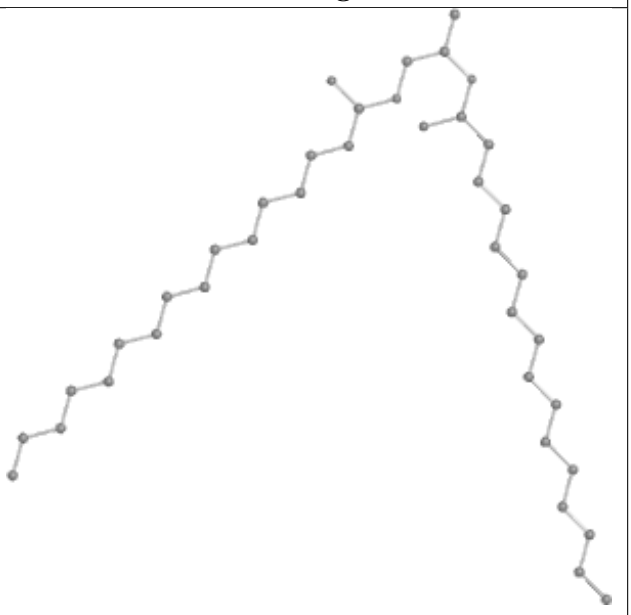
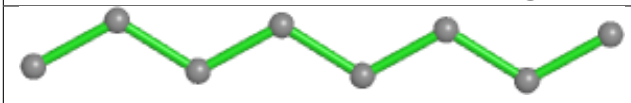


Rings

Ligand MC3 D 404



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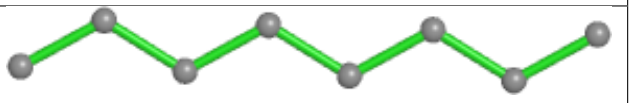
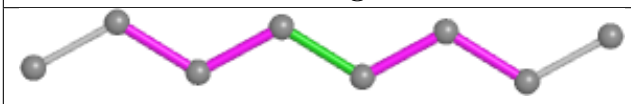


Bond angles



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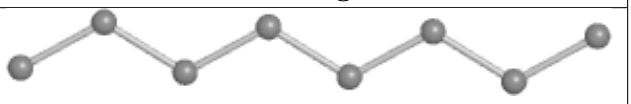
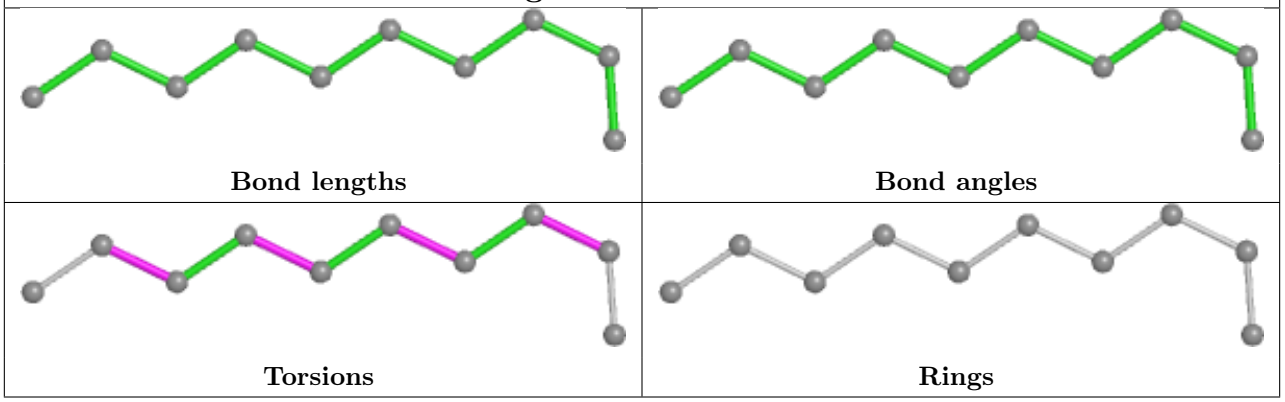


Rings

Ligand MC3 F 408



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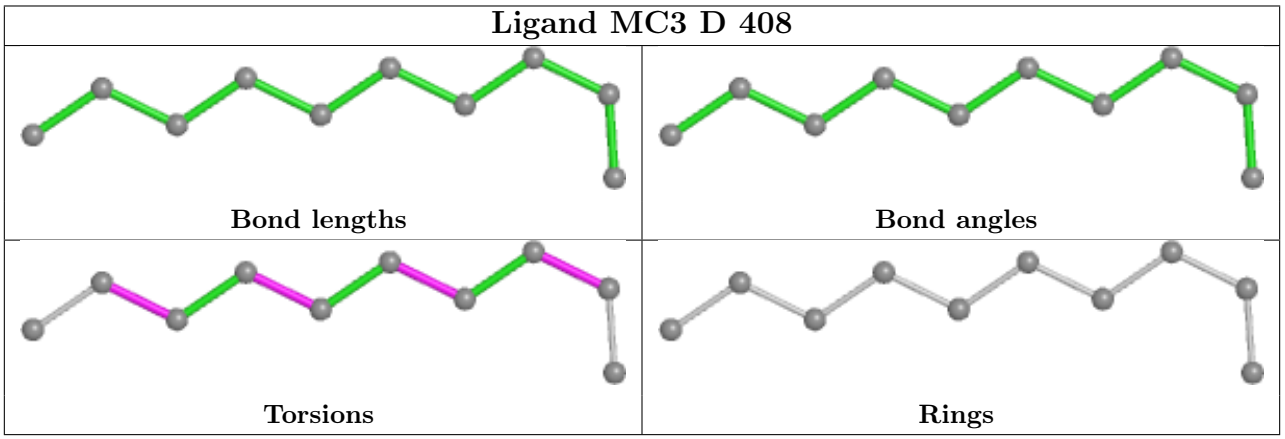
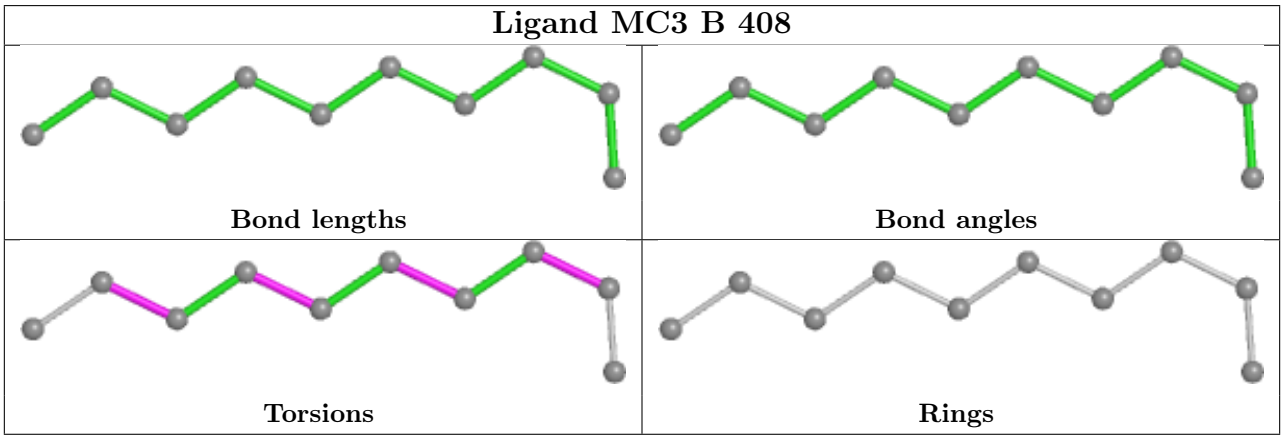
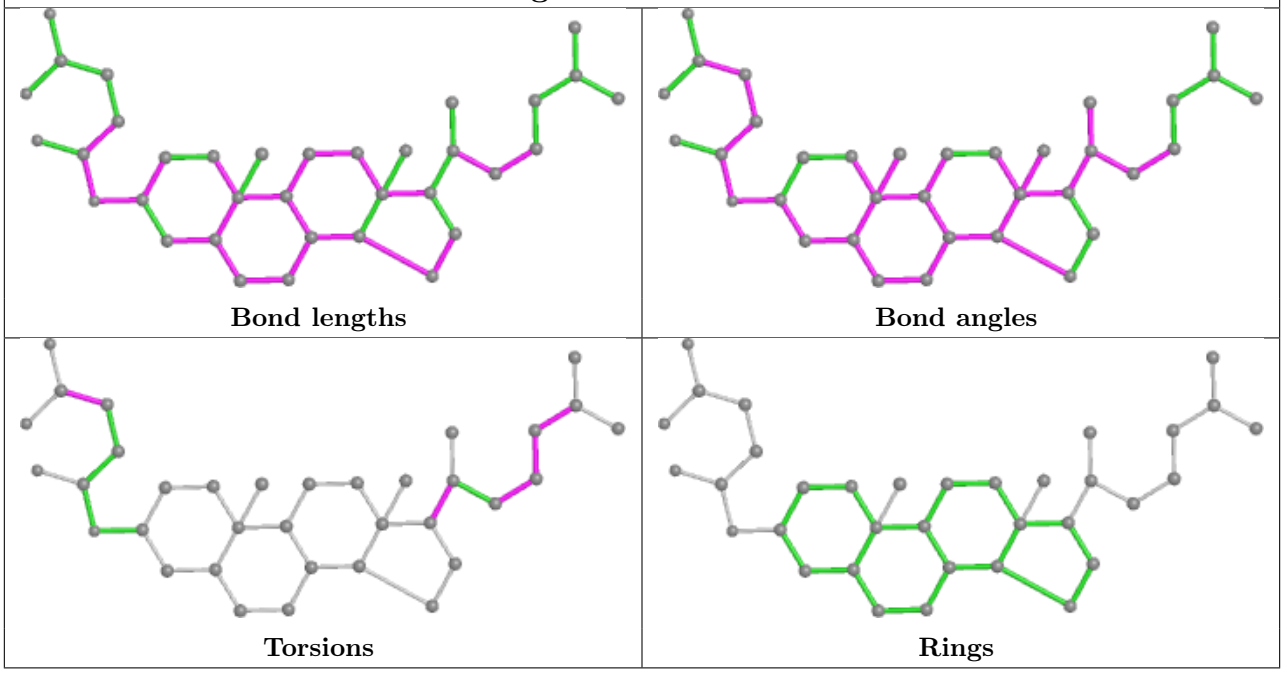


Ligand MC3 B 408



Ligand Y01 C 406



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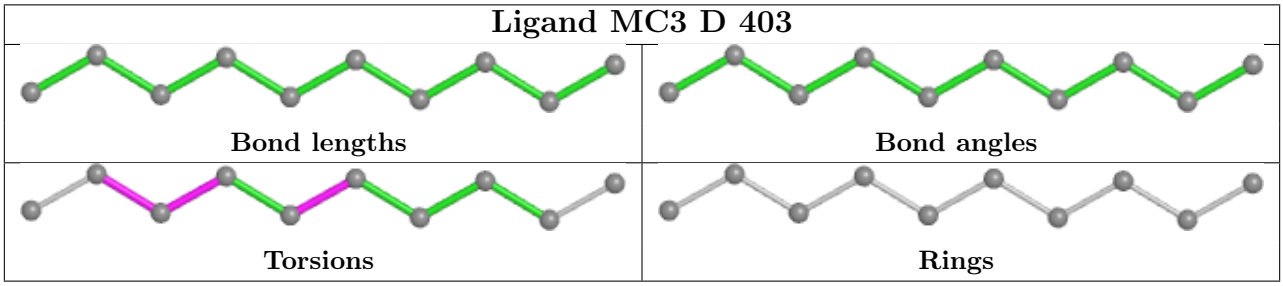

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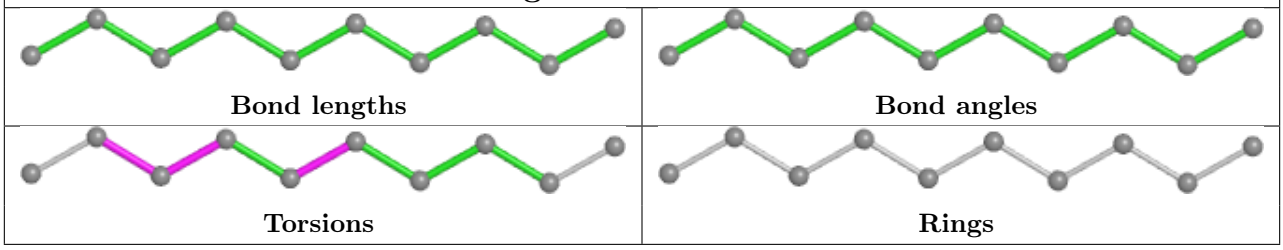
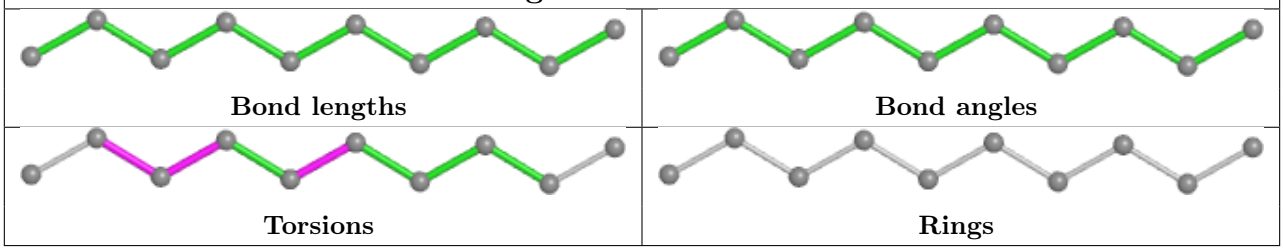


