Full wwPDB EM Validation Report ⓘ

May 26, 2024 – 11:57 AM EDT

PDB ID	:	7S4I
EMDB ID	:	EMD-24827
Title	:	CryoEM structure of Methylococcus capsulatus (Bath) pMMO in a native lipid nanodisc at 2.26 Angstrom resolution
Authors	:	Koo, C.W.; Rosenzweig, A.C.
Deposited on	:	2021-09-09
Resolution	:	2.26 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:

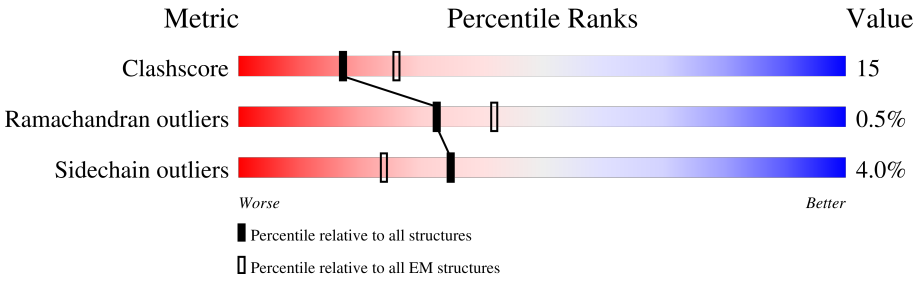
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.26 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	414	75% 16% • 8%
1	E	414	74% 17% • 8%
1	I	414	75% 16% • 8%
2	C	260	61% 28% • 9%
2	G	260	60% 28% • 9%
2	K	260	61% 28% • 9%
3	B	247	72% 24% ••
3	F	247	72% 24% ••

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Mol	Chain	Length	Quality of chain
3	J	247	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
8	P1O	B	308	-	-	X	-
8	P1O	F	308	-	-	X	-
8	P1O	J	301	-	-	X	-

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 25294 atoms, of which 2460 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 Particulate methane monooxygenase alpha subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	382	Total	C	N	O	S	0	0
			3017	1938	513	551	15		
1	E	382	Total	C	N	O	S	0	0
			3017	1938	513	551	15		
1	I	382	Total	C	N	O	S	0	0
			3017	1938	513	551	15		

- Molecule 2 is a protein called Ammonia monooxygenase/methane monooxygenase, subunit C family protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	236	Total	C	N	O	S	0	0
			1972	1339	299	329	5		
2	G	236	Total	C	N	O	S	0	0
			1972	1339	299	329	5		
2	K	236	Total	C	N	O	S	0	0
			1972	1339	299	329	5		

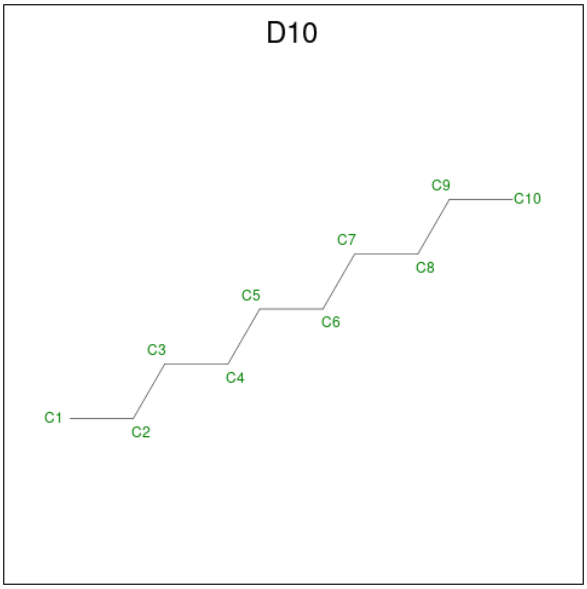
- Molecule 3 is a protein called Particulate methane monooxygenase beta subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	241	Total	C	N	O	S	0	0
			1977	1329	315	322	11		
3	F	241	Total	C	N	O	S	0	0
			1977	1329	315	322	11		
3	J	241	Total	C	N	O	S	0	0
			1977	1329	315	322	11		

- Molecule 4 is COPPER (II) ION (three-letter code: CU) (formula: Cu) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	AltConf
4	A	2	Total Cu 2 2	0
4	C	1	Total Cu 1 1	0
4	G	1	Total Cu 1 1	0
4	K	1	Total Cu 1 1	0
4	E	2	Total Cu 2 2	0
4	I	2	Total Cu 2 2	0

- Molecule 5 is DECANE (three-letter code: D10) (formula: $C_{10}H_{22}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
5	A	1	Total C H 32 10 22	0
5	C	1	Total C H 32 10 22	0
5	B	1	Total C H 32 10 22	0
5	B	1	Total C H 32 10 22	0
5	B	1	Total C H 32 10 22	0

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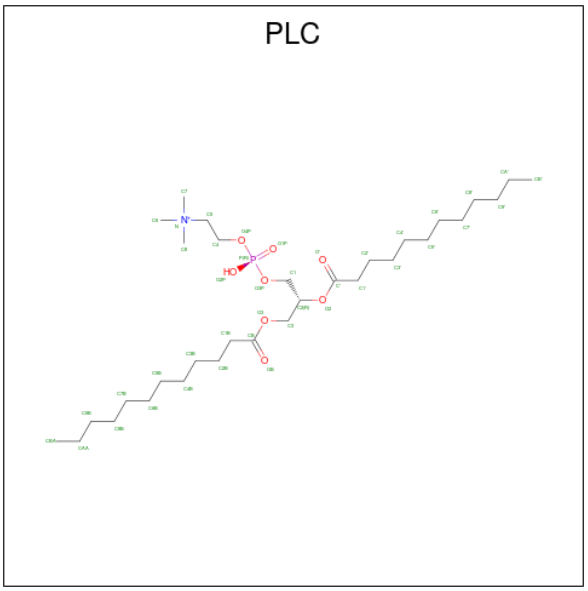
Mol	Chain	Residues	Atoms	AltConf
5	B	1	Total C H 32 10 22	0
5	G	1	Total C H 32 10 22	0
5	K	1	Total C H 32 10 22	0
5	E	1	Total C H 32 10 22	0
5	I	1	Total C H 32 10 22	0
5	F	1	Total C H 32 10 22	0
5	F	1	Total C H 32 10 22	0
5	F	1	Total C H 32 10 22	0
5	F	1	Total C H 32 10 22	0
5	J	1	Total C H 32 10 22	0
5	J	1	Total C H 32 10 22	0
5	J	1	Total C H 32 10 22	0
5	J	1	Total C H 32 10 22	0

- Molecule 6 is DIUNDECYL PHOSPHATIDYL CHOLINE (three-letter code: PLC) (formula: $C_{32}H_{65}NO_8P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
6	C	1	Total	C	H	N	O	P	0
			106	32	64	1	8	1	
6	C	1	Total	C	H	N	O	P	0
			106	32	64	1	8	1	
6	C	1	Total	C	H	N	O	P	0
			106	32	64	1	8	1	
6	C	1	Total	C	H	N	O	P	0
			106	32	64	1	8	1	
6	B	1	Total	C	H	N	O	P	0
			106	32	64	1	8	1	
6	B	1	Total	C	H	N	O	P	0
			106	32	64	1	8	1	
6	G	1	Total	C	H	N	O	P	0
			106	32	64	1	8	1	
6	G	1	Total	C	H	N	O	P	0
			106	32	64	1	8	1	
6	G	1	Total	C	H	N	O	P	0
			106	32	64	1	8	1	
6	G	1	Total	C	H	N	O	P	0
			106	32	64	1	8	1	
6	K	1	Total	C	H	N	O	P	0
			106	32	64	1	8	1	
6	K	1	Total	C	H	N	O	P	0
			106	32	64	1	8	1	
6	K	1	Total	C	H	N	O	P	0
			106	32	64	1	8	1	
6	K	1	Total	C	H	N	O	P	0
			106	32	64	1	8	1	

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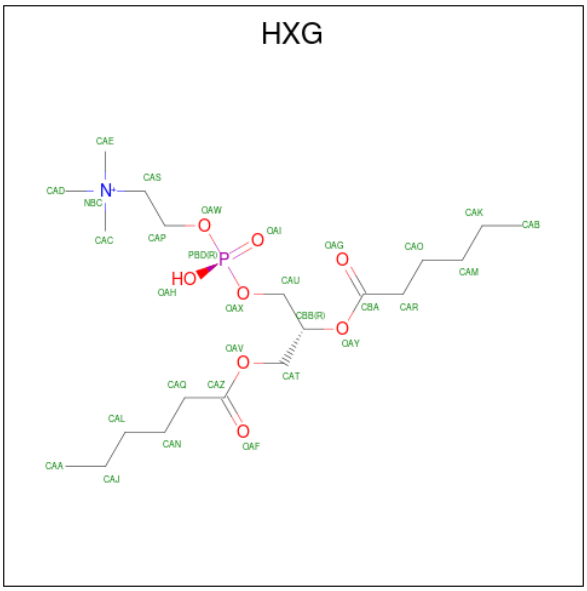
Mol	Chain	Residues	Atoms						AltConf
6	F	1	Total	C	H	N	O	P	0
			106	32	64	1	8	1	
6	F	1	Total	C	H	N	O	P	0
			106	32	64	1	8	1	
6	J	1	Total	C	H	N	O	P	0
			106	32	64	1	8	1	
6	J	1	Total	C	H	N	O	P	0
			106	32	64	1	8	1	

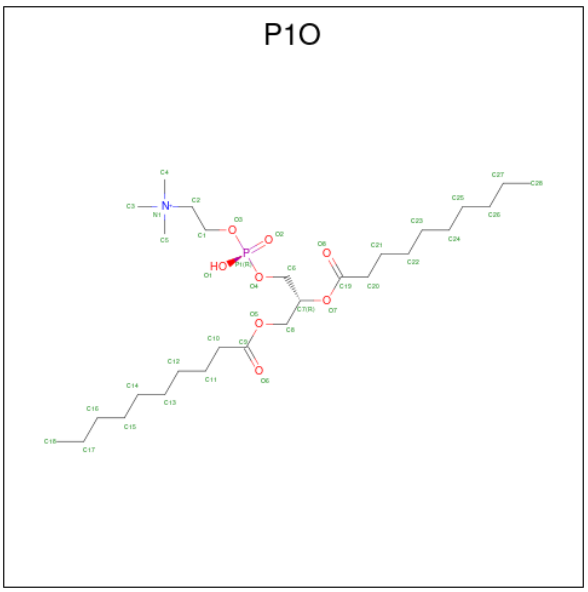
- Molecule 7 is 1,2-dihexanoyl-sn-glycero-3-phosphocholine (three-letter code: HXG) (formula: $C_{20}H_{41}NO_8P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
7	C	1	Total	C	H	N	O	P	0
			70	20	40	1	8	1	
7	C	1	Total	C	H	N	O	P	0
			70	20	40	1	8	1	
7	G	1	Total	C	H	N	O	P	0
			70	20	40	1	8	1	
7	G	1	Total	C	H	N	O	P	0
			70	20	40	1	8	1	
7	K	1	Total	C	H	N	O	P	0
			70	20	40	1	8	1	
7	K	1	Total	C	H	N	O	P	0
			70	20	40	1	8	1	

- Molecule 8 is 1,2-DIDECANOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter

code: P1O) (formula: $C_{28}H_{57}NO_8P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
8	C	1	Total	C	H	N	O	P	0
			94	28	56	1	8	1	
8	C	1	Total	C	H	N	O	P	0
			94	28	56	1	8	1	
8	B	1	Total	C	H	N	O	P	0
			94	28	56	1	8	1	
8	B	1	Total	C	H	N	O	P	0
			94	28	56	1	8	1	
8	G	1	Total	C	H	N	O	P	0
			94	28	56	1	8	1	
8	G	1	Total	C	H	N	O	P	0
			94	28	56	1	8	1	
8	K	1	Total	C	H	N	O	P	0
			94	28	56	1	8	1	
8	K	1	Total	C	H	N	O	P	0
			94	28	56	1	8	1	
8	F	1	Total	C	H	N	O	P	0
			94	28	56	1	8	1	
8	F	1	Total	C	H	N	O	P	0
			94	28	56	1	8	1	
8	J	1	Total	C	H	N	O	P	0
			94	28	56	1	8	1	
8	J	1	Total	C	H	N	O	P	0
			94	28	56	1	8	1	

- Molecule 9 is water.

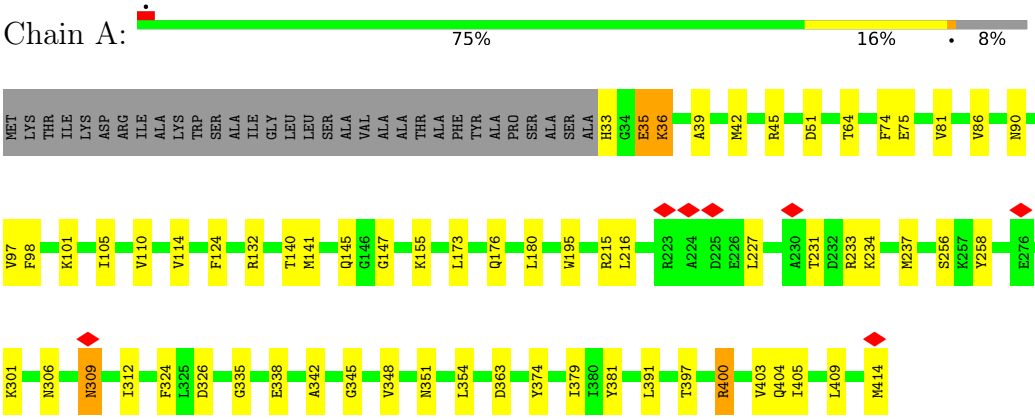
Mol	Chain	Residues	Atoms	AltConf
9	A	70	Total O 70 70	0
9	C	14	Total O 14 14	0
9	B	35	Total O 35 35	0
9	G	14	Total O 14 14	0
9	K	13	Total O 13 13	0
9	E	70	Total O 70 70	0
9	I	69	Total O 69 69	0
9	F	34	Total O 34 34	0
9	J	36	Total O 36 36	0

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.

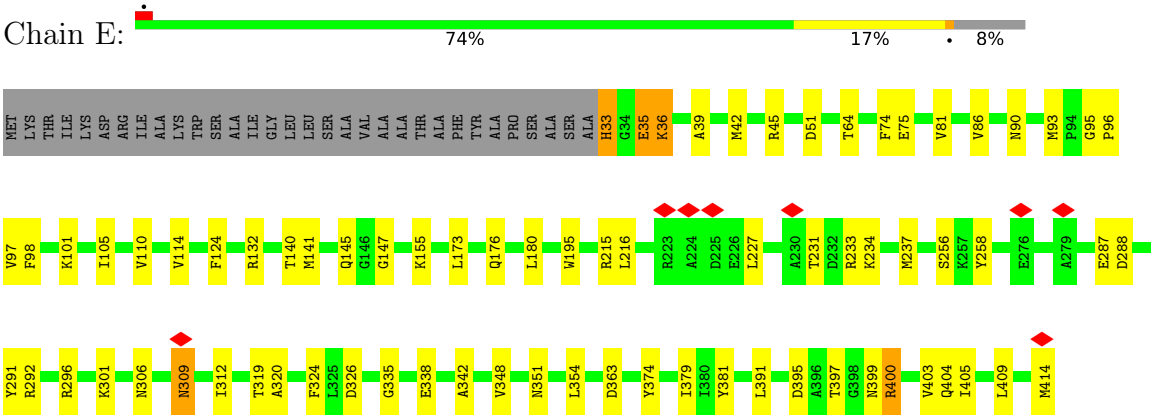
• Molecule 1: Particulate methane monooxygenase alpha subunit

Chain A:



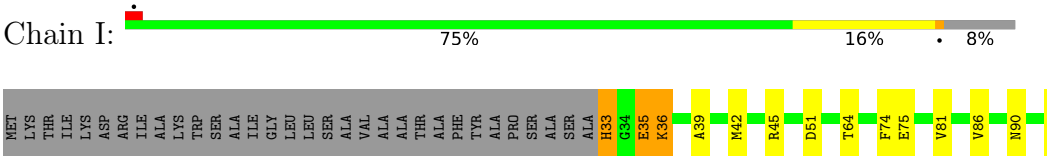
• Molecule 1: Particulate methane monooxygenase alpha subunit

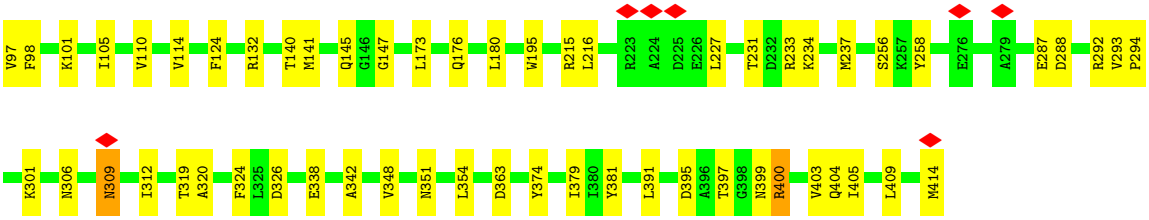
Chain E:



• Molecule 1: Particulate methane monooxygenase alpha subunit

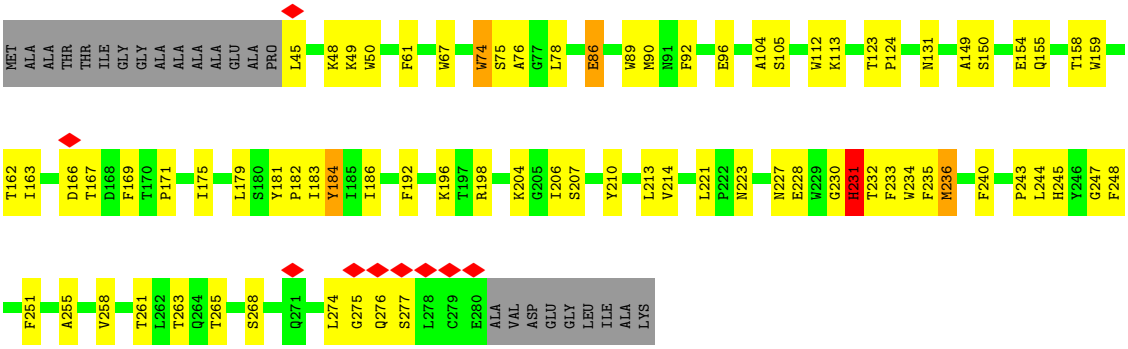
Chain I:





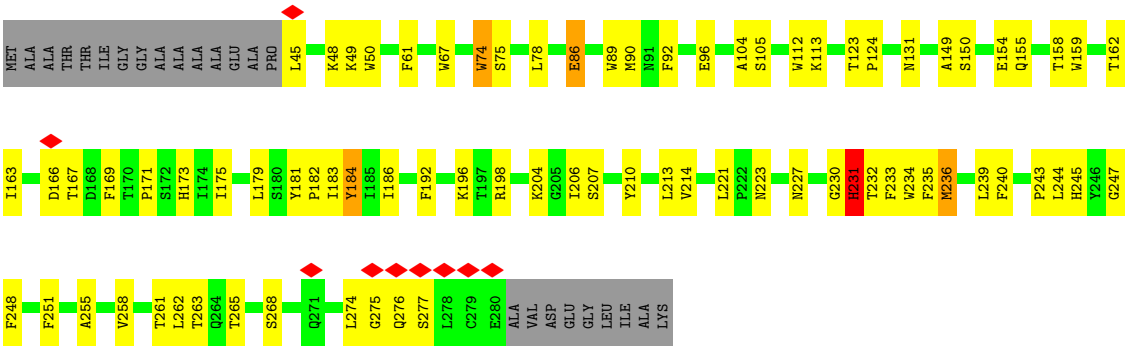
• Molecule 2: Ammonia monooxygenase/methane monooxygenase, subunit C family protein

Chain C:



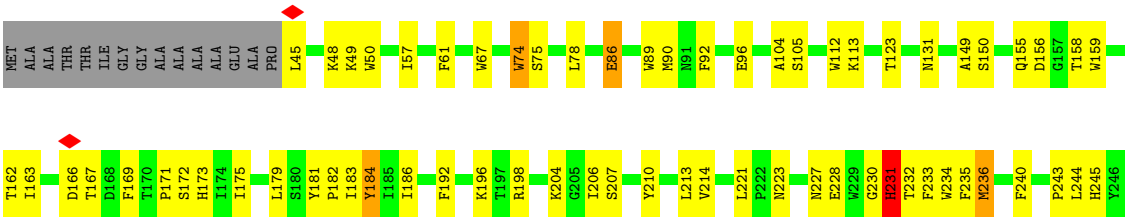
• Molecule 2: Ammonia monooxygenase/methane monooxygenase, subunit C family protein

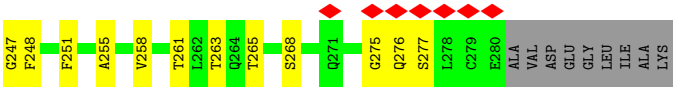
Chain G:



• Molecule 2: Ammonia monooxygenase/methane monooxygenase, subunit C family protein

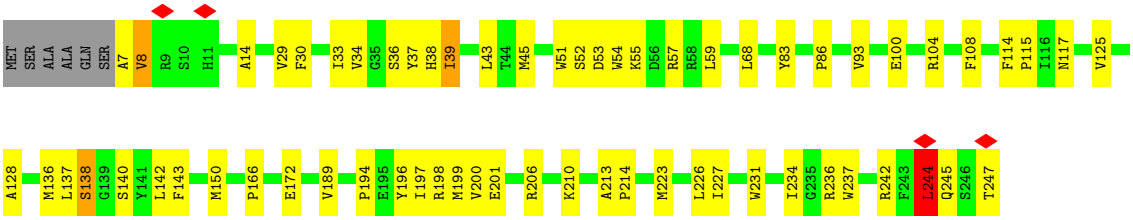
Chain K:





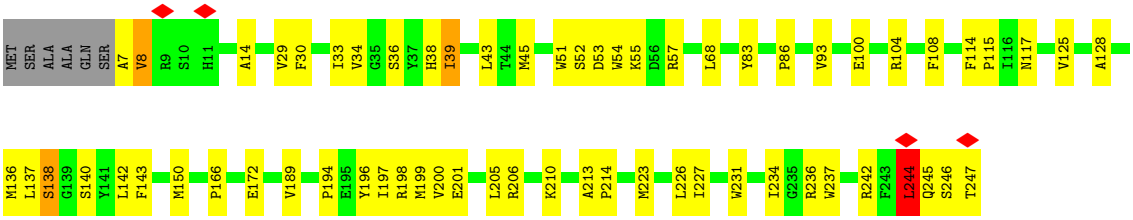
• Molecule 3: Particulate methane monooxygenase beta subunit

Chain B:



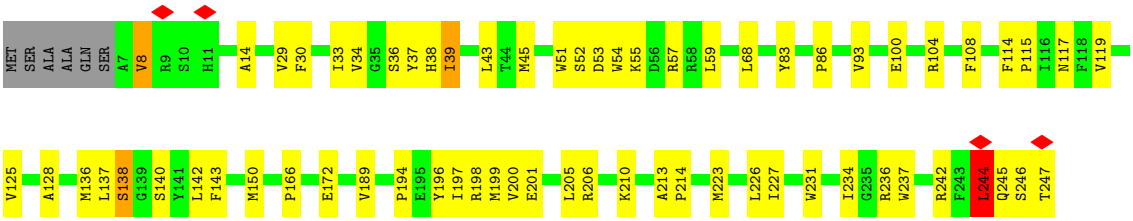
• Molecule 3: Particulate methane monooxygenase beta subunit

Chain F:



• Molecule 3: Particulate methane monooxygenase beta subunit

Chain J:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	1477719	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 ($e^-/Å^2$)	52	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.120	Depositor
Minimum map value	-0.044	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.0229	Depositor
Map size (Å)	204.0, 204.0, 204.0	wwPDB
Map dimensions	432, 432, 432	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.4722222, 0.4722222, 0.4722222	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: D10, P1O, PLC, CU, HXG

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	0.28	0/3099	0.52	1/4215 (0.0%)
1	E	0.28	0/3099	0.52	1/4215 (0.0%)
1	I	0.28	0/3099	0.52	1/4215 (0.0%)
2	C	0.29	0/2051	0.49	0/2810
2	G	0.29	0/2051	0.49	0/2810
2	K	0.29	0/2051	0.49	0/2810
3	B	0.29	0/2053	0.47	0/2810
3	F	0.29	0/2053	0.47	0/2810
3	J	0.29	0/2053	0.47	0/2810
All	All	0.29	0/21609	0.50	3/29505 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	I	288	ASP	CB-CG-OD1	5.41	123.17	118.30
1	E	288	ASP	CB-CG-OD1	5.37	123.13	118.30
1	A	288	ASP	CB-CG-OD1	5.35	123.11	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	3017	0	2980	47	0
1	E	3017	0	2980	50	0
1	I	3017	0	2980	49	0
2	C	1972	0	1904	86	0
2	G	1972	0	1904	90	0
2	K	1972	0	1904	90	0
3	B	1977	0	1936	92	0
3	F	1977	0	1936	97	0
3	J	1977	0	1936	96	0
4	A	2	0	0	0	0
4	C	1	0	0	1	0
4	E	2	0	0	0	0
4	G	1	0	0	1	0
4	I	2	0	0	0	0
4	K	1	0	0	1	0
5	A	10	22	22	0	0
5	B	40	88	88	9	0
5	C	10	22	22	1	0
5	E	10	22	22	0	0
5	F	40	88	88	8	0
5	G	10	22	22	1	0
5	I	10	22	22	0	0
5	J	40	88	88	8	0
5	K	10	22	22	1	0
6	B	84	128	128	3	0
6	C	168	256	256	16	0
6	F	84	128	128	2	0
6	G	168	256	256	18	0
6	J	84	128	128	3	0
6	K	168	256	256	18	0
7	C	60	80	80	23	0
7	G	60	80	80	24	0
7	K	60	80	80	24	0
8	B	76	112	112	35	0
8	C	76	112	112	23	0
8	F	76	112	112	37	0
8	G	76	112	112	21	0
8	J	76	112	112	36	0
8	K	76	112	112	22	0
9	A	70	0	0	4	0
9	B	35	0	0	2	0
9	C	14	0	0	2	0
9	E	70	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	F	34	0	0	5	0
9	G	14	0	0	3	0
9	I	69	0	0	3	0
9	J	36	0	0	2	0
9	K	13	0	0	2	0
All	All	22834	2460	22920	696	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 15.