Ligand MC3 L 403



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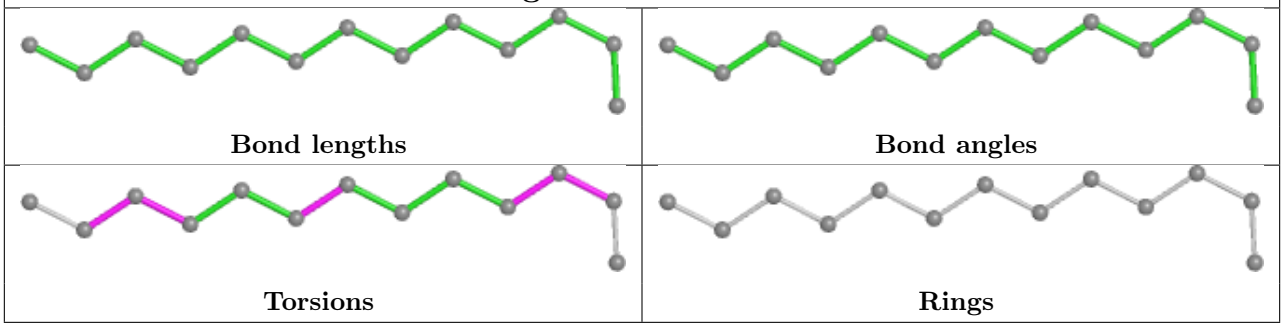

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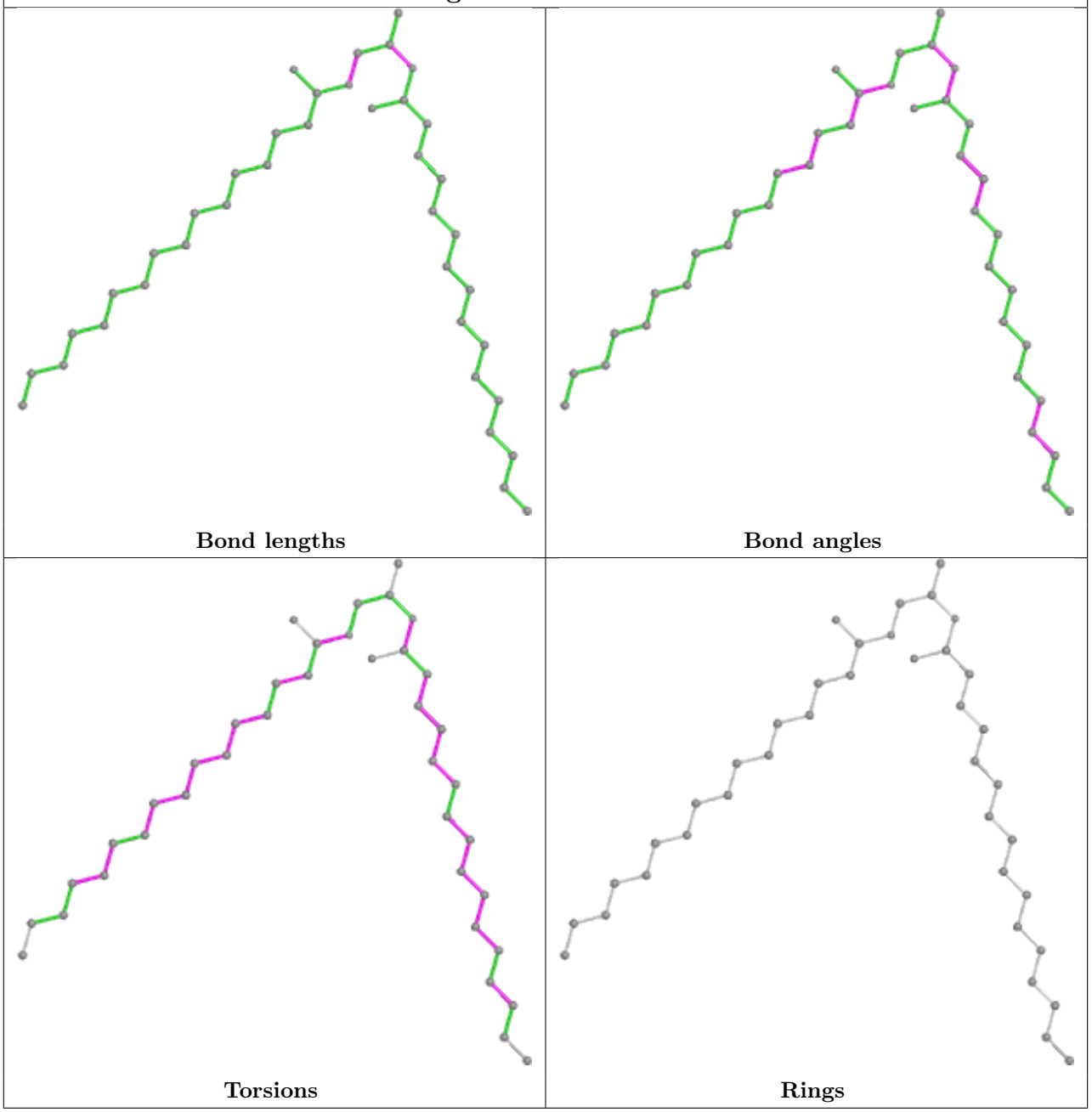

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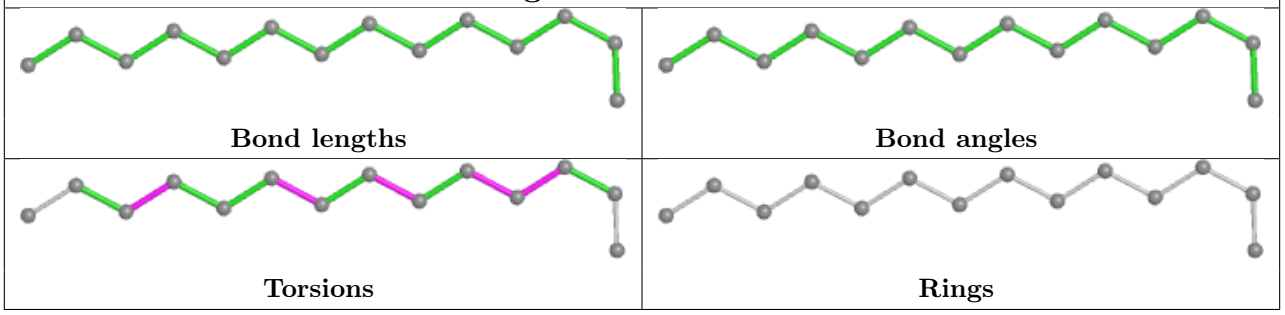
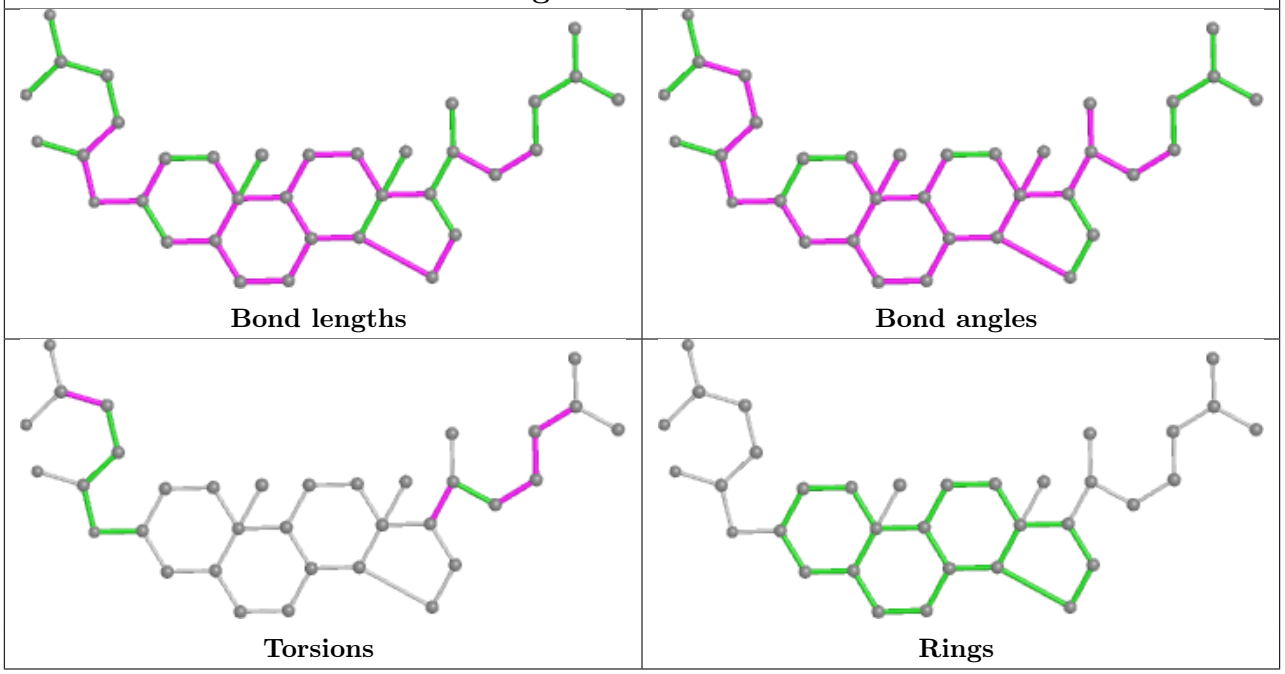
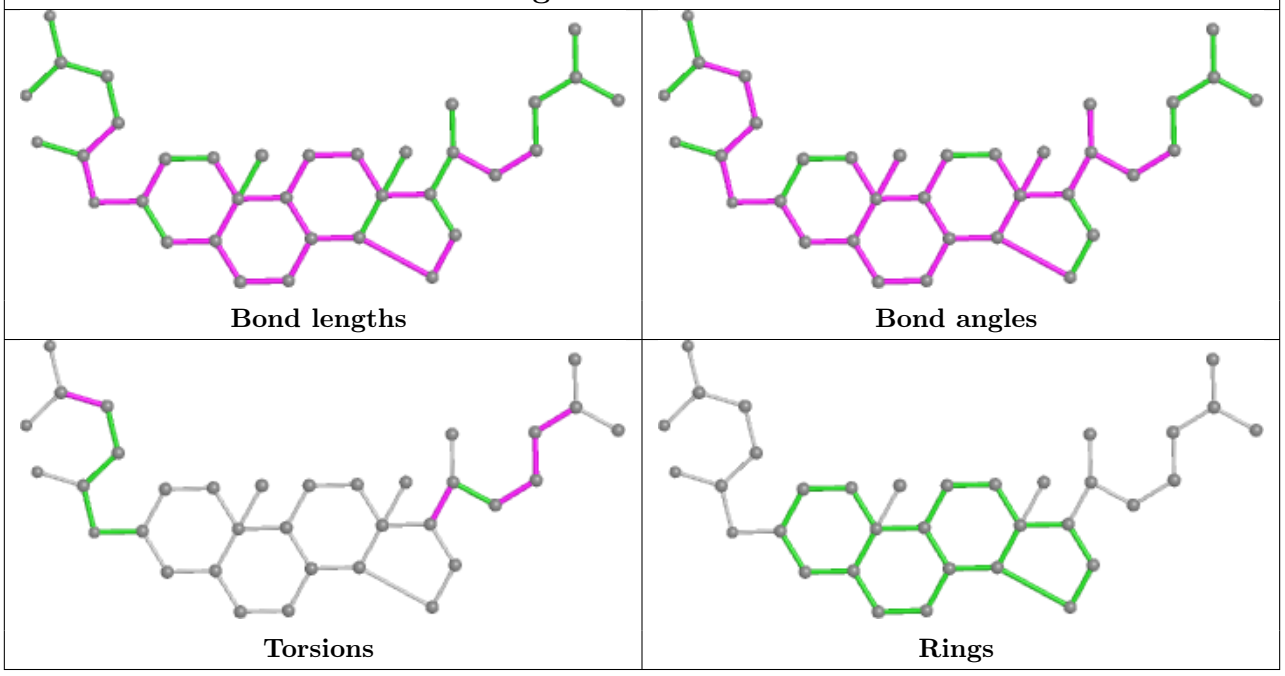