All (696) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:67:TRP:CD1	7:C:306:HXG:H41	1.81	1.16
2:G:67:TRP:CD1	7:G:307:HXG:H41	1.81	1.16
2:K:67:TRP:CD1	7:K:307:HXG:H41	1.81	1.14
6:K:303:PLC:H73	7:K:304:HXG:H36	1.33	1.11
3:B:244:LEU:HD21	8:B:308:P1O:H18	1.34	1.09
3:B:244:LEU:HD21	8:B:308:P1O:C8	1.82	1.08
3:B:244:LEU:CD2	8:B:308:P1O:H18	1.83	1.07
3:F:244:LEU:HD21	8:F:308:P1O:H18	1.37	1.07
2:C:67:TRP:HA	7:C:306:HXG:H39	1.07	1.06
2:K:67:TRP:HA	7:K:307:HXG:H39	1.07	1.06
6:G:303:PLC:H73	7:G:304:HXG:H36	1.32	1.06
6:C:302:PLC:H73	7:C:303:HXG:H36	1.33	1.06
2:G:67:TRP:HA	7:G:307:HXG:H39	1.07	1.06
3:F:244:LEU:HD21	8:F:308:P1O:C8	1.86	1.06
3:F:244:LEU:CD2	8:F:308:P1O:H18	1.87	1.04
3:B:244:LEU:HD23	8:B:308:P1O:C5	1.87	1.03
2:K:67:TRP:CD1	7:K:307:HXG:CAC	2.43	1.01
3:J:244:LEU:HD23	8:J:301:P1O:C5	1.90	1.01
2:G:67:TRP:CD1	7:G:307:HXG:CAC	2.43	1.01
3:F:138:SER:HA	8:F:303:P1O:O8	1.61	1.01
2:C:67:TRP:CD1	7:C:306:HXG:CAC	2.43	1.00
3:J:244:LEU:HD21	8:J:301:P1O:C8	1.91	1.00
2:C:67:TRP:HA	7:C:306:HXG:CAC	1.91	1.00
2:C:67:TRP:CA	7:C:306:HXG:H39	1.90	1.00
3:B:244:LEU:HD23	8:B:308:P1O:H12	1.43	1.00
2:G:67:TRP:CA	7:G:307:HXG:H39	1.91	1.00
2:G:67:TRP:HA	7:G:307:HXG:CAC	1.91	1.00
2:K:67:TRP:CA	7:K:307:HXG:H39	1.91	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:244:LEU:CD2	8:J:301:P1O:H18	1.91	0.99
3:J:138:SER:HA	8:J:304:P1O:O8	1.61	0.99
3:F:244:LEU:HD23	8:F:308:P1O:C5	1.91	0.99
3:J:244:LEU:HD23	8:J:301:P1O:H12	1.45	0.98
3:B:138:SER:HA	8:B:302:P1O:O8	1.61	0.98
2:K:67:TRP:HA	7:K:307:HXG:CAC	1.91	0.98
3:J:244:LEU:HD21	8:J:301:P1O:H18	1.41	0.98
2:G:236:MET:HB3	3:J:206:ARG:HG3	1.45	0.97
2:K:67:TRP:HD1	7:K:307:HXG:H41	1.19	0.97
2:C:50:TRP:CE3	8:C:308:P1O:H39	2.03	0.94
2:C:67:TRP:HD1	7:C:306:HXG:H41	1.18	0.94
3:F:244:LEU:HD23	8:F:308:P1O:H12	1.47	0.93
2:G:67:TRP:HD1	7:G:307:HXG:H41	1.18	0.93
2:G:50:TRP:CE3	8:G:309:P1O:H39	2.03	0.93
2:K:50:TRP:CE3	8:K:309:P1O:H39	2.03	0.93
2:C:236:MET:HB3	3:F:206:ARG:HG3	1.50	0.91
3:B:206:ARG:HG3	2:K:236:MET:HB3	1.51	0.90
3:B:244:LEU:HD11	8:B:308:P1O:H42	1.54	0.89
3:F:244:LEU:HD11	8:F:308:P1O:H42	1.55	0.88
2:G:245:HIS:HE2	4:G:302:CU:CU	0.59	0.88
7:C:303:HXG:H9	5:C:304:D10:H42	1.56	0.88
2:K:245:HIS:HE2	4:K:302:CU:CU	0.59	0.87
2:G:112:TRP:CH2	8:G:310:P1O:H2	2.09	0.87
7:K:304:HXG:H9	5:K:305:D10:H42	1.56	0.87
1:I:36:LYS:HG2	1:I:374:TYR:HA	1.56	0.87
2:C:245:HIS:HE2	4:C:301:CU:CU	0.59	0.87
2:C:112:TRP:CH2	8:C:309:P1O:H2	2.09	0.87
7:G:304:HXG:H9	5:G:305:D10:H42	1.56	0.87
2:K:112:TRP:CH2	8:K:310:P1O:H2	2.09	0.86
1:E:36:LYS:HG2	1:E:374:TYR:HA	1.56	0.86
7:G:307:HXG:H37	7:G:307:HXG:H26	1.58	0.86
1:A:36:LYS:HG2	1:A:374:TYR:HA	1.56	0.85
2:G:67:TRP:HB2	7:G:307:HXG:H40	1.57	0.84
3:B:244:LEU:HD11	8:B:308:P1O:C22	2.08	0.84
2:C:67:TRP:HB2	7:C:306:HXG:H40	1.57	0.84
3:J:244:LEU:HD11	8:J:301:P1O:H42	1.58	0.84
7:K:307:HXG:H37	7:K:307:HXG:H26	1.58	0.84
2:K:67:TRP:HD1	7:K:307:HXG:CAC	1.86	0.84
7:C:306:HXG:H37	7:C:306:HXG:H26	1.58	0.84
2:K:67:TRP:HB2	7:K:307:HXG:H40	1.58	0.83
8:J:304:P1O:O8	8:J:304:P1O:H20	1.79	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:F:303:P1O:O8	8:F:303:P1O:H20	1.79	0.82
3:F:237:TRP:HE1	5:F:306:D10:H32	1.44	0.82
8:B:302:P1O:O8	8:B:302:P1O:H20	1.79	0.82
2:G:67:TRP:HD1	7:G:307:HXG:CAC	1.86	0.81
3:B:237:TRP:HE1	5:B:305:D10:H32	1.44	0.81
3:F:244:LEU:HD11	8:F:308:P1O:C22	2.10	0.81
3:J:237:TRP:HE1	5:J:307:D10:H32	1.44	0.79
1:A:81:VAL:HG13	1:A:147:GLY:HA3	1.65	0.79
2:G:67:TRP:CB	7:G:307:HXG:H40	2.13	0.79
1:I:81:VAL:HG13	1:I:147:GLY:HA3	1.65	0.79
1:E:81:VAL:HG13	1:E:147:GLY:HA3	1.65	0.78
2:C:67:TRP:CB	7:C:306:HXG:H40	2.13	0.78
8:J:304:P1O:H48	8:J:304:P1O:H38	1.66	0.78
2:K:67:TRP:CB	7:K:307:HXG:H40	2.13	0.78
3:F:138:SER:CA	8:F:303:P1O:O8	2.32	0.77
2:G:67:TRP:CB	7:G:307:HXG:CAC	2.63	0.77
3:B:138:SER:CA	8:B:302:P1O:O8	2.32	0.77
2:G:112:TRP:CH2	8:G:310:P1O:C1	2.67	0.77
2:C:67:TRP:CB	7:C:306:HXG:CAC	2.63	0.77
2:C:112:TRP:CH2	8:C:309:P1O:C1	2.67	0.76
8:B:302:P1O:H38	8:B:302:P1O:H48	1.66	0.76
2:K:112:TRP:CH2	8:K:310:P1O:C1	2.67	0.76
3:J:244:LEU:HD11	8:J:301:P1O:C22	2.15	0.76
2:C:112:TRP:CZ2	8:C:309:P1O:C1	2.69	0.76
2:K:112:TRP:CZ2	8:K:310:P1O:C1	2.69	0.76
2:K:67:TRP:CB	7:K:307:HXG:CAC	2.63	0.76
8:F:303:P1O:H38	8:F:303:P1O:H48	1.66	0.76
2:C:48:LYS:HD3	2:C:50:TRP:HD1	1.51	0.76
2:K:48:LYS:HD3	2:K:50:TRP:HD1	1.51	0.76
3:F:7:ALA:CB	9:F:417:HOH:O	2.33	0.76
2:G:112:TRP:CZ2	8:G:310:P1O:C1	2.69	0.76
3:J:138:SER:CA	8:J:304:P1O:O8	2.32	0.76
2:C:67:TRP:HD1	7:C:306:HXG:CAC	1.86	0.75
2:G:48:LYS:HD3	2:G:50:TRP:HD1	1.51	0.75
3:F:138:SER:HB2	8:F:303:P1O:O8	1.87	0.74
8:B:308:P1O:H43	8:B:308:P1O:O6	1.88	0.74
8:F:308:P1O:O6	8:F:308:P1O:H43	1.88	0.74
6:C:310:PLC:H2	3:B:199:MET:SD	2.27	0.74
6:G:301:PLC:H2	3:F:199:MET:SD	2.28	0.74
6:K:301:PLC:H2	3:J:199:MET:SD	2.27	0.73
3:B:138:SER:HB2	8:B:302:P1O:O8	1.87	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:138:SER:HB2	8:J:304:P1O:O8	1.87	0.73
8:J:301:P1O:O6	8:J:301:P1O:H43	1.88	0.72
1:I:93:MET:HE1	1:I:98:PHE:HB2	1.71	0.71
2:K:173:HIS:NE2	9:K:401:HOH:O	2.23	0.71
3:B:244:LEU:HD21	8:B:308:P1O:H17	1.73	0.70
2:G:173:HIS:NE2	9:G:401:HOH:O	2.23	0.70
1:I:215:ARG:HG2	1:I:227:LEU:HD22	1.73	0.70
1:A:93:MET:HE1	1:A:98:PHE:HB2	1.74	0.70
1:E:93:MET:HE1	1:E:98:PHE:HB2	1.74	0.70
1:E:326:ASP:OD2	1:E:351:ASN:ND2	2.25	0.70
3:B:244:LEU:CD2	8:B:308:P1O:H12	2.21	0.70
2:G:112:TRP:CZ2	8:G:310:P1O:H2	2.27	0.69
3:J:138:SER:CB	8:J:304:P1O:O8	2.40	0.69
1:E:215:ARG:HG2	1:E:227:LEU:HD22	1.73	0.69
1:A:75:GLU:OE1	1:A:404:GLN:NE2	2.25	0.69
2:C:112:TRP:CZ2	8:C:309:P1O:H2	2.27	0.69
3:F:138:SER:CB	8:F:303:P1O:O8	2.40	0.69
2:C:67:TRP:CA	7:C:306:HXG:CAC	2.61	0.69
1:I:75:GLU:OE1	1:I:404:GLN:NE2	2.25	0.69
3:F:7:ALA:HB3	9:F:417:HOH:O	1.92	0.69
2:K:112:TRP:CZ2	8:K:310:P1O:H2	2.28	0.69
1:A:215:ARG:HG2	1:A:227:LEU:HD22	1.73	0.69
3:B:138:SER:CB	8:B:302:P1O:O8	2.40	0.69
3:B:244:LEU:HD23	8:B:308:P1O:H18	1.74	0.69
1:I:326:ASP:OD2	1:I:351:ASN:ND2	2.25	0.69
2:G:67:TRP:CG	7:G:307:HXG:CAC	2.76	0.68
2:C:67:TRP:CG	7:C:306:HXG:CAC	2.76	0.68
3:B:142:LEU:HD22	8:J:301:P1O:H48	1.75	0.68
2:K:67:TRP:CG	7:K:307:HXG:CAC	2.76	0.68
1:A:326:ASP:OD2	1:A:351:ASN:ND2	2.25	0.68
2:G:150:SER:OG	3:F:38:HIS:ND1	2.24	0.68
8:B:308:P1O:H48	3:F:142:LEU:HD22	1.76	0.67
3:B:237:TRP:HE1	5:B:305:D10:C3	2.07	0.67
3:J:244:LEU:CD2	8:J:301:P1O:H12	2.23	0.67
8:F:308:P1O:H48	3:J:142:LEU:HD22	1.75	0.67
3:J:237:TRP:HE1	5:J:307:D10:C3	2.07	0.66
1:E:75:GLU:OE1	1:E:404:GLN:NE2	2.25	0.66
1:A:176:GLN:NE2	9:A:601:HOH:O	2.28	0.66
3:F:244:LEU:HD21	8:F:308:P1O:H17	1.75	0.66
6:G:301:PLC:H32	6:G:301:PLC:H1'2	1.78	0.66
3:F:237:TRP:HE1	5:F:306:D10:C3	2.07	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:307:HXG:H37	7:G:307:HXG:CAU	2.26	0.65
6:K:301:PLC:H32	6:K:301:PLC:H1'2	1.78	0.65
7:C:306:HXG:H37	7:C:306:HXG:CAU	2.26	0.65
6:C:310:PLC:H32	6:C:310:PLC:H1'2	1.78	0.65
2:G:236:MET:CB	3:J:206:ARG:HG3	2.25	0.65
7:K:307:HXG:H37	7:K:307:HXG:CAU	2.26	0.65
2:G:67:TRP:CA	7:G:307:HXG:CAC	2.61	0.64
3:F:237:TRP:NE1	5:F:306:D10:H32	2.12	0.64
3:J:237:TRP:NE1	5:J:307:D10:H32	2.12	0.64
8:F:308:P1O:H12	8:F:308:P1O:O3	1.98	0.64
2:K:150:SER:OG	3:J:38:HIS:ND1	2.22	0.64
8:J:301:P1O:H12	8:J:301:P1O:O3	1.98	0.64
3:B:237:TRP:NE1	5:B:305:D10:H32	2.12	0.64
8:B:308:P1O:H12	8:B:308:P1O:O3	1.98	0.63
2:C:261:THR:O	2:C:265:THR:HG23	1.98	0.63
2:K:261:THR:O	2:K:265:THR:HG23	1.98	0.63
3:J:244:LEU:HD21	8:J:301:P1O:H17	1.81	0.63
2:G:261:THR:O	2:G:265:THR:HG23	1.98	0.62
2:G:230:GLY:O	2:G:244:LEU:HD13	2.00	0.62
2:K:67:TRP:CA	7:K:307:HXG:CAC	2.61	0.62
2:K:230:GLY:O	2:K:244:LEU:HD13	2.00	0.62
3:J:138:SER:OG	3:J:138:SER:O	2.17	0.62
2:C:230:GLY:O	2:C:244:LEU:HD13	1.99	0.62
1:E:176:GLN:NE2	9:E:601:HOH:O	2.32	0.62
8:G:309:P1O:H18	8:G:309:P1O:H24	1.82	0.62
3:F:138:SER:O	3:F:138:SER:OG	2.17	0.62
2:G:192:PHE:HB2	2:G:214:VAL:HG21	1.82	0.62
3:F:244:LEU:CD2	8:F:308:P1O:H12	2.24	0.62
8:G:310:P1O:H7	8:G:310:P1O:O8	1.99	0.61
2:C:192:PHE:HB2	2:C:214:VAL:HG21	1.82	0.61
8:C:308:P1O:H18	8:C:308:P1O:H24	1.82	0.61
2:G:232:THR:HA	3:J:206:ARG:O	1.99	0.61
3:F:237:TRP:NE1	5:F:306:D10:H51	2.15	0.61
8:C:309:P1O:O8	8:C:309:P1O:H7	1.99	0.61
3:J:237:TRP:NE1	5:J:307:D10:H51	2.15	0.61
8:K:310:P1O:O8	8:K:310:P1O:H7	1.99	0.61
3:B:138:SER:O	3:B:138:SER:OG	2.17	0.61
8:K:309:P1O:H18	8:K:309:P1O:H24	1.82	0.61
3:B:226:LEU:HD21	2:K:251:PHE:HZ	1.65	0.61
2:G:251:PHE:HZ	3:J:226:LEU:HD21	1.65	0.61
2:K:50:TRP:CZ3	8:K:309:P1O:H39	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:237:TRP:NE1	5:B:305:D10:H51	2.15	0.60
2:G:50:TRP:CZ3	8:G:309:P1O:H39	2.35	0.60
2:K:192:PHE:HB2	2:K:214:VAL:HG21	1.82	0.60
2:C:50:TRP:CZ3	8:C:308:P1O:H39	2.35	0.60
3:J:8:VAL:HG11	3:J:14:ALA:HB2	1.83	0.60
2:C:251:PHE:HZ	3:F:226:LEU:HD21	1.66	0.60
3:F:8:VAL:HG11	3:F:14:ALA:HB2	1.83	0.60
8:C:308:P1O:O2	8:C:308:P1O:H4	2.02	0.60
3:B:8:VAL:HG11	3:B:14:ALA:HB2	1.83	0.60
8:G:309:P1O:O2	8:G:309:P1O:H4	2.02	0.59
2:C:112:TRP:CZ2	8:C:309:P1O:H7	2.38	0.59
8:K:309:P1O:O2	8:K:309:P1O:H4	2.02	0.59
1:I:176:GLN:NE2	9:I:603:HOH:O	2.36	0.59
8:J:301:P1O:H15	8:J:301:P1O:H39	1.83	0.59
8:B:308:P1O:H15	8:B:308:P1O:H39	1.84	0.59
2:K:112:TRP:CZ2	8:K:310:P1O:H7	2.38	0.59
8:F:308:P1O:H15	8:F:308:P1O:H39	1.83	0.59
3:F:244:LEU:HD23	8:F:308:P1O:H18	1.77	0.59
3:J:244:LEU:HD23	8:J:301:P1O:H18	1.82	0.59
2:G:112:TRP:CZ2	8:G:310:P1O:H7	2.38	0.59
3:J:242:ARG:HH21	8:J:301:P1O:C4	2.17	0.58
1:E:291:TYR:HA	9:E:650:HOH:O	2.03	0.58
3:J:242:ARG:HH21	8:J:301:P1O:H9	1.68	0.58
3:B:242:ARG:HH21	8:B:308:P1O:C4	2.17	0.58
8:C:308:P1O:O2	8:C:308:P1O:H6	2.04	0.58
8:B:308:P1O:H17	8:B:308:P1O:H39	1.85	0.58
8:F:308:P1O:H17	8:F:308:P1O:H39	1.85	0.58
1:A:233:ARG:HA	3:B:136:MET:HE1	1.86	0.58
1:I:233:ARG:HA	3:J:136:MET:HE1	1.86	0.57
8:J:301:P1O:H17	8:J:301:P1O:H39	1.85	0.57
2:C:232:THR:HA	3:F:206:ARG:O	2.05	0.57
8:G:309:P1O:O2	8:G:309:P1O:H6	2.04	0.57
8:K:309:P1O:O2	8:K:309:P1O:H6	2.04	0.57
1:E:231:THR:HG22	1:E:234:LYS:HE2	1.87	0.57
6:K:301:PLC:C2	3:J:199:MET:SD	2.93	0.57
2:C:92:PHE:HA	6:C:307:PLC:OB	2.05	0.56
2:C:112:TRP:CH2	8:C:309:P1O:H1	2.40	0.56
2:C:112:TRP:CZ2	8:C:309:P1O:C3	2.88	0.56
1:A:231:THR:HG22	1:A:234:LYS:HE2	1.87	0.56
1:A:309:ASN:OD1	1:A:309:ASN:N	2.39	0.56
3:B:206:ARG:O	2:K:232:THR:HA	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:112:TRP:CZ2	8:G:310:P1O:C3	2.88	0.56
2:G:92:PHE:HA	6:G:308:PLC:OB	2.05	0.56
2:K:112:TRP:CH2	8:K:310:P1O:H1	2.40	0.56
2:K:112:TRP:CZ2	8:K:310:P1O:C3	2.88	0.56
1:E:233:ARG:HA	3:F:136:MET:HE1	1.86	0.56
2:K:92:PHE:HA	6:K:308:PLC:OB	2.05	0.56
1:I:231:THR:HG22	1:I:234:LYS:HE2	1.87	0.56
2:C:236:MET:CB	3:F:206:ARG:HG3	2.30	0.56
3:B:213:ALA:HB3	6:B:301:PLC:H11	1.88	0.56
2:G:112:TRP:HB2	8:G:310:P1O:H40	1.88	0.56
6:G:301:PLC:H63	6:G:301:PLC:O4P	2.06	0.55
1:E:309:ASN:N	1:E:309:ASN:OD1	2.39	0.55
2:K:112:TRP:HB2	8:K:310:P1O:H40	1.88	0.55
2:C:112:TRP:HB2	8:C:309:P1O:H40	1.88	0.55
3:B:244:LEU:HD11	8:B:308:P1O:H43	1.86	0.55
6:C:310:PLC:C2	3:B:199:MET:SD	2.94	0.55
6:G:301:PLC:C2	3:F:199:MET:SD	2.95	0.55
1:E:45:ARG:HB3	1:E:74:PHE:CD2	2.42	0.55
1:I:309:ASN:OD1	1:I:309:ASN:N	2.39	0.55
3:B:244:LEU:HD21	8:B:308:P1O:H15	1.88	0.55
2:G:112:TRP:CH2	8:G:310:P1O:H1	2.40	0.55
3:J:244:LEU:HD23	8:J:301:P1O:H13	1.87	0.55
3:B:206:ARG:HG3	2:K:236:MET:CB	2.31	0.55
1:A:45:ARG:HB3	1:A:74:PHE:CD2	2.42	0.55
2:G:67:TRP:CD1	7:G:307:HXG:H40	2.39	0.55
1:I:45:ARG:HB3	1:I:74:PHE:CD2	2.42	0.55
3:F:242:ARG:HH21	8:F:308:P1O:C4	2.21	0.55
3:B:244:LEU:HD21	8:B:308:P1O:C6	2.37	0.54
3:F:244:LEU:HD11	8:F:308:P1O:H43	1.89	0.54
6:C:310:PLC:O4P	6:C:310:PLC:H63	2.06	0.54
3:B:242:ARG:HH21	8:B:308:P1O:H9	1.71	0.54
3:B:244:LEU:CD2	8:B:308:P1O:C8	2.57	0.54
3:F:213:ALA:HB3	6:F:302:PLC:H11	1.88	0.54
2:K:50:TRP:CD2	8:K:309:P1O:H16	2.43	0.54
6:K:301:PLC:O4P	6:K:301:PLC:H63	2.06	0.54
2:C:150:SER:OG	3:B:38:HIS:ND1	2.25	0.54
2:C:50:TRP:CD2	8:C:308:P1O:H16	2.43	0.54
2:C:234:TRP:HH2	2:C:243:PRO:HB2	1.73	0.54
3:J:213:ALA:HB3	6:J:303:PLC:H11	1.88	0.54
3:J:244:LEU:HD21	8:J:301:P1O:H15	1.90	0.53
3:J:244:LEU:CD2	8:J:301:P1O:C8	2.66	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:50:TRP:CD2	8:G:309:P1O:H16	2.43	0.53
3:F:242:ARG:HH21	8:F:308:P1O:H9	1.73	0.53
3:F:244:LEU:CD1	8:F:308:P1O:H42	2.35	0.53
2:K:67:TRP:CD1	7:K:307:HXG:H40	2.39	0.53
3:J:242:ARG:NH2	8:J:301:P1O:C4	2.72	0.53
3:F:244:LEU:HD21	8:F:308:P1O:H15	1.91	0.53
1:A:292:ARG:NH1	1:A:414:MET:O	2.42	0.53
3:B:244:LEU:CD1	8:B:308:P1O:H42	2.33	0.52
3:F:244:LEU:CD2	8:F:308:P1O:C8	2.61	0.52
2:C:67:TRP:CD1	7:C:306:HXG:H40	2.39	0.52
2:C:183:ILE:HG12	6:C:307:PLC:HEA3	1.92	0.52
2:K:234:TRP:HH2	2:K:243:PRO:HB2	1.73	0.52
7:K:304:HXG:H17	7:K:304:HXG:H10	1.92	0.52
2:G:183:ILE:HG12	6:G:308:PLC:HEA3	1.92	0.52
1:I:39:ALA:HB3	1:I:42:MET:HG3	1.92	0.52
3:F:143:PHE:CD2	8:F:303:P1O:H26	2.45	0.52
3:J:143:PHE:CD2	8:J:304:P1O:H26	2.45	0.52
3:B:143:PHE:CD2	8:B:302:P1O:H26	2.45	0.52
2:G:234:TRP:HH2	2:G:243:PRO:HB2	1.73	0.52
6:C:310:PLC:H9'1	6:K:303:PLC:HTA1	1.93	0.51
1:E:39:ALA:HB3	1:E:42:MET:HG3	1.92	0.51
7:G:304:HXG:H10	7:G:304:HXG:H17	1.92	0.51
6:C:302:PLC:HTA1	6:G:301:PLC:H9'1	1.93	0.51
2:G:192:PHE:HZ	2:G:206:ILE:HG23	1.75	0.51
6:G:303:PLC:HTA1	6:K:301:PLC:H9'1	1.93	0.51
3:F:100:GLU:O	3:F:104:ARG:HG2	2.11	0.51
1:E:292:ARG:NH1	1:E:414:MET:O	2.42	0.51
3:J:100:GLU:O	3:J:104:ARG:HG2	2.11	0.51
3:J:244:LEU:HD21	8:J:301:P1O:C6	2.41	0.51
2:G:112:TRP:CE2	8:G:310:P1O:C3	2.94	0.51
2:K:183:ILE:HG12	6:K:308:PLC:HEA3	1.92	0.51
1:I:292:ARG:NH1	1:I:414:MET:O	2.42	0.51
2:C:112:TRP:CE2	8:C:309:P1O:C3	2.94	0.51
2:C:112:TRP:CE2	8:C:309:P1O:H6	2.46	0.51
2:C:245:HIS:HB3	3:B:43:LEU:HD13	1.92	0.51
2:K:192:PHE:HZ	2:K:206:ILE:HG23	1.75	0.51
2:C:131:ASN:OD1	2:C:268:SER:OG	2.29	0.50
7:C:303:HXG:H17	7:C:303:HXG:H10	1.92	0.50
8:C:309:P1O:H12	8:C:309:P1O:H16	1.93	0.50
3:B:45:MET:HE3	3:B:68:LEU:HD11	1.93	0.50
2:K:75:SER:OG	2:K:75:SER:O	2.28	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:112:TRP:CE2	8:K:310:P1O:C3	2.94	0.50
2:G:112:TRP:CE2	8:G:310:P1O:H6	2.46	0.50
2:G:236:MET:H	7:G:304:HXG:H37	1.76	0.50
2:K:112:TRP:CE2	8:K:310:P1O:H6	2.46	0.50
2:K:236:MET:H	7:K:304:HXG:H37	1.76	0.50
2:C:236:MET:H	7:C:303:HXG:H37	1.76	0.50
1:E:124:PHE:CE2	1:E:140:THR:HG21	2.47	0.50
1:A:39:ALA:HB3	1:A:42:MET:HG3	1.92	0.50
1:A:155:LYS:NZ	1:A:335:GLY:O	2.35	0.50
3:B:86:PRO:HA	9:B:426:HOH:O	2.11	0.50
3:B:242:ARG:NH2	8:B:308:P1O:C4	2.75	0.50
2:G:245:HIS:HB3	3:F:43:LEU:HD13	1.94	0.50
2:K:206:ILE:HD13	3:J:247:THR:HG23	1.93	0.50
3:F:45:MET:HE3	3:F:68:LEU:HD11	1.93	0.50
3:F:244:LEU:HD21	8:F:308:P1O:C6	2.41	0.50
3:F:244:LEU:HD23	8:F:308:P1O:H13	1.87	0.50
2:C:192:PHE:HZ	2:C:206:ILE:HG23	1.75	0.50
6:C:302:PLC:C7	7:C:303:HXG:H36	2.24	0.50
8:G:310:P1O:H16	8:G:310:P1O:H12	1.93	0.50
2:K:131:ASN:OD1	2:K:268:SER:OG	2.29	0.50
3:F:7:ALA:HB2	9:F:417:HOH:O	2.05	0.50
2:G:131:ASN:OD1	2:G:268:SER:OG	2.29	0.50
8:K:310:P1O:H16	8:K:310:P1O:H12	1.93	0.50
3:B:30:PHE:O	3:B:34:VAL:HG23	2.12	0.50
3:J:30:PHE:O	3:J:34:VAL:HG23	2.12	0.50
3:B:100:GLU:O	3:B:104:ARG:HG2	2.11	0.50
2:K:206:ILE:HD12	3:J:245:GLN:O	2.12	0.50
2:K:206:ILE:CD1	3:J:246:SER:HA	2.42	0.49
2:C:75:SER:OG	2:C:75:SER:O	2.28	0.49
6:K:301:PLC:OB	6:K:301:PLC:H81	2.12	0.49
6:G:301:PLC:OB	6:G:301:PLC:H81	2.12	0.49
1:I:124:PHE:CE2	1:I:140:THR:HG21	2.47	0.49
1:A:124:PHE:CE2	1:A:140:THR:HG21	2.47	0.49
3:F:86:PRO:HA	9:F:423:HOH:O	2.11	0.49
1:A:90:ASN:HB3	1:A:141:MET:HG3	1.95	0.49
1:E:105:ILE:HD12	1:E:114:VAL:HG21	1.94	0.49
6:C:310:PLC:H81	6:C:310:PLC:OB	2.12	0.49
1:A:105:ILE:HD12	1:A:114:VAL:HG21	1.94	0.48
1:E:90:ASN:HB3	1:E:141:MET:HG3	1.95	0.48
1:I:105:ILE:HD12	1:I:114:VAL:HG21	1.94	0.48
3:F:30:PHE:O	3:F:34:VAL:HG23	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:666:HOH:O	3:B:57:ARG:HG3	2.11	0.48
1:E:155:LYS:NZ	1:E:335:GLY:O	2.35	0.48
3:F:236:ARG:HA	3:F:236:ARG:HD3	1.65	0.48
3:F:52:SER:HA	3:F:55:LYS:HG3	1.96	0.48
6:G:303:PLC:H2A2	6:G:303:PLC:H4'1	1.95	0.48
1:E:145:GLN:HA	3:F:196:TYR:CE1	2.49	0.48
1:I:348:VAL:HB	1:I:351:ASN:HB2	1.96	0.48
3:B:237:TRP:CD1	5:B:305:D10:H51	2.49	0.48
2:G:234:TRP:CH2	2:G:243:PRO:HB2	2.49	0.48
2:G:104:ALA:HB2	2:G:186:ILE:HG12	1.96	0.48
6:K:303:PLC:H2A2	6:K:303:PLC:H4'1	1.95	0.48
1:I:93:MET:HG3	1:I:95:GLY:O	2.14	0.48
3:F:138:SER:O	3:F:140:SER:N	2.47	0.48
3:F:237:TRP:CD1	5:F:306:D10:H51	2.49	0.48
1:A:348:VAL:HB	1:A:351:ASN:HB2	1.96	0.48
2:K:104:ALA:HB2	2:K:186:ILE:HG12	1.96	0.48
2:K:149:ALA:HB1	3:J:39:ILE:HG13	1.95	0.48
1:E:93:MET:HG3	1:E:95:GLY:O	2.14	0.48
3:F:242:ARG:NH2	8:F:308:P1O:C4	2.77	0.48
3:J:86:PRO:HA	9:J:423:HOH:O	2.13	0.48
1:A:93:MET:HG3	1:A:95:GLY:O	2.14	0.48
1:A:173:LEU:HD21	3:B:172:GLU:HB2	1.96	0.48
1:I:90:ASN:HB3	1:I:141:MET:HG3	1.95	0.48
3:J:244:LEU:HD11	8:J:301:P1O:H43	1.94	0.48
9:A:615:HOH:O	3:B:189:VAL:HG13	2.14	0.47
2:C:104:ALA:HB2	2:C:186:ILE:HG12	1.96	0.47
2:C:275:GLY:HA3	2:C:276:GLN:HA	1.50	0.47
3:B:52:SER:HA	3:B:55:LYS:HG3	1.96	0.47
9:I:615:HOH:O	3:J:189:VAL:HG13	2.14	0.47
1:A:145:GLN:HA	3:B:196:TYR:CE1	2.49	0.47
3:B:226:LEU:HD21	2:K:251:PHE:CZ	2.48	0.47
3:B:236:ARG:HA	3:B:236:ARG:HD3	1.65	0.47
2:K:74:TRP:HA	2:K:78:LEU:HG	1.96	0.47
2:K:234:TRP:CH2	2:K:243:PRO:HB2	2.49	0.47
3:J:52:SER:HA	3:J:55:LYS:HG3	1.96	0.47
2:G:74:TRP:HA	2:G:78:LEU:HG	1.96	0.47
2:K:175:ILE:O	2:K:179:LEU:HB3	2.15	0.47
3:J:138:SER:O	3:J:140:SER:N	2.47	0.47
3:J:237:TRP:CD1	5:J:307:D10:H51	2.49	0.47
2:C:175:ILE:O	2:C:179:LEU:HB3	2.15	0.47
3:B:138:SER:O	3:B:140:SER:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:206:ILE:HD13	3:F:247:THR:HG23	1.95	0.47
1:E:348:VAL:HB	1:E:351:ASN:HB2	1.96	0.47
1:A:51:ASP:CG	1:A:400:ARG:HH22	2.18	0.47
2:C:74:TRP:HA	2:C:78:LEU:HG	1.97	0.47
2:C:234:TRP:CH2	2:C:243:PRO:HB2	2.49	0.47
3:J:242:ARG:NH2	8:J:301:P1O:H8	2.30	0.47
1:A:195:TRP:HB3	3:B:125:VAL:HB	1.97	0.47
2:G:255:ALA:HB3	3:F:36:SER:HB3	1.97	0.47
1:E:173:LEU:HD21	3:F:172:GLU:HB2	1.97	0.47
1:I:173:LEU:HD21	3:J:172:GLU:HB2	1.96	0.47
3:J:54:TRP:HH2	3:J:197:ILE:HG22	1.80	0.47
2:C:206:ILE:HD12	3:B:245:GLN:O	2.15	0.47
3:B:242:ARG:NH2	8:B:308:P1O:H8	2.30	0.47
2:G:112:TRP:CZ2	8:G:310:P1O:H1	2.50	0.47
3:J:45:MET:HE3	3:J:68:LEU:HD11	1.97	0.47
2:C:183:ILE:HG12	6:C:307:PLC:CBA	2.45	0.47
3:B:54:TRP:HH2	3:B:197:ILE:HG22	1.80	0.47
2:K:61:PHE:HA	6:K:308:PLC:H8'1	1.96	0.47
1:I:145:GLN:HA	3:J:196:TYR:CE1	2.50	0.47
1:I:292:ARG:HE	1:I:292:ARG:HB3	1.61	0.47
1:I:306:ASN:ND2	1:I:354:LEU:O	2.48	0.47
3:F:54:TRP:HH2	3:F:197:ILE:HG22	1.80	0.47
2:C:61:PHE:HA	6:C:307:PLC:H8'1	1.96	0.46
6:C:302:PLC:H4'1	6:C:302:PLC:H2A2	1.96	0.46
2:G:206:ILE:HD12	3:F:245:GLN:O	2.15	0.46
2:G:175:ILE:O	2:G:179:LEU:HB3	2.15	0.46
2:K:230:GLY:O	2:K:244:LEU:HD22	2.15	0.46
2:K:263:THR:HG21	9:J:406:HOH:O	2.14	0.46
2:K:275:GLY:HA3	2:K:276:GLN:HA	1.50	0.46
1:E:147:GLY:O	3:J:205:LEU:HB2	2.15	0.46
3:J:237:TRP:HB2	5:J:306:D10:H51	1.97	0.46
2:G:183:ILE:HG12	6:G:308:PLC:CBA	2.45	0.46
3:B:237:TRP:HB2	5:B:304:D10:H51	1.97	0.46
2:G:61:PHE:HA	6:G:308:PLC:H8'1	1.96	0.46
2:K:255:ALA:HB3	3:J:36:SER:HB3	1.97	0.46
2:K:245:HIS:HB3	3:J:43:LEU:HD13	1.97	0.46
1:E:105:ILE:HG13	1:E:110:VAL:HG21	1.98	0.46
1:I:105:ILE:HG13	1:I:110:VAL:HG21	1.98	0.46
1:A:258:TYR:CE2	3:B:166:PRO:HG3	2.51	0.46
1:A:379:ILE:HG21	1:A:409:LEU:HD23	1.98	0.46
2:C:206:ILE:HD13	3:B:247:THR:HG23	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:230:GLY:O	2:G:244:LEU:HD22	2.15	0.46
2:K:183:ILE:HG12	6:K:308:PLC:CBA	2.45	0.46
6:K:303:PLC:C7	7:K:304:HXG:H36	2.24	0.46
1:A:35:GLU:O	1:A:36:LYS:HB2	2.16	0.46
2:G:263:THR:HG21	9:F:407:HOH:O	2.15	0.46
2:K:221:LEU:HG	6:K:306:PLC:HE'3	1.98	0.46
1:E:51:ASP:CG	1:E:400:ARG:HH22	2.18	0.46
1:I:35:GLU:O	1:I:36:LYS:HB2	2.16	0.46
1:A:237:MET:HG3	3:B:137:LEU:HD11	1.98	0.46
2:C:86:GLU:HA	2:C:90:MET:HB2	1.98	0.46
1:E:35:GLU:O	1:E:36:LYS:HB2	2.16	0.46
1:A:306:ASN:ND2	1:A:354:LEU:O	2.48	0.46
2:K:155:GLN:HA	2:K:158:THR:HG22	1.98	0.46
3:F:237:TRP:HB2	5:F:305:D10:H51	1.97	0.46
2:C:230:GLY:O	2:C:244:LEU:HD22	2.15	0.46
3:B:244:LEU:HD23	8:B:308:P1O:H13	1.86	0.46
2:G:75:SER:O	2:G:75:SER:OG	2.28	0.46
2:C:255:ALA:HB3	3:B:36:SER:HB3	1.98	0.45
2:G:221:LEU:HG	6:G:306:PLC:HE'3	1.98	0.45
1:E:306:ASN:ND2	1:E:354:LEU:O	2.48	0.45
1:I:258:TYR:CE2	3:J:166:PRO:HG3	2.50	0.45
3:J:104:ARG:HA	3:J:108:PHE:HB2	1.98	0.45
2:G:162:THR:HG21	3:F:114:PHE:HE2	1.81	0.45
9:G:406:HOH:O	3:J:150:MET:CE	2.65	0.45
1:I:195:TRP:HB3	3:J:125:VAL:HB	1.97	0.45
3:F:104:ARG:HA	3:F:108:PHE:HB2	1.98	0.45
2:C:181:TYR:HA	2:C:184:TYR:CE2	2.51	0.45
1:E:195:TRP:HB3	3:F:125:VAL:HB	1.97	0.45
3:F:237:TRP:NE1	5:F:306:D10:C3	2.76	0.45
2:C:155:GLN:HA	2:C:158:THR:HG22	1.98	0.45
2:C:236:MET:HG2	7:C:303:HXG:CAE	2.47	0.45
2:G:181:TYR:HA	2:G:184:TYR:CE2	2.51	0.45
1:I:51:ASP:CG	1:I:400:ARG:HH22	2.18	0.45
3:J:138:SER:HA	8:J:304:P1O:C19	2.42	0.45
1:A:381:TYR:CZ	3:F:210:LYS:HA	2.52	0.45
2:G:149:ALA:HB1	3:F:39:ILE:HG13	1.98	0.45
1:I:216:LEU:HB2	3:J:83:TYR:CE2	2.52	0.45
2:K:181:TYR:HA	2:K:184:TYR:CE2	2.51	0.45
2:G:86:GLU:HA	2:G:90:MET:HB2	1.98	0.45
2:K:236:MET:HG2	7:K:304:HXG:CAE	2.47	0.45
1:E:51:ASP:OD2	1:E:400:ARG:NH2	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:379:ILE:HG21	1:E:409:LEU:HD23	1.98	0.45
1:I:379:ILE:HG21	1:I:409:LEU:HD23	1.98	0.45
1:A:105:ILE:HG13	1:A:110:VAL:HG21	1.98	0.45
2:G:155:GLN:HA	2:G:158:THR:HG22	1.98	0.45
2:G:236:MET:HG2	7:G:304:HXG:CAE	2.47	0.45
2:K:86:GLU:HA	2:K:90:MET:HB2	1.98	0.45
1:E:237:MET:HG3	3:F:137:LEU:HD11	1.99	0.45
3:J:231:TRP:HA	3:J:234:ILE:HB	1.99	0.45
2:C:221:LEU:HG	6:C:305:PLC:HE'3	1.98	0.44
3:B:210:LYS:HA	1:I:381:TYR:CZ	2.52	0.44
1:E:258:TYR:CE2	3:F:166:PRO:HG3	2.51	0.44
3:F:231:TRP:HA	3:F:234:ILE:HB	1.99	0.44
3:B:104:ARG:HA	3:B:108:PHE:HB2	1.98	0.44
2:K:67:TRP:CG	7:K:307:HXG:H40	2.51	0.44
1:E:216:LEU:HB2	3:F:83:TYR:CE2	2.52	0.44
1:I:101:LYS:HD2	1:I:101:LYS:HA	1.80	0.44
2:C:162:THR:HG21	3:B:114:PHE:HE2	1.82	0.44
2:C:251:PHE:CZ	3:F:226:LEU:HD21	2.49	0.44
9:C:405:HOH:O	3:F:150:MET:CE	2.65	0.44
3:B:150:MET:CE	9:K:406:HOH:O	2.65	0.44
3:B:231:TRP:HA	3:B:234:ILE:HB	1.99	0.44
2:K:235:PHE:HA	7:K:304:HXG:H41	2.00	0.44
1:I:287:GLU:O	1:I:301:LYS:HB3	2.18	0.44
2:G:248:PHE:HB2	3:F:43:LEU:HD12	2.00	0.44
1:A:287:GLU:O	1:A:301:LYS:HB3	2.18	0.44
2:C:235:PHE:HA	7:C:303:HXG:H41	2.00	0.44
2:G:235:PHE:HA	7:G:304:HXG:H41	2.00	0.44
2:K:248:PHE:HB2	3:J:43:LEU:HD12	2.00	0.44
1:I:237:MET:HG3	3:J:137:LEU:HD11	1.99	0.44
2:C:124:PRO:HB2	3:B:7:ALA:N	2.32	0.44
2:C:263:THR:HG21	9:B:408:HOH:O	2.17	0.44
1:E:381:TYR:CZ	3:J:210:LYS:HA	2.52	0.44
1:A:51:ASP:OD2	1:A:400:ARG:NH2	2.49	0.44
3:F:29:VAL:HG13	3:F:33:ILE:HD12	2.00	0.44
1:A:306:ASN:HB2	1:A:354:LEU:HD23	2.00	0.43
2:K:162:THR:HG21	3:J:114:PHE:HE2	1.83	0.43
3:F:138:SER:HA	8:F:303:P1O:C19	2.42	0.43
3:J:37:TYR:OH	3:J:68:LEU:O	2.29	0.43
2:C:154:GLU:OE2	3:B:38:HIS:NE2	2.42	0.43
1:E:97:VAL:HA	1:E:132:ARG:HB2	2.00	0.43
1:I:51:ASP:OD2	1:I:400:ARG:NH2	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:29:VAL:HG13	3:B:33:ILE:HD12	2.00	0.43
3:B:37:TYR:OH	3:B:68:LEU:O	2.29	0.43
2:G:158:THR:O	2:G:162:THR:HG23	2.19	0.43
2:K:213:LEU:HD22	2:K:258:VAL:HA	2.00	0.43
1:E:287:GLU:O	1:E:301:LYS:HB3	2.18	0.43
2:G:96:GLU:HA	6:G:308:PLC:H7A1	2.01	0.43
2:G:181:TYR:HB2	2:G:182:PRO:HD3	2.01	0.43
2:K:112:TRP:CZ2	8:K:310:P1O:H1	2.50	0.43
3:F:54:TRP:CH2	3:F:197:ILE:HG22	2.54	0.43
3:F:242:ARG:NH2	8:F:308:P1O:H8	2.34	0.43
3:J:54:TRP:CH2	3:J:197:ILE:HG22	2.54	0.43
8:J:301:P1O:H15	8:J:301:P1O:C20	2.47	0.43
1:A:216:LEU:HB2	3:B:83:TYR:CE2	2.53	0.43
2:C:181:TYR:HB2	2:C:182:PRO:HD3	2.01	0.43
9:C:405:HOH:O	3:F:150:MET:HE3	2.17	0.43
2:G:158:THR:HB	3:F:108:PHE:CE2	2.54	0.43
2:G:206:ILE:CD1	3:F:246:SER:HA	2.49	0.43
2:K:96:GLU:HA	6:K:308:PLC:H7A1	2.01	0.43
1:E:306:ASN:HB2	1:E:354:LEU:HD23	2.00	0.43
3:J:236:ARG:HA	3:J:236:ARG:HD3	1.65	0.43
1:A:312:ILE:HG12	1:A:354:LEU:HB3	2.01	0.43
2:C:96:GLU:HA	6:C:307:PLC:H7A1	2.01	0.43
2:K:181:TYR:HB2	2:K:182:PRO:HD3	2.01	0.43
1:E:324:PHE:HA	1:E:342:ALA:HB3	2.01	0.43
3:B:115:PRO:HB2	3:B:117:ASN:OD1	2.19	0.43
2:K:158:THR:O	2:K:162:THR:HG23	2.19	0.43
2:K:198:ARG:HH21	8:K:309:P1O:H2	1.84	0.43
1:E:312:ILE:HG12	1:E:354:LEU:HB3	2.01	0.43
2:C:158:THR:HB	3:B:108:PHE:CE2	2.53	0.43
2:G:198:ARG:HH21	8:G:309:P1O:H2	1.84	0.43
6:G:303:PLC:C7	7:G:304:HXG:H36	2.24	0.43
1:I:96:PRO:HG3	3:J:114:PHE:CE1	2.53	0.43
1:I:312:ILE:HG12	1:I:354:LEU:HB3	2.01	0.43
3:J:29:VAL:HG13	3:J:33:ILE:HD12	2.00	0.43
2:C:248:PHE:HB2	3:B:43:LEU:HD12	2.01	0.43
2:G:154:GLU:OE2	3:F:38:HIS:NE2	2.43	0.43
2:C:223:ASN:OD1	2:C:247:GLY:HA3	2.19	0.42
3:B:237:TRP:NE1	5:B:305:D10:C3	2.76	0.42
5:B:306:D10:H103	5:J:308:D10:H103	2.00	0.42
8:B:308:P1O:H43	8:B:308:P1O:H17	2.01	0.42
9:G:406:HOH:O	3:J:150:MET:HE3	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:227:ASN:ND2	2:K:228:GLU:OE2	2.45	0.42
1:E:96:PRO:HG3	3:F:114:PHE:CE1	2.54	0.42
1:I:324:PHE:HA	1:I:342:ALA:HB3	2.01	0.42
1:A:324:PHE:HA	1:A:342:ALA:HB3	2.01	0.42
2:G:223:ASN:OD1	2:G:247:GLY:HA3	2.19	0.42
6:G:303:PLC:H1A1	3:J:59:LEU:HD11	2.00	0.42
3:J:214:PRO:HA	6:J:303:PLC:H2'1	2.02	0.42
3:J:237:TRP:NE1	5:J:307:D10:C3	2.76	0.42
8:J:301:P1O:H43	8:J:301:P1O:H17	2.01	0.42
1:A:96:PRO:HG3	3:B:114:PHE:CE1	2.54	0.42
1:A:147:GLY:O	3:F:205:LEU:HB2	2.19	0.42
2:C:149:ALA:HB1	3:B:39:ILE:HG13	2.00	0.42
3:B:57:ARG:HH21	3:B:201:GLU:CD	2.23	0.42
3:J:59:LEU:HD13	3:J:59:LEU:HA	1.91	0.42
3:J:115:PRO:HB2	3:J:117:ASN:OD1	2.19	0.42
2:C:158:THR:O	2:C:162:THR:HG23	2.19	0.42
3:B:54:TRP:CH2	3:B:197:ILE:HG22	2.54	0.42
3:B:93:VAL:HG21	3:B:128:ALA:HB2	2.01	0.42
2:G:251:PHE:CZ	3:J:226:LEU:HD21	2.50	0.42
2:G:262:LEU:HD23	2:G:262:LEU:HA	1.91	0.42
3:F:57:ARG:HH21	3:F:201:GLU:CD	2.23	0.42
8:F:308:P1O:H43	8:F:308:P1O:H17	2.01	0.42
2:G:213:LEU:HD22	2:G:258:VAL:HA	2.00	0.42
1:I:306:ASN:HB2	1:I:354:LEU:HD23	2.00	0.42
3:F:198:ARG:HG2	3:F:200:VAL:HG13	2.01	0.42
3:J:93:VAL:HG21	3:J:128:ALA:HB2	2.01	0.42
1:A:97:VAL:HA	1:A:132:ARG:HB2	2.00	0.42
2:K:158:THR:HB	3:J:108:PHE:CE2	2.54	0.42
6:K:301:PLC:O2	3:J:199:MET:SD	2.77	0.42
3:F:115:PRO:HB2	3:F:117:ASN:OD1	2.19	0.42
3:F:194:PRO:HG2	3:F:197:ILE:HG13	2.01	0.42
3:F:214:PRO:HA	6:F:302:PLC:H2'1	2.02	0.42
3:J:198:ARG:HG2	3:J:200:VAL:HG13	2.01	0.42
3:J:213:ALA:HB3	6:J:303:PLC:C1	2.50	0.42
3:J:244:LEU:CD1	8:J:301:P1O:H42	2.39	0.42
1:A:195:TRP:O	3:B:125:VAL:HG11	2.20	0.42
2:C:113:LYS:HB3	2:C:113:LYS:HE2	1.60	0.42
3:B:214:PRO:HA	6:B:301:PLC:H2'1	2.02	0.42
6:G:303:PLC:H1A1	6:G:303:PLC:H31	1.83	0.42
1:I:97:VAL:HA	1:I:132:ARG:HB2	2.00	0.42
2:G:236:MET:H	2:G:236:MET:HG2	1.64	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:113:LYS:HB3	2:K:113:LYS:HE2	1.60	0.42
9:E:613:HOH:O	3:F:189:VAL:HG13	2.18	0.42
1:I:293:VAL:HA	1:I:294:PRO:HA	1.92	0.42
2:C:89:TRP:CE2	2:C:171:PRO:HB3	2.55	0.42
2:C:213:LEU:HD22	2:C:258:VAL:HA	2.00	0.42
2:G:124:PRO:HB2	3:F:7:ALA:N	2.35	0.42
1:E:86:VAL:HB	1:E:145:GLN:HB2	2.02	0.42
1:E:391:LEU:HB2	1:E:403:VAL:HG22	2.02	0.42
1:A:405:ILE:HA	9:A:632:HOH:O	2.19	0.42
2:G:89:TRP:CE2	2:G:171:PRO:HB3	2.55	0.42
2:K:223:ASN:OD1	2:K:247:GLY:HA3	2.19	0.42
1:E:195:TRP:O	3:F:125:VAL:HG11	2.20	0.42
1:I:86:VAL:HB	1:I:145:GLN:HB2	2.01	0.42
1:I:319:THR:HG23	1:I:320:ALA:H	1.85	0.42
2:K:227:ASN:O	2:K:231:HIS:HB2	2.20	0.41
3:F:104:ARG:HA	3:F:104:ARG:HD3	1.87	0.41
2:C:112:TRP:CZ2	8:C:309:P1O:H1	2.50	0.41
2:C:198:ARG:HH21	8:C:308:P1O:H2	1.84	0.41
2:G:275:GLY:HA3	2:G:276:GLN:HA	1.50	0.41
1:E:405:ILE:HA	9:E:634:HOH:O	2.20	0.41
2:C:227:ASN:ND2	2:C:228:GLU:OE2	2.45	0.41
2:G:112:TRP:CE2	8:G:310:P1O:H7	2.56	0.41
3:F:93:VAL:HG21	3:F:128:ALA:HB2	2.01	0.41
3:J:57:ARG:HH21	3:J:201:GLU:CD	2.23	0.41
3:J:194:PRO:HG2	3:J:197:ILE:HG13	2.02	0.41
2:C:167:THR:HG23	2:C:169:PHE:H	1.86	0.41
3:B:51:TRP:HB2	3:B:54:TRP:CD1	2.56	0.41
3:B:213:ALA:HB3	6:B:301:PLC:C1	2.50	0.41
2:K:78:LEU:HB3	1:I:33:HIS:HD2	1.85	0.41
2:K:206:ILE:HB	3:J:244:LEU:O	2.20	0.41
1:E:319:THR:HG23	1:E:320:ALA:H	1.85	0.41
3:J:51:TRP:HB2	3:J:54:TRP:CD1	2.56	0.41
1:A:86:VAL:HB	1:A:145:GLN:HB2	2.02	0.41
2:C:112:TRP:CZ2	8:C:309:P1O:C2	3.04	0.41
3:B:194:PRO:HG2	3:B:197:ILE:HG13	2.02	0.41
2:G:78:LEU:HB3	1:E:33:HIS:HD2	1.85	0.41
2:G:159:TRP:O	2:G:163:ILE:HG13	2.21	0.41
2:K:89:TRP:CE2	2:K:171:PRO:HB3	2.55	0.41
7:K:304:HXG:H40	7:K:304:HXG:OAW	2.21	0.41
1:I:36:LYS:HG3	1:I:374:TYR:CD2	2.56	0.41
1:I:195:TRP:O	3:J:125:VAL:HG11	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:391:LEU:HB2	1:A:403:VAL:HG22	2.02	0.41
8:C:308:P1O:H7	8:C:308:P1O:H1	1.85	0.41
3:B:198:ARG:HG2	3:B:200:VAL:HG13	2.01	0.41
2:G:113:LYS:HB3	2:G:113:LYS:HE2	1.61	0.41
2:G:227:ASN:O	2:G:231:HIS:HB2	2.20	0.41
7:G:304:HXG:OAW	7:G:304:HXG:H40	2.21	0.41
2:K:112:TRP:CE2	8:K:310:P1O:H7	2.56	0.41
2:K:57:ILE:HD12	2:K:57:ILE:HA	1.90	0.41
1:E:395:ASP:OD2	1:E:399:ASN:ND2	2.54	0.41
8:F:308:P1O:H17	8:F:308:P1O:C20	2.51	0.41
1:A:36:LYS:HG3	1:A:374:TYR:CD2	2.56	0.41
1:A:338:GLU:H	1:A:338:GLU:CD	2.24	0.41
2:C:227:ASN:O	2:C:231:HIS:HB2	2.20	0.41
7:C:303:HXG:H40	7:C:303:HXG:OAW	2.21	0.41
3:B:68:LEU:HD23	3:B:68:LEU:HA	1.83	0.41
3:B:223:MET:O	3:B:227:ILE:HG12	2.20	0.41
2:K:48:LYS:HD3	2:K:50:TRP:CD1	2.41	0.41
2:K:159:TRP:O	2:K:163:ILE:HG13	2.21	0.41
1:I:338:GLU:H	1:I:338:GLU:CD	2.24	0.41
1:I:395:ASP:OD2	1:I:399:ASN:ND2	2.54	0.41
3:F:51:TRP:HB2	3:F:54:TRP:CD1	2.56	0.41
8:F:308:P1O:H15	8:F:308:P1O:C20	2.47	0.41
3:J:223:MET:O	3:J:227:ILE:HG12	2.21	0.41
2:C:75:SER:O	2:C:76:ALA:HB3	2.21	0.41
3:B:53:ASP:O	3:B:198:ARG:HD2	2.21	0.41
8:B:308:P1O:H15	8:B:308:P1O:C20	2.47	0.41
2:G:274:LEU:HD11	2:G:276:GLN:HE22	1.86	0.41
1:I:405:ILE:HA	9:I:632:HOH:O	2.20	0.41
3:F:223:MET:O	3:F:227:ILE:HG12	2.21	0.41
8:F:308:P1O:C6	8:F:308:P1O:C20	2.99	0.41
2:C:274:LEU:HD11	2:C:276:GLN:HE22	1.86	0.40
2:G:67:TRP:CG	7:G:307:HXG:H40	2.51	0.40
1:E:101:LYS:HD2	1:E:101:LYS:HA	1.80	0.40
1:A:101:LYS:HD2	1:A:101:LYS:HA	1.80	0.40
1:A:342:ALA:HB1	1:A:345:GLY:HA3	2.04	0.40
3:B:59:LEU:HD11	6:K:303:PLC:H1A1	2.03	0.40
2:K:156:ASP:HA	2:K:172:SER:OG	2.21	0.40
2:K:167:THR:HG23	2:K:169:PHE:H	1.85	0.40
3:J:53:ASP:O	3:J:198:ARG:HD2	2.21	0.40
1:E:36:LYS:HG3	1:E:374:TYR:CD2	2.56	0.40
1:E:338:GLU:CD	1:E:338:GLU:H	2.24	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:53:ASP:O	3:F:198:ARG:HD2	2.21	0.40
3:F:68:LEU:HD23	3:F:68:LEU:HA	1.83	0.40
8:J:301:P1O:H17	8:J:301:P1O:C20	2.51	0.40
2:C:112:TRP:CE2	8:C:309:P1O:H7	2.56	0.40
2:C:159:TRP:O	2:C:163:ILE:HG13	2.21	0.40
5:B:306:D10:H103	5:F:307:D10:H103	2.03	0.40
2:G:167:THR:HG23	2:G:169:PHE:H	1.86	0.40
2:G:239:LEU:HD11	3:F:199:MET:HE2	2.02	0.40
8:B:302:P1O:H2	8:B:302:P1O:H12	1.85	0.40
2:K:112:TRP:CZ2	8:K:310:P1O:C2	3.04	0.40
1:I:391:LEU:HB2	1:I:403:VAL:HG22	2.02	0.40
3:J:115:PRO:O	3:J:119:VAL:HG22	2.22	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	380/414 (92%)	365 (96%)	15 (4%)	0	100	100
1	E	380/414 (92%)	365 (96%)	15 (4%)	0	100	100
1	I	380/414 (92%)	365 (96%)	15 (4%)	0	100	100
2	C	234/260 (90%)	212 (91%)	19 (8%)	3 (1%)	12	8
2	G	234/260 (90%)	212 (91%)	19 (8%)	3 (1%)	12	8
2	K	234/260 (90%)	213 (91%)	18 (8%)	3 (1%)	12	8
3	B	239/247 (97%)	227 (95%)	11 (5%)	1 (0%)	34	37
3	F	239/247 (97%)	227 (95%)	11 (5%)	1 (0%)	34	37
3	J	239/247 (97%)	227 (95%)	11 (5%)	1 (0%)	34	37
All	All	2559/2763 (93%)	2413 (94%)	134 (5%)	12 (0%)	32	29