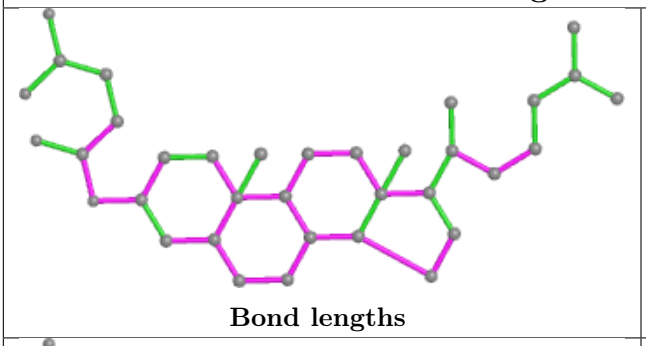
Ligand Y01 E 406



Ligand Y01 F 406



Ligand Y01 B 406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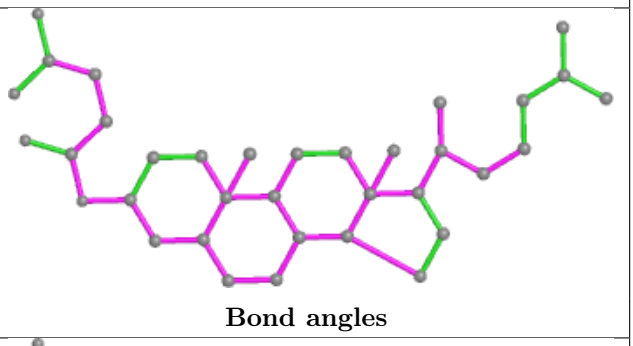
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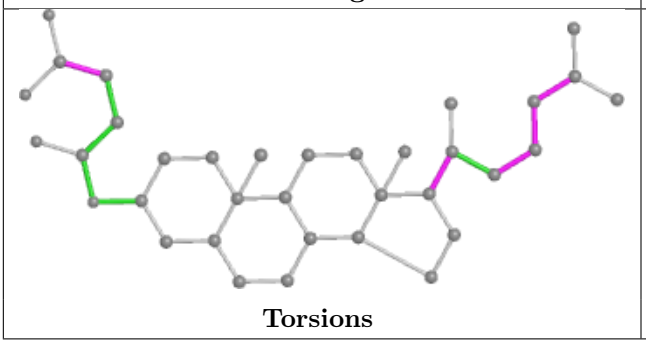
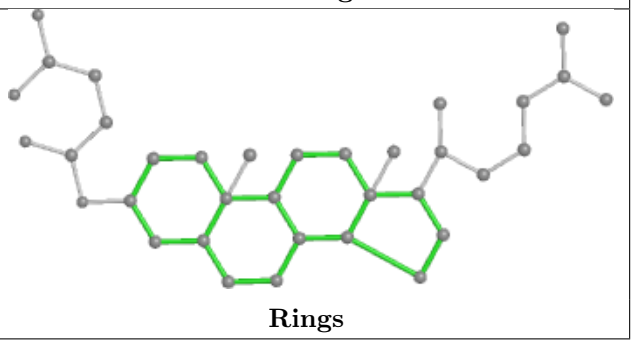
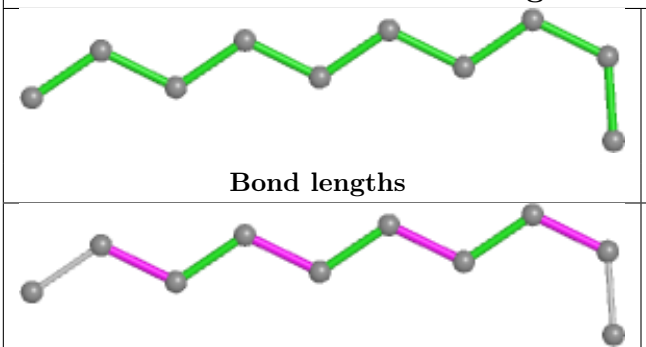

Torsions


Rings

Ligand MC3 J 408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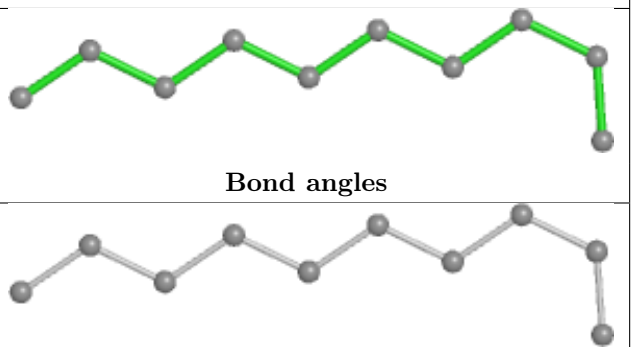
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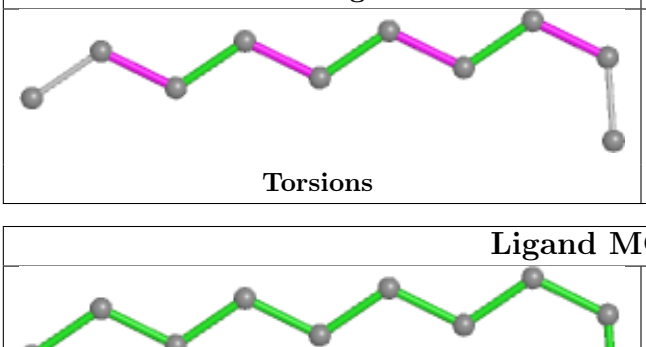
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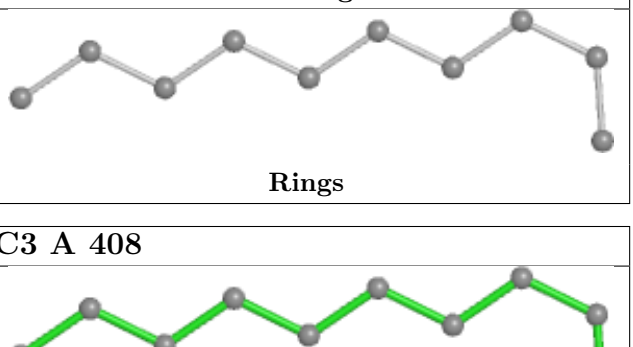
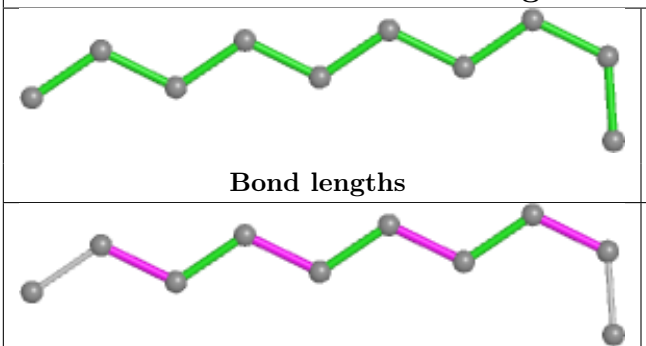

Rings

Ligand MC3 A 408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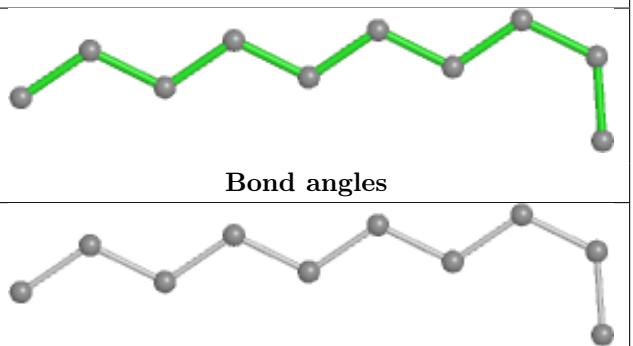
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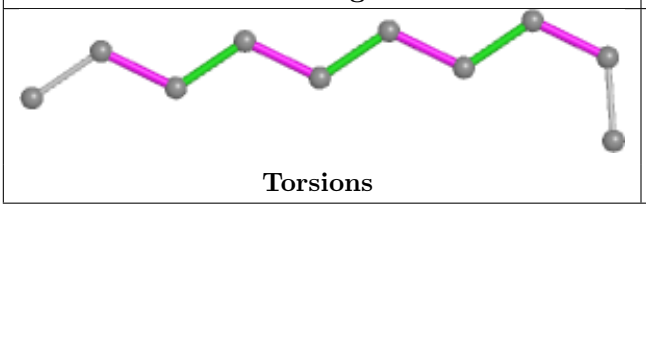
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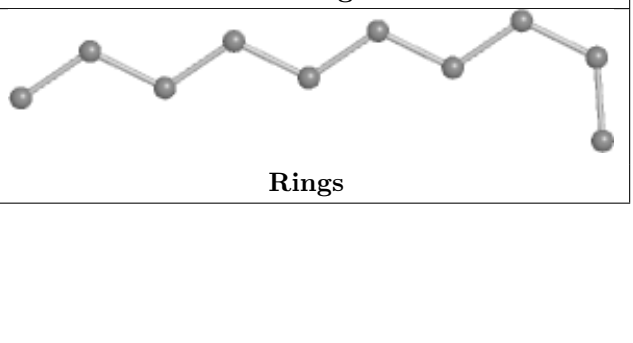
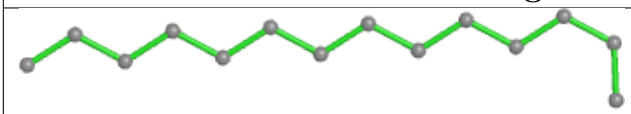

Rings

Ligand MC3 F 401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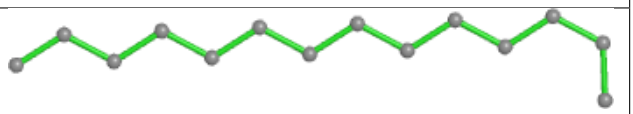
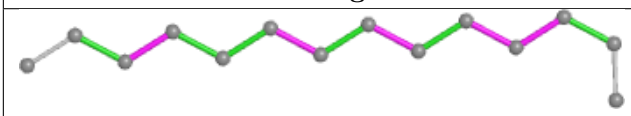

Bond angles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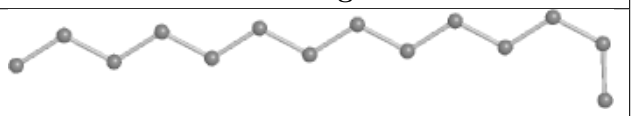
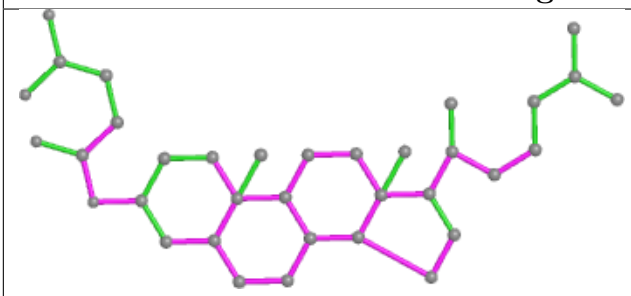
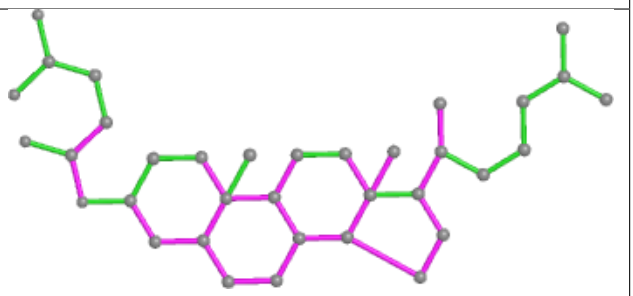

Rings

Ligand Y01 I 405


Bond lengths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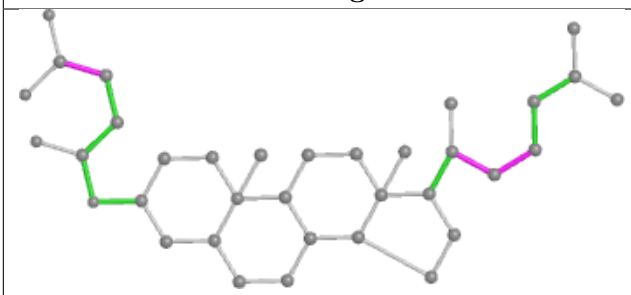
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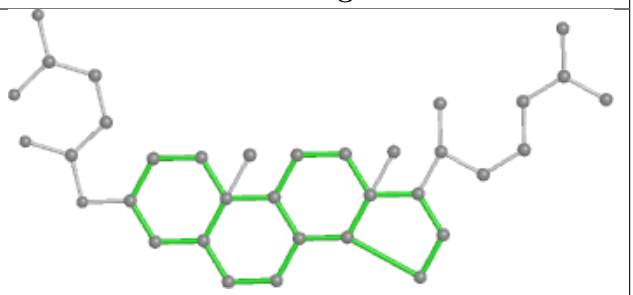
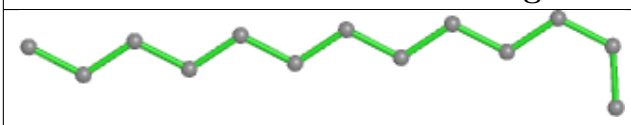