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	277	SER
2	G	277	SER
2	K	277	SER
2	C	231	HIS
3	B	244	LEU
2	G	231	HIS
2	K	231	HIS
3	F	244	LEU
3	J	244	LEU
2	C	233	PHE
2	G	233	PHE
2	K	233	PHE

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	323/345 (94%)	313 (97%)	10 (3%)	40	49
1	E	323/345 (94%)	312 (97%)	11 (3%)	37	45
1	I	323/345 (94%)	313 (97%)	10 (3%)	40	49
2	C	200/212 (94%)	185 (92%)	15 (8%)	13	12
2	G	200/212 (94%)	185 (92%)	15 (8%)	13	12
2	K	200/212 (94%)	185 (92%)	15 (8%)	13	12
3	B	206/210 (98%)	202 (98%)	4 (2%)	57	66
3	F	206/210 (98%)	202 (98%)	4 (2%)	57	66
3	J	206/210 (98%)	202 (98%)	4 (2%)	57	66
All	All	2187/2301 (95%)	2099 (96%)	88 (4%)	35	37

All (88) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	HIS

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Mol	Chain	Res	Type
1	A	35	GLU
1	A	36	LYS
1	A	64	THR
1	A	180	LEU
1	A	256	SER
1	A	309	ASN
1	A	363	ASP
1	A	397	THR
1	A	400	ARG
2	C	45	LEU
2	C	49	LYS
2	C	74	TRP
2	C	86	GLU
2	C	105	SER
2	C	123	THR
2	C	166	ASP
2	C	184	TYR
2	C	196	LYS
2	C	204	LYS
2	C	207	SER
2	C	210	TYR
2	C	231	HIS
2	C	236	MET
2	C	240	PHE
3	B	8	VAL
3	B	39	ILE
3	B	138	SER
3	B	244	LEU
2	G	45	LEU
2	G	49	LYS
2	G	74	TRP
2	G	86	GLU
2	G	105	SER
2	G	123	THR
2	G	166	ASP
2	G	184	TYR
2	G	196	LYS
2	G	204	LYS
2	G	207	SER
2	G	210	TYR
2	G	231	HIS
2	G	236	MET

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Mol	Chain	Res	Type
2	G	240	PHE
2	K	45	LEU
2	K	49	LYS
2	K	74	TRP
2	K	86	GLU
2	K	105	SER
2	K	123	THR
2	K	166	ASP
2	K	184	TYR
2	K	196	LYS
2	K	204	LYS
2	K	207	SER
2	K	210	TYR
2	K	231	HIS
2	K	236	MET
2	K	240	PHE
1	E	33	HIS
1	E	35	GLU
1	E	36	LYS
1	E	64	THR
1	E	180	LEU
1	E	256	SER
1	E	296	ARG
1	E	309	ASN
1	E	363	ASP
1	E	397	THR
1	E	400	ARG
1	I	33	HIS
1	I	35	GLU
1	I	36	LYS
1	I	64	THR
1	I	180	LEU
1	I	256	SER
1	I	309	ASN
1	I	363	ASP
1	I	397	THR
1	I	400	ARG
3	F	8	VAL
3	F	39	ILE
3	F	138	SER
3	F	244	LEU
3	J	8	VAL

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Mol	Chain	Res	Type
3	J	39	ILE
3	J	138	SER
3	J	244	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 63 ligands modelled in this entry, 9 are monoatomic - leaving 54 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	PLC	K	308	-	41,41,41	0.85	0	47,49,49	0.68	2 (4%)
6	PLC	K	306	-	41,41,41	0.86	0	47,49,49	0.68	1 (2%)
6	PLC	C	305	-	41,41,41	0.86	0	47,49,49	0.68	1 (2%)
5	D10	F	304	-	9,9,9	0.21	0	8,8,8	0.56	0
5	D10	B	305	-	9,9,9	0.22	0	8,8,8	0.55	0
6	PLC	G	303	-	41,41,41	1.05	2 (4%)	47,49,49	1.09	3 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
8	P1O	B	308	-	37,37,37	1.11	2 (5%)	43,45,45	1.09	3 (6%)
7	HXG	G	307	-	29,29,29	0.35	0	35,37,37	0.36	0
5	D10	B	306	-	9,9,9	0.21	0	8,8,8	0.56	0
7	HXG	G	304	-	29,29,29	0.35	0	35,37,37	0.36	0
6	PLC	K	301	-	41,41,41	1.05	2 (4%)	47,49,49	1.04	3 (6%)
5	D10	J	306	-	9,9,9	0.21	0	8,8,8	0.56	0
6	PLC	K	303	-	41,41,41	1.05	2 (4%)	47,49,49	1.09	3 (6%)
5	D10	G	305	-	9,9,9	0.21	0	8,8,8	0.55	0
8	P1O	G	310	-	37,37,37	1.11	2 (5%)	43,45,45	1.12	3 (6%)
8	P1O	J	304	-	37,37,37	1.11	2 (5%)	43,45,45	1.10	3 (6%)
5	D10	K	305	-	9,9,9	0.21	0	8,8,8	0.56	0
6	PLC	G	306	-	41,41,41	0.86	0	47,49,49	0.68	1 (2%)
5	D10	J	308	-	9,9,9	0.21	0	8,8,8	0.56	0
6	PLC	J	302	-	41,41,41	0.80	0	47,49,49	0.75	1 (2%)
5	D10	F	305	-	9,9,9	0.21	0	8,8,8	0.56	0
5	D10	A	503	-	9,9,9	0.21	0	8,8,8	0.55	0
8	P1O	G	309	-	37,37,37	1.11	2 (5%)	43,45,45	1.12	3 (6%)
8	P1O	J	301	-	37,37,37	1.11	2 (5%)	43,45,45	1.09	3 (6%)
8	P1O	F	303	-	37,37,37	1.11	2 (5%)	43,45,45	1.10	3 (6%)
8	P1O	F	308	-	37,37,37	1.11	2 (5%)	43,45,45	1.08	2 (4%)
5	D10	I	503	-	9,9,9	0.21	0	8,8,8	0.55	0
7	HXG	K	304	-	29,29,29	0.35	0	35,37,37	0.36	0
6	PLC	B	301	-	41,41,41	0.87	0	47,49,49	0.84	1 (2%)
5	D10	B	303	-	9,9,9	0.21	0	8,8,8	0.56	0
5	D10	C	304	-	9,9,9	0.21	0	8,8,8	0.56	0
5	D10	F	306	-	9,9,9	0.22	0	8,8,8	0.55	0
8	P1O	B	302	-	37,37,37	1.11	2 (5%)	43,45,45	1.10	3 (6%)
8	P1O	K	310	-	37,37,37	1.11	2 (5%)	43,45,45	1.12	3 (6%)
8	P1O	K	309	-	37,37,37	1.11	2 (5%)	43,45,45	1.11	3 (6%)
5	D10	F	307	-	9,9,9	0.20	0	8,8,8	0.56	0
7	HXG	C	303	-	29,29,29	0.35	0	35,37,37	0.36	0
6	PLC	C	307	-	41,41,41	0.85	0	47,49,49	0.68	2 (4%)
7	HXG	K	307	-	29,29,29	0.35	0	35,37,37	0.36	0
5	D10	B	304	-	9,9,9	0.21	0	8,8,8	0.55	0
6	PLC	G	301	-	41,41,41	1.05	2 (4%)	47,49,49	1.04	3 (6%)
8	P1O	C	309	-	37,37,37	1.11	2 (5%)	43,45,45	1.12	3 (6%)
7	HXG	C	306	-	29,29,29	0.35	0	35,37,37	0.36	0
6	PLC	F	301	-	41,41,41	0.80	0	47,49,49	0.75	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	PLC	F	302	-	41,41,41	0.87	0	47,49,49	0.83	1 (2%)
6	PLC	J	303	-	41,41,41	0.87	0	47,49,49	0.83	1 (2%)
6	PLC	C	310	-	41,41,41	1.05	2 (4%)	47,49,49	1.04	3 (6%)
6	PLC	B	307	-	41,41,41	0.80	0	47,49,49	0.75	1 (2%)
6	PLC	C	302	-	41,41,41	1.05	2 (4%)	47,49,49	1.09	3 (6%)
8	P1O	C	308	-	37,37,37	1.11	2 (5%)	43,45,45	1.11	3 (6%)
6	PLC	G	308	-	41,41,41	0.85	0	47,49,49	0.68	2 (4%)
5	D10	J	305	-	9,9,9	0.20	0	8,8,8	0.56	0
5	D10	E	503	-	9,9,9	0.21	0	8,8,8	0.55	0
5	D10	J	307	-	9,9,9	0.22	0	8,8,8	0.55	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
6	PLC	K	308	-	-	17/45/45/45	-
6	PLC	K	306	-	-	13/45/45/45	-
6	PLC	C	305	-	-	13/45/45/45	-
5	D10	F	304	-	-	0/7/7/7	-
5	D10	B	305	-	-	6/7/7/7	-
6	PLC	G	303	-	-	22/45/45/45	-
8	P1O	B	308	-	-	20/41/41/41	-
7	HXG	G	307	-	-	7/33/33/33	-
5	D10	B	306	-	-	5/7/7/7	-
7	HXG	G	304	-	-	9/33/33/33	-
6	PLC	K	301	-	-	26/45/45/45	-
5	D10	J	306	-	-	2/7/7/7	-
6	PLC	K	303	-	-	22/45/45/45	-
5	D10	G	305	-	-	0/7/7/7	-
8	P1O	G	310	-	-	26/41/41/41	-
8	P1O	J	304	-	-	25/41/41/41	-
5	D10	K	305	-	-	0/7/7/7	-
6	PLC	G	306	-	-	13/45/45/45	-
5	D10	J	308	-	-	5/7/7/7	-
6	PLC	J	302	-	-	15/45/45/45	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	D10	F	305	-	-	2/7/7/7	-
5	D10	A	503	-	-	0/7/7/7	-
8	P1O	G	309	-	-	18/41/41/41	-
8	P1O	J	301	-	-	20/41/41/41	-
8	P1O	F	303	-	-	25/41/41/41	-
8	P1O	F	308	-	-	20/41/41/41	-
5	D10	I	503	-	-	0/7/7/7	-
7	HXG	K	304	-	-	9/33/33/33	-
6	PLC	B	301	-	-	15/45/45/45	-
5	D10	B	303	-	-	0/7/7/7	-
5	D10	C	304	-	-	0/7/7/7	-
5	D10	F	306	-	-	6/7/7/7	-
8	P1O	B	302	-	-	25/41/41/41	-
8	P1O	K	310	-	-	26/41/41/41	-
8	P1O	K	309	-	-	18/41/41/41	-
5	D10	F	307	-	-	5/7/7/7	-
7	HXG	C	303	-	-	9/33/33/33	-
6	PLC	C	307	-	-	17/45/45/45	-
7	HXG	K	307	-	-	7/33/33/33	-
5	D10	B	304	-	-	2/7/7/7	-
6	PLC	G	301	-	-	26/45/45/45	-
8	P1O	C	309	-	-	26/41/41/41	-
7	HXG	C	306	-	-	7/33/33/33	-
6	PLC	F	301	-	-	15/45/45/45	-
6	PLC	F	302	-	-	15/45/45/45	-
6	PLC	J	303	-	-	15/45/45/45	-
6	PLC	C	310	-	-	26/45/45/45	-
6	PLC	B	307	-	-	15/45/45/45	-
6	PLC	C	302	-	-	22/45/45/45	-
8	P1O	C	308	-	-	19/41/41/41	-
6	PLC	G	308	-	-	17/45/45/45	-
5	D10	J	305	-	-	0/7/7/7	-
5	D10	E	503	-	-	0/7/7/7	-
5	D10	J	307	-	-	6/7/7/7	-

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	K	301	PLC	O3-CB	4.30	1.45	1.33
8	B	302	P1O	O5-C9	4.30	1.45	1.33
8	J	304	P1O	O5-C9	4.28	1.45	1.33
6	G	301	PLC	O3-CB	4.28	1.45	1.33
8	C	308	P1O	O5-C9	4.28	1.45	1.33
8	F	303	P1O	O5-C9	4.27	1.45	1.33
8	F	308	P1O	O5-C9	4.27	1.45	1.33
6	C	310	PLC	O3-CB	4.27	1.45	1.33
8	B	308	P1O	O5-C9	4.27	1.45	1.33
8	K	309	P1O	O5-C9	4.26	1.45	1.33
8	J	301	P1O	O5-C9	4.26	1.45	1.33
8	G	309	P1O	O5-C9	4.26	1.45	1.33
6	G	303	PLC	O3-CB	4.25	1.45	1.33
6	C	302	PLC	O3-CB	4.24	1.45	1.33
8	K	310	P1O	O5-C9	4.24	1.45	1.33
6	K	303	PLC	O3-CB	4.24	1.45	1.33
8	C	309	P1O	O5-C9	4.23	1.45	1.33
8	G	310	P1O	O5-C9	4.23	1.45	1.33
8	J	301	P1O	O7-C19	4.16	1.46	1.34
8	F	308	P1O	O7-C19	4.16	1.46	1.34
8	G	310	P1O	O7-C19	4.15	1.46	1.34
8	B	308	P1O	O7-C19	4.14	1.46	1.34
8	C	309	P1O	O7-C19	4.13	1.46	1.34
6	K	301	PLC	O2-C'	4.10	1.45	1.34
6	C	310	PLC	O2-C'	4.09	1.45	1.34
8	K	310	P1O	O7-C19	4.09	1.45	1.34
6	G	301	PLC	O2-C'	4.09	1.45	1.34
8	B	302	P1O	O7-C19	4.08	1.45	1.34
8	F	303	P1O	O7-C19	4.08	1.45	1.34
6	K	303	PLC	O2-C'	4.08	1.45	1.34
6	G	303	PLC	O2-C'	4.07	1.45	1.34
8	J	304	P1O	O7-C19	4.07	1.45	1.34
6	C	302	PLC	O2-C'	4.07	1.45	1.34
8	G	309	P1O	O7-C19	4.06	1.45	1.34
8	K	309	P1O	O7-C19	4.06	1.45	1.34
8	C	308	P1O	O7-C19	4.05	1.45	1.34

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	B	308	P1O	O7-C19-C20	4.24	120.63	111.50
8	J	301	P1O	O7-C19-C20	4.23	120.62	111.50
8	F	308	P1O	O7-C19-C20	4.22	120.59	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	K	310	P1O	O7-C19-C20	4.18	120.50	111.50
8	C	309	P1O	O7-C19-C20	4.17	120.49	111.50
8	G	309	P1O	O7-C19-C20	4.17	120.48	111.50
8	G	310	P1O	O7-C19-C20	4.16	120.47	111.50
8	J	304	P1O	O7-C19-C20	4.15	120.44	111.50
8	C	308	P1O	O7-C19-C20	4.15	120.44	111.50
8	F	303	P1O	O7-C19-C20	4.13	120.41	111.50
8	B	302	P1O	O7-C19-C20	4.13	120.41	111.50
8	K	309	P1O	O7-C19-C20	4.12	120.39	111.50
6	G	303	PLC	O2-C'-C1'	4.11	120.36	111.50
6	C	302	PLC	O2-C'-C1'	4.10	120.35	111.50
6	K	303	PLC	O2-C'-C1'	4.09	120.33	111.50
6	C	310	PLC	O2-C'-C1'	4.08	120.29	111.50
6	G	301	PLC	O2-C'-C1'	4.08	120.29	111.50
6	K	301	PLC	O2-C'-C1'	4.06	120.26	111.50
6	J	302	PLC	O2-C'-C1'	3.83	119.75	111.50
6	F	301	PLC	O2-C'-C1'	3.82	119.74	111.50
6	B	307	PLC	O2-C'-C1'	3.81	119.70	111.50
6	B	301	PLC	O2-C'-C1'	3.71	119.51	111.50
6	F	302	PLC	O2-C'-C1'	3.69	119.45	111.50
6	J	303	PLC	O2-C'-C1'	3.68	119.43	111.50
6	K	308	PLC	O2-C'-C1'	3.16	118.31	111.50
6	C	307	PLC	O2-C'-C1'	3.14	118.26	111.50
6	G	308	PLC	O2-C'-C1'	3.14	118.26	111.50
6	G	303	PLC	O3-CB-C1B	2.74	120.49	111.91
6	K	303	PLC	O3-CB-C1B	2.73	120.48	111.91
6	C	302	PLC	O3-CB-C1B	2.73	120.48	111.91
8	J	304	P1O	O5-C9-C10	2.69	120.36	111.91
8	B	308	P1O	O5-C9-C10	2.69	120.35	111.91
8	J	301	P1O	O5-C9-C10	2.69	120.34	111.91
6	C	310	PLC	O3-CB-C1B	2.69	120.34	111.91
8	B	302	P1O	O5-C9-C10	2.68	120.33	111.91
8	F	308	P1O	O5-C9-C10	2.68	120.33	111.91
8	F	303	P1O	O5-C9-C10	2.68	120.32	111.91
8	G	309	P1O	O5-C9-C10	2.68	120.31	111.91
6	G	301	PLC	O3-CB-C1B	2.67	120.29	111.91
8	K	309	P1O	O5-C9-C10	2.67	120.28	111.91
8	C	308	P1O	O5-C9-C10	2.67	120.28	111.91
6	K	301	PLC	O3-CB-C1B	2.66	120.25	111.91
8	K	310	P1O	O5-C9-C10	2.62	120.14	111.91
8	G	310	P1O	O5-C9-C10	2.62	120.13	111.91
8	C	309	P1O	O5-C9-C10	2.61	120.11	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	G	306	PLC	O2-C'-C1'	2.45	116.78	111.50
6	C	305	PLC	O2-C'-C1'	2.45	116.78	111.50
6	K	306	PLC	O2-C'-C1'	2.44	116.76	111.50
8	G	310	P1O	C7-O7-C19	-2.40	111.88	117.79
8	K	310	P1O	C7-O7-C19	-2.39	111.91	117.79
8	C	309	P1O	C7-O7-C19	-2.39	111.92	117.79
6	C	302	PLC	C2-O2-C'	-2.38	111.93	117.79
6	G	303	PLC	C2-O2-C'	-2.37	111.96	117.79
6	K	303	PLC	C2-O2-C'	-2.37	111.96	117.79
8	B	302	P1O	C7-O7-C19	-2.32	112.09	117.79
8	F	303	P1O	C7-O7-C19	-2.31	112.11	117.79
8	J	304	P1O	C7-O7-C19	-2.30	112.13	117.79
8	G	309	P1O	C7-O7-C19	-2.23	112.31	117.79
8	C	308	P1O	C7-O7-C19	-2.22	112.33	117.79
8	K	309	P1O	C7-O7-C19	-2.20	112.37	117.79
6	K	308	PLC	O2-C'-O'	-2.18	118.42	123.70
6	G	308	PLC	O2-C'-O'	-2.18	118.43	123.70
6	C	307	PLC	O2-C'-O'	-2.18	118.44	123.70
6	G	301	PLC	C2-O2-C'	-2.10	112.63	117.79
6	K	301	PLC	C2-O2-C'	-2.10	112.63	117.79
6	C	310	PLC	C2-O2-C'	-2.09	112.64	117.79
8	B	308	P1O	O7-C19-O8	-2.01	118.84	123.70
8	J	301	P1O	O7-C19-O8	-2.00	118.87	123.70

There are no chirality outliers.

All (679) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	302	PLC	O4P-C4-C5-N
6	C	302	PLC	C1'-C'-O2-C2
6	C	302	PLC	C1B-CB-O3-C3
6	C	302	PLC	OB-CB-O3-C3
6	C	302	PLC	C1-O3P-P-O2P
6	C	302	PLC	C4-O4P-P-O2P
6	C	305	PLC	C1'-C'-O2-C2
6	C	305	PLC	C4-O4P-P-O1P
6	C	305	PLC	C4-O4P-P-O3P
6	C	307	PLC	C1'-C'-O2-C2
6	C	307	PLC	O'-C'-O2-C2
6	C	307	PLC	C1-O3P-P-O1P
6	C	310	PLC	C1'-C'-O2-C2
6	C	310	PLC	C4-O4P-P-O3P

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Mol	Chain	Res	Type	Atoms
6	B	301	PLC	C1'-C'-O2-C2
6	B	301	PLC	C1-O3P-P-O2P
6	B	307	PLC	C1'-C'-O2-C2
6	B	307	PLC	C1-O3P-P-O1P
6	B	307	PLC	C4-O4P-P-O1P
6	G	301	PLC	C1'-C'-O2-C2
6	G	301	PLC	C4-O4P-P-O3P
6	G	303	PLC	O4P-C4-C5-N
6	G	303	PLC	C1'-C'-O2-C2
6	G	303	PLC	C1B-CB-O3-C3
6	G	303	PLC	OB-CB-O3-C3
6	G	303	PLC	C1-O3P-P-O2P
6	G	303	PLC	C4-O4P-P-O2P
6	G	306	PLC	C1'-C'-O2-C2
6	G	306	PLC	C4-O4P-P-O1P
6	G	306	PLC	C4-O4P-P-O3P
6	G	308	PLC	C1'-C'-O2-C2
6	G	308	PLC	O'-C'-O2-C2
6	G	308	PLC	C1-O3P-P-O1P
6	K	301	PLC	C1'-C'-O2-C2
6	K	301	PLC	C4-O4P-P-O3P
6	K	303	PLC	O4P-C4-C5-N
6	K	303	PLC	C1'-C'-O2-C2
6	K	303	PLC	C1B-CB-O3-C3
6	K	303	PLC	OB-CB-O3-C3
6	K	303	PLC	C1-O3P-P-O2P
6	K	303	PLC	C4-O4P-P-O2P
6	K	306	PLC	C1'-C'-O2-C2
6	K	306	PLC	C4-O4P-P-O1P
6	K	306	PLC	C4-O4P-P-O3P
6	K	308	PLC	C1'-C'-O2-C2
6	K	308	PLC	O'-C'-O2-C2
6	K	308	PLC	C1-O3P-P-O1P
6	F	301	PLC	C1'-C'-O2-C2
6	F	301	PLC	C1-O3P-P-O1P
6	F	301	PLC	C4-O4P-P-O1P
6	F	302	PLC	C1'-C'-O2-C2
6	F	302	PLC	C1-O3P-P-O2P
6	J	302	PLC	C1'-C'-O2-C2
6	J	302	PLC	C1-O3P-P-O1P
6	J	302	PLC	C4-O4P-P-O1P
6	J	303	PLC	C1'-C'-O2-C2

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Mol	Chain	Res	Type	Atoms
6	J	303	PLC	C1-O3P-P-O2P
7	C	303	HXG	CAU-OAX-PBD-OAW
7	C	306	HXG	OAW-CAP-CAS-NBC
7	G	304	HXG	CAU-OAX-PBD-OAW
7	G	307	HXG	OAW-CAP-CAS-NBC
7	K	304	HXG	CAU-OAX-PBD-OAW
7	K	307	HXG	OAW-CAP-CAS-NBC
8	C	308	P1O	C1-O3-P1-O1
8	C	308	P1O	C2-C1-O3-P1
8	C	308	P1O	O3-C1-C2-N1
8	C	308	P1O	O6-C9-O5-C8
8	C	308	P1O	C10-C9-O5-C8
8	C	308	P1O	O8-C19-O7-C7
8	C	309	P1O	C1-O3-P1-O1
8	C	309	P1O	C1-O3-P1-O2
8	C	309	P1O	C6-O4-P1-O1
8	C	309	P1O	C6-O4-P1-O2
8	B	302	P1O	C1-O3-P1-O1
8	B	302	P1O	C1-O3-P1-O2
8	B	302	P1O	C1-O3-P1-O4
8	B	302	P1O	C6-O4-P1-O1
8	B	302	P1O	C6-O4-P1-O2
8	B	308	P1O	C6-O4-P1-O1
8	B	308	P1O	C6-O4-P1-O2
8	B	308	P1O	C6-O4-P1-O3
8	B	308	P1O	O8-C19-O7-C7
8	G	309	P1O	C1-O3-P1-O1
8	G	309	P1O	C2-C1-O3-P1
8	G	309	P1O	O3-C1-C2-N1
8	G	309	P1O	O6-C9-O5-C8
8	G	309	P1O	C10-C9-O5-C8
8	G	309	P1O	O8-C19-O7-C7
8	G	310	P1O	C1-O3-P1-O1
8	G	310	P1O	C1-O3-P1-O2
8	G	310	P1O	C6-O4-P1-O1
8	G	310	P1O	C6-O4-P1-O2
8	K	309	P1O	C1-O3-P1-O1
8	K	309	P1O	C2-C1-O3-P1
8	K	309	P1O	O3-C1-C2-N1
8	K	309	P1O	O6-C9-O5-C8
8	K	309	P1O	C10-C9-O5-C8
8	K	309	P1O	O8-C19-O7-C7

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Mol	Chain	Res	Type	Atoms
8	K	310	P1O	C1-O3-P1-O1
8	K	310	P1O	C1-O3-P1-O2
8	K	310	P1O	C6-O4-P1-O1
8	K	310	P1O	C6-O4-P1-O2
8	F	303	P1O	C1-O3-P1-O1
8	F	303	P1O	C1-O3-P1-O2
8	F	303	P1O	C1-O3-P1-O4
8	F	303	P1O	C6-O4-P1-O1
8	F	303	P1O	C6-O4-P1-O2
8	F	308	P1O	C6-O4-P1-O1
8	F	308	P1O	C6-O4-P1-O2
8	F	308	P1O	C6-O4-P1-O3
8	F	308	P1O	O8-C19-O7-C7
8	J	301	P1O	C6-O4-P1-O1
8	J	301	P1O	C6-O4-P1-O2
8	J	301	P1O	C6-O4-P1-O3
8	J	301	P1O	O8-C19-O7-C7
8	J	304	P1O	C1-O3-P1-O1
8	J	304	P1O	C1-O3-P1-O2
8	J	304	P1O	C1-O3-P1-O4
8	J	304	P1O	C6-O4-P1-O1
8	J	304	P1O	C6-O4-P1-O2
6	B	301	PLC	OB-CB-O3-C3
6	F	302	PLC	OB-CB-O3-C3
6	J	303	PLC	OB-CB-O3-C3
6	C	305	PLC	C2-C3-O3-CB
6	G	306	PLC	C2-C3-O3-CB
6	K	306	PLC	C2-C3-O3-CB
6	B	301	PLC	C1B-CB-O3-C3
6	F	302	PLC	C1B-CB-O3-C3
6	J	303	PLC	C1B-CB-O3-C3
8	B	302	P1O	C10-C9-O5-C8
8	F	303	P1O	C10-C9-O5-C8
8	J	304	P1O	C10-C9-O5-C8
6	C	305	PLC	OB-CB-O3-C3
6	C	307	PLC	OB-CB-O3-C3
6	B	307	PLC	OB-CB-O3-C3
6	G	306	PLC	OB-CB-O3-C3
6	G	308	PLC	OB-CB-O3-C3
6	K	306	PLC	OB-CB-O3-C3
6	K	308	PLC	OB-CB-O3-C3
6	F	301	PLC	OB-CB-O3-C3

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Mol	Chain	Res	Type	Atoms
6	J	302	PLC	OB-CB-O3-C3
8	B	302	P1O	O6-C9-O5-C8
8	F	303	P1O	O6-C9-O5-C8
8	J	304	P1O	O6-C9-O5-C8
6	C	302	PLC	O'-C'-O2-C2
6	C	305	PLC	O'-C'-O2-C2
6	C	310	PLC	O'-C'-O2-C2
6	B	301	PLC	O'-C'-O2-C2
6	B	307	PLC	O'-C'-O2-C2
6	G	301	PLC	O'-C'-O2-C2
6	G	303	PLC	O'-C'-O2-C2
6	G	306	PLC	O'-C'-O2-C2
6	K	301	PLC	O'-C'-O2-C2
6	K	303	PLC	O'-C'-O2-C2
6	K	306	PLC	O'-C'-O2-C2
6	F	301	PLC	O'-C'-O2-C2
6	F	302	PLC	O'-C'-O2-C2
6	J	302	PLC	O'-C'-O2-C2
6	J	303	PLC	O'-C'-O2-C2
6	B	301	PLC	C2-C3-O3-CB
6	F	302	PLC	C2-C3-O3-CB
6	J	303	PLC	C2-C3-O3-CB
6	C	305	PLC	C1B-CB-O3-C3
6	C	307	PLC	C1B-CB-O3-C3
6	G	306	PLC	C1B-CB-O3-C3
6	G	308	PLC	C1B-CB-O3-C3
6	K	306	PLC	C1B-CB-O3-C3
6	K	308	PLC	C1B-CB-O3-C3
8	C	308	P1O	C20-C19-O7-C7
8	B	308	P1O	C20-C19-O7-C7
8	G	309	P1O	C20-C19-O7-C7
8	K	309	P1O	C20-C19-O7-C7
8	F	308	P1O	C20-C19-O7-C7
8	J	301	P1O	C20-C19-O7-C7
6	B	307	PLC	C1B-CB-O3-C3
6	F	301	PLC	C1B-CB-O3-C3
6	J	302	PLC	C1B-CB-O3-C3
6	C	310	PLC	C4-C5-N-C6
6	G	301	PLC	C4-C5-N-C6
6	K	301	PLC	C4-C5-N-C6
6	C	310	PLC	C1B-CB-O3-C3
6	G	301	PLC	C1B-CB-O3-C3

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Mol	Chain	Res	Type	Atoms
6	K	301	PLC	C1B-CB-O3-C3
8	C	308	P1O	C9-C10-C11-C12
8	G	309	P1O	C9-C10-C11-C12
8	K	309	P1O	C9-C10-C11-C12
7	C	303	HXG	CAL-CAN-CAQ-CAZ
7	G	304	HXG	CAL-CAN-CAQ-CAZ
7	K	304	HXG	CAL-CAN-CAQ-CAZ
8	C	309	P1O	C10-C9-O5-C8
8	G	310	P1O	C10-C9-O5-C8
8	K	310	P1O	C10-C9-O5-C8
7	C	306	HXG	CAM-CAO-CAR-CBA
7	G	307	HXG	CAM-CAO-CAR-CBA
7	K	307	HXG	CAM-CAO-CAR-CBA
8	B	308	P1O	C19-C20-C21-C22
8	F	308	P1O	C19-C20-C21-C22
8	J	301	P1O	C19-C20-C21-C22
8	C	309	P1O	C7-C6-O4-P1
8	G	310	P1O	C7-C6-O4-P1
8	K	310	P1O	C7-C6-O4-P1
6	C	310	PLC	OB-CB-O3-C3
6	G	301	PLC	OB-CB-O3-C3
6	K	301	PLC	OB-CB-O3-C3
6	C	302	PLC	C1-O3P-P-O4P
6	C	302	PLC	C4-O4P-P-O3P
6	B	301	PLC	C1-O3P-P-O4P
6	G	303	PLC	C1-O3P-P-O4P
6	G	303	PLC	C4-O4P-P-O3P
6	K	303	PLC	C1-O3P-P-O4P
6	K	303	PLC	C4-O4P-P-O3P
6	F	302	PLC	C1-O3P-P-O4P
6	J	303	PLC	C1-O3P-P-O4P
7	C	303	HXG	CAP-OAW-PBD-OAX
7	G	304	HXG	CAP-OAW-PBD-OAX
7	K	304	HXG	CAP-OAW-PBD-OAX
8	C	308	P1O	C1-O3-P1-O4
8	C	308	P1O	C6-O4-P1-O3
8	C	309	P1O	C1-O3-P1-O4
8	C	309	P1O	C6-O4-P1-O3
8	B	302	P1O	C6-O4-P1-O3
8	G	309	P1O	C1-O3-P1-O4
8	G	309	P1O	C6-O4-P1-O3
8	G	310	P1O	C1-O3-P1-O4