Rings

Ligand MC3 E 407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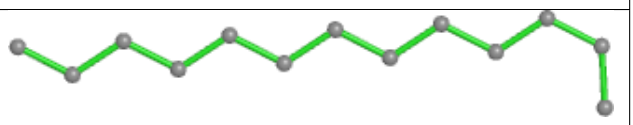
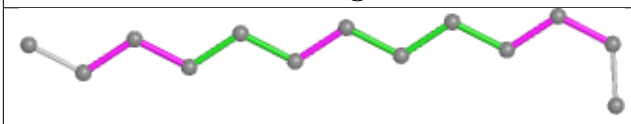
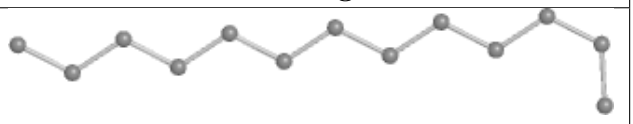
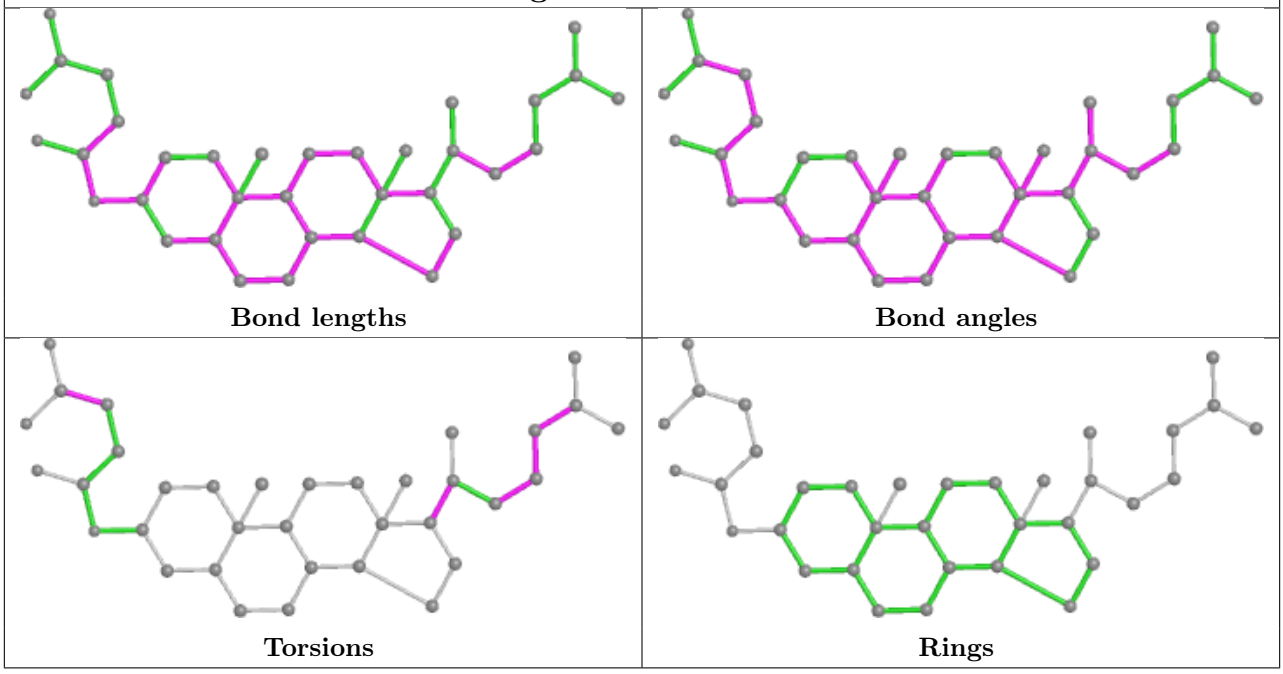

Bond angles

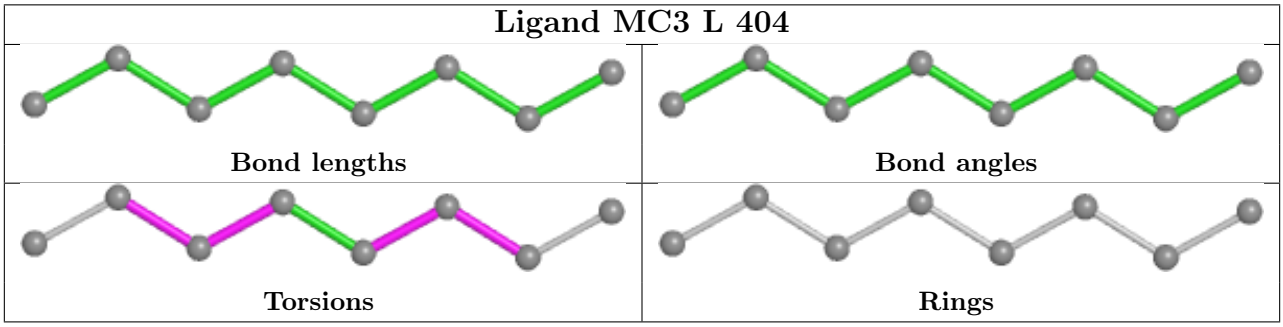

Torsions


Rings

Ligand Y01 H 406



Ligand MC3 L 404



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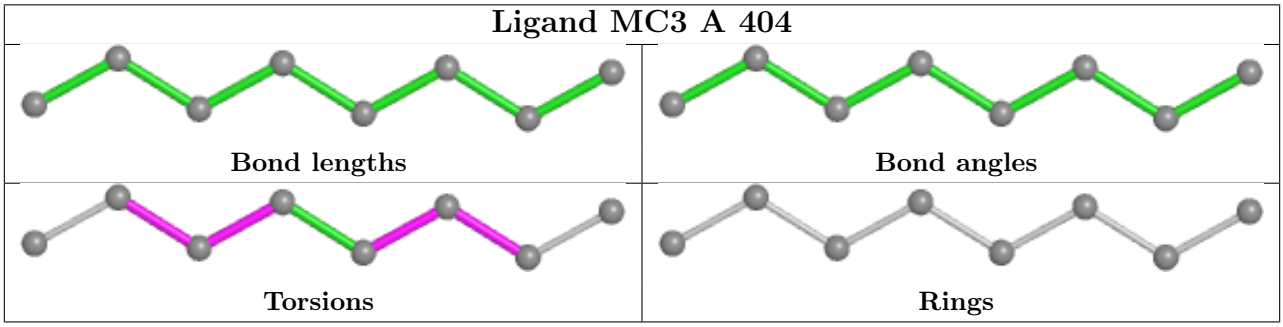

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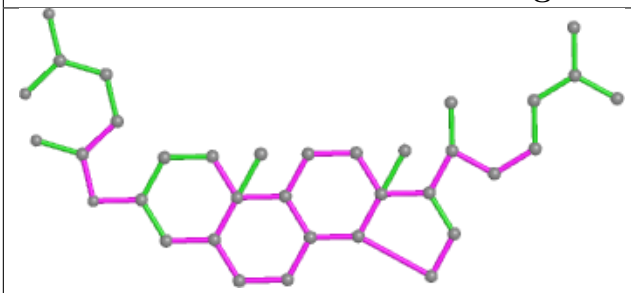

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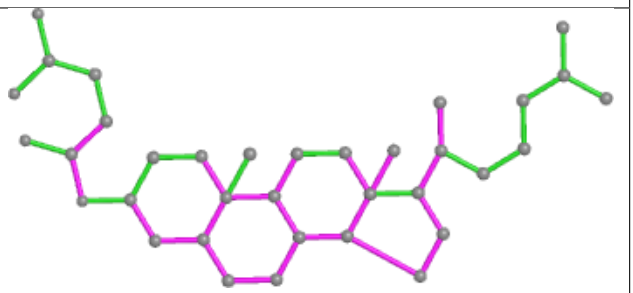
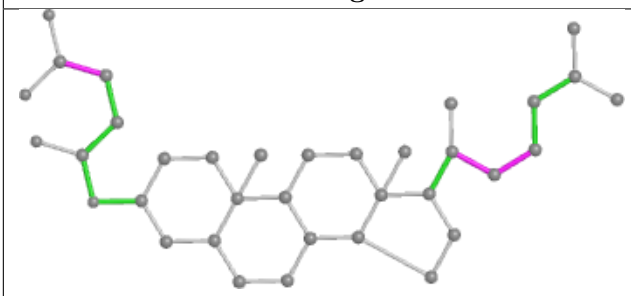
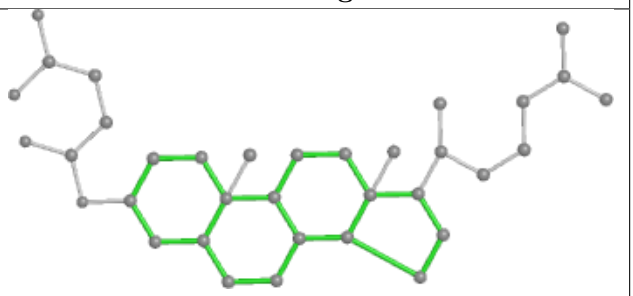