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Mol	Chain	Res	Type	Atoms
8	G	310	P1O	C6-O4-P1-O3
8	K	309	P1O	C1-O3-P1-O4
8	K	309	P1O	C6-O4-P1-O3
8	K	310	P1O	C1-O3-P1-O4
8	K	310	P1O	C6-O4-P1-O3
8	F	303	P1O	C6-O4-P1-O3
8	J	304	P1O	C6-O4-P1-O3
6	C	310	PLC	CB-C1B-C2B-C3B
6	G	301	PLC	CB-C1B-C2B-C3B
6	K	301	PLC	CB-C1B-C2B-C3B
6	C	310	PLC	C4-C5-N-C7
6	G	301	PLC	C4-C5-N-C7
6	K	301	PLC	C4-C5-N-C7
8	G	309	P1O	C21-C22-C23-C24
8	B	302	P1O	C20-C19-O7-C7
8	F	303	P1O	C20-C19-O7-C7
8	J	304	P1O	C20-C19-O7-C7
6	C	310	PLC	C2B-C3B-C4B-C5B
6	G	301	PLC	C2B-C3B-C4B-C5B
6	K	301	PLC	C2B-C3B-C4B-C5B
8	C	308	P1O	C21-C22-C23-C24
8	C	309	P1O	C13-C14-C15-C16
8	B	302	P1O	C11-C12-C13-C14
8	G	310	P1O	C13-C14-C15-C16
8	K	309	P1O	C21-C22-C23-C24
8	F	303	P1O	C11-C12-C13-C14
8	J	304	P1O	C11-C12-C13-C14
6	C	302	PLC	C6B-C7B-C8B-C9B
6	G	303	PLC	C6B-C7B-C8B-C9B
6	K	303	PLC	C6B-C7B-C8B-C9B
8	K	310	P1O	C13-C14-C15-C16
6	C	305	PLC	C3-C2-O2-C'
6	G	306	PLC	C3-C2-O2-C'
6	K	306	PLC	C3-C2-O2-C'
8	B	302	P1O	O8-C19-O7-C7
8	F	303	P1O	O8-C19-O7-C7
8	J	304	P1O	O8-C19-O7-C7
8	C	309	P1O	O6-C9-O5-C8
8	G	310	P1O	O6-C9-O5-C8
8	K	310	P1O	O6-C9-O5-C8
8	B	308	P1O	C23-C24-C25-C26
8	F	308	P1O	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
8	J	301	P1O	C23-C24-C25-C26
8	B	308	P1O	C9-C10-C11-C12
8	F	308	P1O	C9-C10-C11-C12
8	J	301	P1O	C9-C10-C11-C12
5	B	305	D10	C5-C6-C7-C8
5	F	306	D10	C5-C6-C7-C8
5	J	307	D10	C5-C6-C7-C8
6	C	310	PLC	C3B-C4B-C5B-C6B
6	G	301	PLC	C3B-C4B-C5B-C6B
6	K	301	PLC	C3B-C4B-C5B-C6B
8	C	309	P1O	C24-C25-C26-C27
8	B	302	P1O	C21-C22-C23-C24
8	B	308	P1O	C14-C15-C16-C17
8	K	310	P1O	C24-C25-C26-C27
8	F	303	P1O	C21-C22-C23-C24
8	F	308	P1O	C14-C15-C16-C17
8	J	301	P1O	C14-C15-C16-C17
8	J	304	P1O	C21-C22-C23-C24
8	G	310	P1O	C24-C25-C26-C27
8	F	303	P1O	C13-C14-C15-C16
8	B	302	P1O	C13-C14-C15-C16
8	J	304	P1O	C13-C14-C15-C16
6	C	310	PLC	C4-C5-N-C8
6	G	301	PLC	C4-C5-N-C8
6	K	301	PLC	C4-C5-N-C8
6	C	310	PLC	C4B-C5B-C6B-C7B
6	B	301	PLC	C5'-C6'-C7'-C8'
6	G	301	PLC	C4B-C5B-C6B-C7B
6	F	302	PLC	C5'-C6'-C7'-C8'
6	J	303	PLC	C5'-C6'-C7'-C8'
6	K	301	PLC	C4B-C5B-C6B-C7B
8	B	308	P1O	C13-C14-C15-C16
8	F	308	P1O	C13-C14-C15-C16
8	J	301	P1O	C13-C14-C15-C16
6	C	302	PLC	C3B-C4B-C5B-C6B
6	C	310	PLC	C6'-C7'-C8'-C9'
6	B	307	PLC	C1'-C2'-C3'-C4'
6	G	301	PLC	C6'-C7'-C8'-C9'
6	G	303	PLC	C3B-C4B-C5B-C6B
6	K	301	PLC	C6'-C7'-C8'-C9'
6	K	303	PLC	C3B-C4B-C5B-C6B
6	F	301	PLC	C1'-C2'-C3'-C4'

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Mol	Chain	Res	Type	Atoms
6	J	302	PLC	C1'-C2'-C3'-C4'
6	C	302	PLC	C1'-C2'-C3'-C4'
6	G	303	PLC	C1'-C2'-C3'-C4'
6	K	303	PLC	C1'-C2'-C3'-C4'
5	F	307	D10	C5-C6-C7-C8
5	J	308	D10	C5-C6-C7-C8
7	C	303	HXG	CAR-CBA-OAY-CBB
7	G	304	HXG	CAR-CBA-OAY-CBB
7	K	304	HXG	CAR-CBA-OAY-CBB
5	B	306	D10	C5-C6-C7-C8
8	C	309	P1O	C21-C22-C23-C24
8	G	310	P1O	C21-C22-C23-C24
8	K	310	P1O	C21-C22-C23-C24
8	C	309	P1O	C12-C13-C14-C15
8	G	310	P1O	C12-C13-C14-C15
8	K	310	P1O	C12-C13-C14-C15
6	C	310	PLC	C4'-C5'-C6'-C7'
6	G	301	PLC	C4'-C5'-C6'-C7'
6	K	301	PLC	C4'-C5'-C6'-C7'
6	C	302	PLC	C6'-C7'-C8'-C9'
6	G	303	PLC	C6'-C7'-C8'-C9'
6	K	303	PLC	C6'-C7'-C8'-C9'
8	B	302	P1O	C23-C24-C25-C26
8	F	303	P1O	C23-C24-C25-C26
8	J	304	P1O	C23-C24-C25-C26
6	C	305	PLC	CB-C1B-C2B-C3B
6	G	306	PLC	CB-C1B-C2B-C3B
6	K	306	PLC	CB-C1B-C2B-C3B
8	C	309	P1O	C10-C11-C12-C13
8	K	310	P1O	C10-C11-C12-C13
8	G	310	P1O	C10-C11-C12-C13
7	C	303	HXG	OAG-CBA-OAY-CBB
7	G	304	HXG	OAG-CBA-OAY-CBB
7	K	304	HXG	OAG-CBA-OAY-CBB
6	C	302	PLC	CB-C1B-C2B-C3B
6	G	303	PLC	CB-C1B-C2B-C3B
6	K	303	PLC	CB-C1B-C2B-C3B
8	B	308	P1O	C12-C13-C14-C15
8	F	308	P1O	C12-C13-C14-C15
8	J	301	P1O	C12-C13-C14-C15
8	B	308	P1O	C22-C23-C24-C25
8	F	308	P1O	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
8	J	301	P1O	C22-C23-C24-C25
6	C	302	PLC	C4B-C5B-C6B-C7B
6	G	303	PLC	C4B-C5B-C6B-C7B
6	K	303	PLC	C4B-C5B-C6B-C7B
8	C	309	P1O	C20-C19-O7-C7
8	G	310	P1O	C20-C19-O7-C7
8	K	310	P1O	C20-C19-O7-C7
6	F	302	PLC	C4'-C5'-C6'-C7'
6	B	301	PLC	C4'-C5'-C6'-C7'
6	J	303	PLC	C4'-C5'-C6'-C7'
8	C	309	P1O	O8-C19-O7-C7
8	G	310	P1O	O8-C19-O7-C7
8	K	310	P1O	O8-C19-O7-C7
5	B	304	D10	C5-C6-C7-C8
5	B	305	D10	C4-C5-C6-C7
5	B	306	D10	C4-C5-C6-C7
5	F	305	D10	C5-C6-C7-C8
5	F	306	D10	C4-C5-C6-C7
5	F	307	D10	C4-C5-C6-C7
5	J	306	D10	C5-C6-C7-C8
5	J	307	D10	C4-C5-C6-C7
5	J	308	D10	C4-C5-C6-C7
6	B	307	PLC	C1-O3P-P-O4P
6	F	301	PLC	C1-O3P-P-O4P
6	J	302	PLC	C1-O3P-P-O4P
8	C	308	P1O	C22-C23-C24-C25
8	G	309	P1O	C22-C23-C24-C25
8	K	309	P1O	C22-C23-C24-C25
7	C	303	HXG	OAX-CAU-CBB-CAT
7	G	304	HXG	OAX-CAU-CBB-CAT
7	K	304	HXG	OAX-CAU-CBB-CAT
8	B	302	P1O	C20-C21-C22-C23
8	F	303	P1O	C20-C21-C22-C23
8	J	304	P1O	C20-C21-C22-C23
6	C	307	PLC	C4'-C5'-C6'-C7'
6	G	308	PLC	C4'-C5'-C6'-C7'
6	K	308	PLC	C4'-C5'-C6'-C7'
5	B	306	D10	C6-C7-C8-C9
5	J	308	D10	C6-C7-C8-C9
5	F	307	D10	C6-C7-C8-C9
6	C	310	PLC	C6B-C7B-C8B-C9B
6	G	301	PLC	C6B-C7B-C8B-C9B

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Mol	Chain	Res	Type	Atoms
6	K	301	PLC	C6B-C7B-C8B-C9B
5	B	305	D10	C2-C3-C4-C5
5	B	306	D10	C2-C3-C4-C5
5	F	306	D10	C2-C3-C4-C5
5	F	307	D10	C2-C3-C4-C5
5	J	307	D10	C2-C3-C4-C5
5	J	308	D10	C2-C3-C4-C5
8	B	308	P1O	C15-C16-C17-C18
8	F	308	P1O	C15-C16-C17-C18
8	J	301	P1O	C15-C16-C17-C18
8	B	308	P1O	C6-C7-O7-C19
8	F	308	P1O	C6-C7-O7-C19
8	J	301	P1O	C6-C7-O7-C19
6	C	310	PLC	C7B-C8B-C9B-CAA
6	G	301	PLC	C7B-C8B-C9B-CAA
6	K	301	PLC	C7B-C8B-C9B-CAA
6	C	302	PLC	O2-C2-C3-O3
6	G	303	PLC	O2-C2-C3-O3
6	K	303	PLC	O2-C2-C3-O3
5	F	306	D10	C6-C7-C8-C9
5	J	307	D10	C6-C7-C8-C9
5	B	305	D10	C6-C7-C8-C9
6	C	307	PLC	C7'-C8'-C9'-CA'
6	G	308	PLC	C7'-C8'-C9'-CA'
6	K	308	PLC	C7'-C8'-C9'-CA'
6	K	303	PLC	C8B-C9B-CAA-CBA
6	C	302	PLC	C8B-C9B-CAA-CBA
6	G	303	PLC	C8B-C9B-CAA-CBA
8	C	309	P1O	O4-C6-C7-C8
8	G	310	P1O	O4-C6-C7-C8
8	K	310	P1O	O4-C6-C7-C8
6	F	301	PLC	C'-C1'-C2'-C3'
6	J	302	PLC	C'-C1'-C2'-C3'
6	B	307	PLC	C'-C1'-C2'-C3'
6	B	301	PLC	C1-C2-C3-O3
6	F	302	PLC	C1-C2-C3-O3
6	J	303	PLC	C1-C2-C3-O3
6	C	307	PLC	C1B-C2B-C3B-C4B
6	G	308	PLC	C1B-C2B-C3B-C4B
6	K	308	PLC	C1B-C2B-C3B-C4B
8	C	309	P1O	C19-C20-C21-C22
8	G	310	P1O	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
8	K	310	P1O	C19-C20-C21-C22
8	B	302	P1O	C12-C13-C14-C15
8	F	303	P1O	C12-C13-C14-C15
8	J	304	P1O	C12-C13-C14-C15
6	G	303	PLC	C8'-C9'-CA'-CB'
6	C	302	PLC	C8'-C9'-CA'-CB'
6	K	303	PLC	C8'-C9'-CA'-CB'
8	C	309	P1O	C15-C16-C17-C18
8	G	310	P1O	C15-C16-C17-C18
8	K	310	P1O	C15-C16-C17-C18
5	B	305	D10	C3-C4-C5-C6
5	F	306	D10	C3-C4-C5-C6
5	J	307	D10	C3-C4-C5-C6
6	B	307	PLC	C5B-C6B-C7B-C8B
6	F	301	PLC	C5B-C6B-C7B-C8B
6	J	302	PLC	C5B-C6B-C7B-C8B
6	C	302	PLC	C3'-C4'-C5'-C6'
6	C	302	PLC	C1B-C2B-C3B-C4B
6	G	303	PLC	C3'-C4'-C5'-C6'
6	G	303	PLC	C1B-C2B-C3B-C4B
6	K	303	PLC	C3'-C4'-C5'-C6'
6	K	303	PLC	C1B-C2B-C3B-C4B
6	C	310	PLC	O3P-C1-C2-C3
6	G	301	PLC	O3P-C1-C2-C3
6	K	301	PLC	O3P-C1-C2-C3
8	G	310	P1O	C14-C15-C16-C17
8	C	309	P1O	C14-C15-C16-C17
8	C	309	P1O	C22-C23-C24-C25
8	G	310	P1O	C22-C23-C24-C25
8	K	310	P1O	C14-C15-C16-C17
8	K	310	P1O	C22-C23-C24-C25
8	C	308	P1O	C11-C12-C13-C14
8	G	309	P1O	C11-C12-C13-C14
8	K	309	P1O	C11-C12-C13-C14
6	C	310	PLC	C3-C2-O2-C'
6	B	307	PLC	C1-C2-O2-C'
6	G	301	PLC	C3-C2-O2-C'
6	K	301	PLC	C3-C2-O2-C'
6	F	301	PLC	C1-C2-O2-C'
6	J	302	PLC	C1-C2-O2-C'
7	C	306	HXG	CAT-CBB-OAY-CBA
7	G	307	HXG	CAT-CBB-OAY-CBA

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Mol	Chain	Res	Type	Atoms
7	K	307	HXG	CAT-CBB-OAY-CBA
8	J	304	P1O	C9-C10-C11-C12
6	C	310	PLC	O3P-C1-C2-O2
6	G	301	PLC	O3P-C1-C2-O2
6	K	301	PLC	O3P-C1-C2-O2
8	C	309	P1O	O4-C6-C7-O7
8	G	310	P1O	O4-C6-C7-O7
8	K	310	P1O	O4-C6-C7-O7
8	B	302	P1O	C9-C10-C11-C12
8	F	303	P1O	C9-C10-C11-C12
8	C	309	P1O	O7-C7-C8-O5
8	G	310	P1O	O7-C7-C8-O5
8	K	310	P1O	O7-C7-C8-O5
8	B	302	P1O	C24-C25-C26-C27
8	F	303	P1O	C24-C25-C26-C27
8	J	304	P1O	C24-C25-C26-C27
8	B	302	P1O	C15-C16-C17-C18
8	F	303	P1O	C15-C16-C17-C18
8	J	304	P1O	C15-C16-C17-C18
6	C	307	PLC	C1-O3P-P-O4P
6	G	308	PLC	C1-O3P-P-O4P
6	K	308	PLC	C1-O3P-P-O4P
6	C	307	PLC	C2-C1-O3P-P
6	G	308	PLC	C2-C1-O3P-P
6	K	308	PLC	C2-C1-O3P-P
6	C	310	PLC	C4-O4P-P-O2P
6	B	301	PLC	C1-O3P-P-O1P
6	B	307	PLC	C1-O3P-P-O2P
6	G	301	PLC	C4-O4P-P-O2P
6	K	301	PLC	C4-O4P-P-O2P
6	F	301	PLC	C1-O3P-P-O2P
6	F	302	PLC	C1-O3P-P-O1P
6	J	302	PLC	C1-O3P-P-O2P
6	J	303	PLC	C1-O3P-P-O1P
7	C	303	HXG	CAU-OAX-PBD-OAH
7	C	303	HXG	CAP-OAW-PBD-OAI
7	G	304	HXG	CAU-OAX-PBD-OAH
7	G	304	HXG	CAP-OAW-PBD-OAI
7	K	304	HXG	CAU-OAX-PBD-OAH
7	K	304	HXG	CAP-OAW-PBD-OAI
8	C	308	P1O	C6-O4-P1-O2
8	B	302	P1O	C1-C2-N1-C5

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Mol	Chain	Res	Type	Atoms
8	B	308	P1O	C1-O3-P1-O1
8	G	309	P1O	C6-O4-P1-O2
8	K	309	P1O	C6-O4-P1-O2
8	F	303	P1O	C1-C2-N1-C5
8	F	308	P1O	C1-O3-P1-O1
8	J	301	P1O	C1-O3-P1-O1
8	J	304	P1O	C1-C2-N1-C5
6	C	305	PLC	C7B-C8B-C9B-CAA
6	K	306	PLC	C7B-C8B-C9B-CAA
6	C	307	PLC	C5-C4-O4P-P
6	B	307	PLC	C5-C4-O4P-P
6	G	308	PLC	C5-C4-O4P-P
6	K	308	PLC	C5-C4-O4P-P
6	F	301	PLC	C5-C4-O4P-P
6	J	302	PLC	C5-C4-O4P-P
8	B	308	P1O	C21-C22-C23-C24
8	F	308	P1O	C21-C22-C23-C24
8	J	301	P1O	C21-C22-C23-C24
6	G	306	PLC	C7B-C8B-C9B-CAA
5	B	306	D10	C3-C4-C5-C6
8	B	302	P1O	C10-C11-C12-C13
8	F	303	P1O	C10-C11-C12-C13
8	J	304	P1O	C10-C11-C12-C13
7	C	303	HXG	OAX-CAU-CBB-OAY
7	G	304	HXG	OAX-CAU-CBB-OAY
7	K	304	HXG	OAX-CAU-CBB-OAY
5	F	307	D10	C3-C4-C5-C6
5	J	308	D10	C3-C4-C5-C6
8	B	302	P1O	C1-C2-N1-C4
8	F	303	P1O	C1-C2-N1-C4
8	J	304	P1O	C1-C2-N1-C4
6	C	302	PLC	C1-C2-C3-O3
6	B	307	PLC	O4P-C4-C5-N
6	G	303	PLC	C1-C2-C3-O3
6	K	303	PLC	C1-C2-C3-O3
6	F	301	PLC	O4P-C4-C5-N
6	J	302	PLC	O4P-C4-C5-N
6	B	301	PLC	O2-C2-C3-O3
6	F	302	PLC	O2-C2-C3-O3
6	J	303	PLC	O2-C2-C3-O3
6	K	301	PLC	C3'-C4'-C5'-C6'
6	G	301	PLC	C3'-C4'-C5'-C6'

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Mol	Chain	Res	Type	Atoms
7	C	306	HXG	CBB-CAU-OAX-PBD
7	G	307	HXG	CBB-CAU-OAX-PBD
7	K	307	HXG	CBB-CAU-OAX-PBD
6	C	310	PLC	C3'-C4'-C5'-C6'
6	K	306	PLC	C3B-C4B-C5B-C6B
6	G	306	PLC	C3B-C4B-C5B-C6B
6	C	307	PLC	C'-C1'-C2'-C3'
6	K	308	PLC	C'-C1'-C2'-C3'
6	C	305	PLC	C3B-C4B-C5B-C6B
6	G	308	PLC	C'-C1'-C2'-C3'
8	G	309	P1O	C24-C25-C26-C27
8	C	308	P1O	C24-C25-C26-C27
8	K	309	P1O	C24-C25-C26-C27
8	C	309	P1O	C6-C7-C8-O5
8	G	310	P1O	C6-C7-C8-O5
8	K	310	P1O	C6-C7-C8-O5
6	C	302	PLC	C5B-C6B-C7B-C8B
6	G	303	PLC	C5B-C6B-C7B-C8B
6	K	303	PLC	C5B-C6B-C7B-C8B
6	C	305	PLC	C5B-C6B-C7B-C8B
6	G	306	PLC	C5B-C6B-C7B-C8B
6	K	306	PLC	C5B-C6B-C7B-C8B
6	G	301	PLC	C5'-C6'-C7'-C8'
6	K	301	PLC	C5'-C6'-C7'-C8'
6	C	310	PLC	C5'-C6'-C7'-C8'
5	J	307	D10	C7-C8-C9-C10
5	B	305	D10	C7-C8-C9-C10
5	F	306	D10	C7-C8-C9-C10
7	C	306	HXG	OAV-CAT-CBB-OAY
7	G	307	HXG	OAV-CAT-CBB-OAY
7	K	307	HXG	OAV-CAT-CBB-OAY
8	B	302	P1O	O7-C7-C8-O5
8	F	303	P1O	O7-C7-C8-O5
8	J	304	P1O	O7-C7-C8-O5
8	C	309	P1O	C23-C24-C25-C26
8	G	310	P1O	C23-C24-C25-C26
8	K	310	P1O	C23-C24-C25-C26
6	C	307	PLC	C3-C2-O2-C'
6	G	308	PLC	C3-C2-O2-C'
6	K	308	PLC	C3-C2-O2-C'
8	B	302	P1O	C1-C2-N1-C3
8	F	303	P1O	C1-C2-N1-C3

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Mol	Chain	Res	Type	Atoms
8	J	304	P1O	C1-C2-N1-C3
6	C	305	PLC	C8B-C9B-CAA-CBA
6	G	306	PLC	C8B-C9B-CAA-CBA
6	K	306	PLC	C8B-C9B-CAA-CBA
6	C	307	PLC	C6B-C7B-C8B-C9B
6	K	308	PLC	C6B-C7B-C8B-C9B
6	G	308	PLC	C6B-C7B-C8B-C9B
6	B	307	PLC	C7B-C8B-C9B-CAA
6	J	302	PLC	C7B-C8B-C9B-CAA
6	F	301	PLC	C7B-C8B-C9B-CAA
8	G	310	P1O	C9-C10-C11-C12
8	K	310	P1O	C9-C10-C11-C12
8	C	309	P1O	C9-C10-C11-C12
6	C	310	PLC	C1-O3P-P-O4P
6	G	301	PLC	C1-O3P-P-O4P
6	K	301	PLC	C1-O3P-P-O4P
8	B	308	P1O	O7-C19-C20-C21
6	C	310	PLC	C2B-C1B-CB-O3
6	G	301	PLC	C2B-C1B-CB-O3
6	K	301	PLC	C2B-C1B-CB-O3
8	F	308	P1O	O7-C19-C20-C21
8	J	301	P1O	O7-C19-C20-C21
7	G	307	HXG	OAG-CBA-OAY-CBB
6	C	307	PLC	O2-C'-C1'-C2'
6	G	308	PLC	O2-C'-C1'-C2'
6	K	308	PLC	O2-C'-C1'-C2'
5	B	304	D10	C7-C8-C9-C10
5	F	305	D10	C7-C8-C9-C10
5	J	306	D10	C7-C8-C9-C10
8	B	308	P1O	C25-C26-C27-C28
8	F	308	P1O	C25-C26-C27-C28
8	J	301	P1O	C25-C26-C27-C28
8	K	309	P1O	C10-C11-C12-C13
6	C	307	PLC	O'-C'-C1'-C2'
6	G	308	PLC	O'-C'-C1'-C2'
8	C	308	P1O	C10-C11-C12-C13
8	G	309	P1O	C10-C11-C12-C13
7	C	306	HXG	OAG-CBA-OAY-CBB
7	K	307	HXG	OAG-CBA-OAY-CBB
8	C	308	P1O	C7-C6-O4-P1
8	G	309	P1O	C7-C6-O4-P1
8	K	309	P1O	C7-C6-O4-P1

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Mol	Chain	Res	Type	Atoms
6	K	308	PLC	O'-C'-C1'-C2'
7	C	306	HXG	CAU-OAX-PBD-OAI
7	G	307	HXG	CAU-OAX-PBD-OAI
7	K	307	HXG	CAU-OAX-PBD-OAI
8	B	308	P1O	C1-O3-P1-O2
8	F	308	P1O	C1-O3-P1-O2
8	J	301	P1O	C1-O3-P1-O2
8	C	308	P1O	C11-C10-C9-O5
8	G	309	P1O	C11-C10-C9-O5
8	K	309	P1O	C11-C10-C9-O5
6	C	307	PLC	C1-C2-O2-C'
6	B	301	PLC	C1-C2-O2-C'
6	B	301	PLC	C3-C2-O2-C'
6	G	308	PLC	C1-C2-O2-C'
6	K	308	PLC	C1-C2-O2-C'
6	F	302	PLC	C1-C2-O2-C'
6	F	302	PLC	C3-C2-O2-C'
6	J	303	PLC	C1-C2-O2-C'
6	J	303	PLC	C3-C2-O2-C'
8	B	308	P1O	O8-C19-C20-C21
8	F	308	P1O	O8-C19-C20-C21
8	J	301	P1O	O8-C19-C20-C21
8	B	302	P1O	C11-C10-C9-O5
8	F	303	P1O	C11-C10-C9-O5
8	J	304	P1O	C11-C10-C9-O5
6	K	301	PLC	C2B-C1B-CB-OB
6	C	310	PLC	C2B-C1B-CB-OB
6	G	301	PLC	C2B-C1B-CB-OB
6	C	310	PLC	O2-C'-C1'-C2'
6	K	301	PLC	O2-C'-C1'-C2'
6	F	302	PLC	C6'-C7'-C8'-C9'
6	B	301	PLC	C6'-C7'-C8'-C9'
6	G	301	PLC	O2-C'-C1'-C2'
6	J	303	PLC	C6'-C7'-C8'-C9'
8	C	308	P1O	C11-C10-C9-O6

There are no ring outliers.

45 monomers are involved in 319 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	K	308	PLC	5	0
6	K	306	PLC	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	305	PLC	1	0
5	B	305	D10	6	0
6	G	303	PLC	6	0
8	B	308	P1O	27	0
7	G	307	HXG	16	0
5	B	306	D10	2	0
7	G	304	HXG	8	0
6	K	301	PLC	7	0
5	J	306	D10	1	0
6	K	303	PLC	5	0
5	G	305	D10	1	0
8	G	310	P1O	14	0
8	J	304	P1O	8	0
5	K	305	D10	1	0
6	G	306	PLC	1	0
5	J	308	D10	1	0
5	F	305	D10	1	0
8	G	309	P1O	7	0
8	J	301	P1O	28	0
8	F	303	P1O	8	0
8	F	308	P1O	29	0
7	K	304	HXG	8	0
6	B	301	PLC	3	0
5	C	304	D10	1	0
5	F	306	D10	6	0
8	B	302	P1O	8	0
8	K	310	P1O	15	0
8	K	309	P1O	7	0
5	F	307	D10	1	0
7	C	303	HXG	8	0
6	C	307	PLC	5	0
7	K	307	HXG	16	0
5	B	304	D10	1	0
6	G	301	PLC	6	0
8	C	309	P1O	15	0
7	C	306	HXG	15	0
6	F	302	PLC	2	0
6	J	303	PLC	3	0
6	C	310	PLC	6	0
6	C	302	PLC	4	0
8	C	308	P1O	8	0
6	G	308	PLC	5	0

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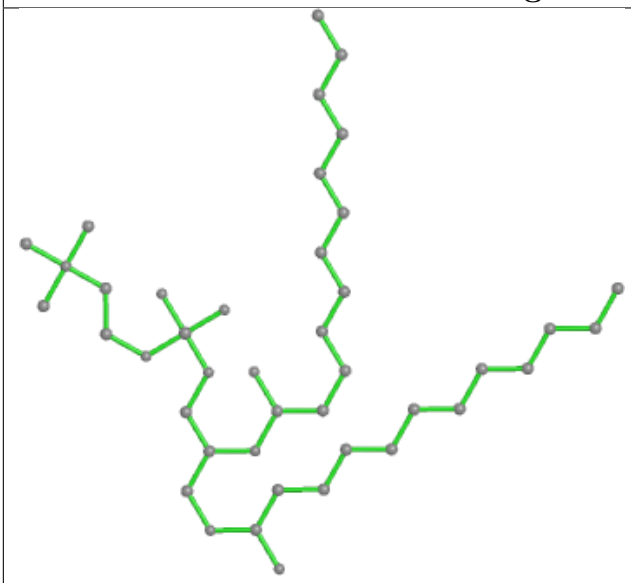
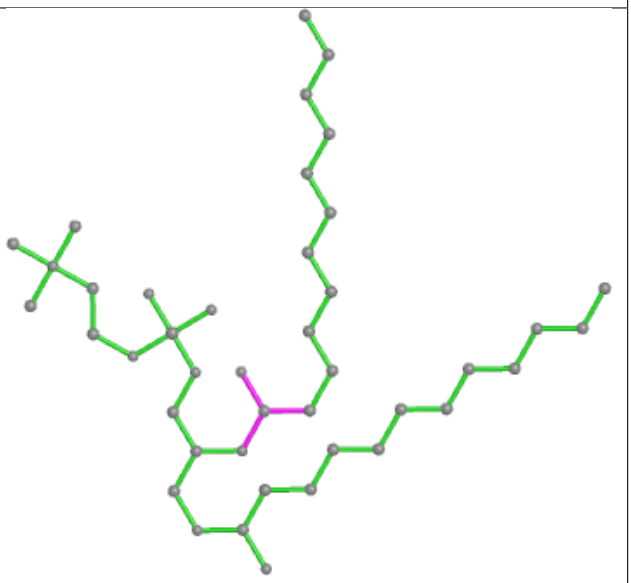
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	J	307	D10	6	0

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.

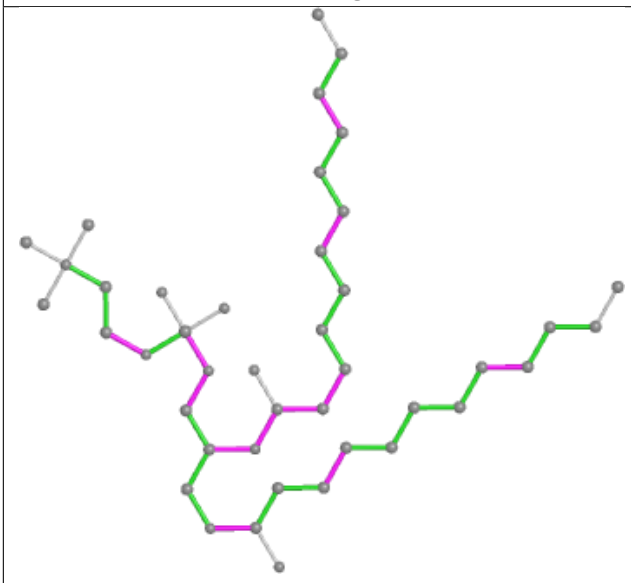
Ligand PLC K 308



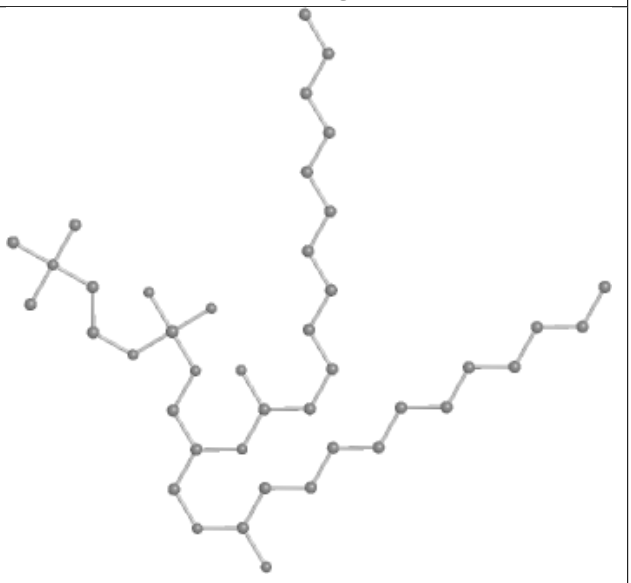
Bond lengths



Bond angles

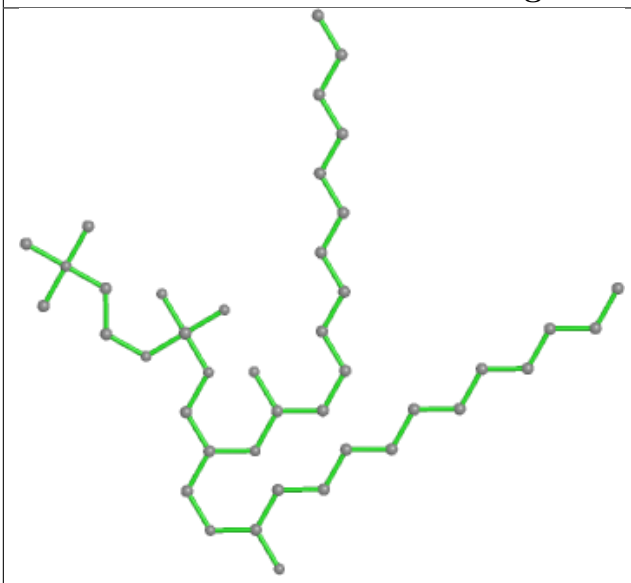


Torsions

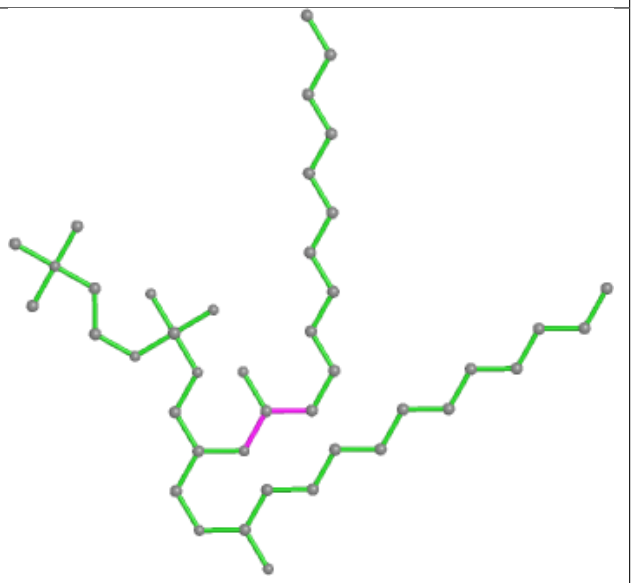


Rings

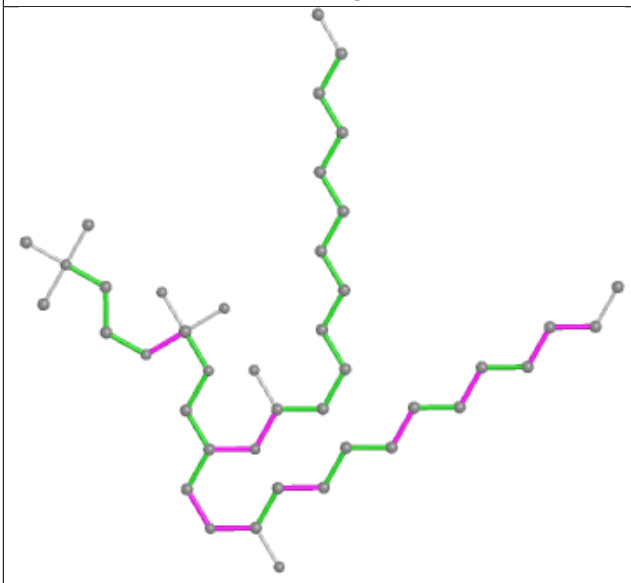
Ligand PLC K 306



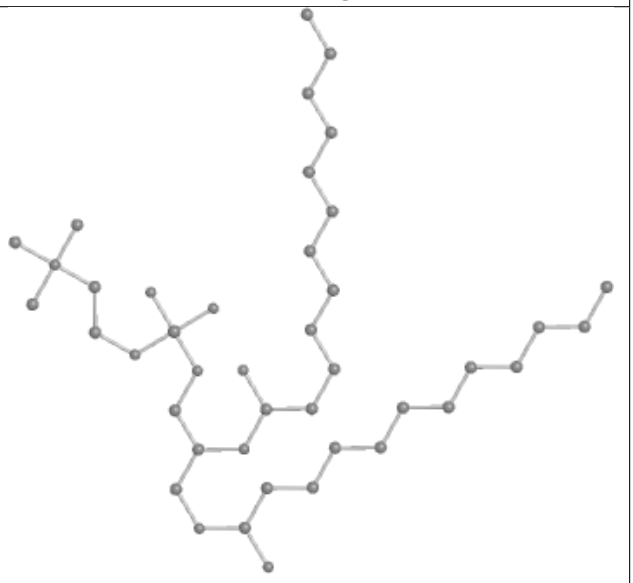
Bond lengths



Bond angles

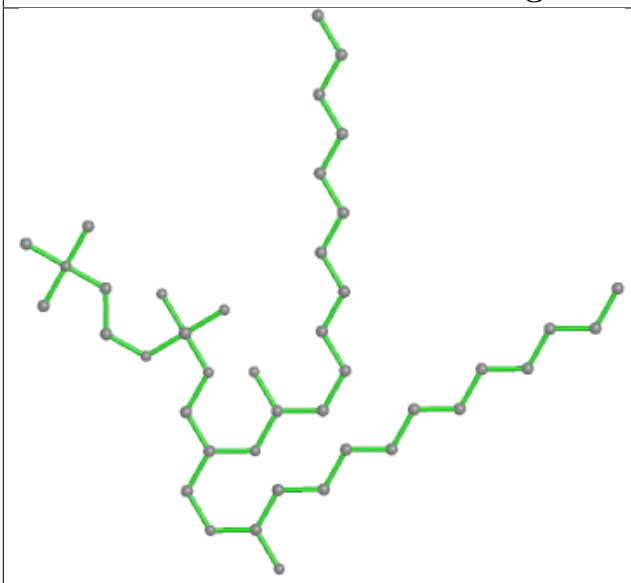


Torsions

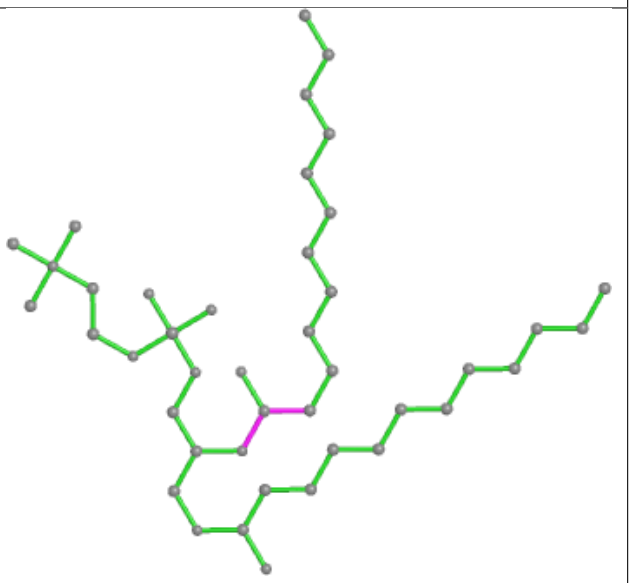


Rings

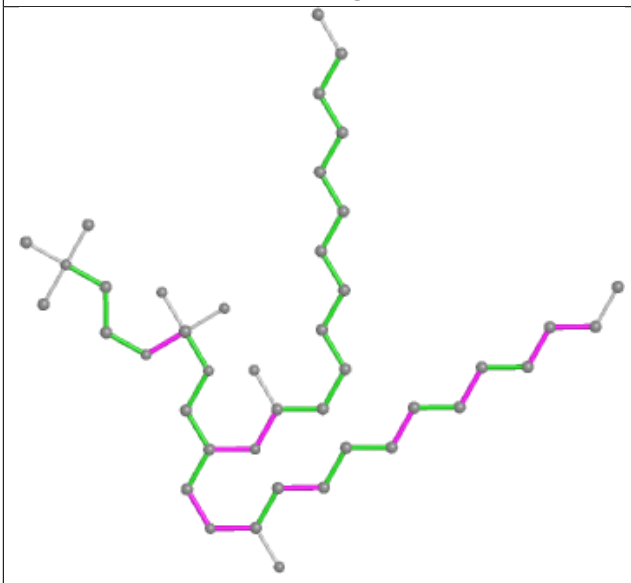
Ligand PLC C 305



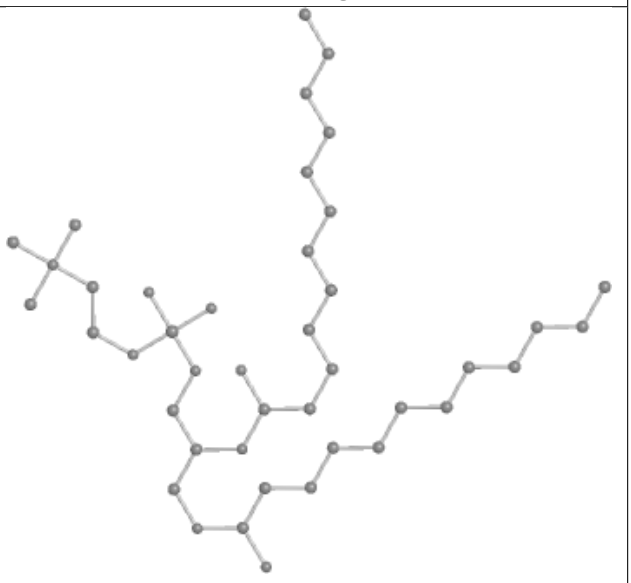
Bond lengths



Bond angles

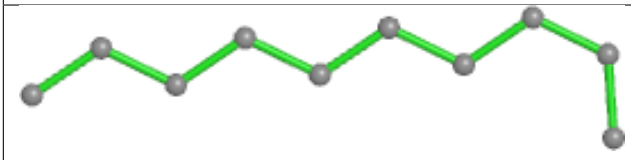


Torsions

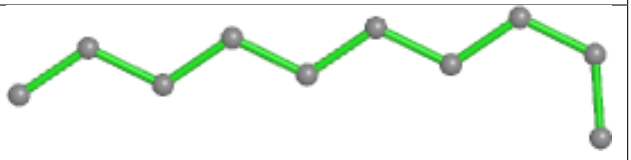


Rings

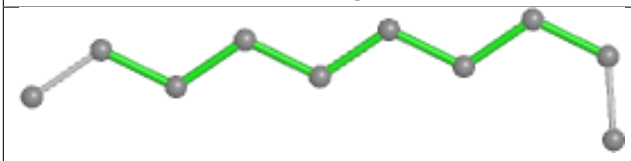
Ligand D10 F 304



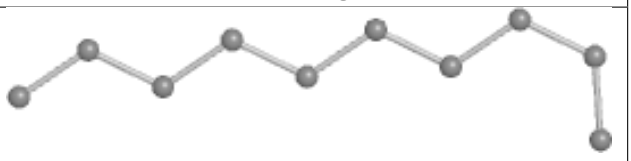
Bond lengths



Bond angles

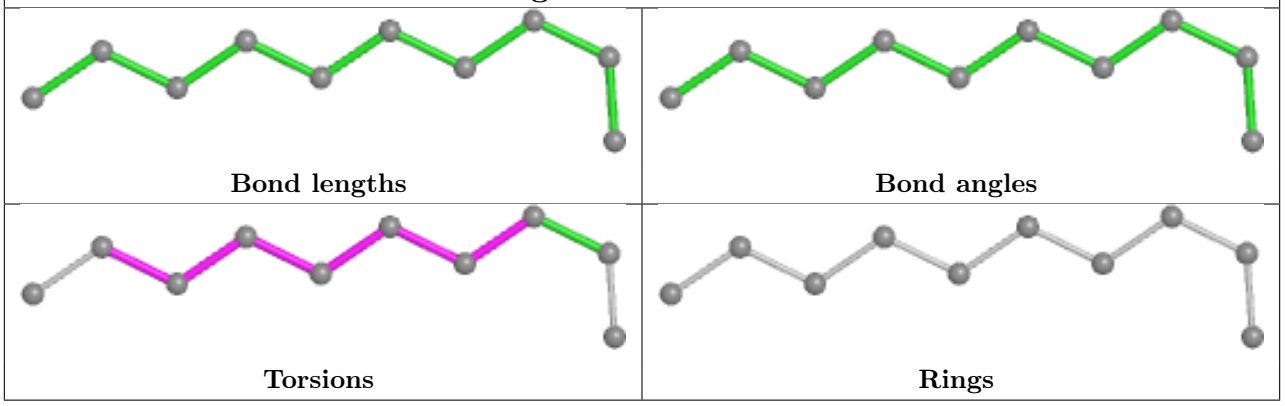


Torsions

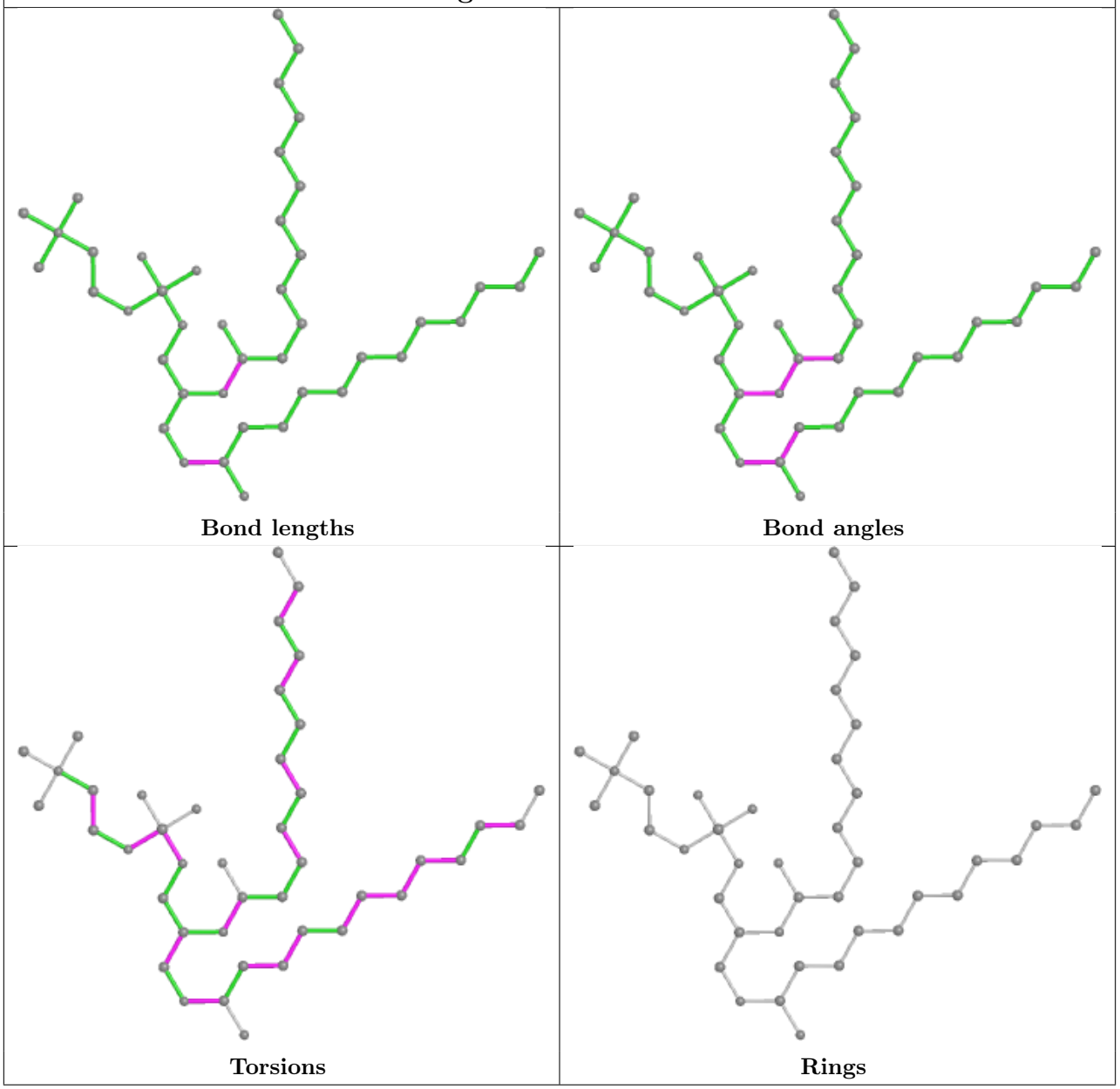


Rings

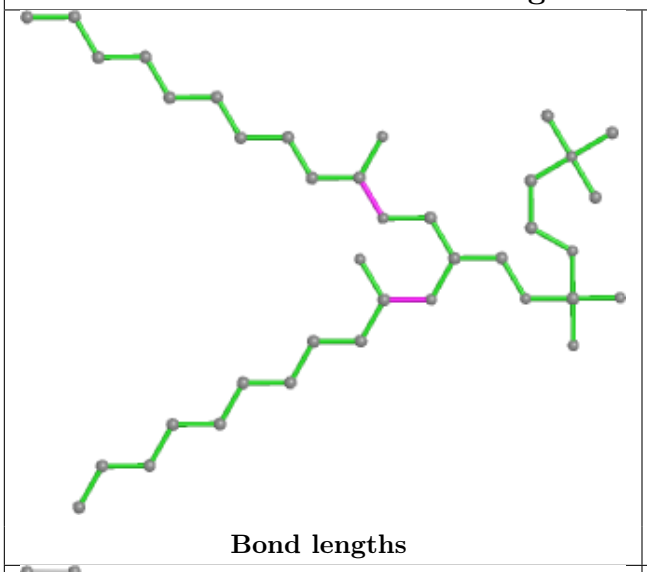
Ligand D10 B 305



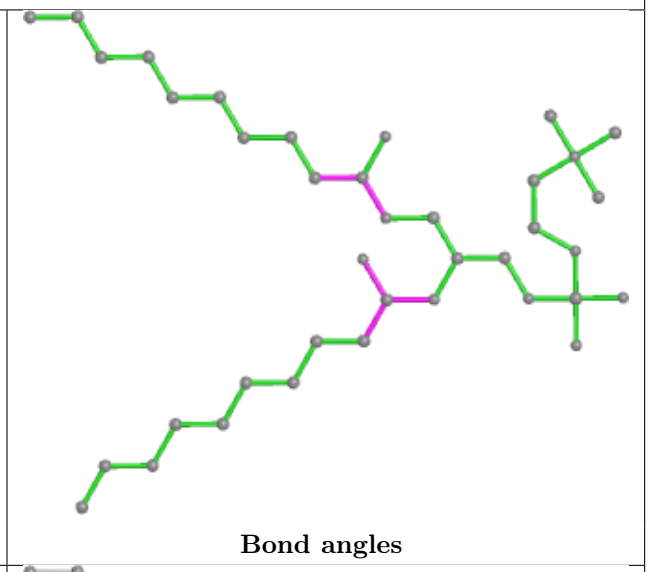
Ligand PLC G 303



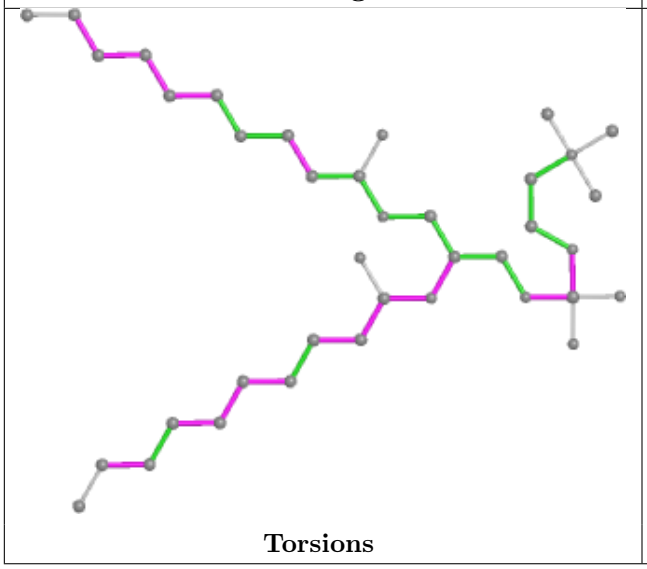
Ligand P1O B 308



Bond lengths



Bond angles



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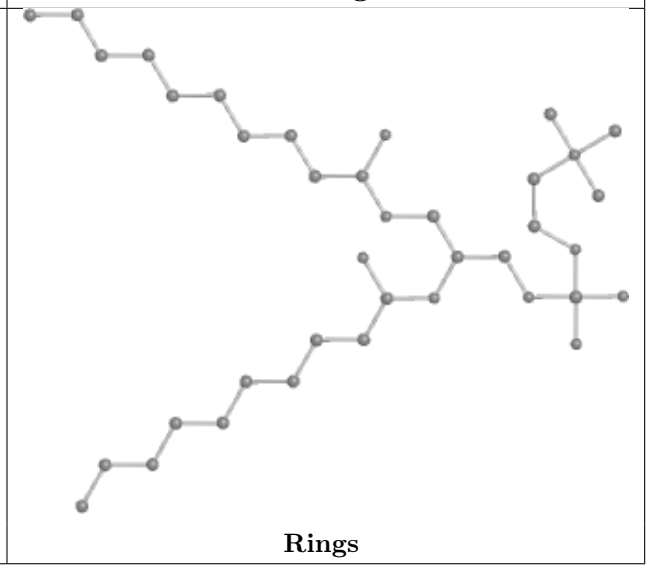
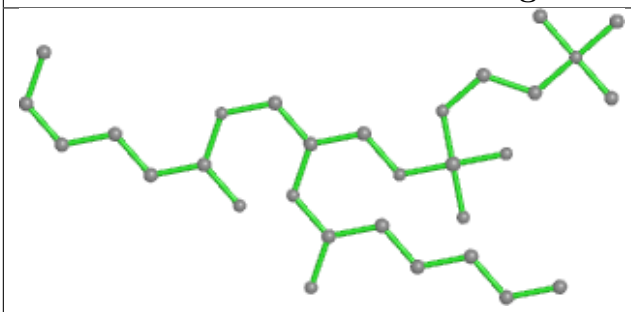
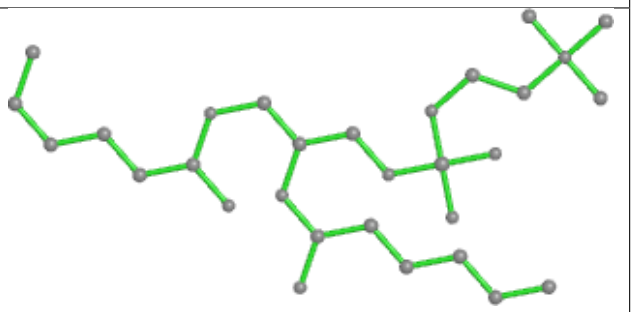


Rings

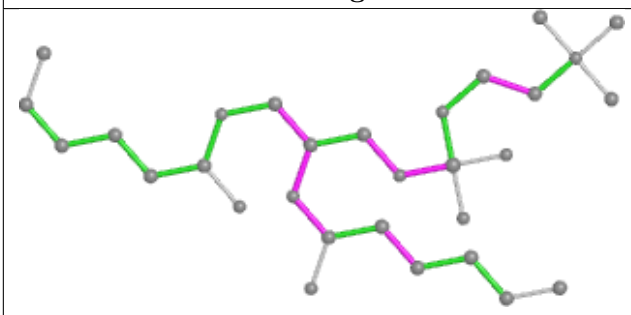
Ligand HXG G 307



Bond lengths



Bond angles



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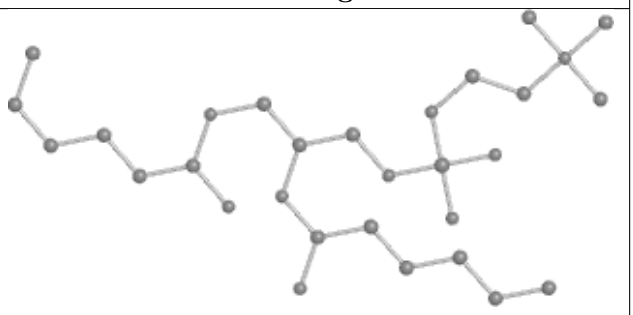
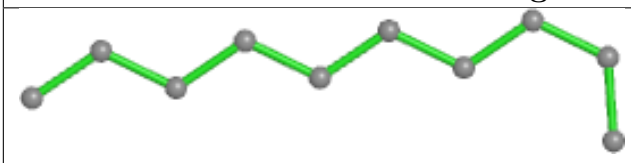
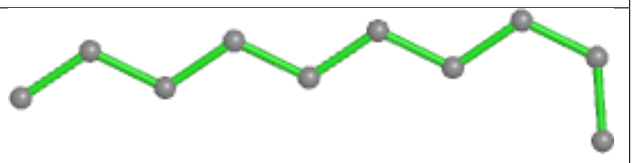


Rings

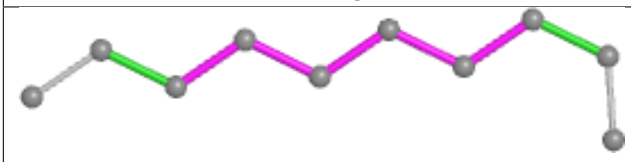
Ligand D10 B 306



Bond lengths



Bond angles



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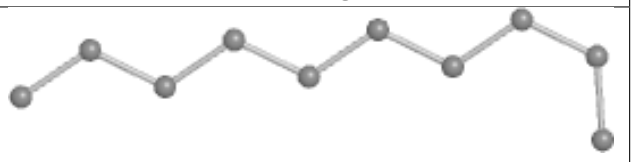
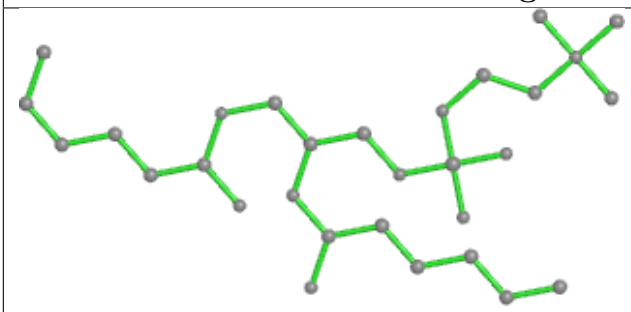
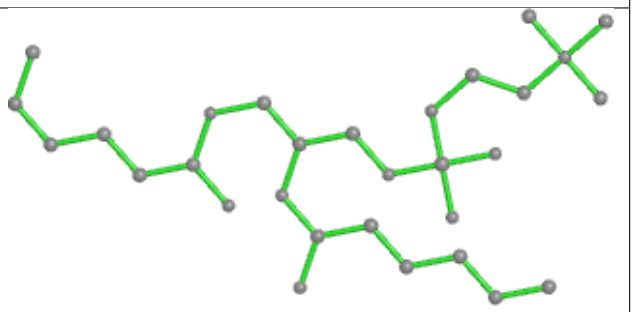