Bond angles

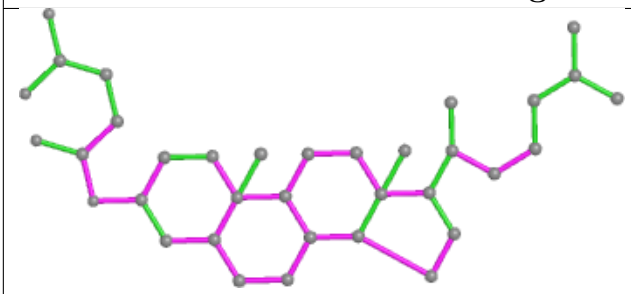


Torsions

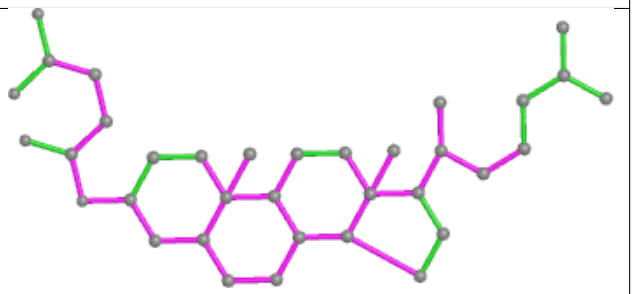


Rings

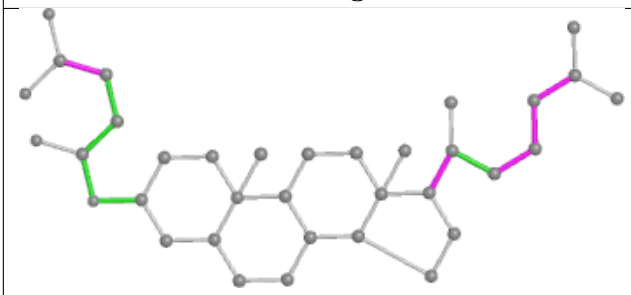
Ligand Y01 K 406



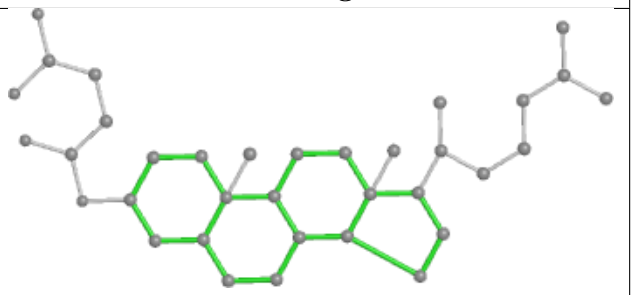
Bond lengths



Bond angles



Torsions



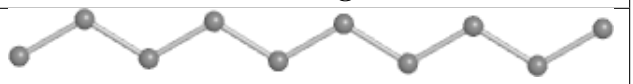
Rings

Ligand MC3 C 403

Bond lengths

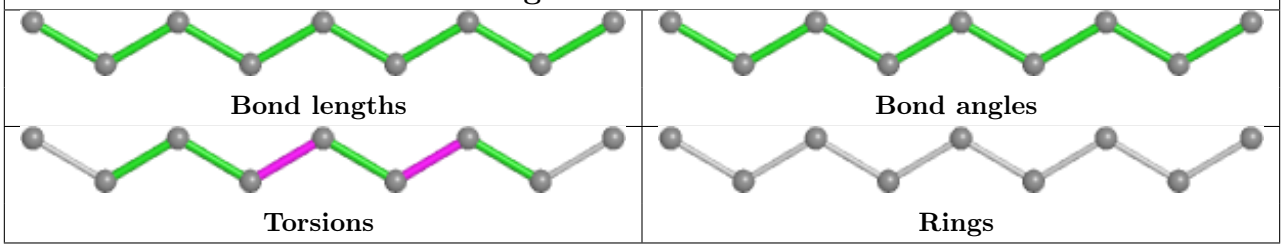
Bond angles

Torsions



Rings

Ligand MC3 B 402



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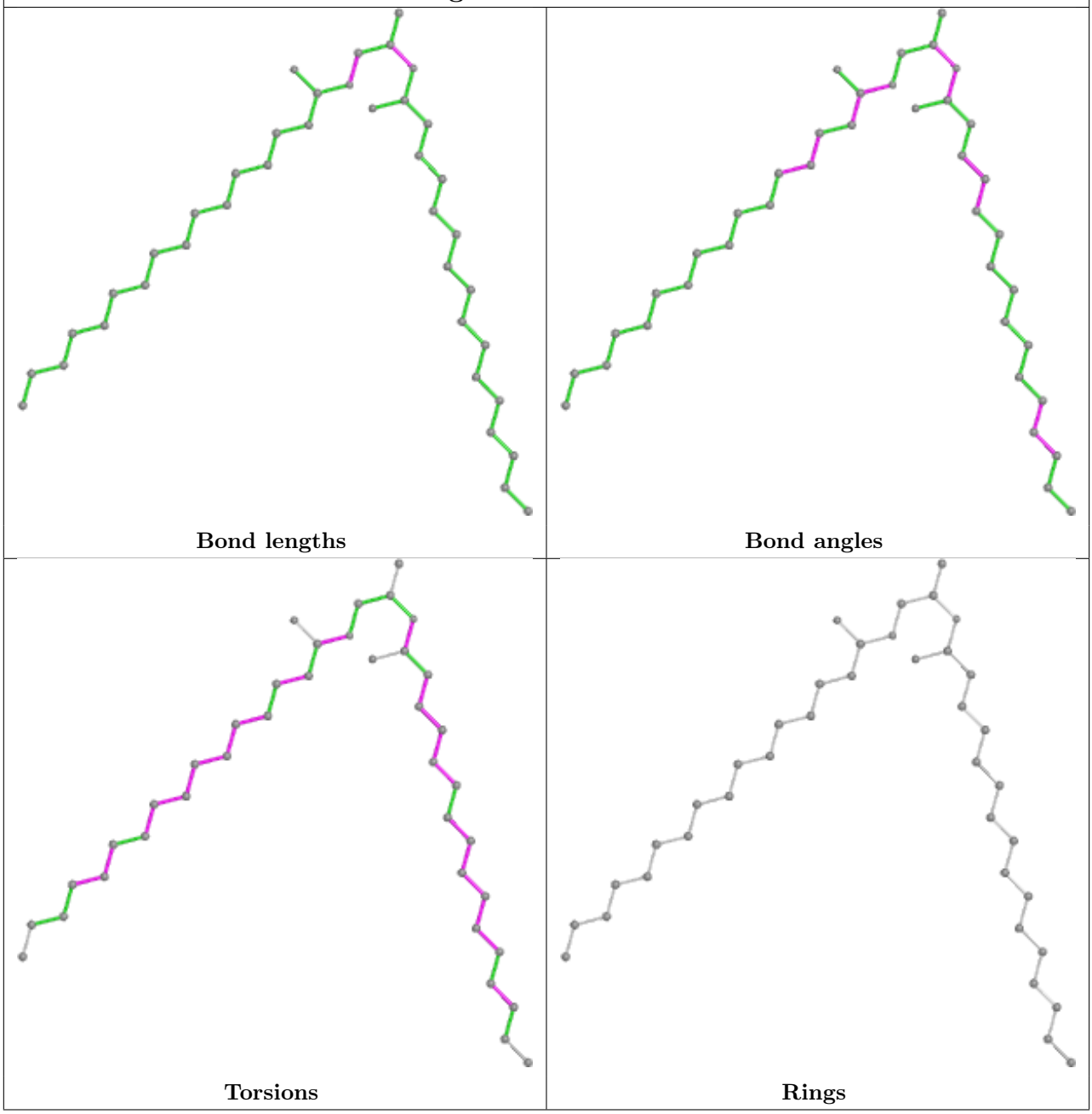

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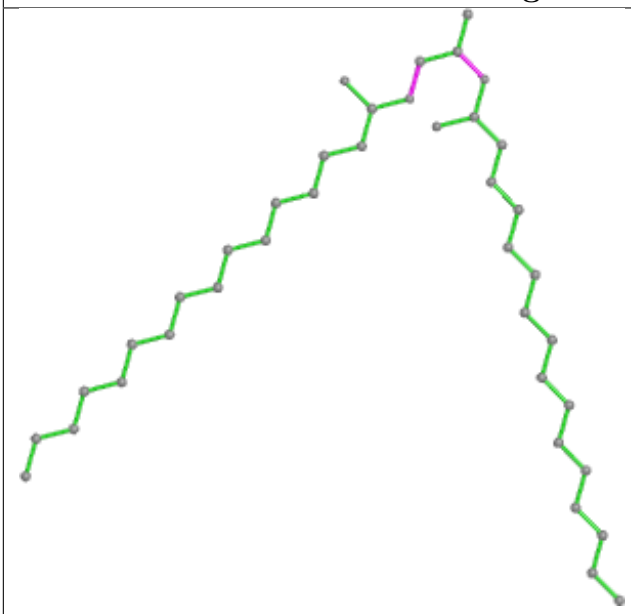

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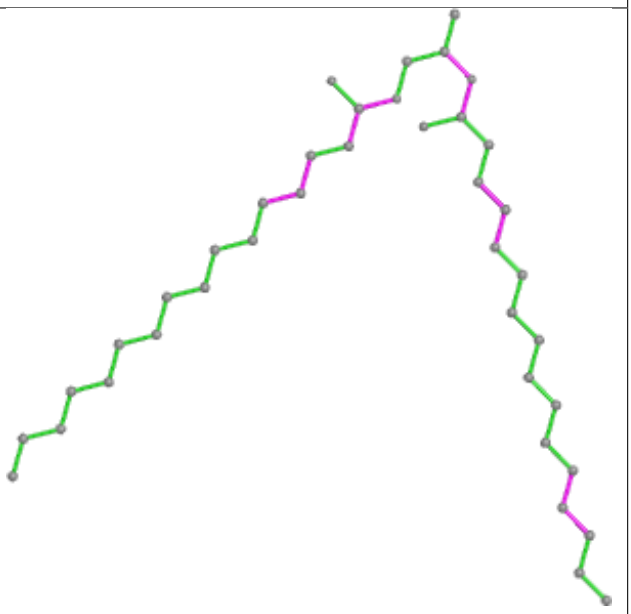
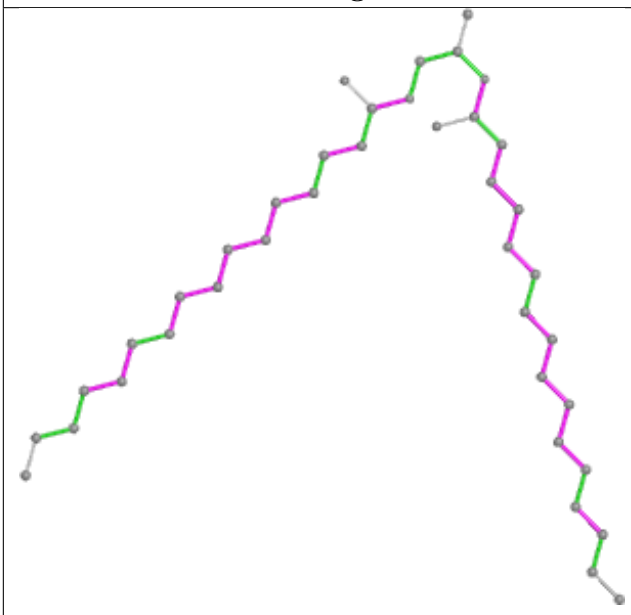


Bond angles



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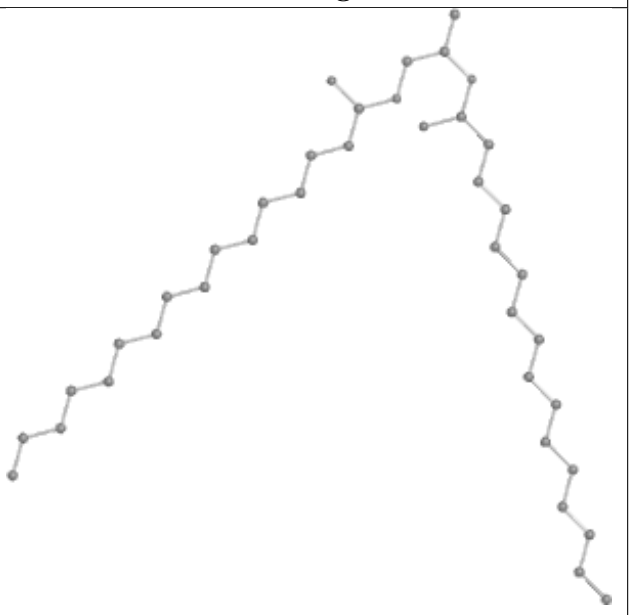
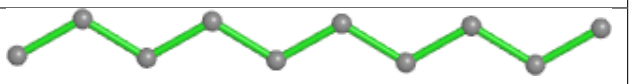


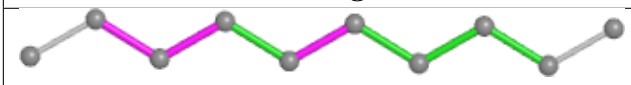
Rings

Ligand MC3 A 403

Bond lengths



Bond angles



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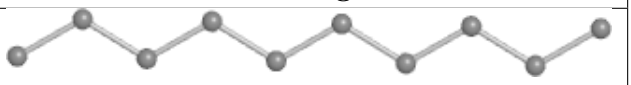
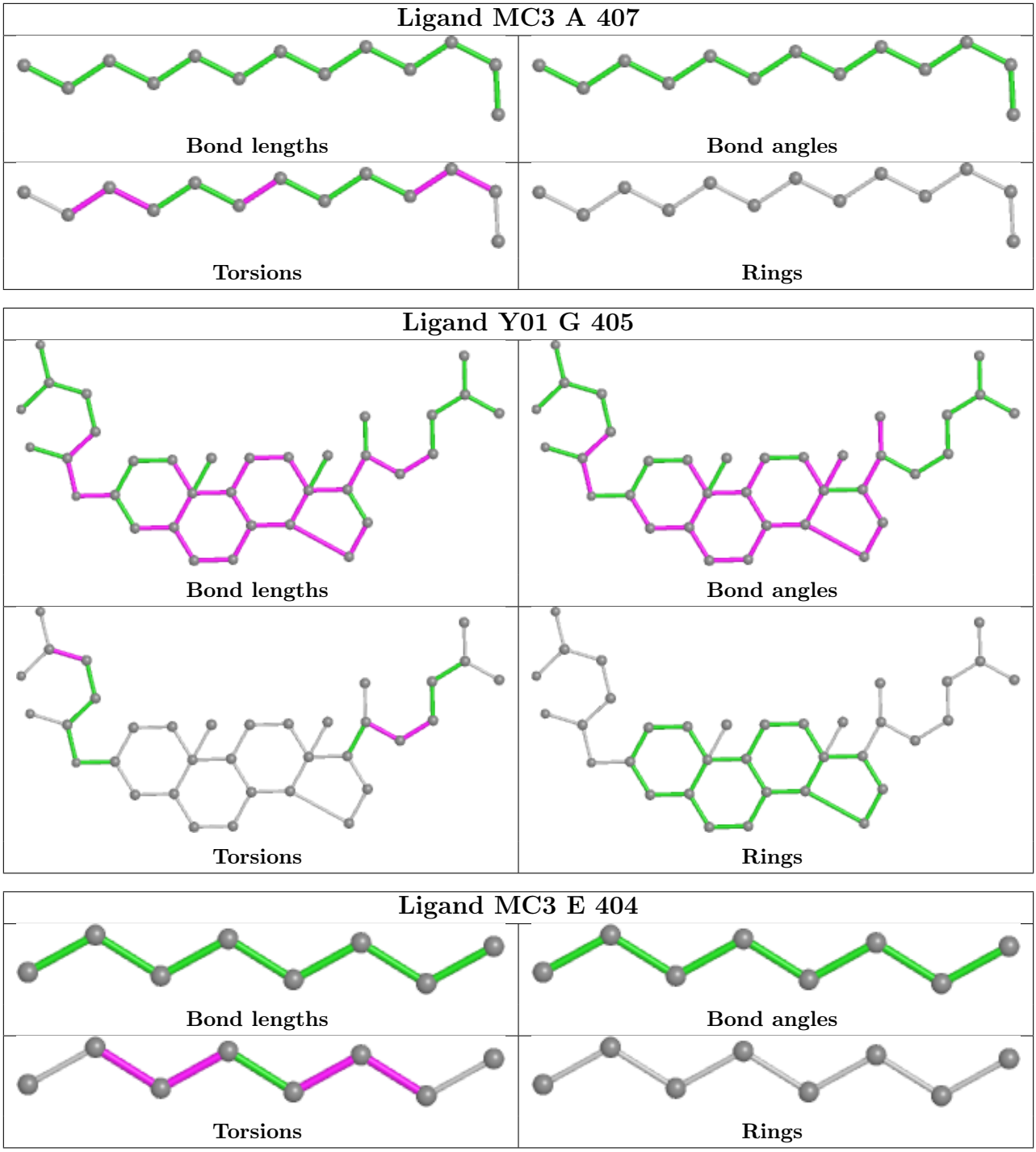


Rings



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

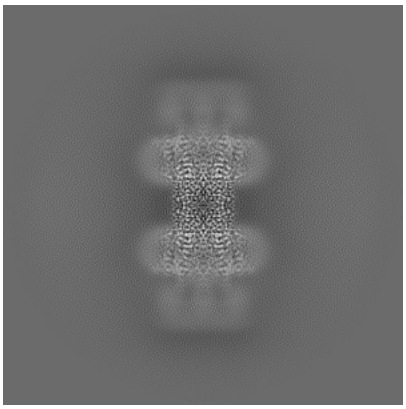
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-33270. These allow visual inspection of the internal detail of the map and identification of artifacts.

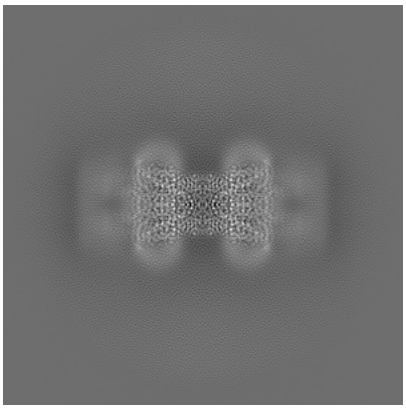
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

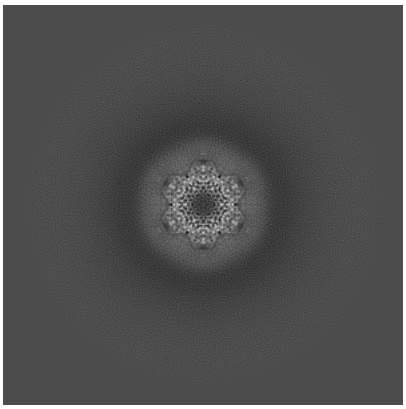
6.1.1 Primary map



X

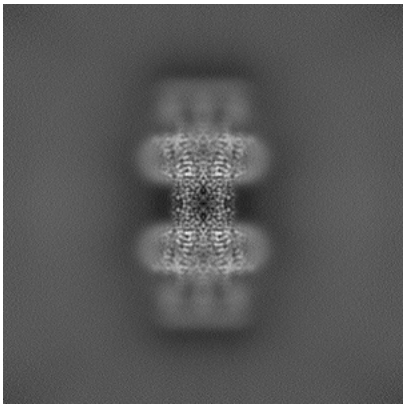


Y

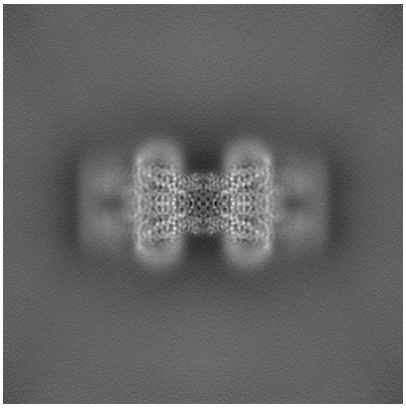


Z

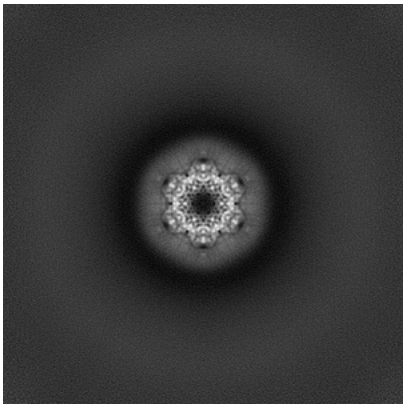
6.1.2 Raw map



X



Y

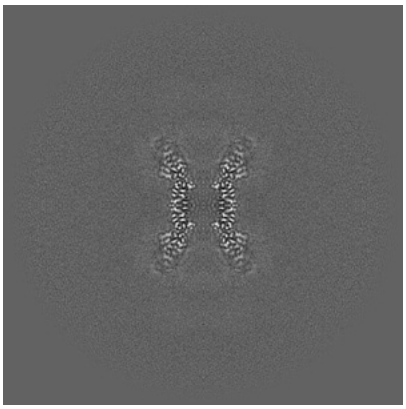


Z

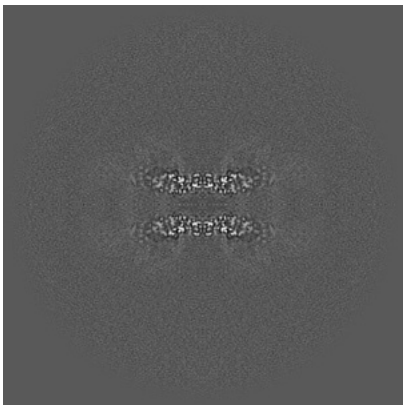
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

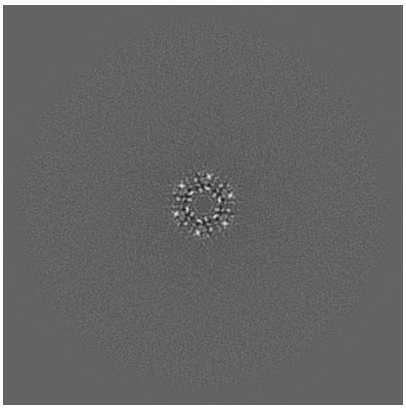
6.2.1 Primary map



X Index: 270

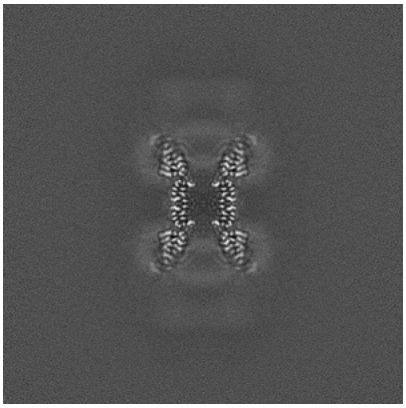


Y Index: 270

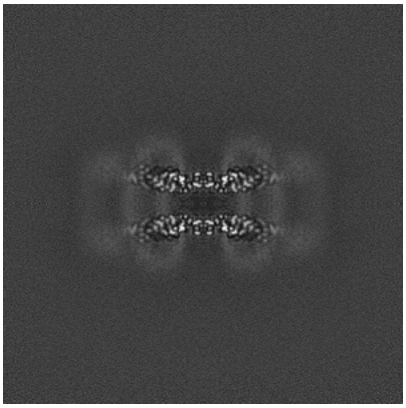


Z Index: 270

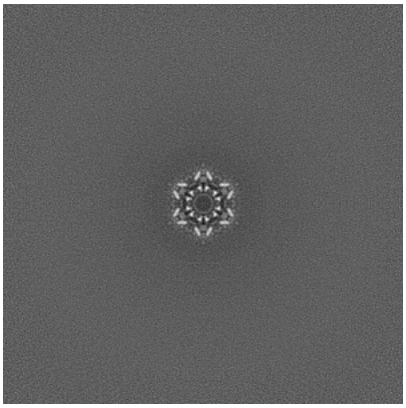
6.2.2 Raw map



X Index: 270



Y Index: 270

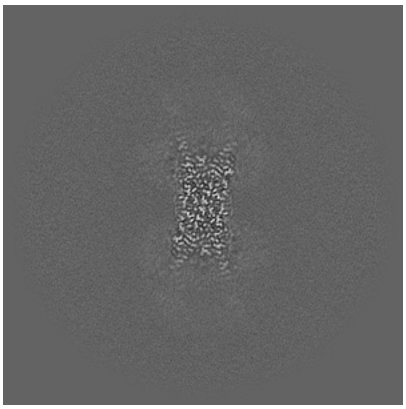


Z Index: 270

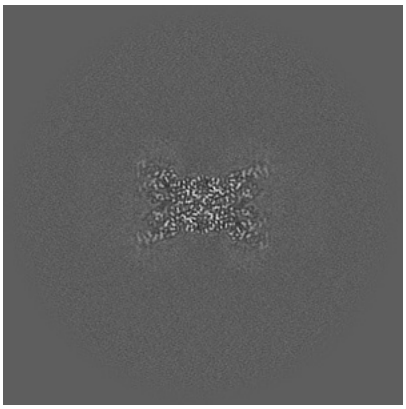
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

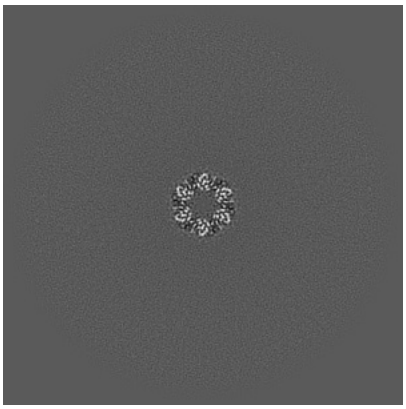
6.3.1 Primary map



X Index: 295

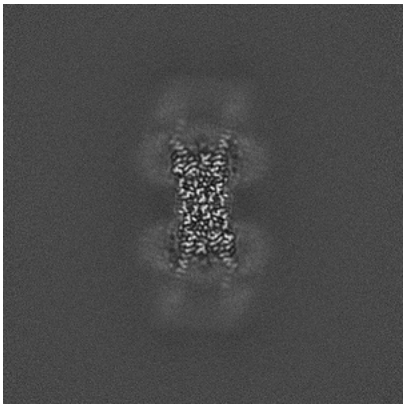


Y Index: 292

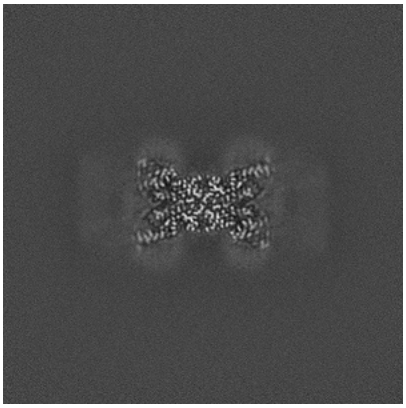


Z Index: 255

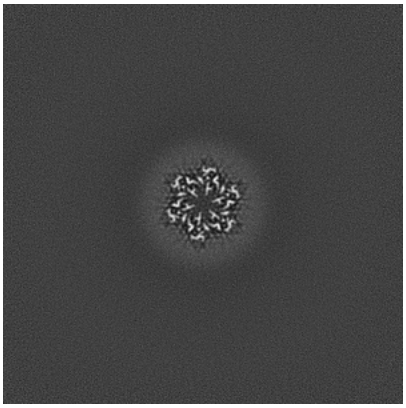
6.3.2 Raw map



X Index: 295



Y Index: 248

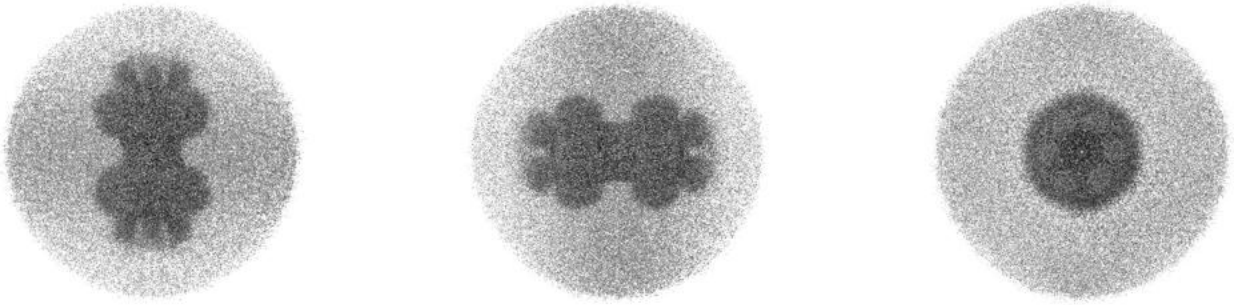


Z Index: 308

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

6.4 Orthogonal surface views (i)

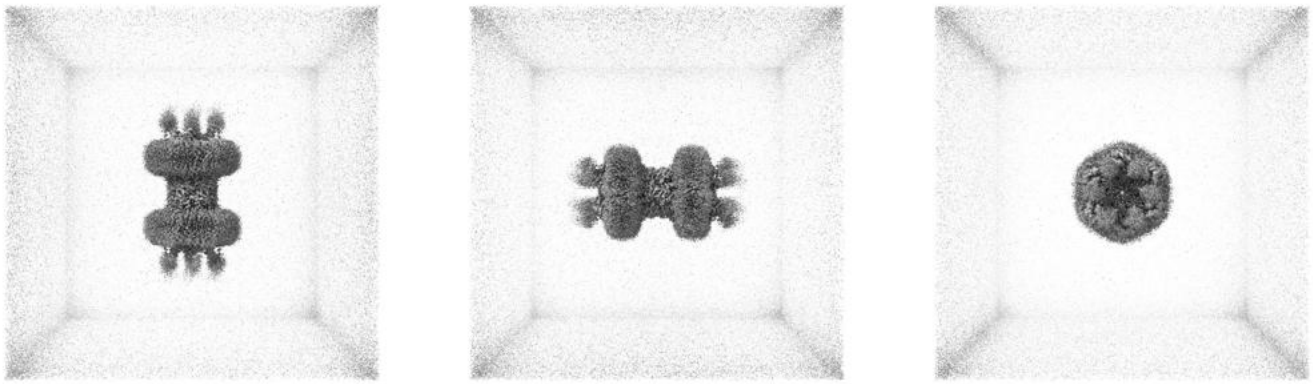
6.4.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.45. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