Rings

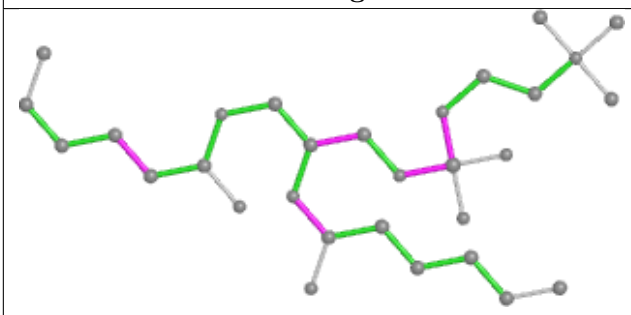
Ligand HXG G 304



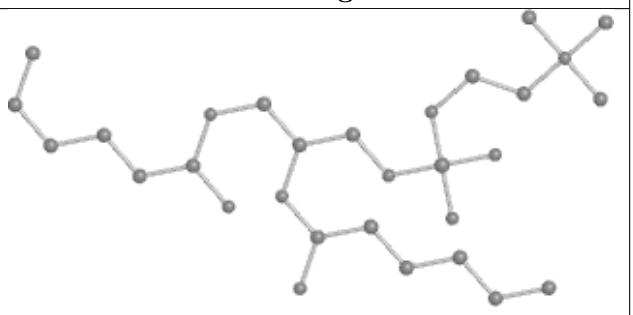
Bond lengths



Bond angles

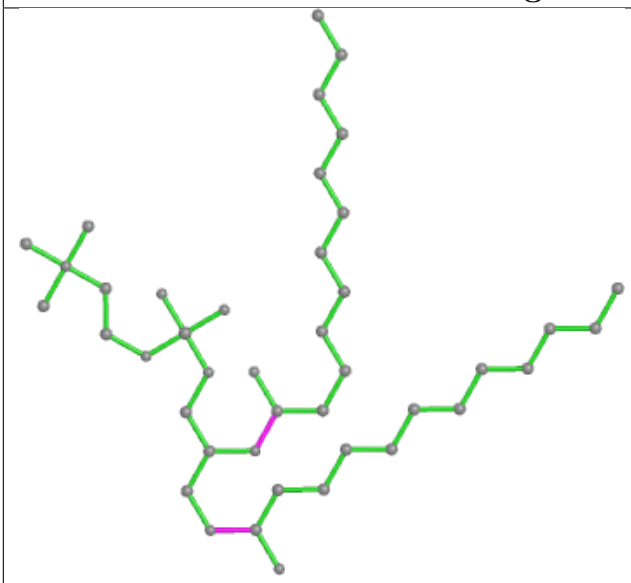


Torsions

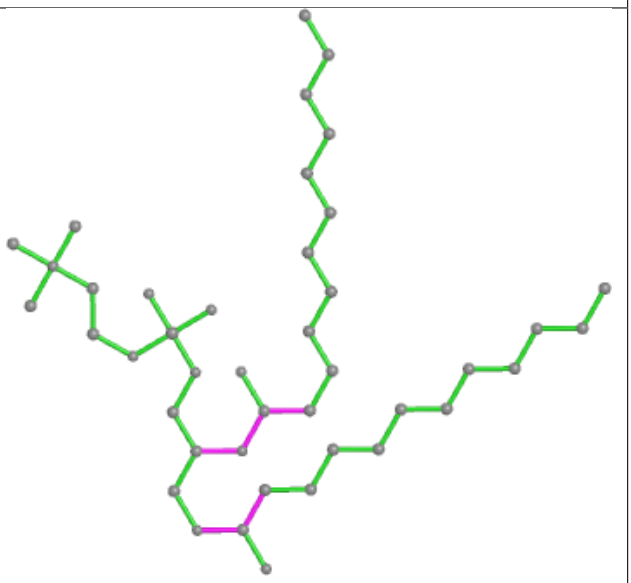


Rings

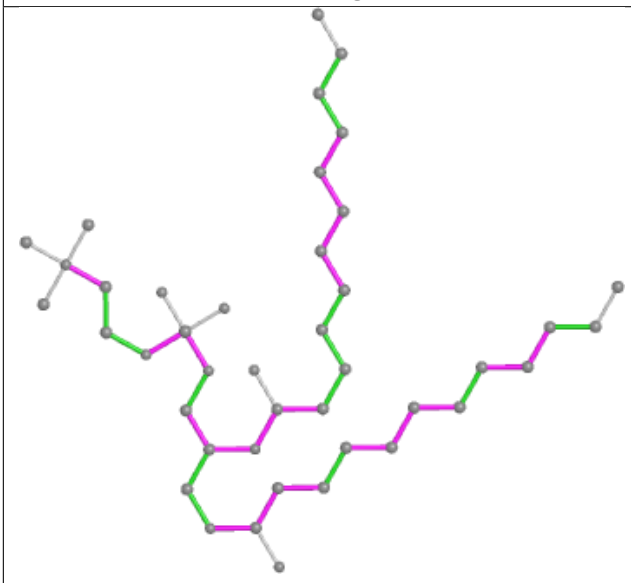
Ligand PLC K 301



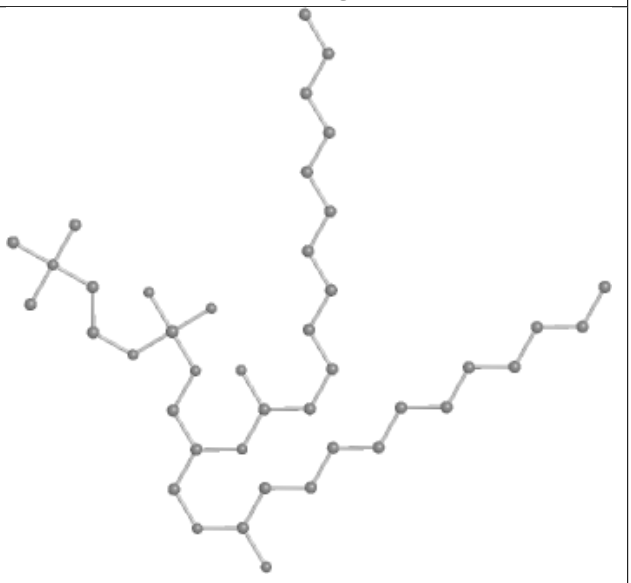
Bond lengths



Bond angles

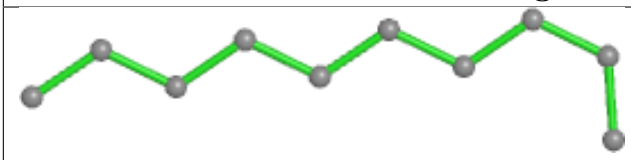


Torsions

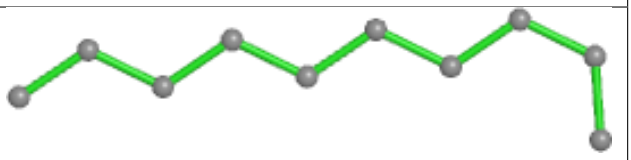


Rings

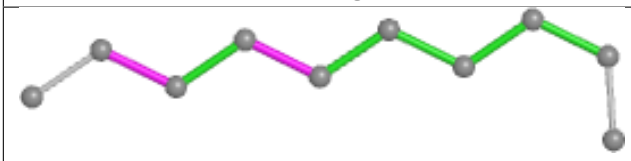
Ligand D10 J 306



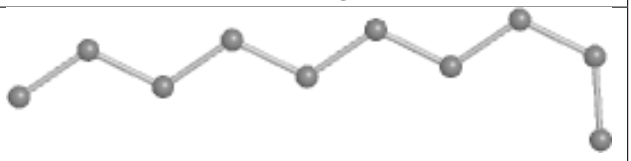
Bond lengths



Bond angles

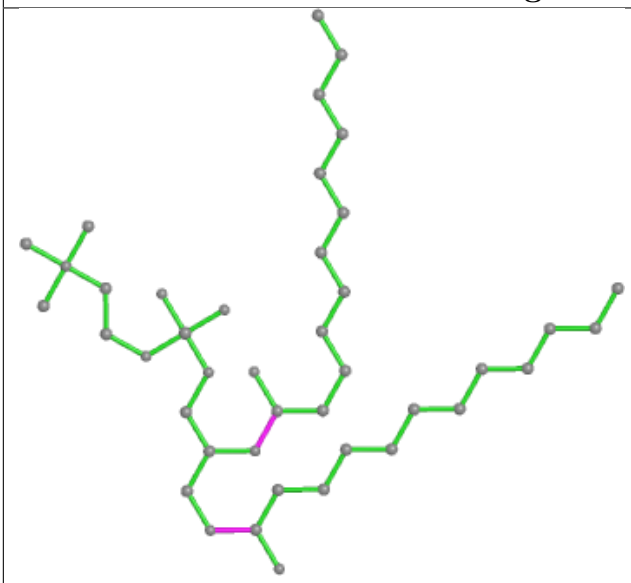


Torsions

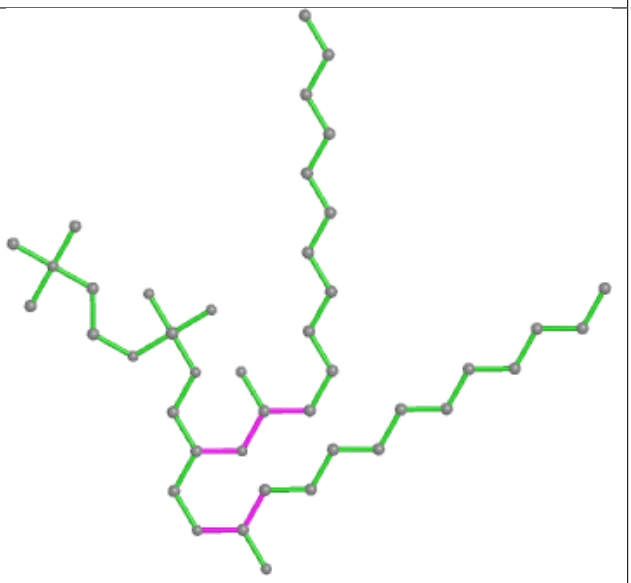


Rings

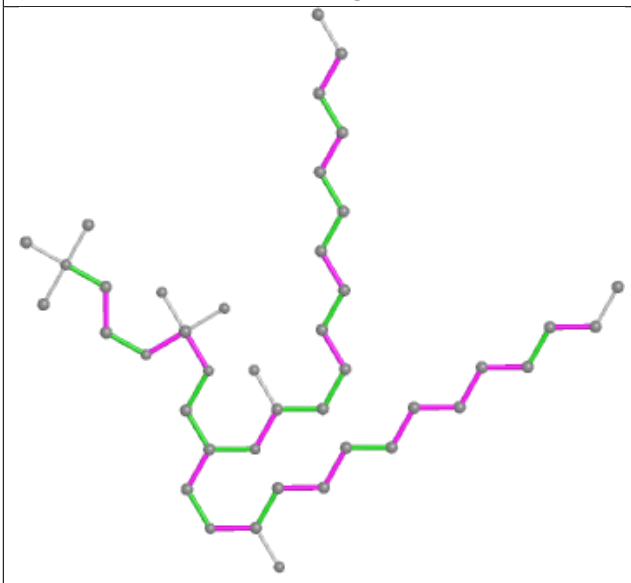
Ligand PLC K 303



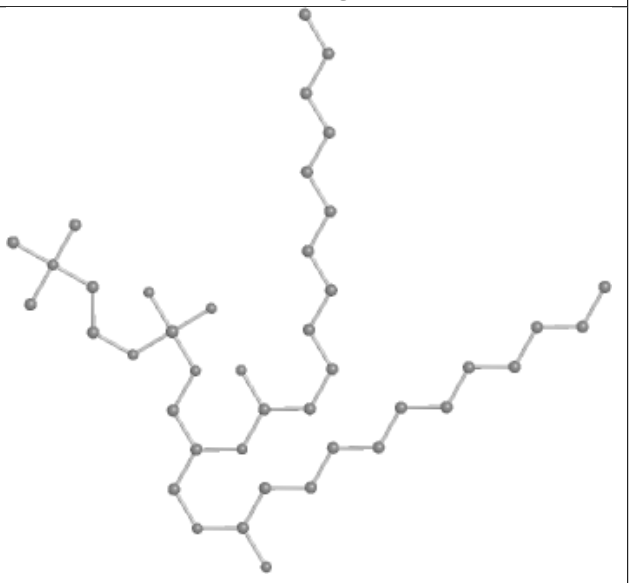
Bond lengths



Bond angles

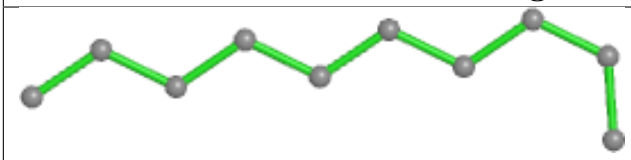


Torsions

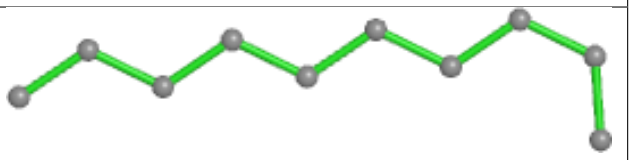


Rings

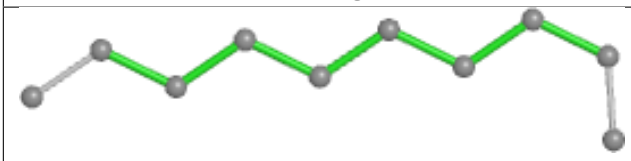
Ligand D10 G 305



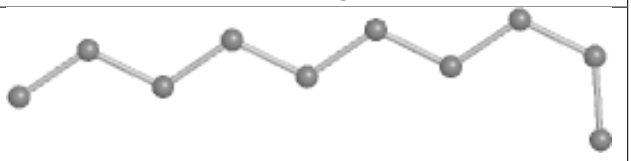
Bond lengths



Bond angles

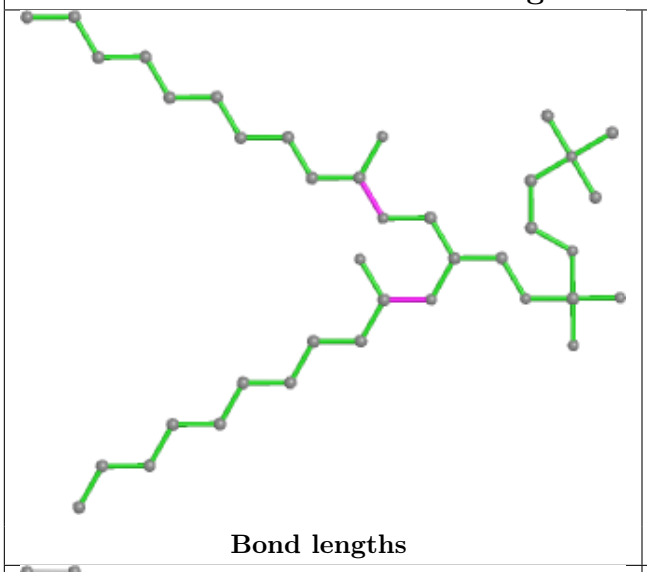


Torsions

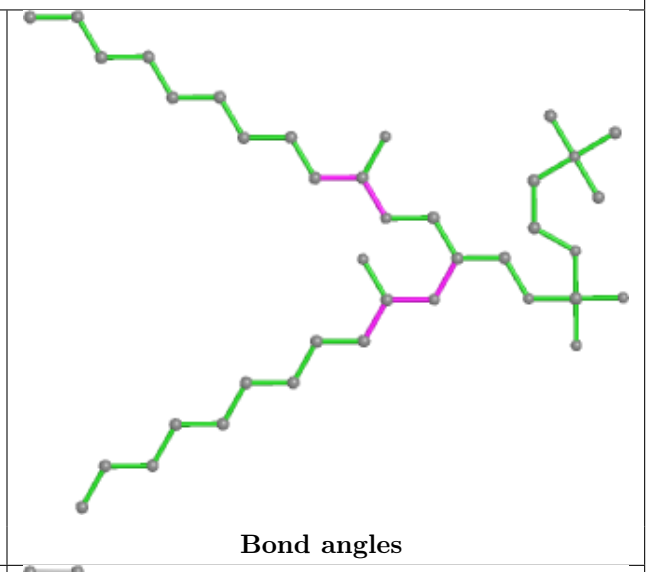


Rings

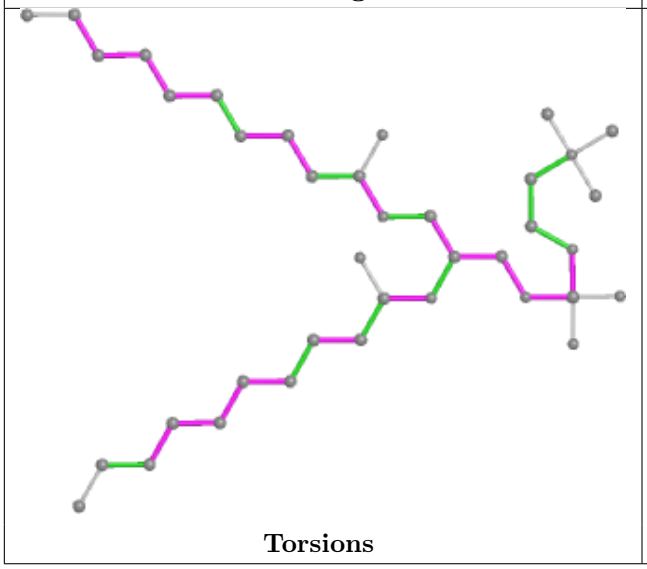
Ligand P1O G 310



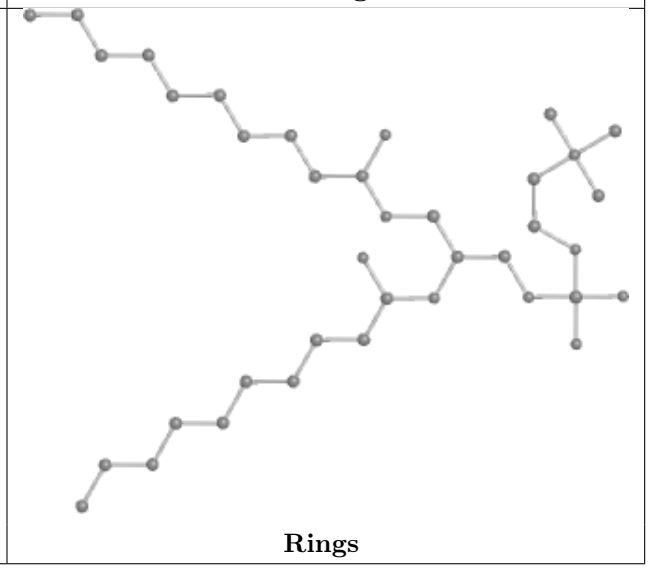
Bond lengths



Bond angles

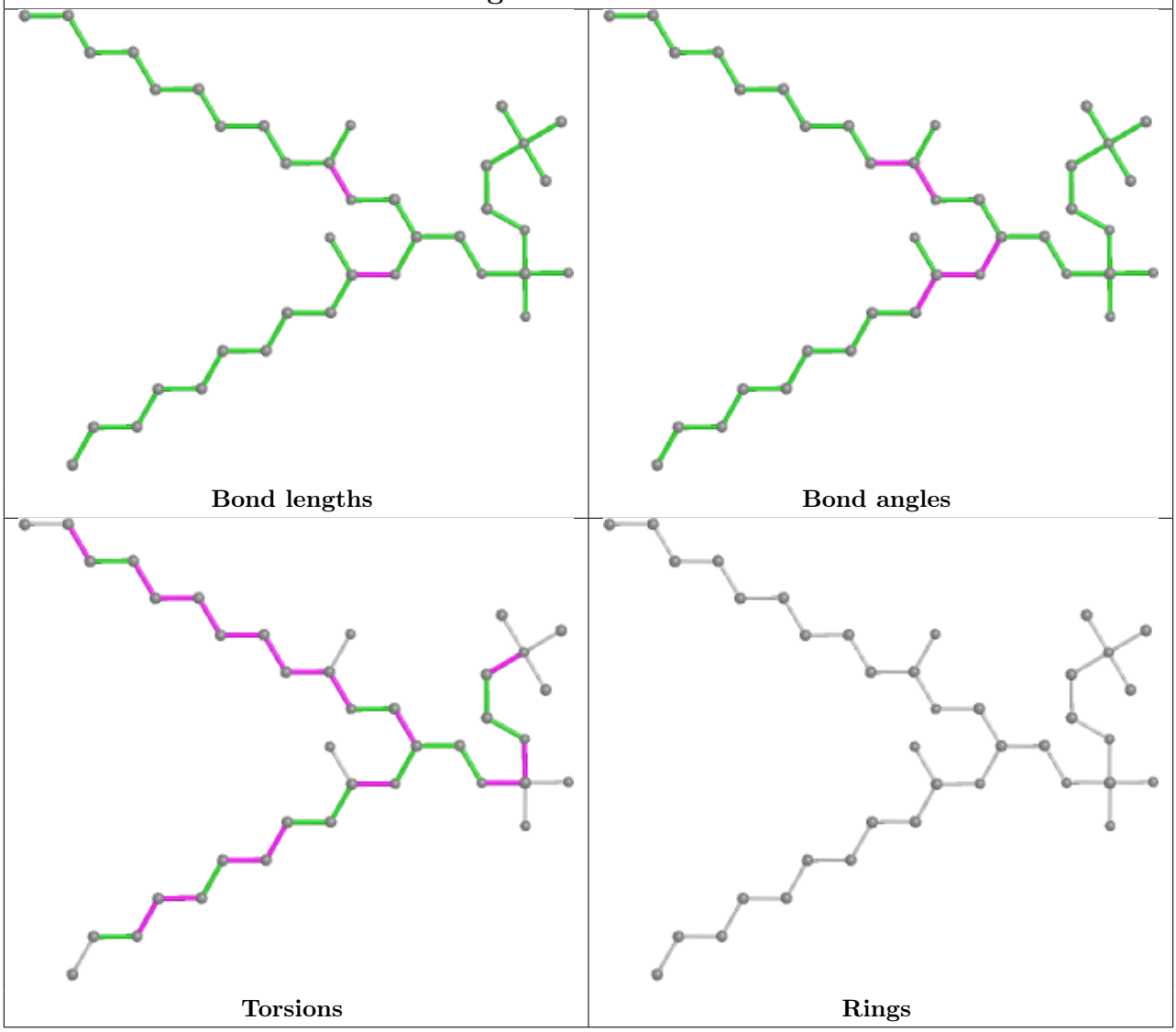


Torsions

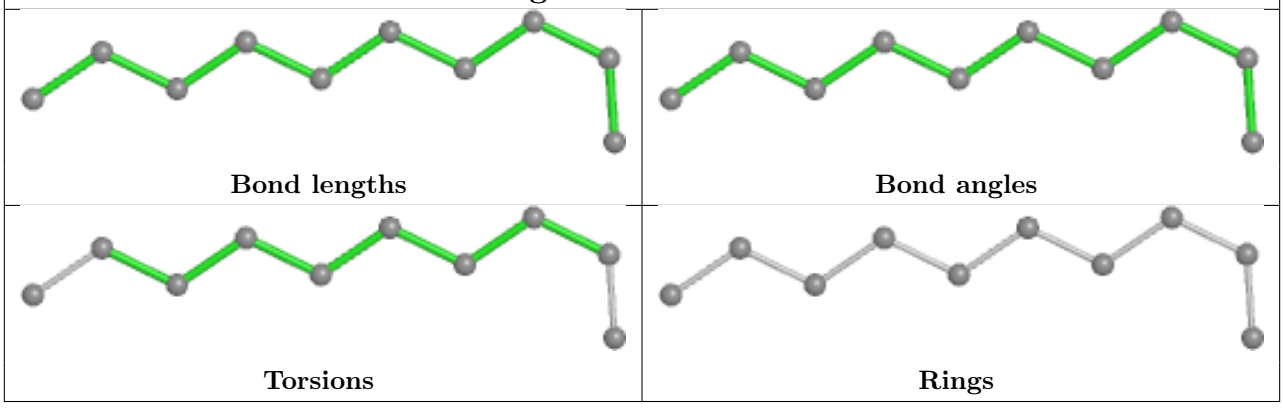


Rings

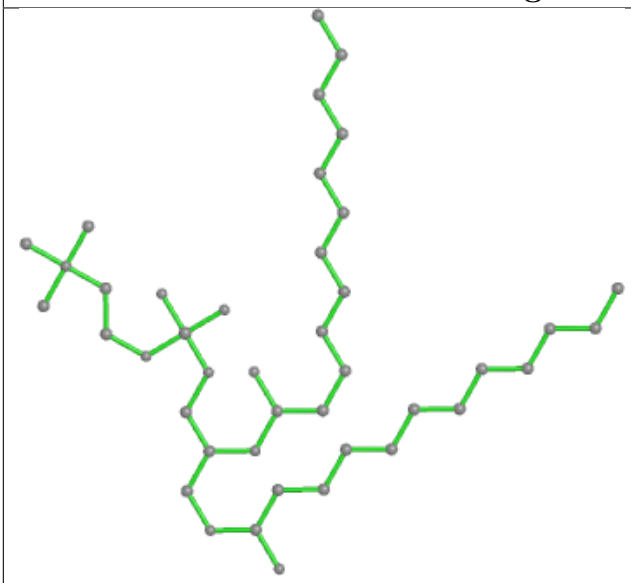
Ligand P1O J 304



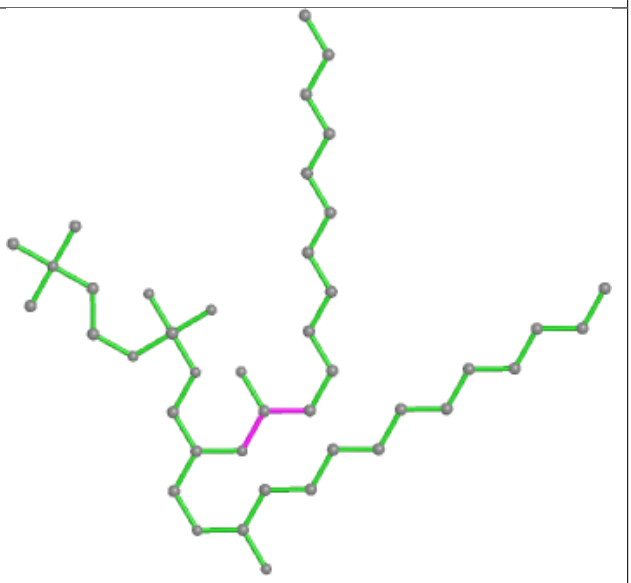
Ligand D10 K 305



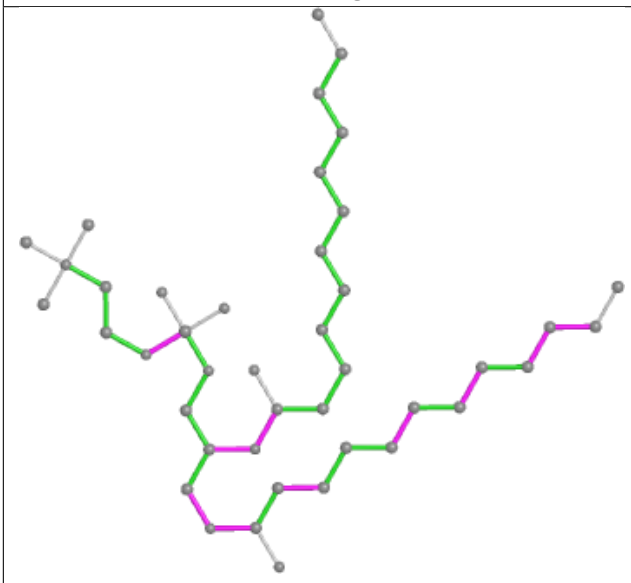
Ligand PLC G 306



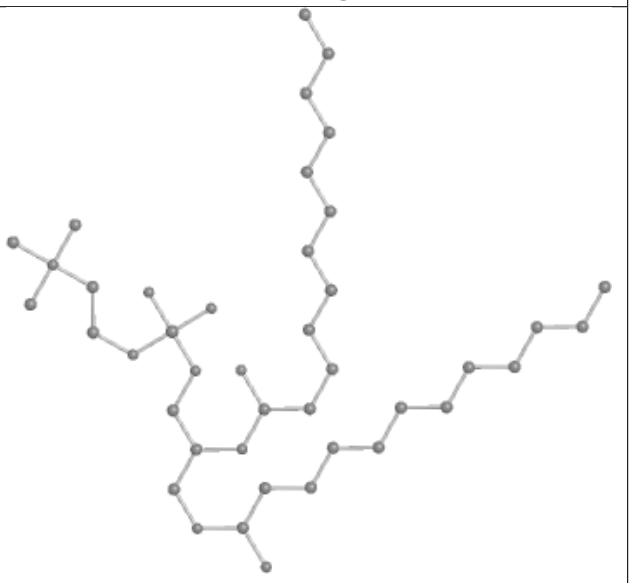
Bond lengths



Bond angles

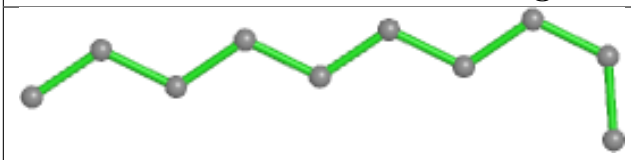


Torsions

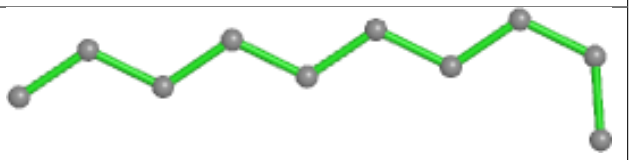


Rings

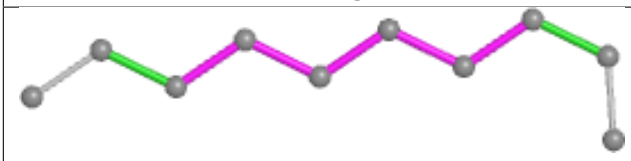
Ligand D10 J 308



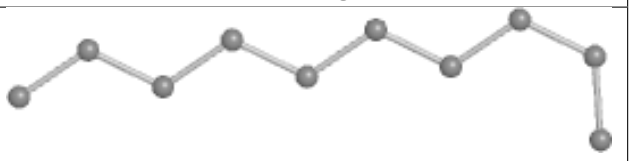
Bond lengths



Bond angles

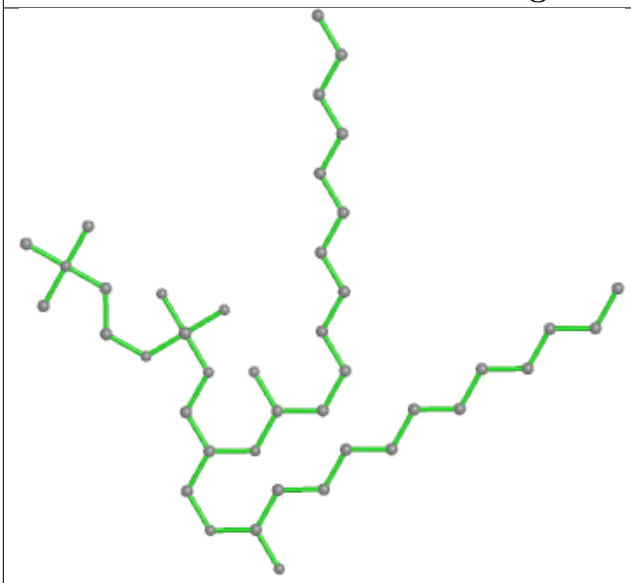


Torsions



Rings

Ligand PLC J 302



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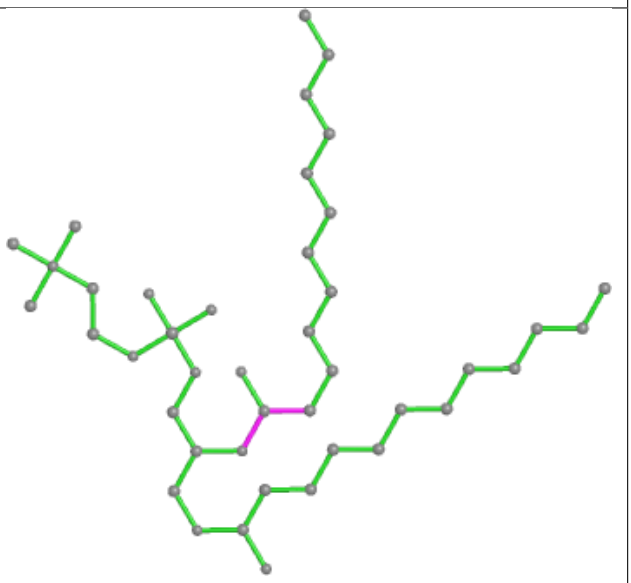
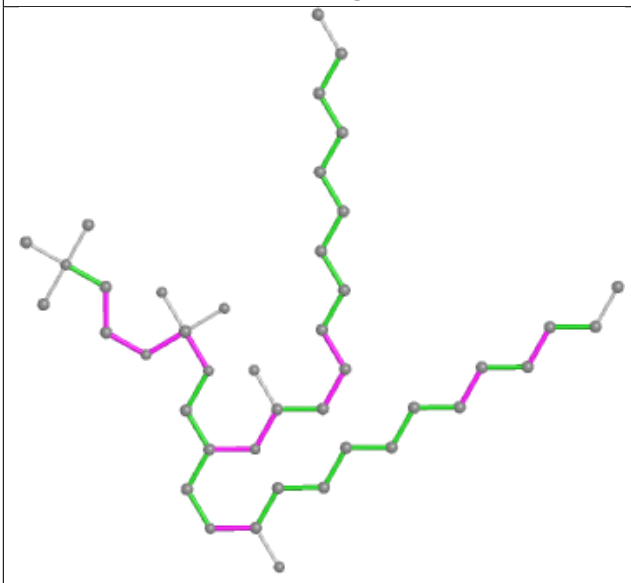
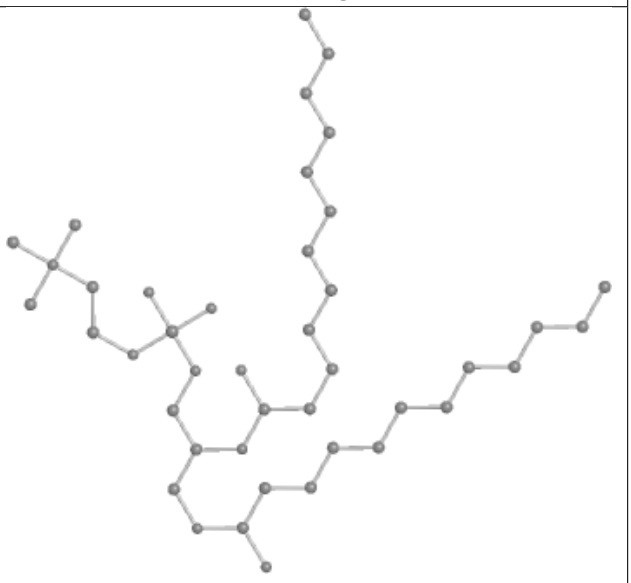


Bond angles

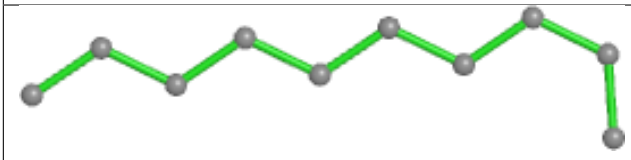


Torsions

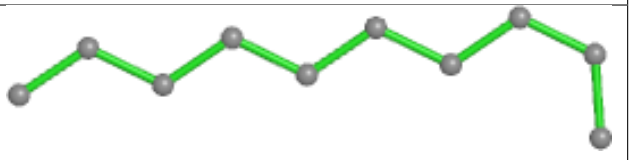


Rings

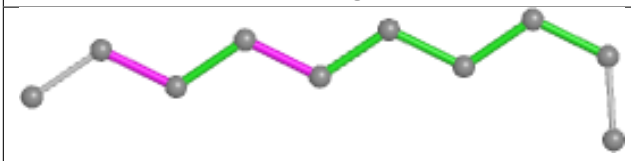
Ligand D10 F 305



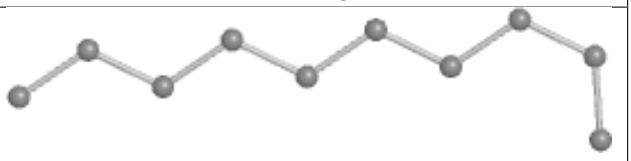
Bond lengths



Bond angles

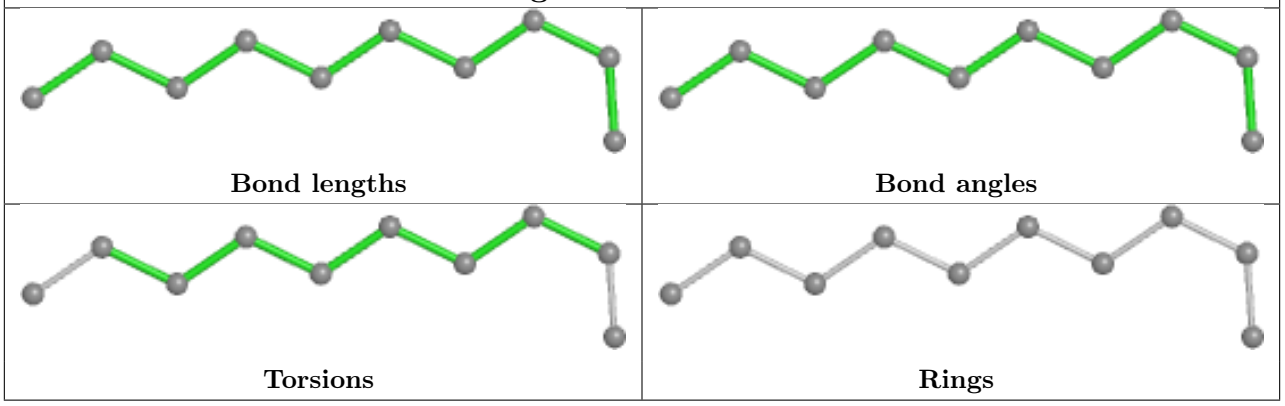


Torsions

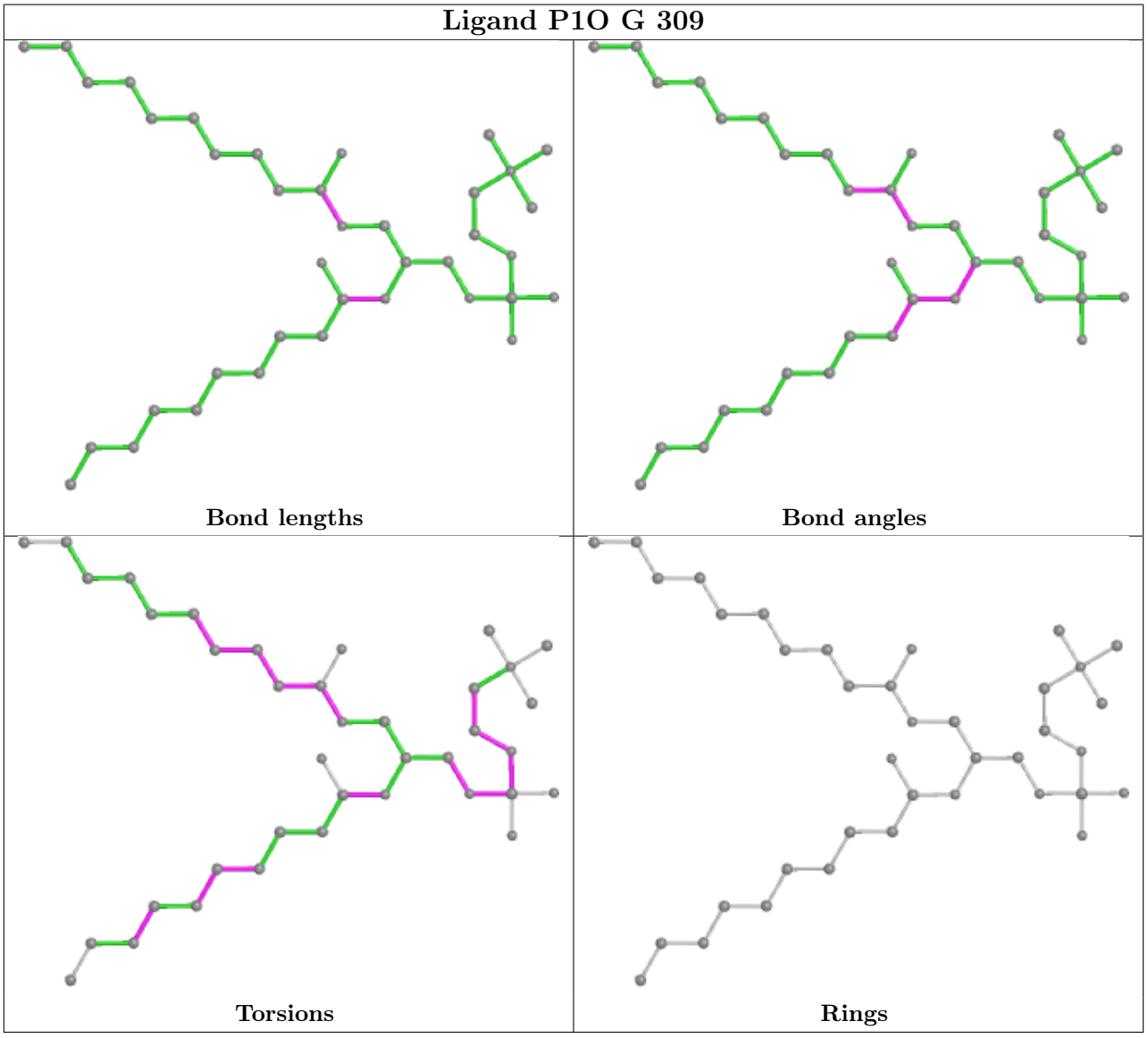


Rings

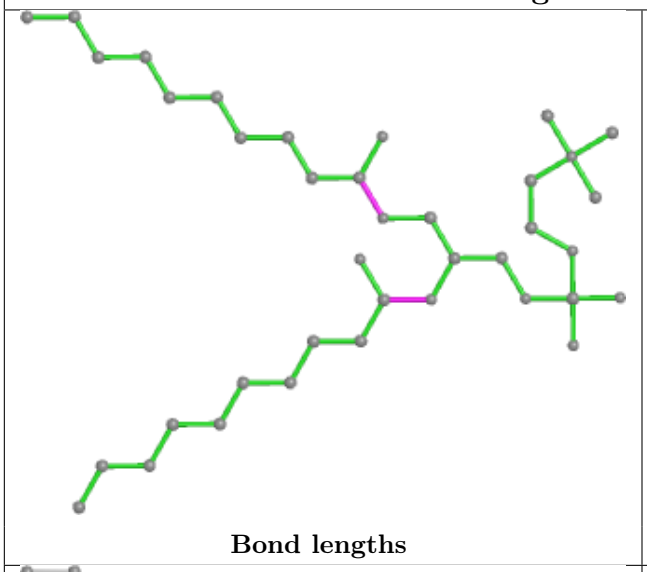
Ligand D10 A 503



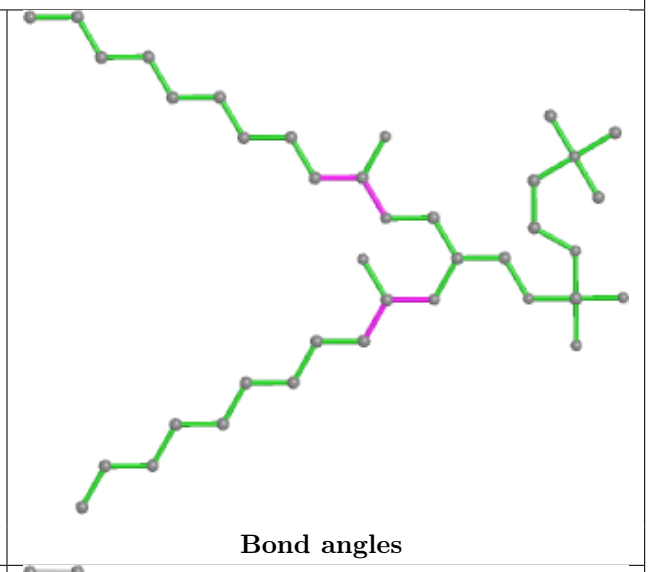
Ligand P1O G 309



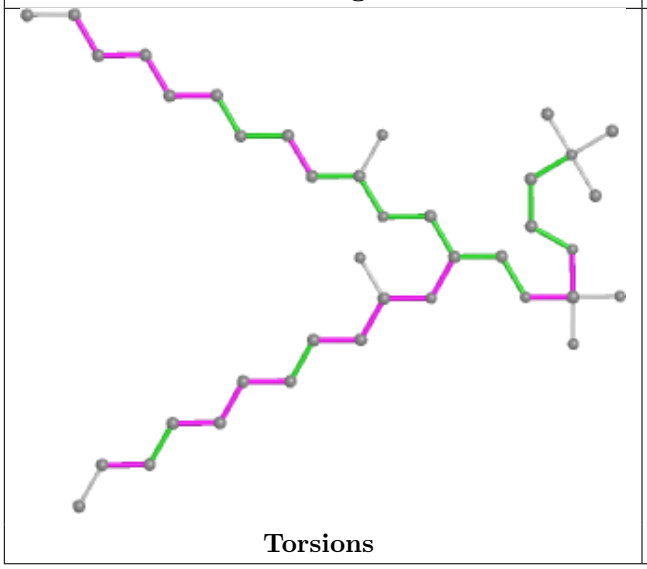
Ligand P1O J 301



Bond lengths



Bond angles



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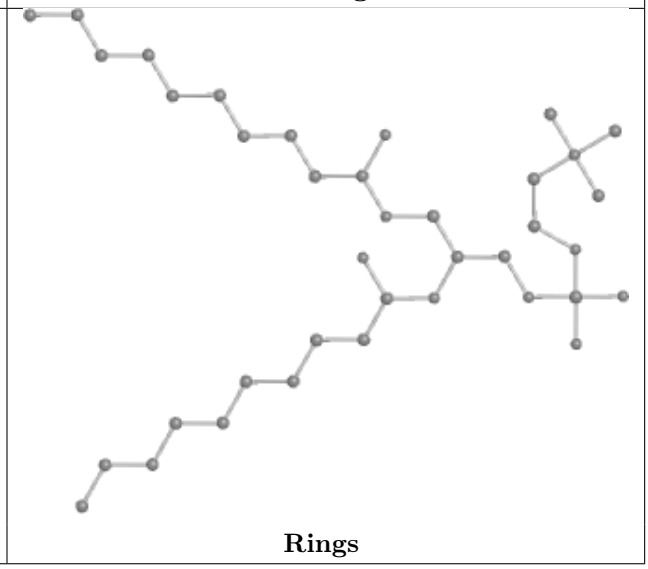
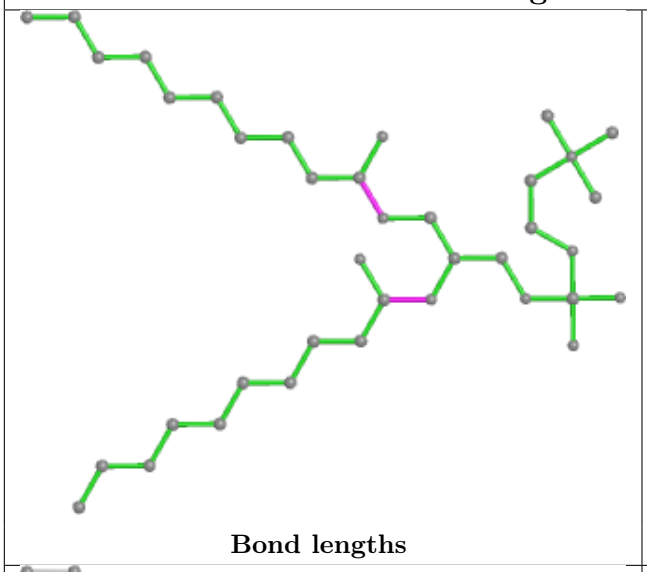
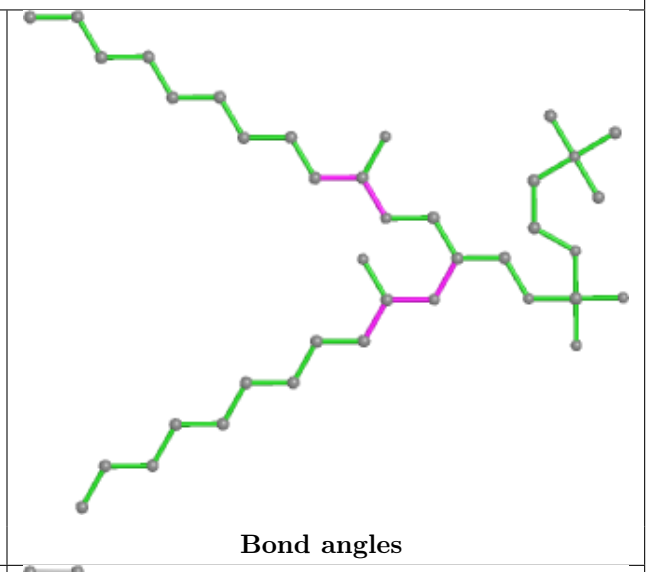


Rings

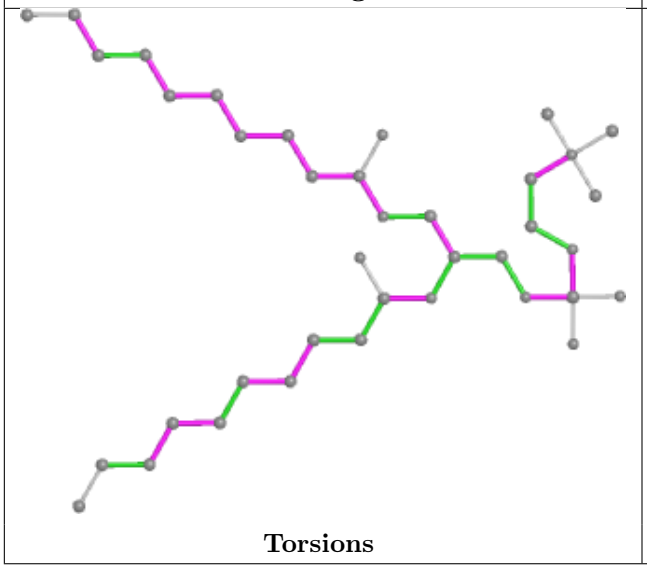
Ligand P1O F 303



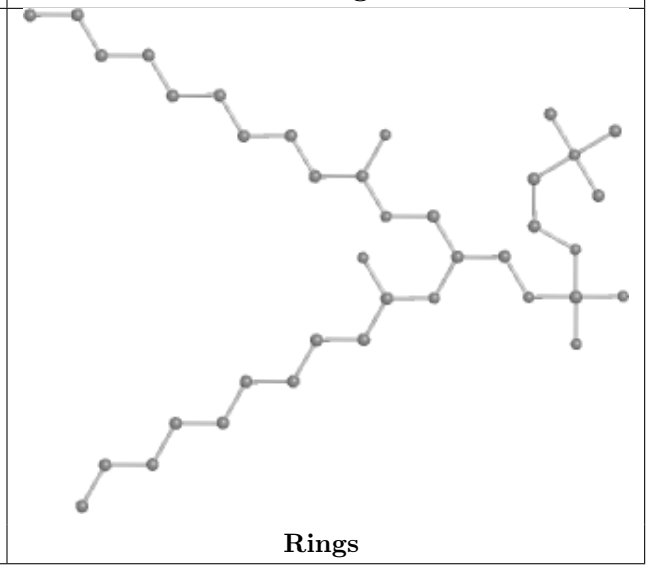
Bond lengths



Bond angles

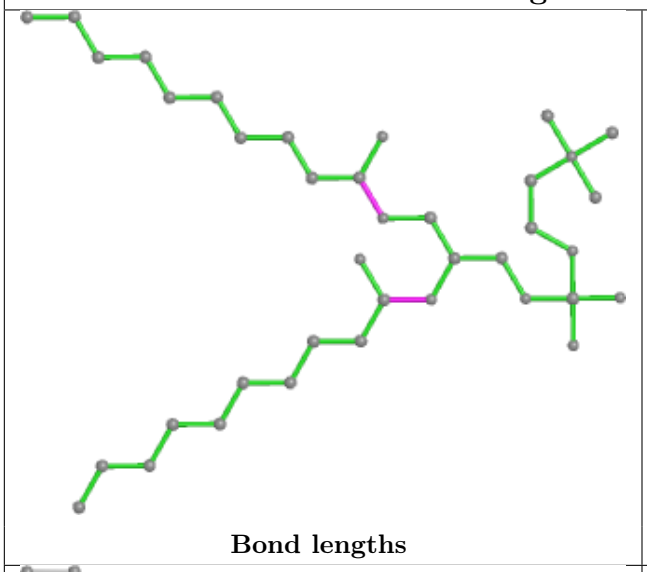


Torsions

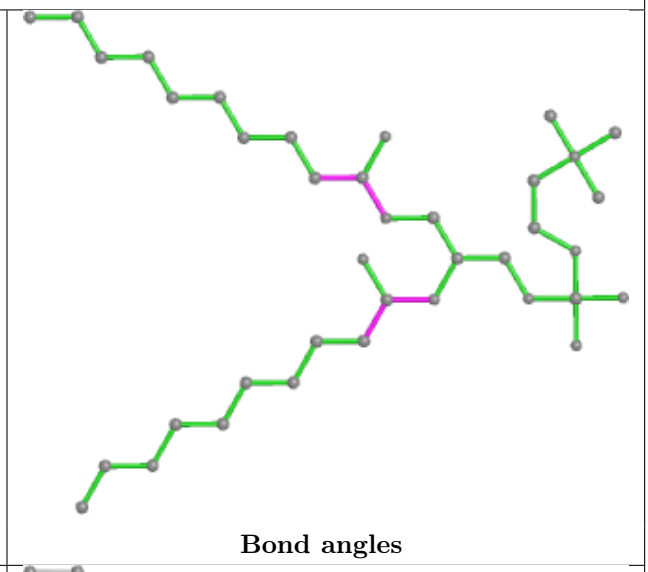


Rings

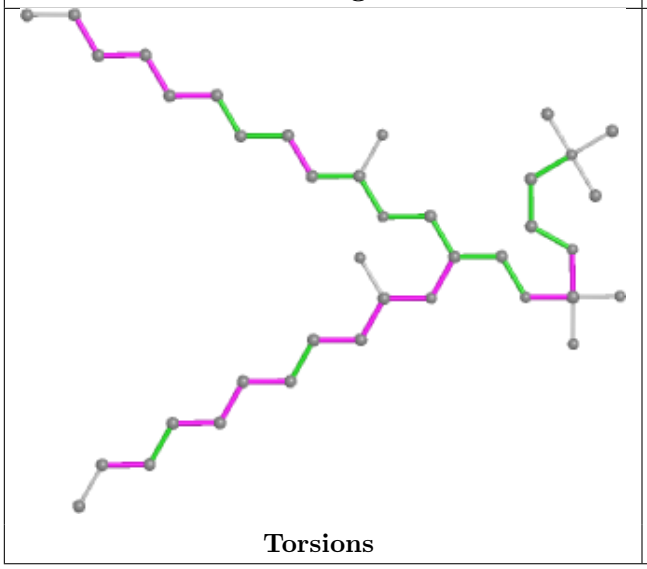
Ligand P1O F 308



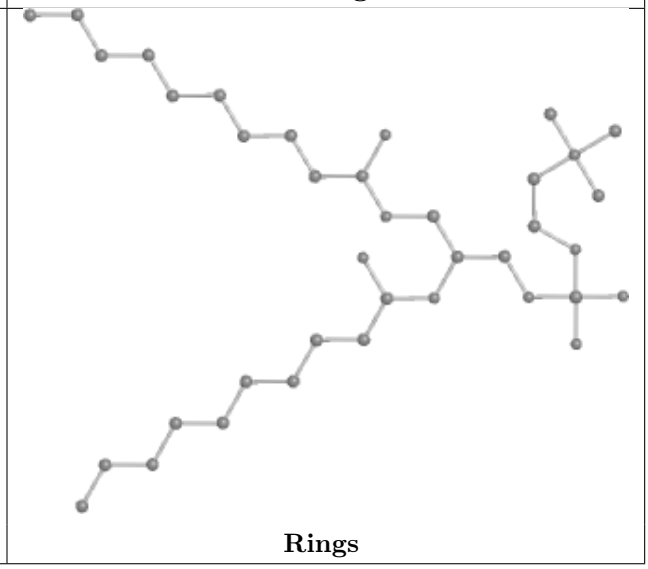
Bond lengths



Bond angles

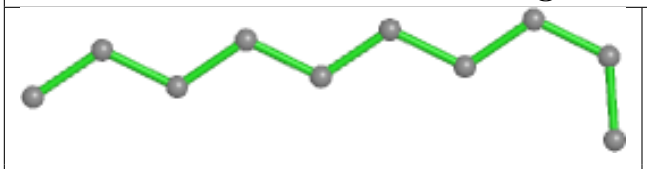


Torsions

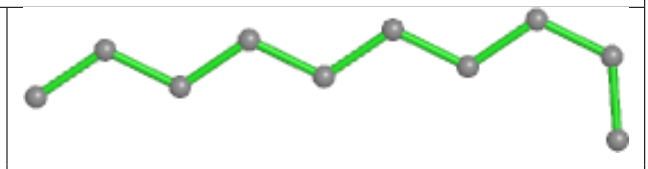


Rings

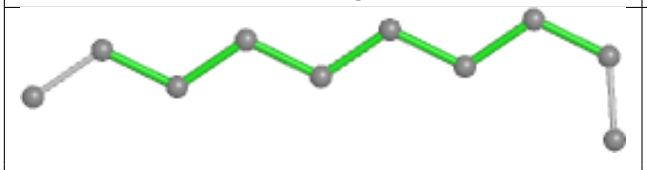
Ligand D10 I 503



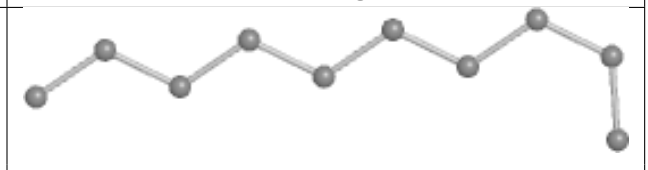
Bond lengths



Bond angles

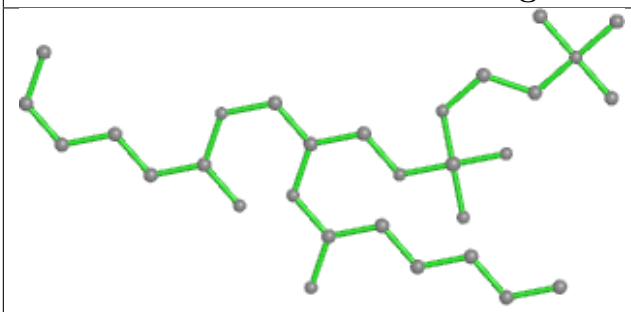


Torsions

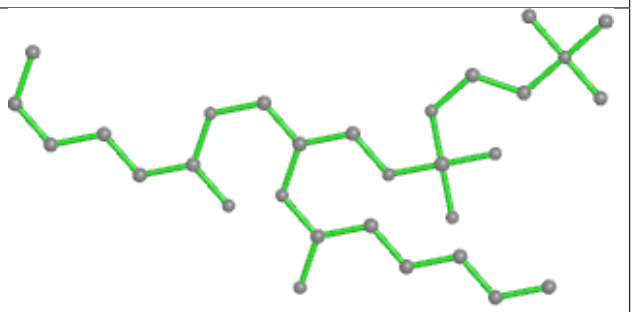


Rings

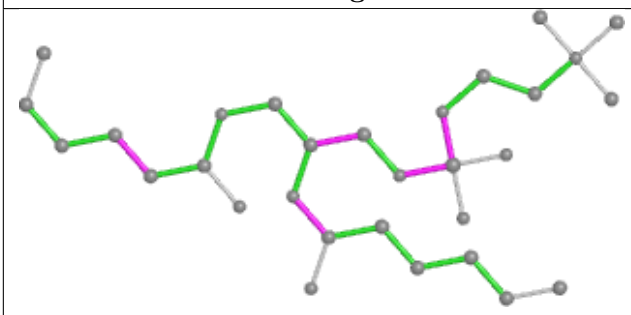
Ligand HXG K 304



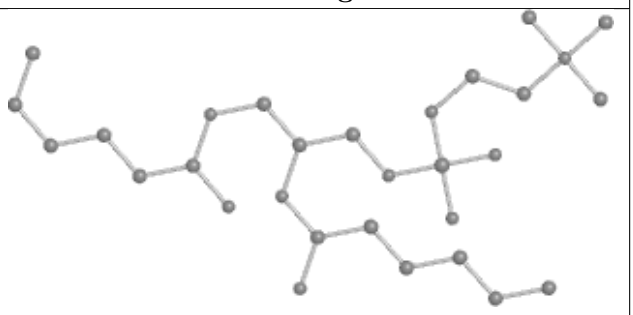
Bond lengths



Bond angles

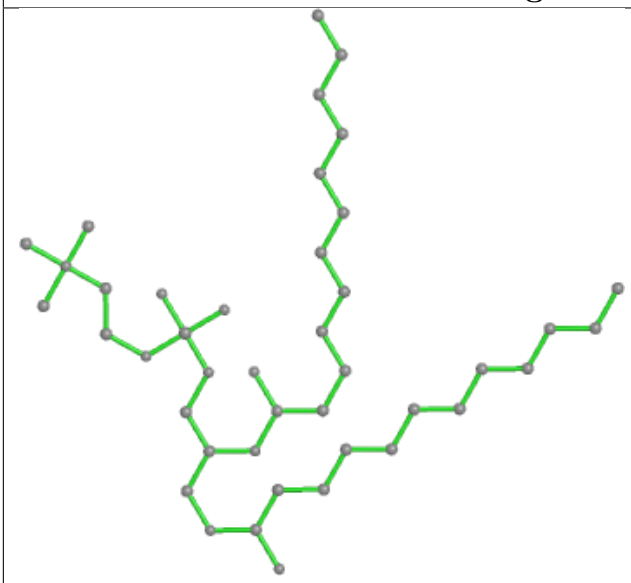


Torsions

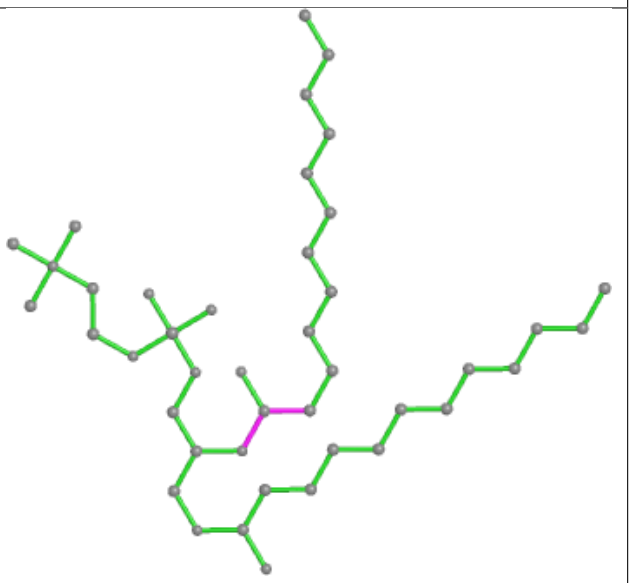


Rings

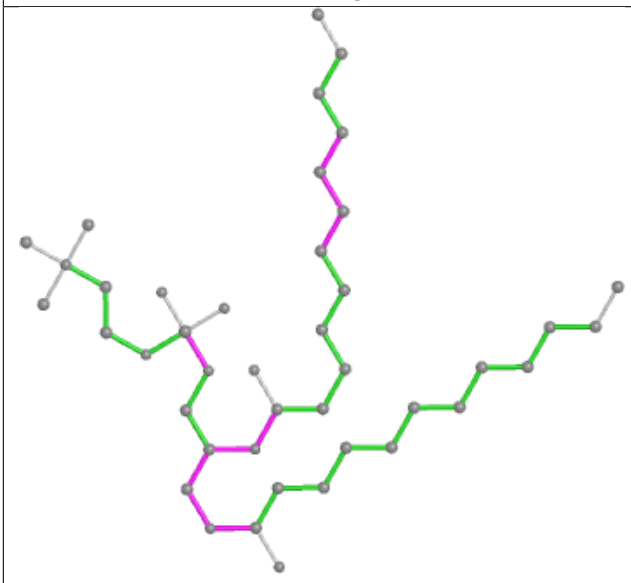
Ligand PLC B 301



Bond lengths



Bond angles



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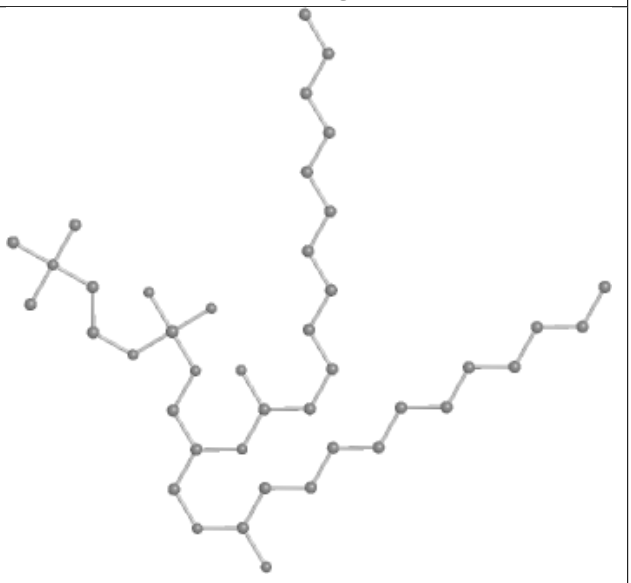
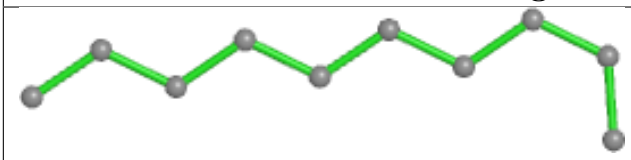
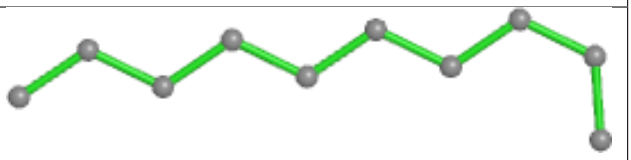


Rings

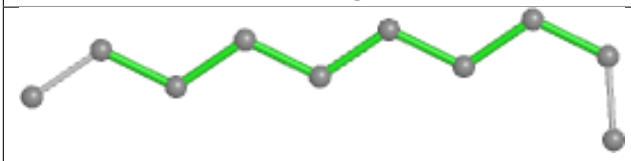
Ligand D10 B 303



Bond lengths



Bond angles



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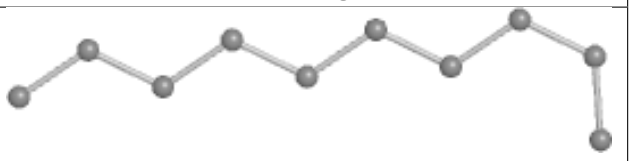
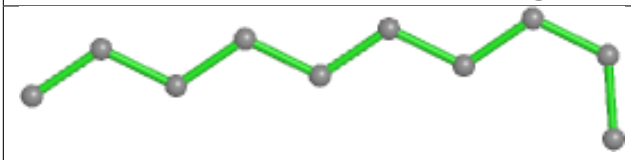
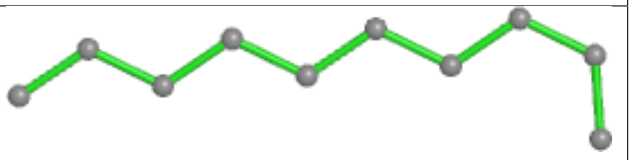
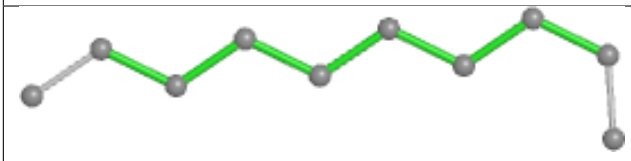
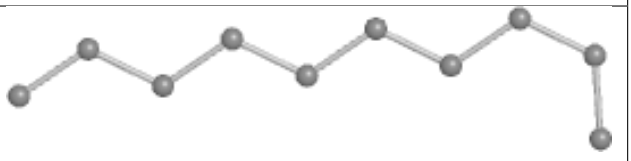
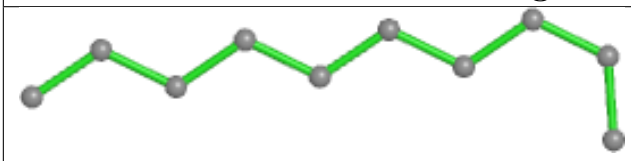
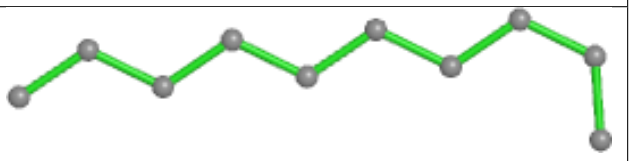
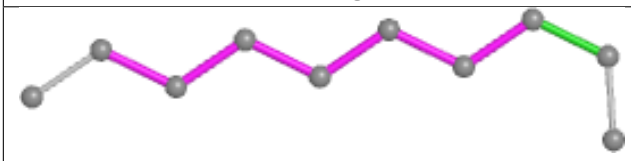
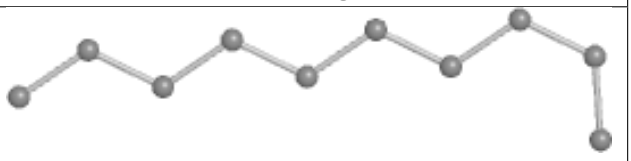
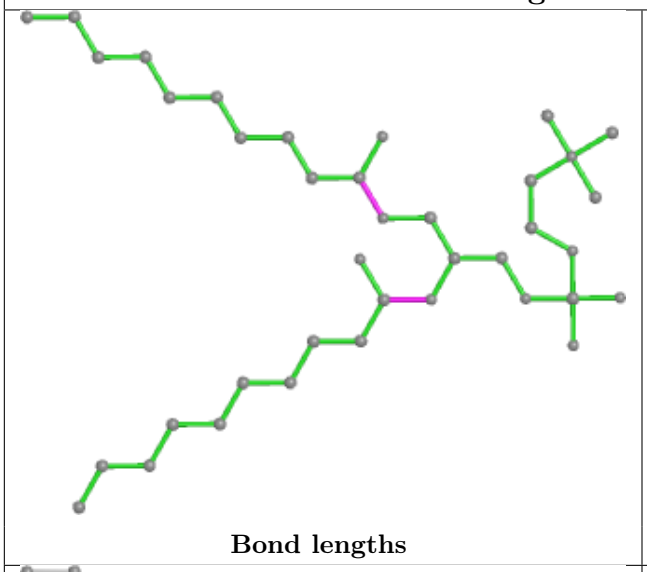


Rings

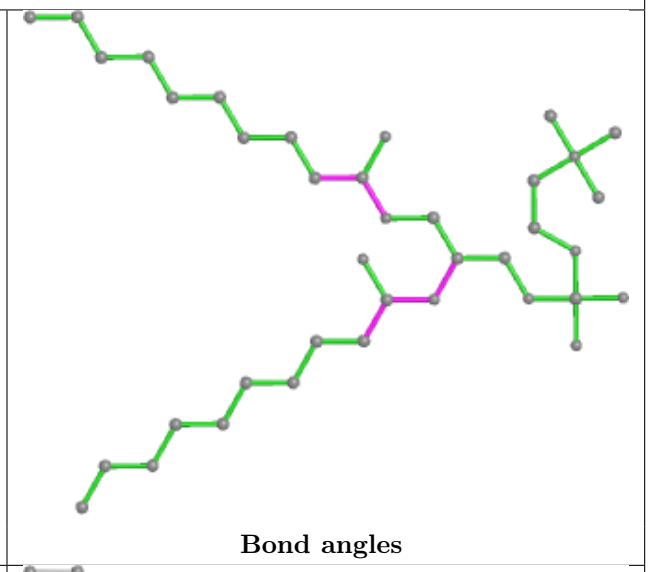
Ligand D10 C 304	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand D10 F 306	
 Bond lengths	 Bond angles
 Torsions	 Rings

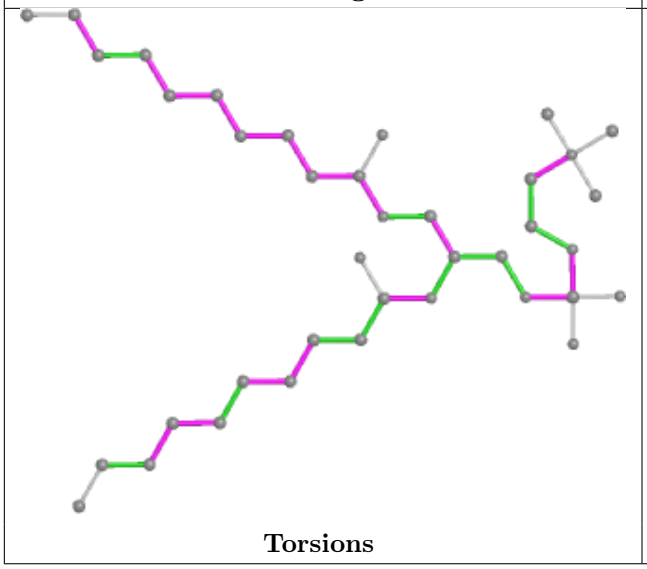
Ligand P1O B 302



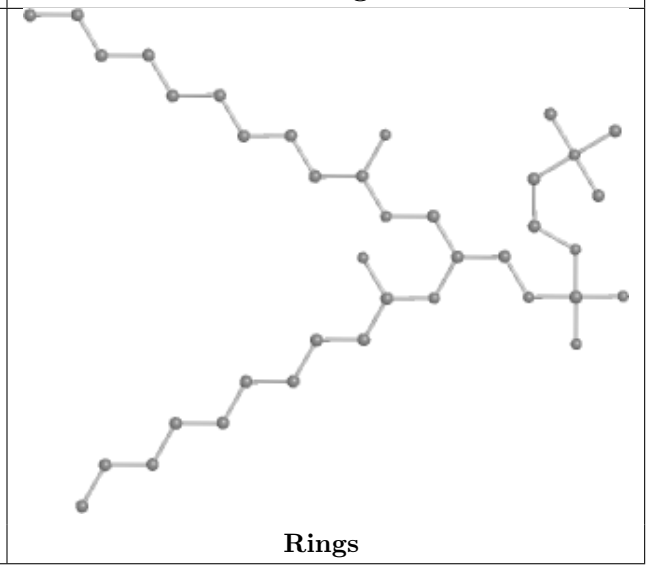
Bond lengths



Bond angles

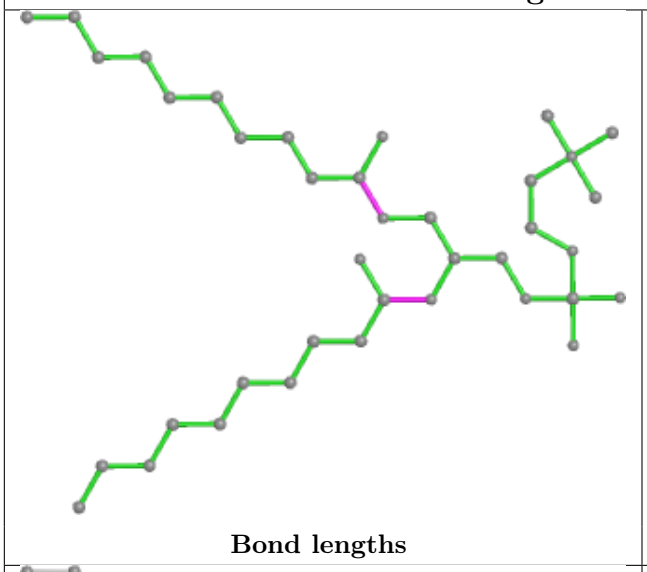


Torsions

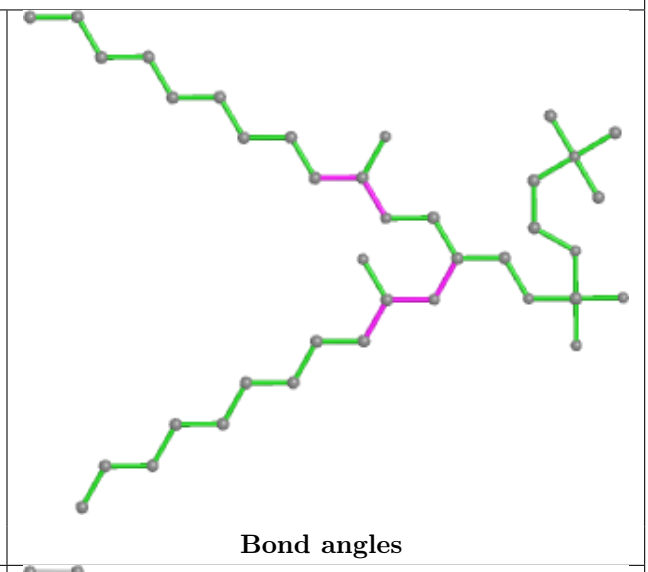


Rings

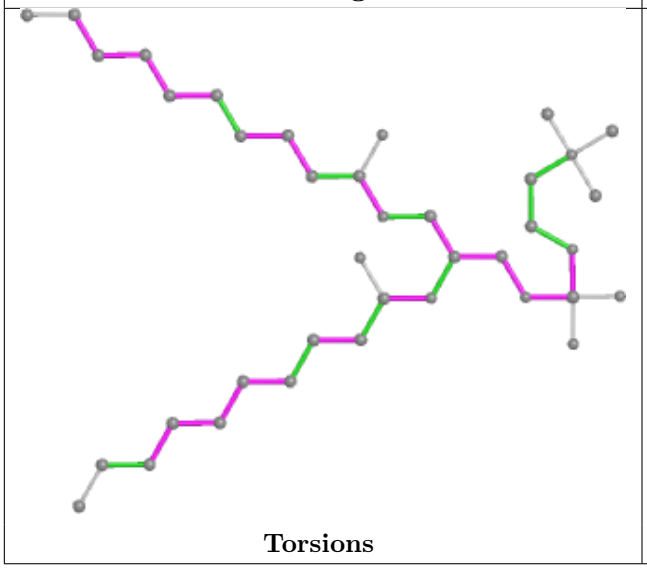
Ligand P1O K 310



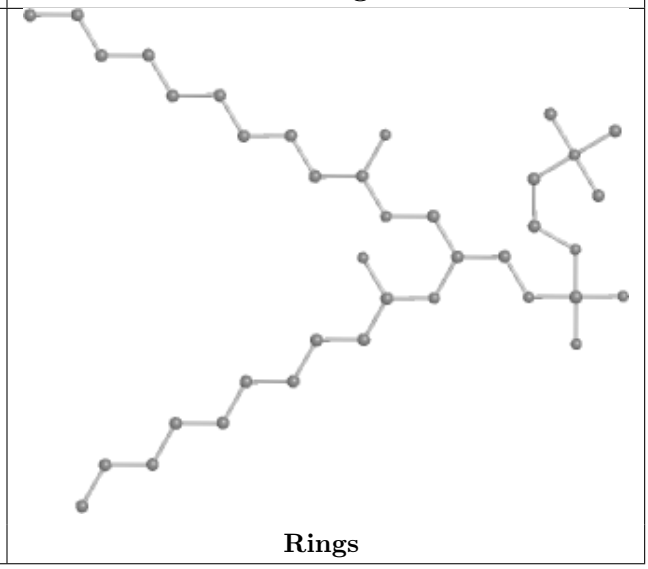
Bond lengths



Bond angles

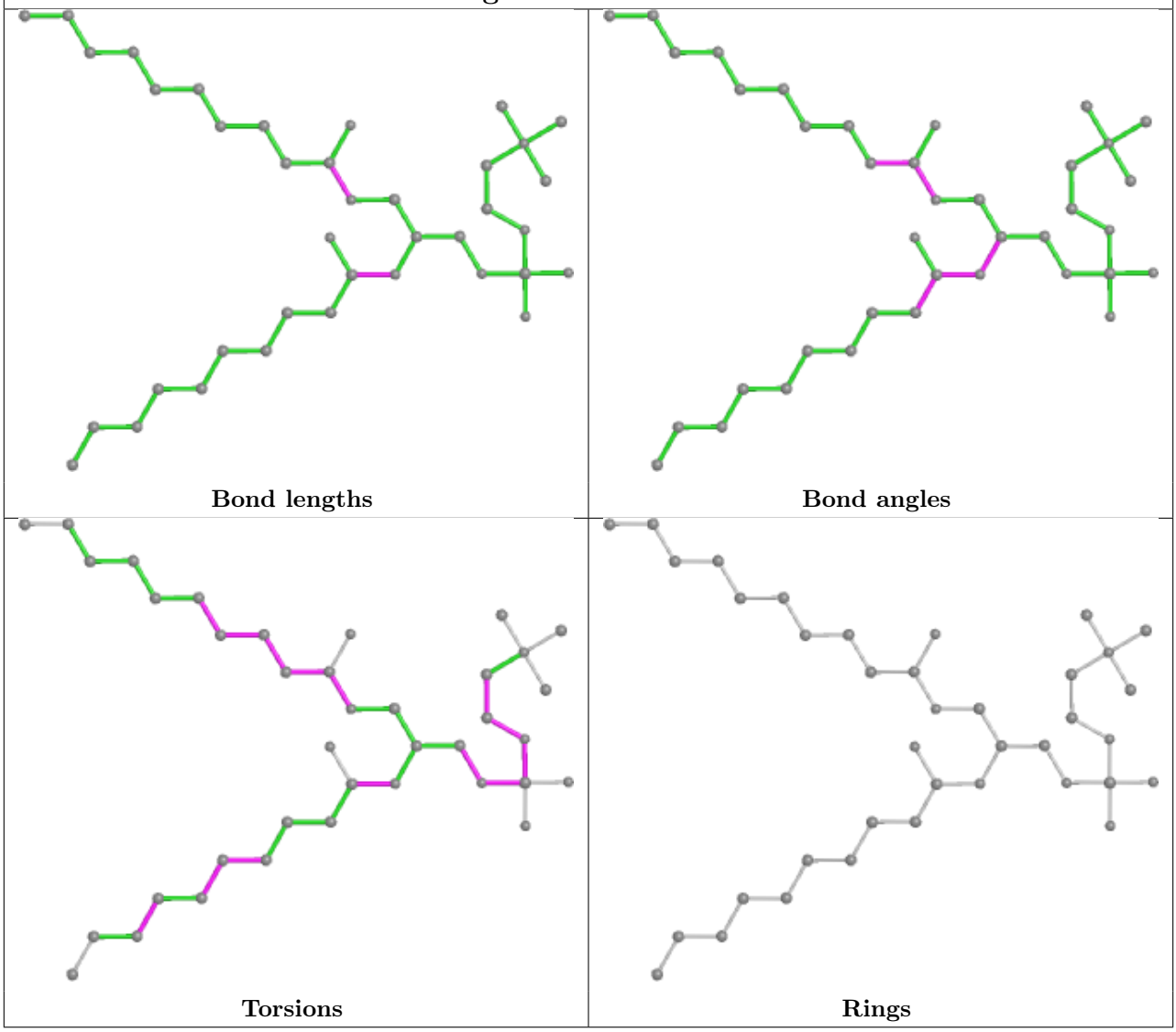


Torsions

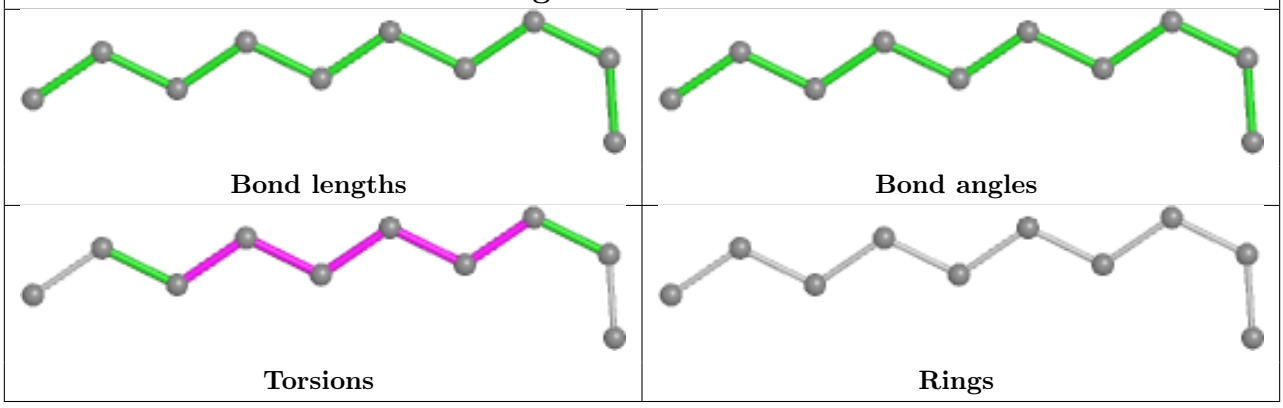


Rings

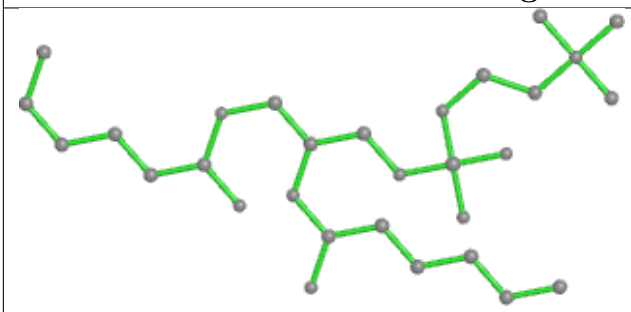
Ligand P1O K 309



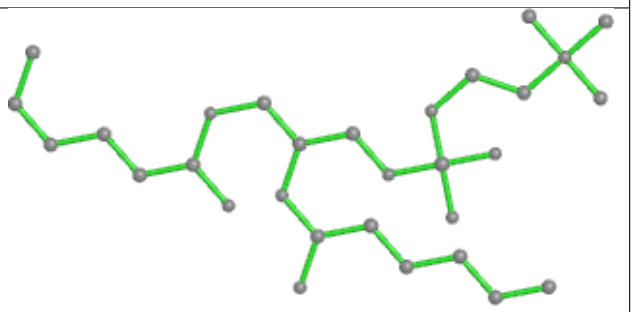
Ligand D10 F 307



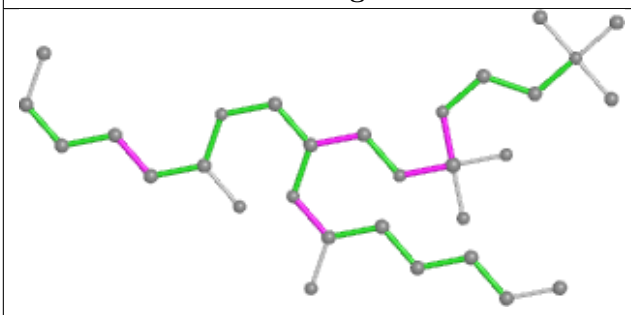
Ligand HXG C 303



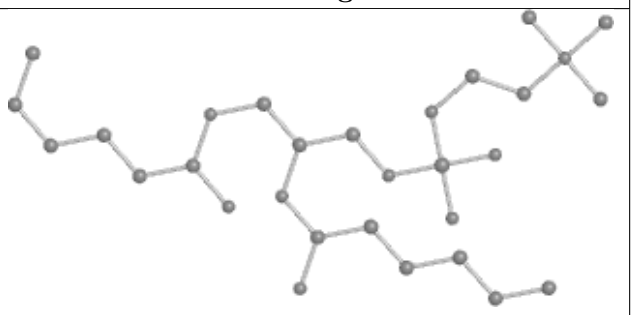
Bond lengths



Bond angles

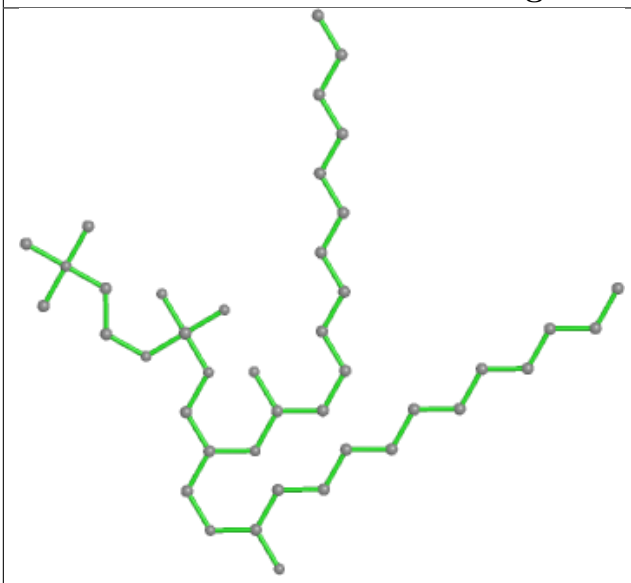


Torsions

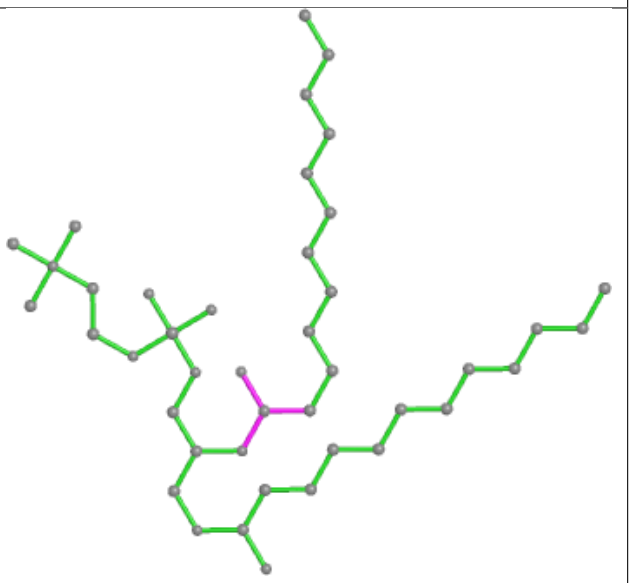


Rings

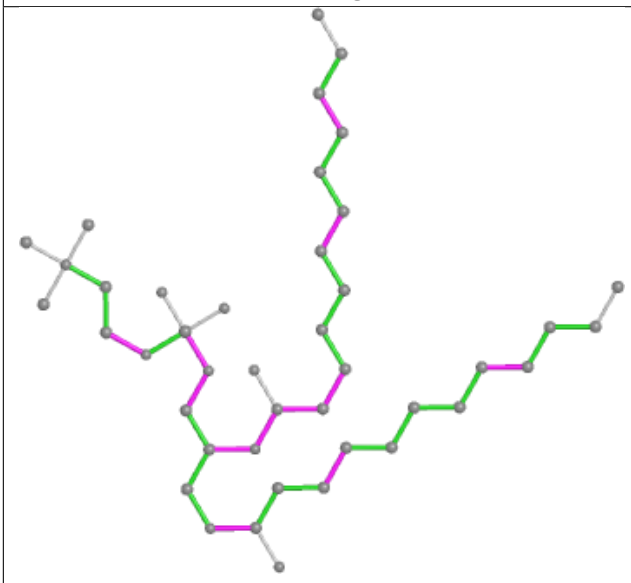
Ligand PLC C 307



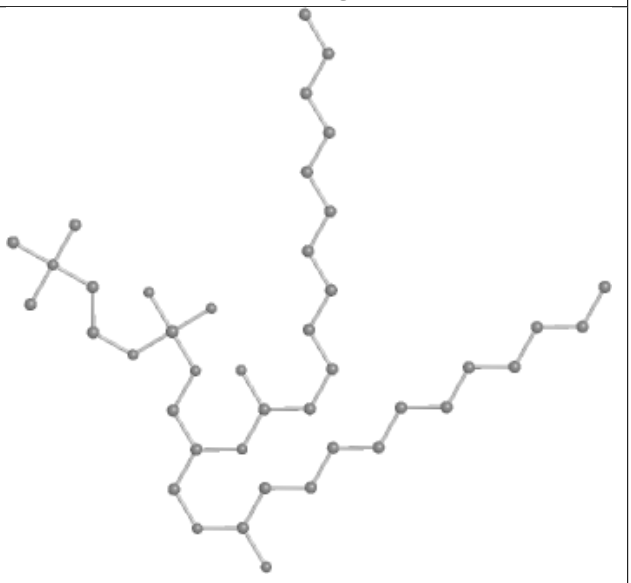
Bond lengths



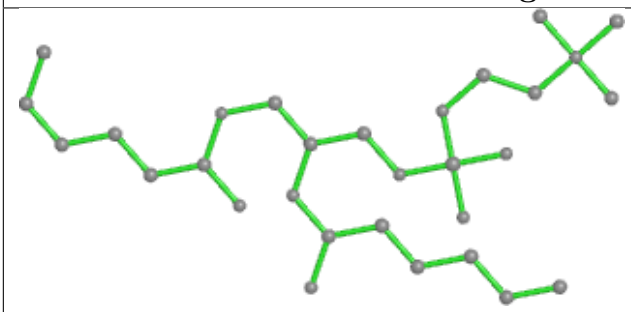
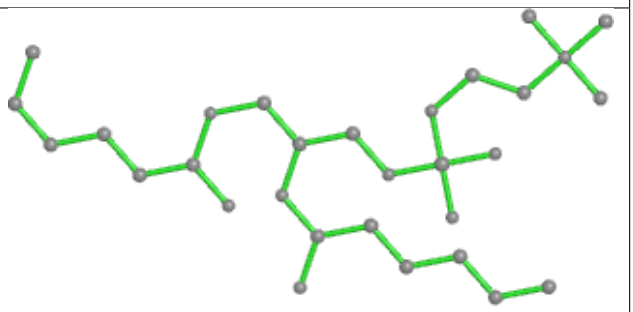
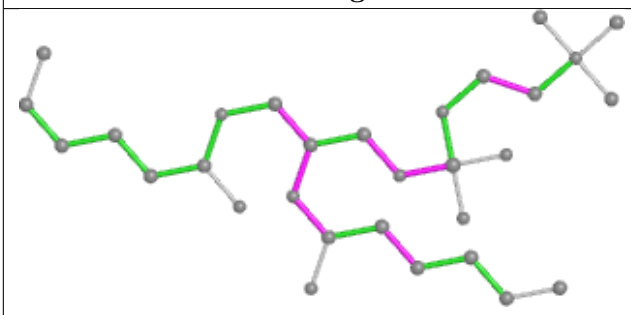
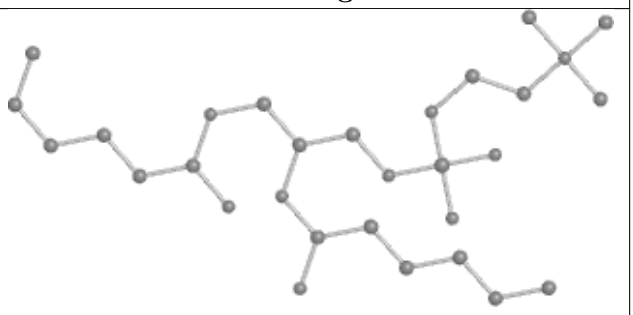
Bond angles

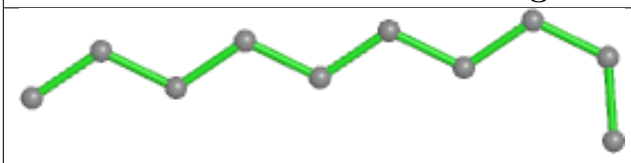
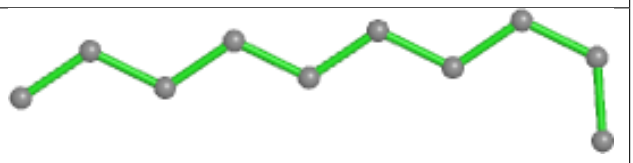
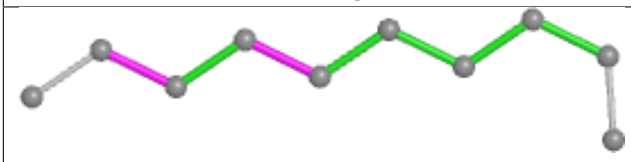
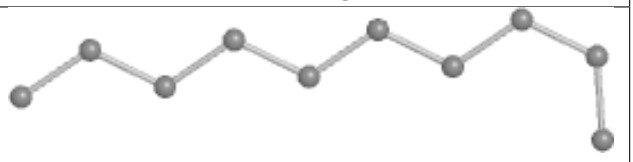


Torsions

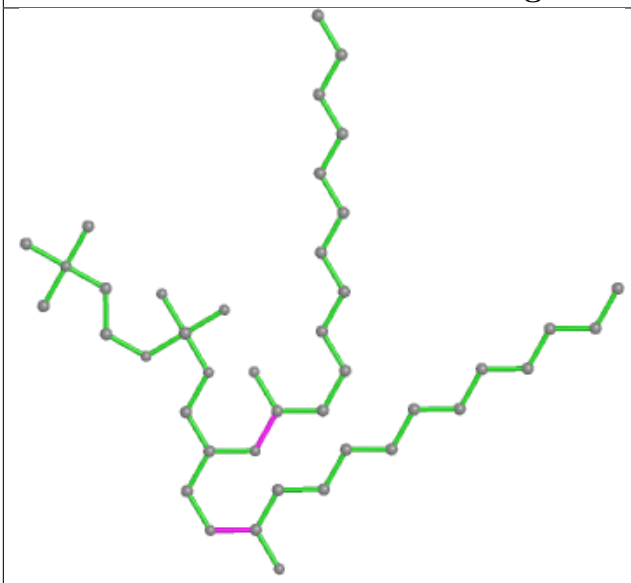


Rings

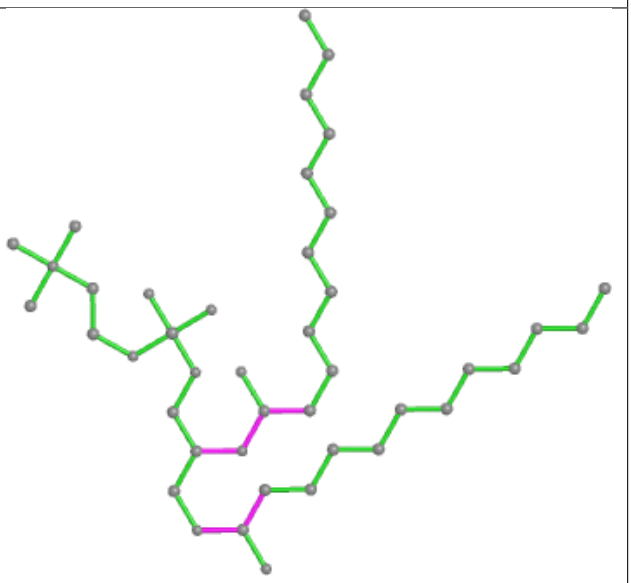
Ligand HXG K 307	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand D10 B 304	
 Bond lengths	 Bond angles
 Torsions	 Rings