X Y Z

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

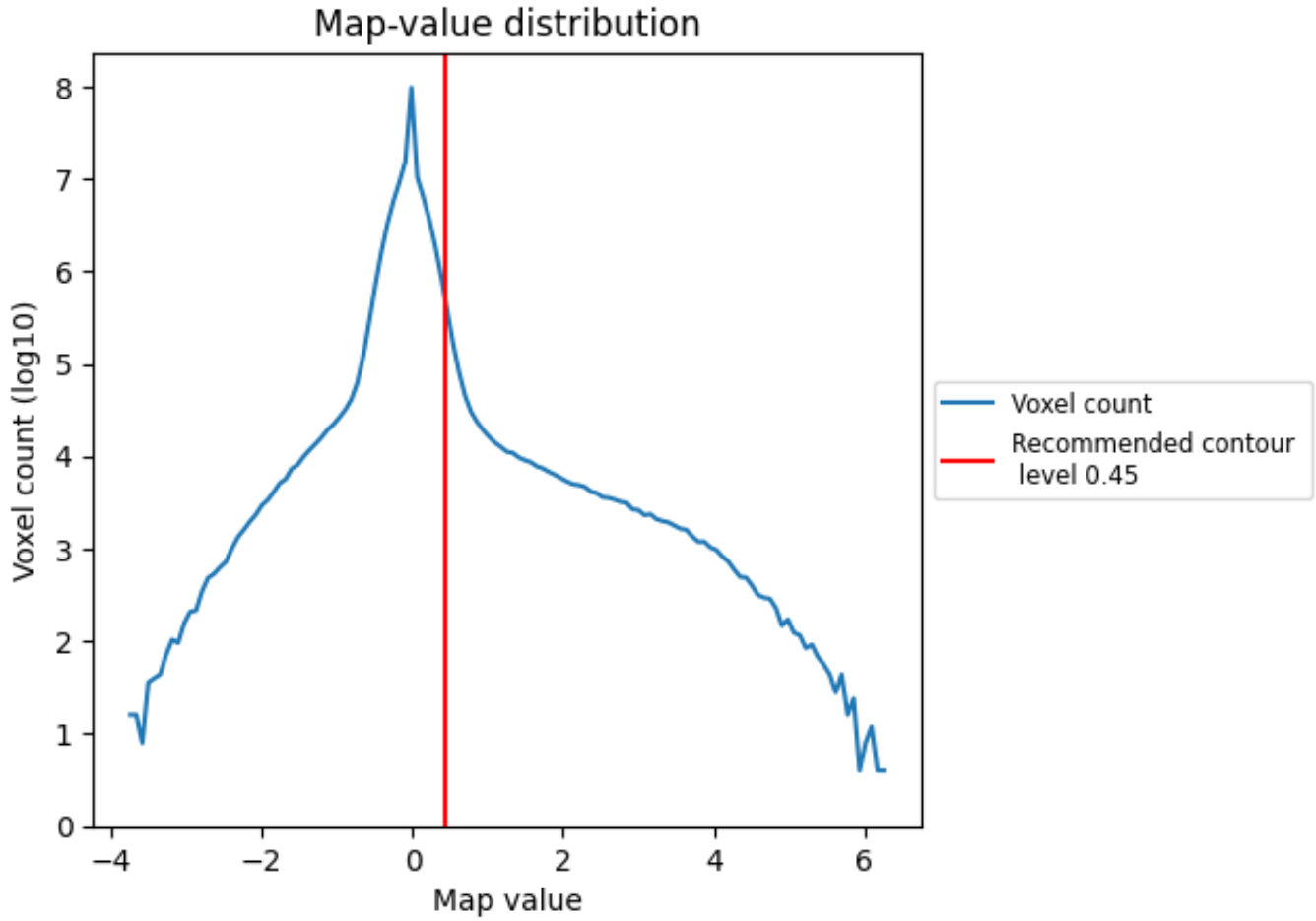
6.5 Mask visualisation (i)

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

7 Map analysis

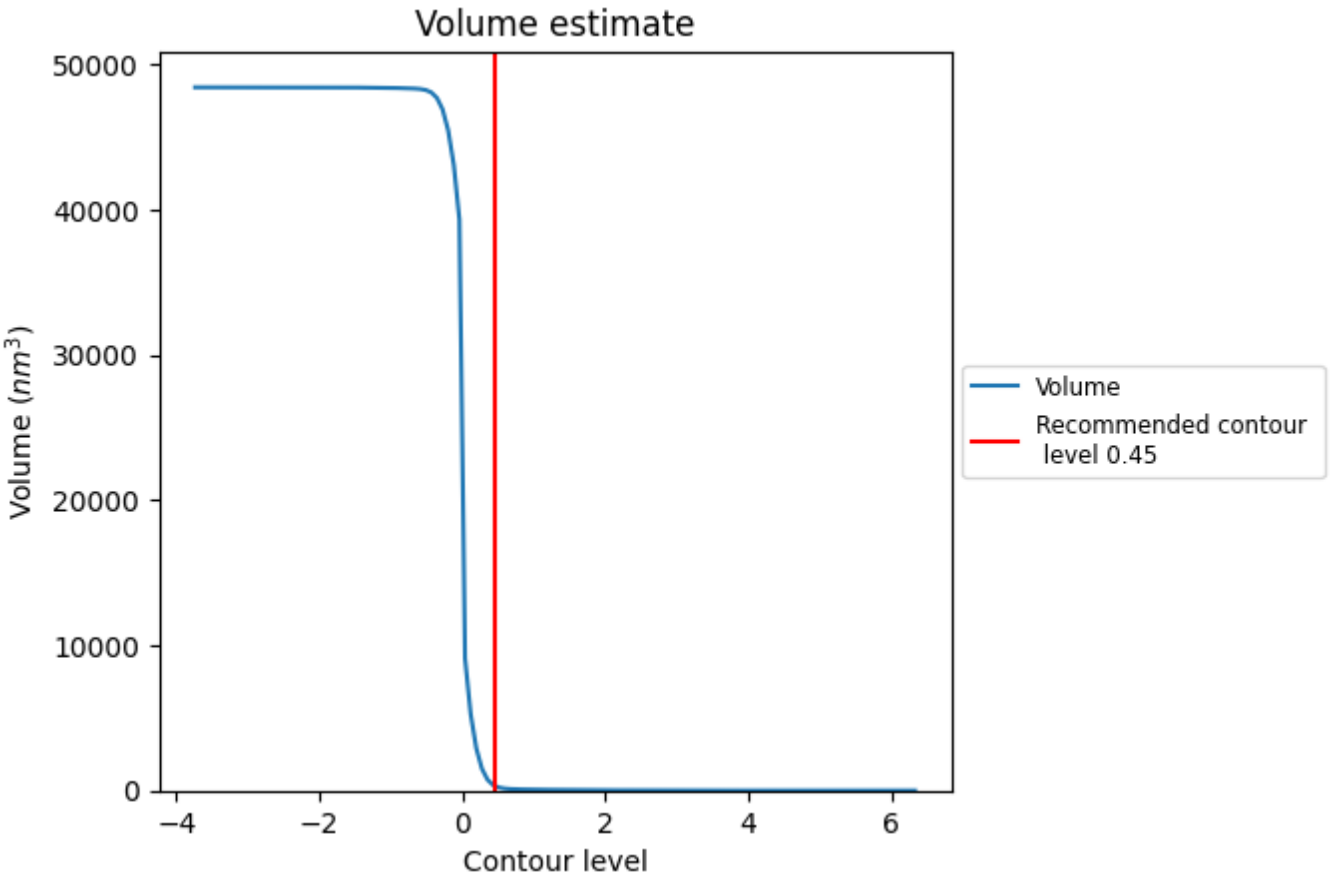
This section contains the results of statistical analysis of the map.

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.

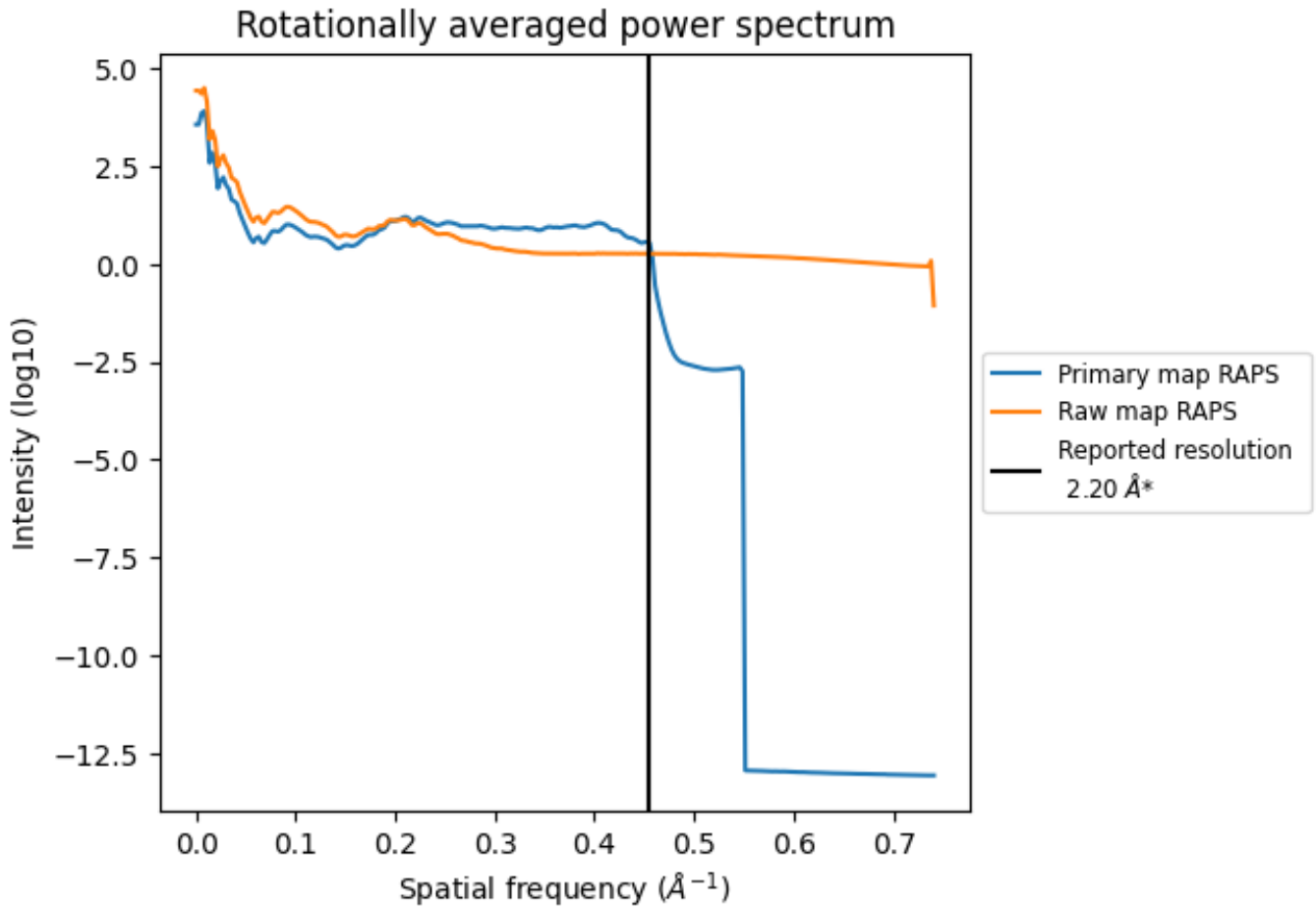
7.2 Volume estimate



The volume at the recommended contour level is 337 nm^3; this corresponds to an approximate mass of 304 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)

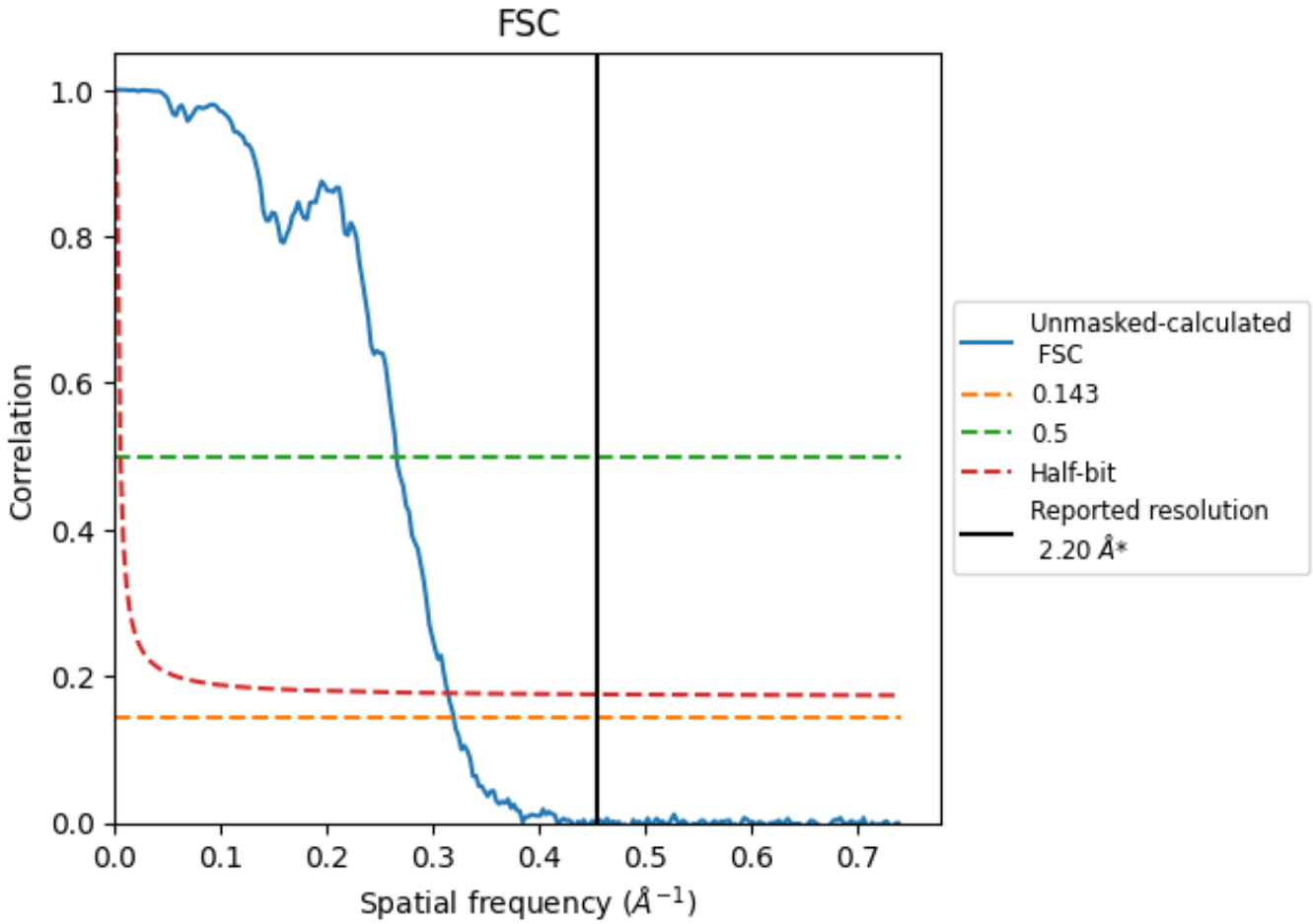


*Reported resolution corresponds to spatial frequency of 0.455 Å^{-1}

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 0.455 Å^{-1}

8.2 Resolution estimates (i)

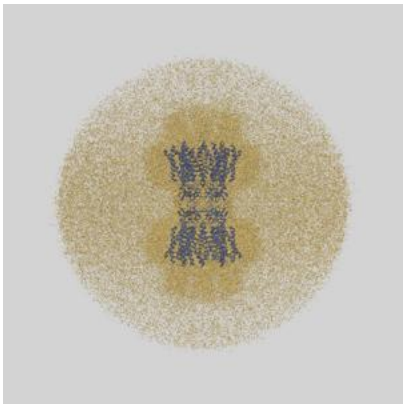
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.20	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.13	3.77	3.19

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.13 differs from the reported value 2.2 by more than 10 %

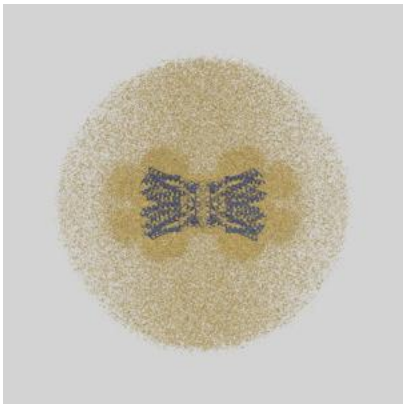
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-33270 and PDB model 7XKT. Per-residue inclusion information can be found in section 3 on page 16.

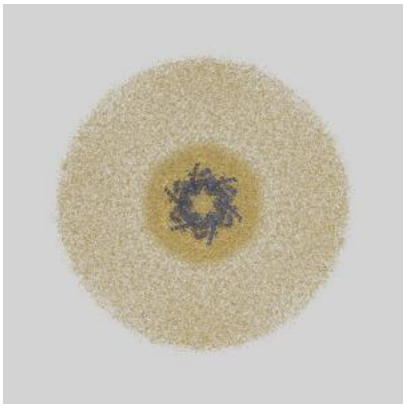
9.1 Map-model overlay



X



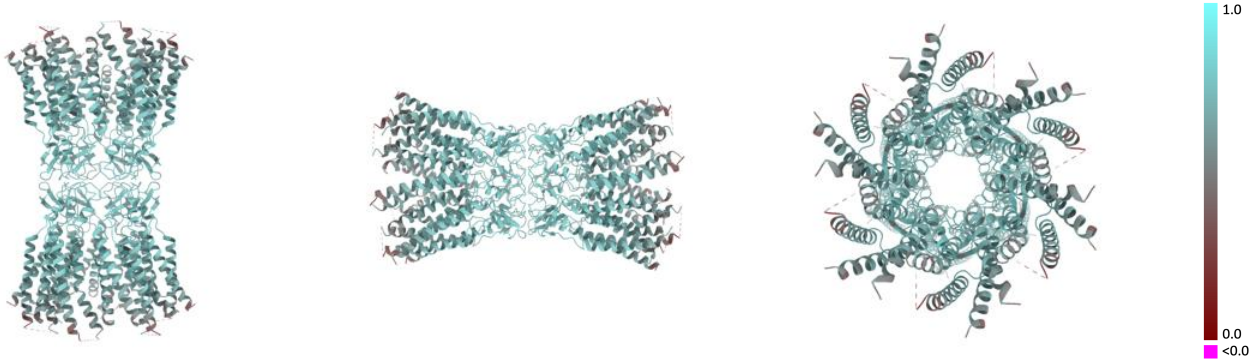
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.45 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

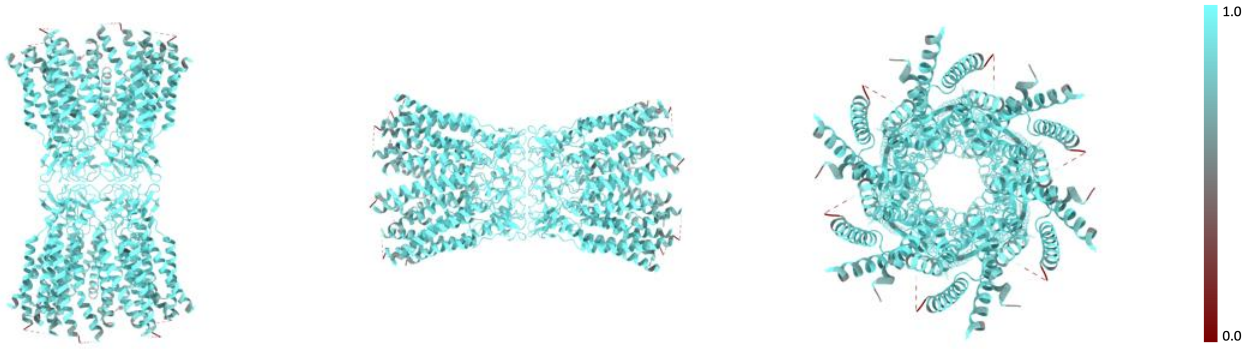
9.2 Q-score mapped to coordinate model



X Y Z

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

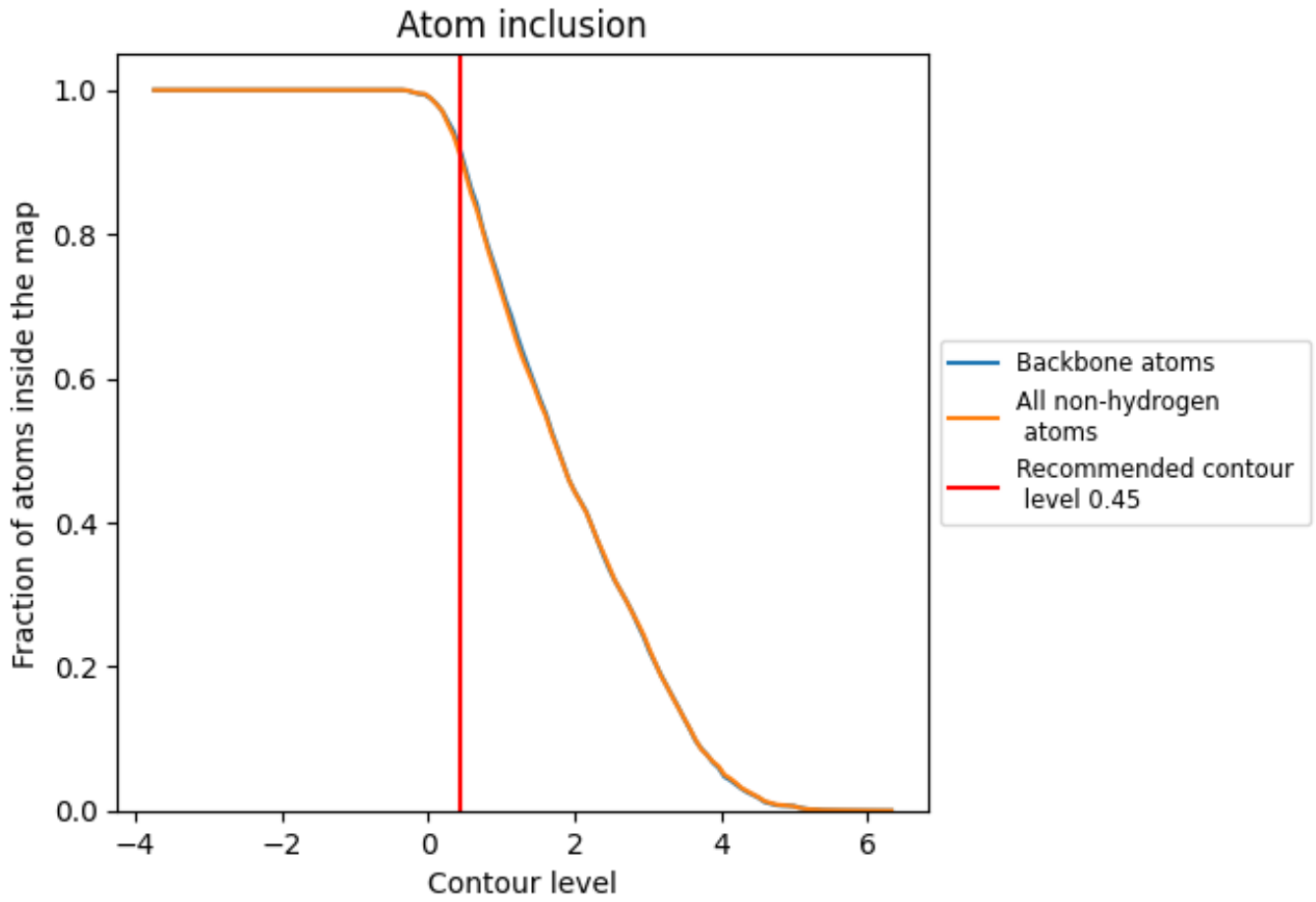
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.45).

9.4 Atom inclusion (i)



At the recommended contour level, 91% of all backbone atoms, 91% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.45) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9064	0.6490
A	0.9124	0.6490
B	0.9130	0.6490
C	0.9110	0.6490
D	0.9130	0.6480
E	0.9124	0.6470
F	0.9110	0.6480
G	0.9124	0.6490
H	0.9124	0.6490
I	0.9110	0.6490
J	0.9124	0.6480
K	0.9130	0.6480
L	0.9110	0.6480