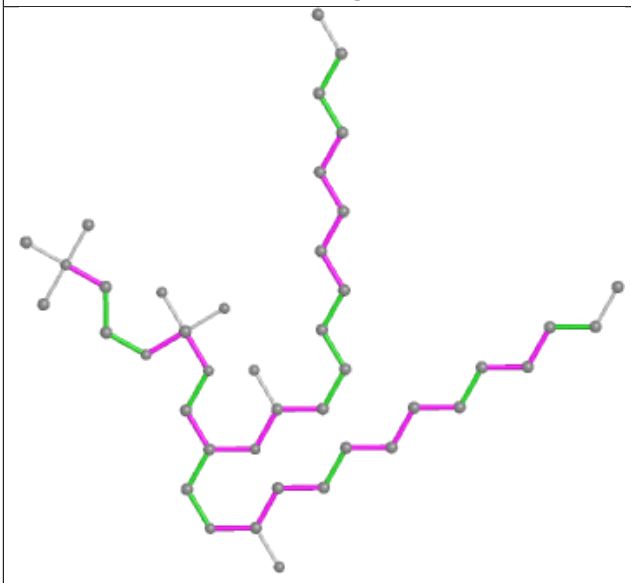
Ligand PLC G 301



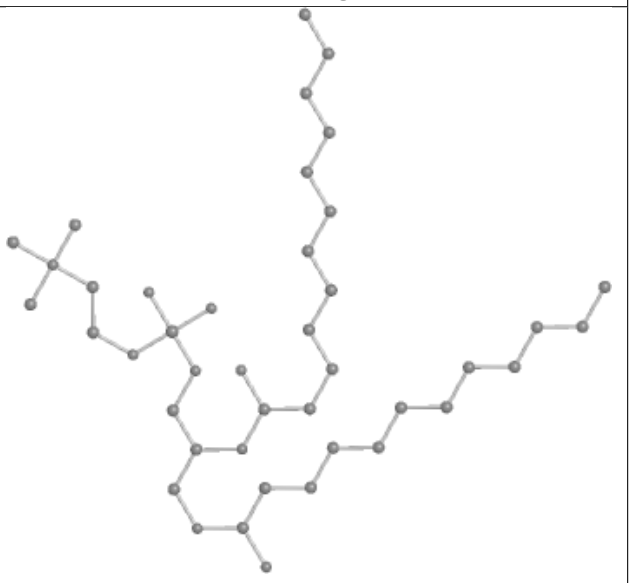
Bond lengths



Bond angles

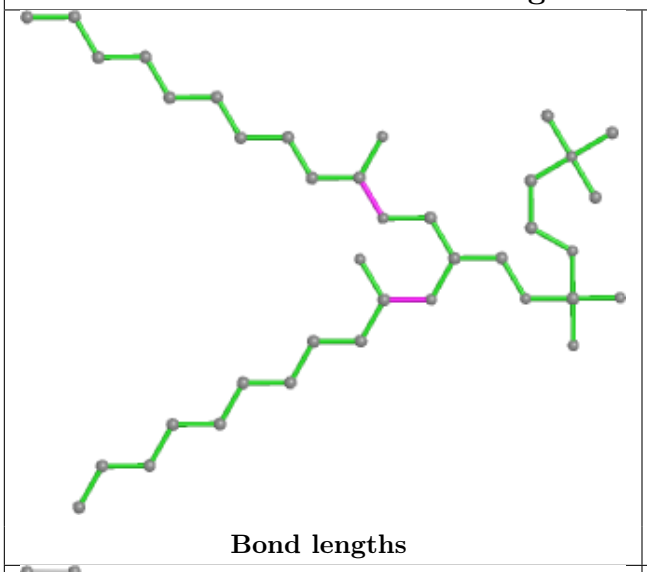


Torsions

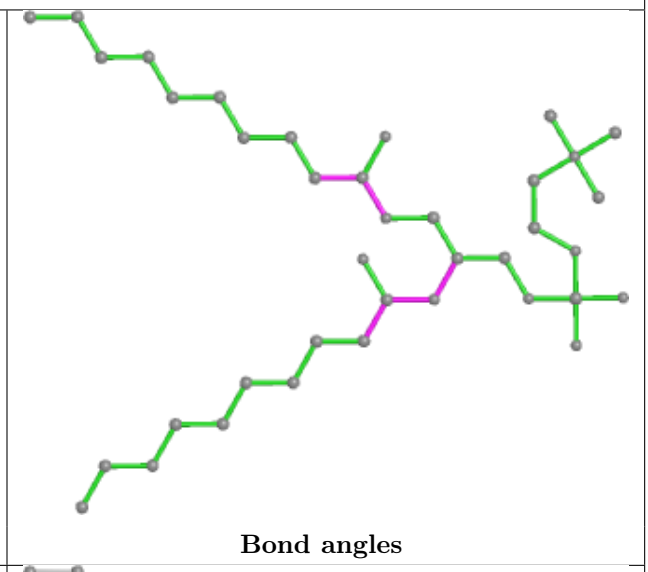


Rings

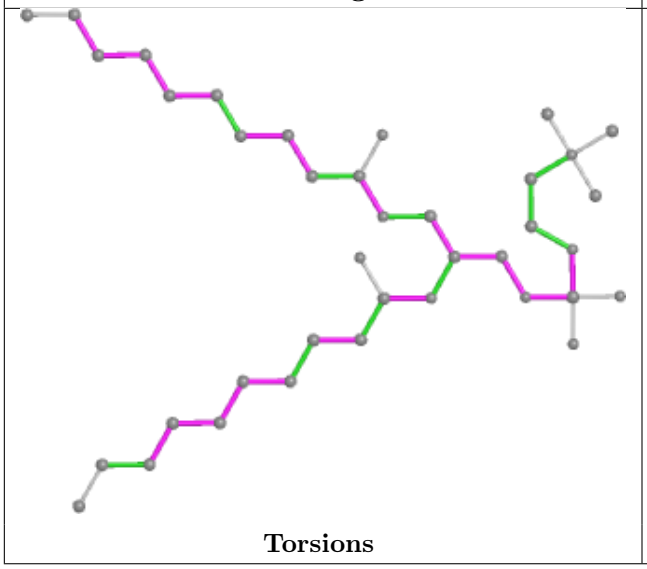
Ligand P1O C 309



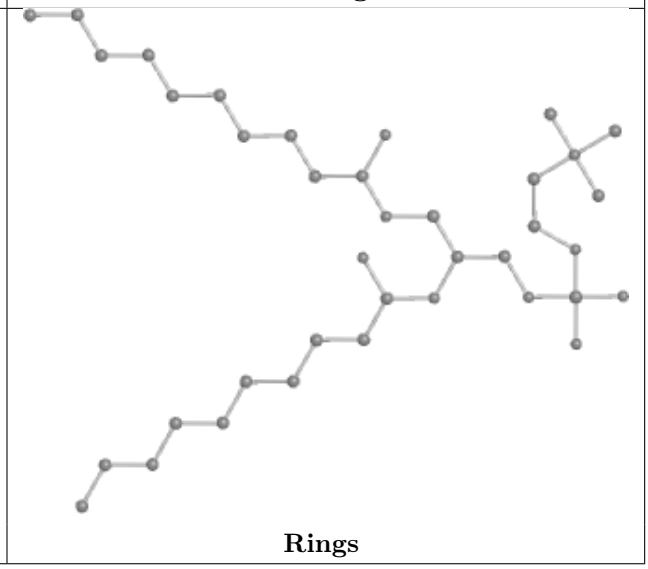
Bond lengths



Bond angles

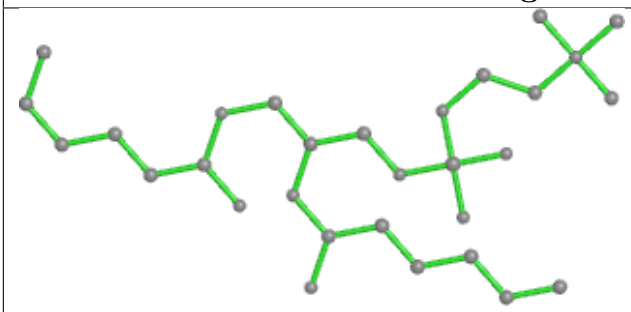


Torsions

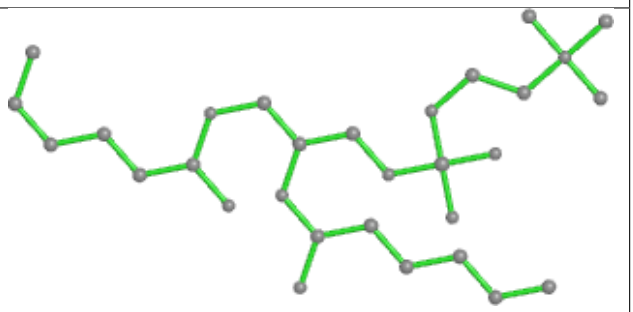


Rings

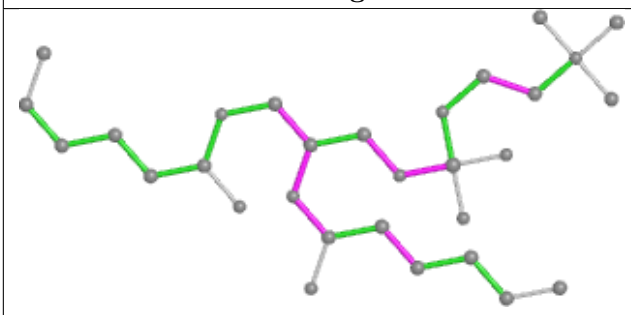
Ligand HXG C 306



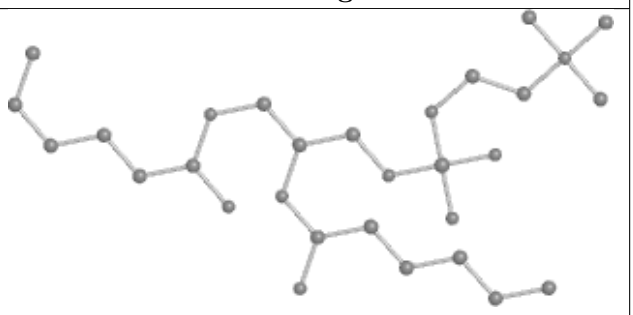
Bond lengths



Bond angles

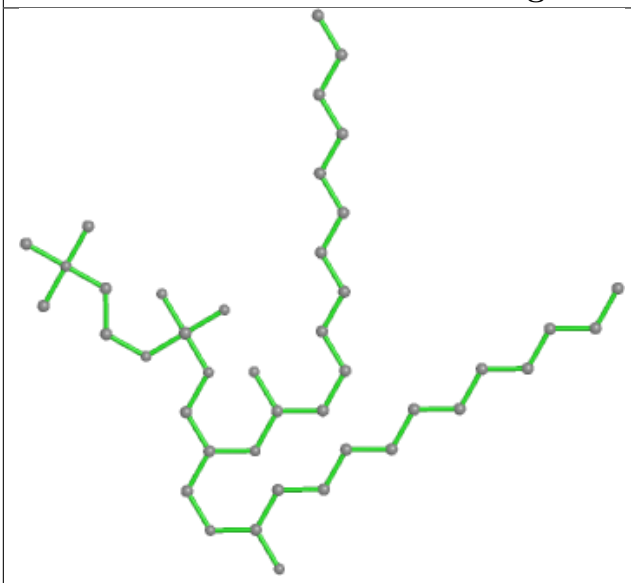


Torsions

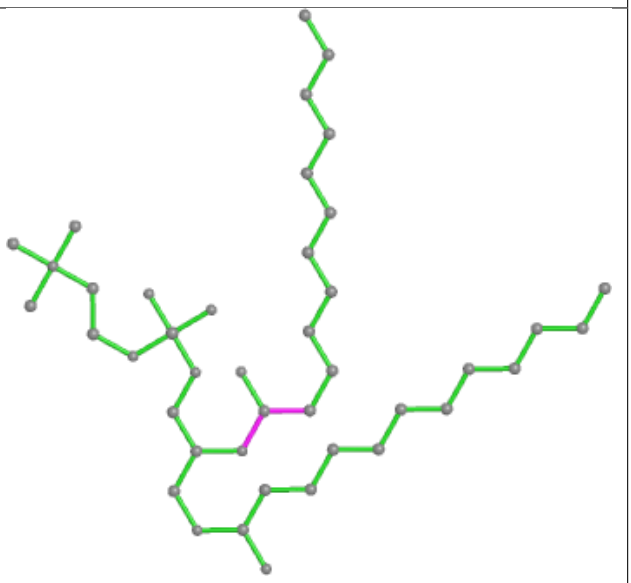


Rings

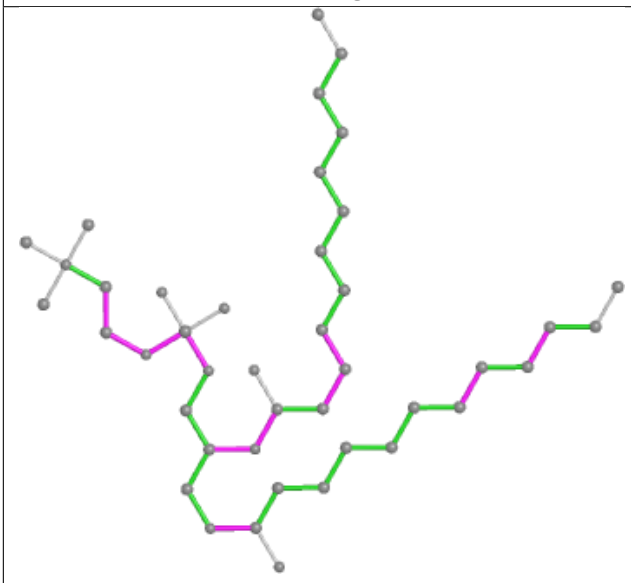
Ligand PLC F 301



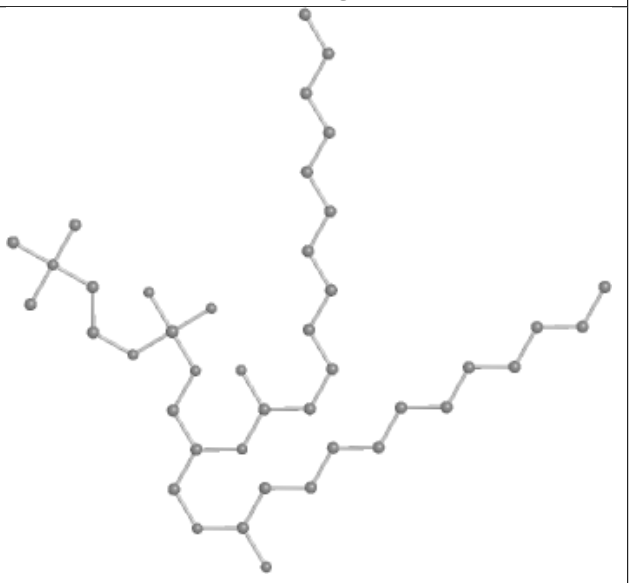
Bond lengths



Bond angles

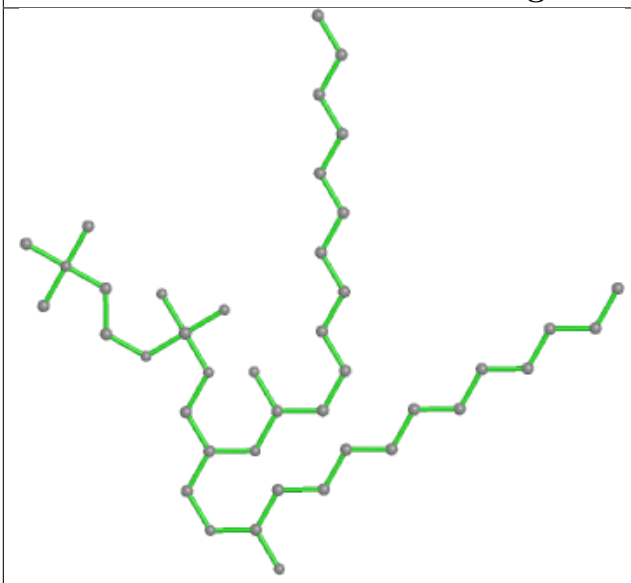


Torsions

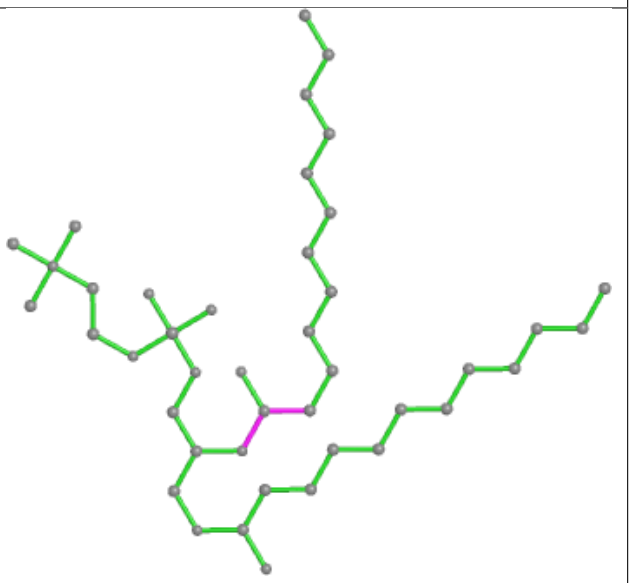


Rings

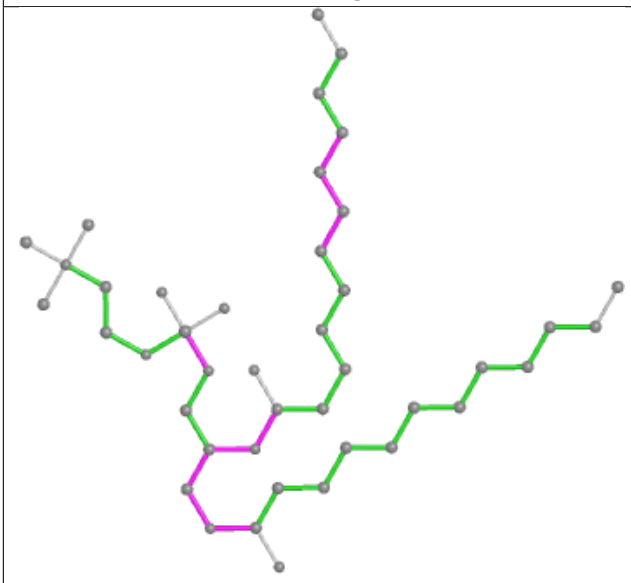
Ligand PLC F 302



Bond lengths



Bond angles



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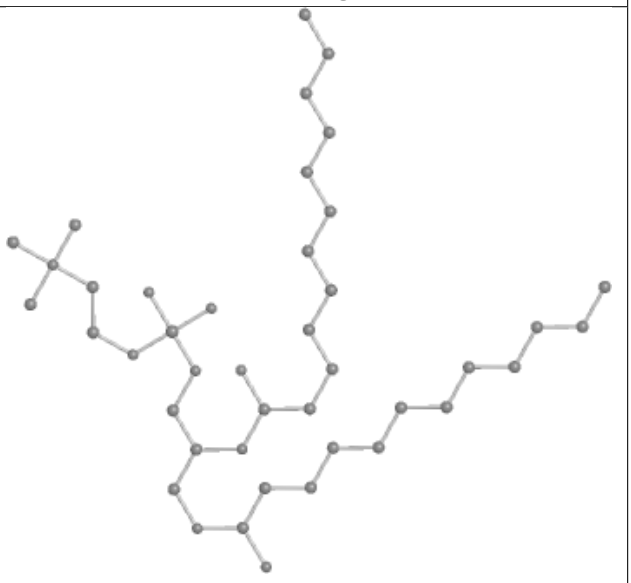
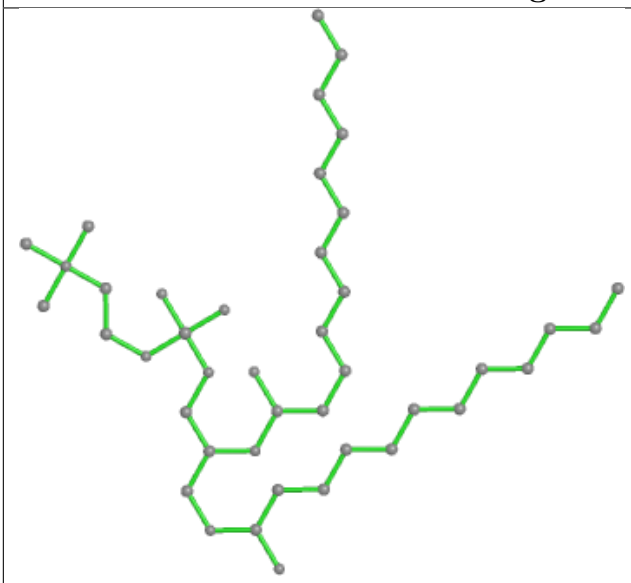


Rings

Ligand PLC J 303



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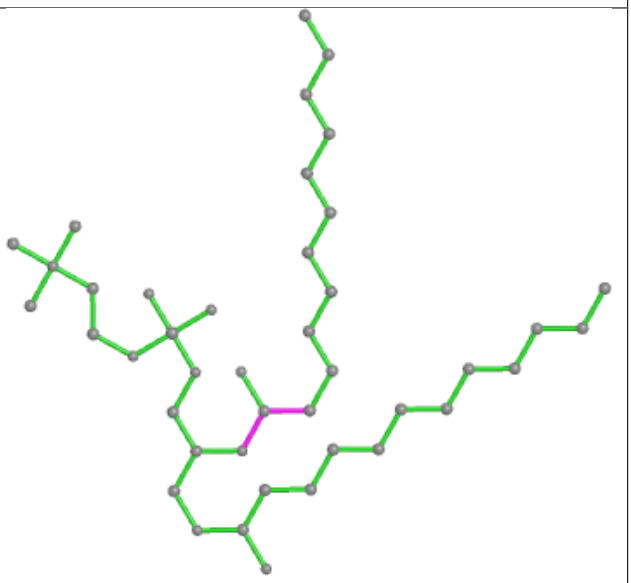
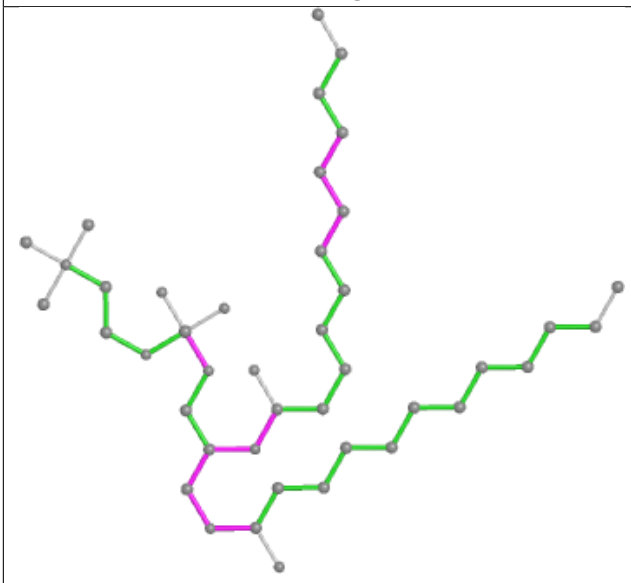
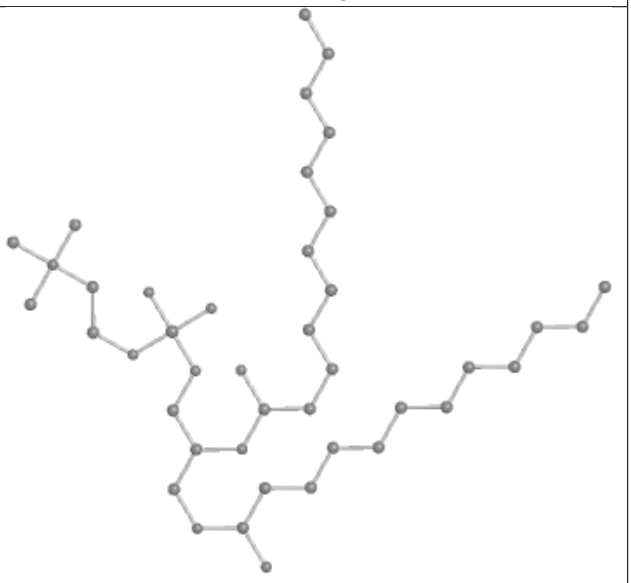


Bond angles

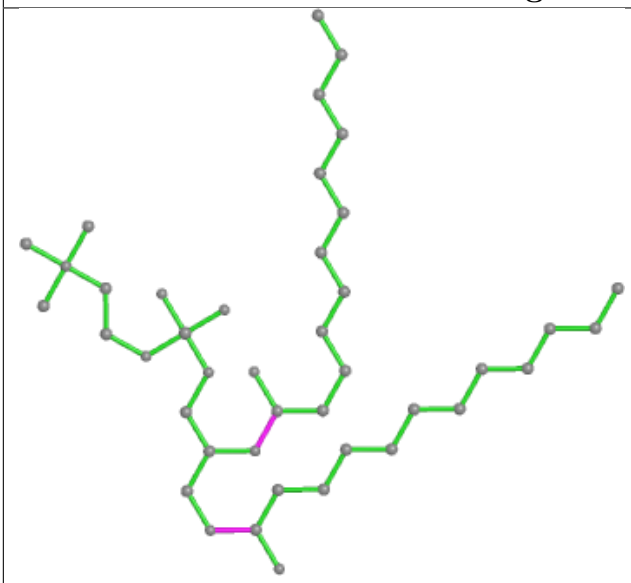


Torsions



Rings

Ligand PLC C 310



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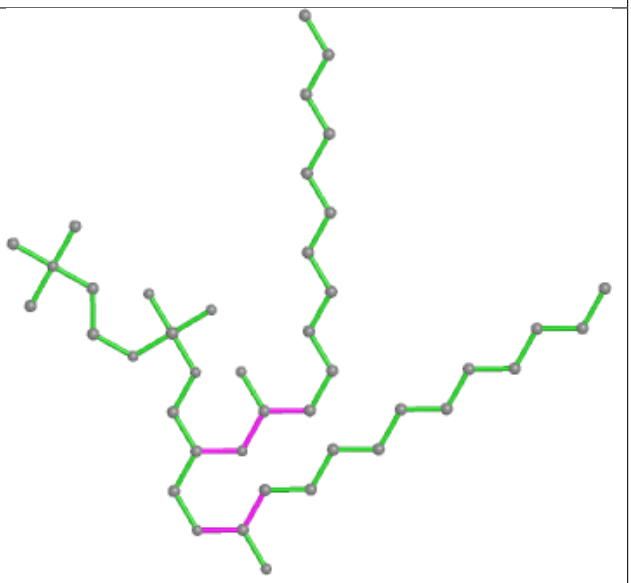
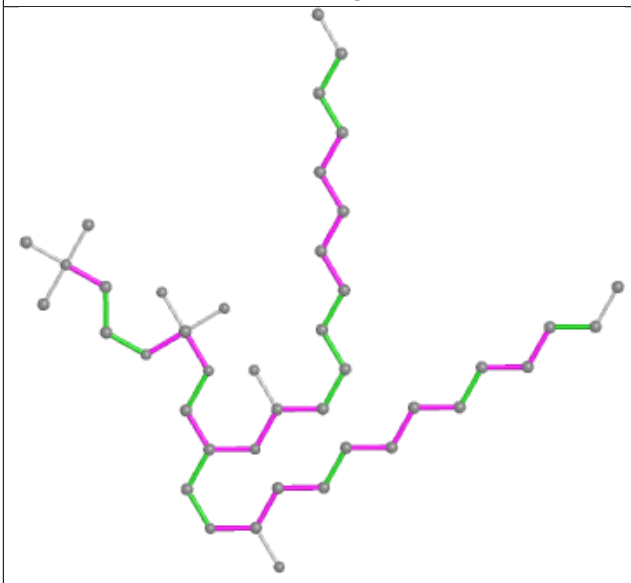
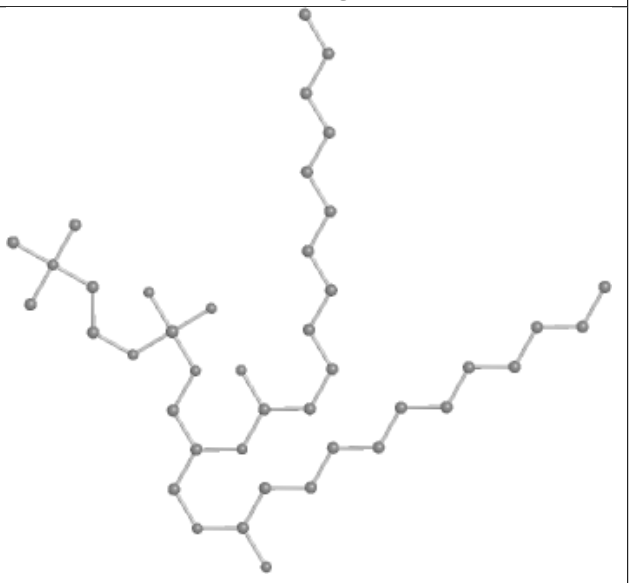


Bond angles

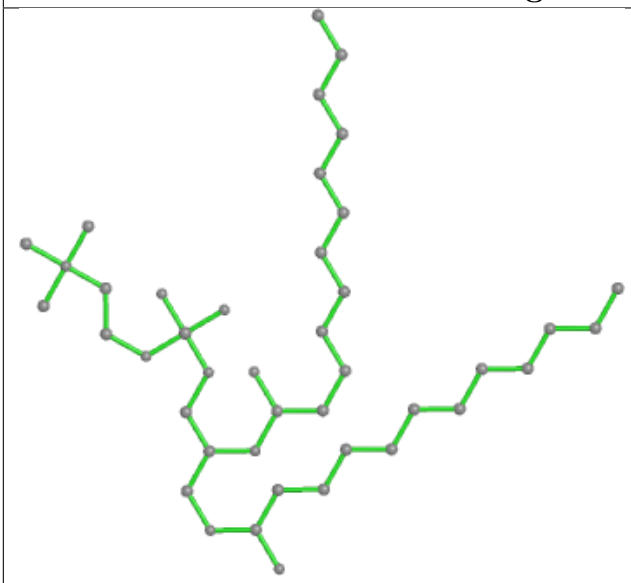


Torsions

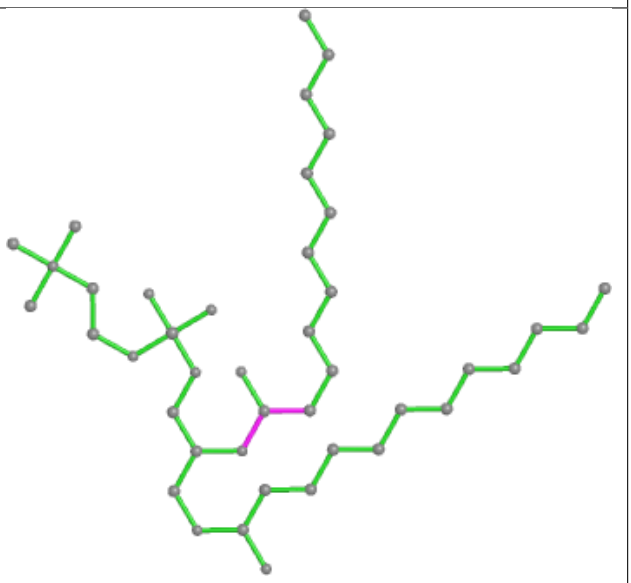


Rings

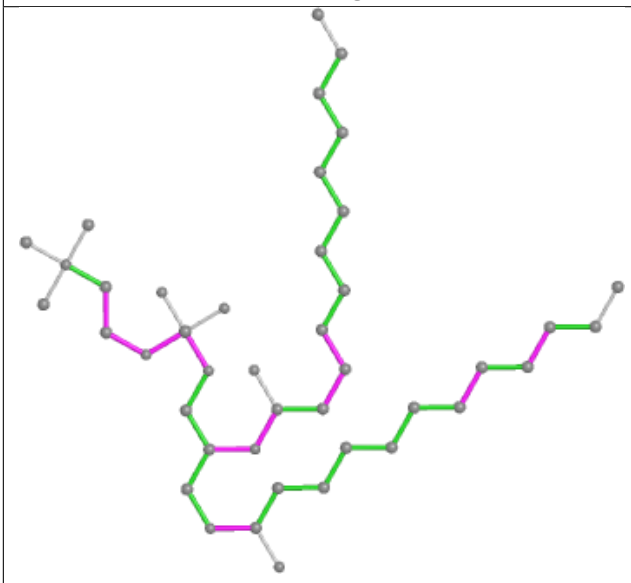
Ligand PLC B 307



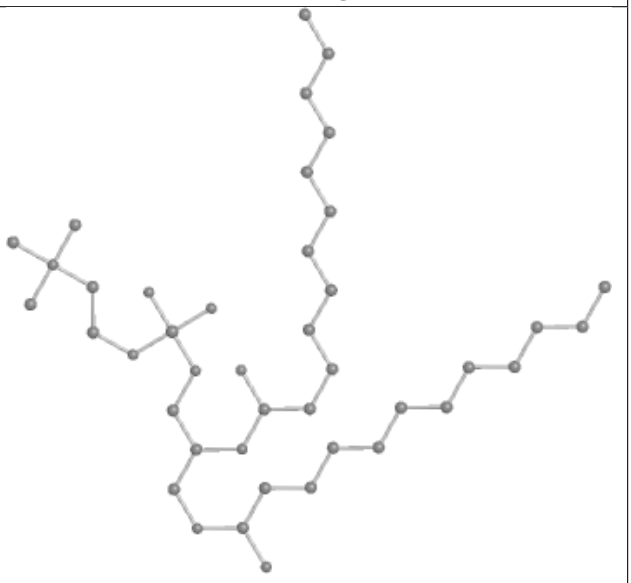
Bond lengths



Bond angles

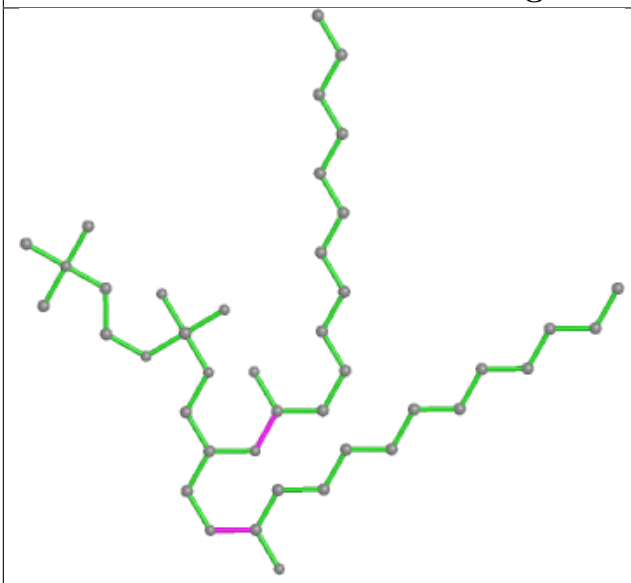


Torsions

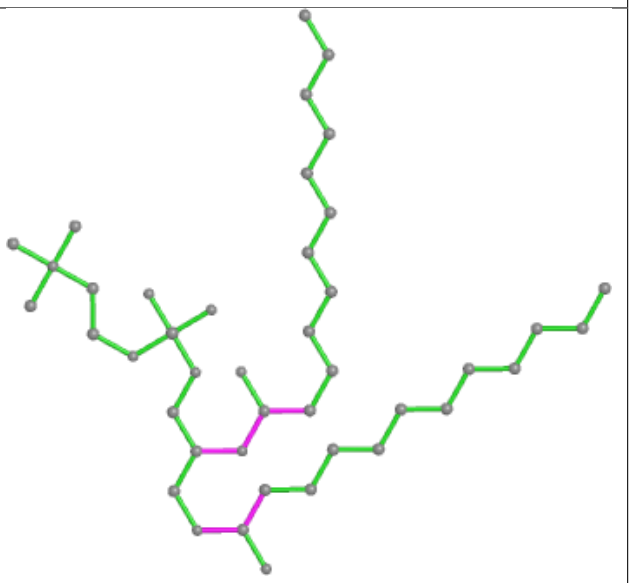


Rings

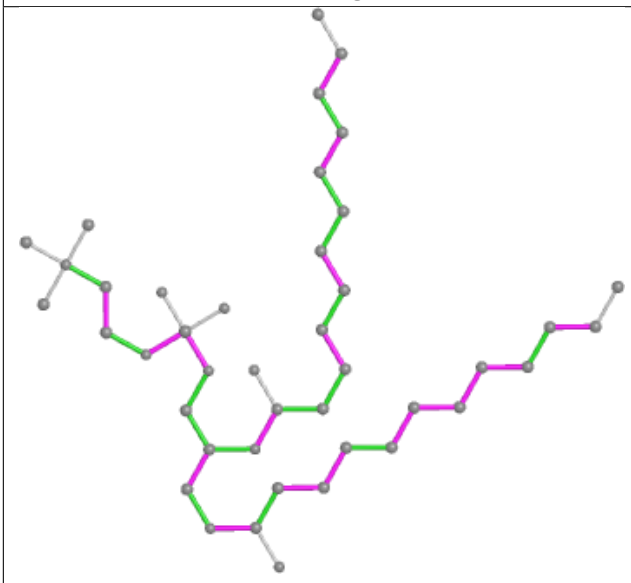
Ligand PLC C 302



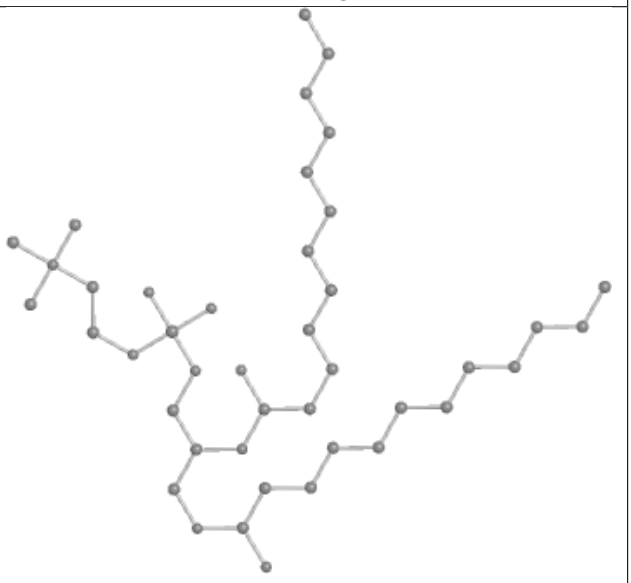
Bond lengths



Bond angles

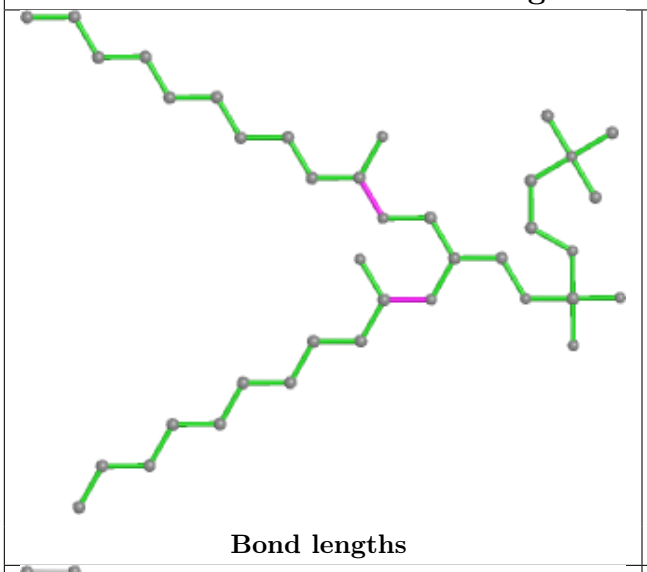


Torsions

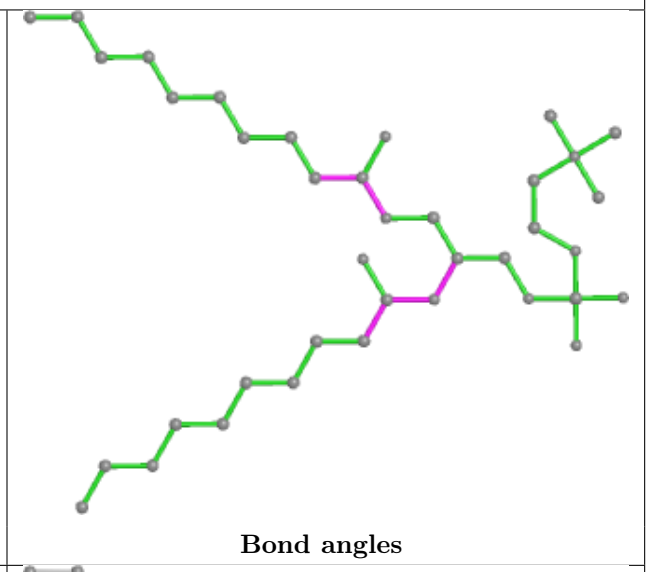


Rings

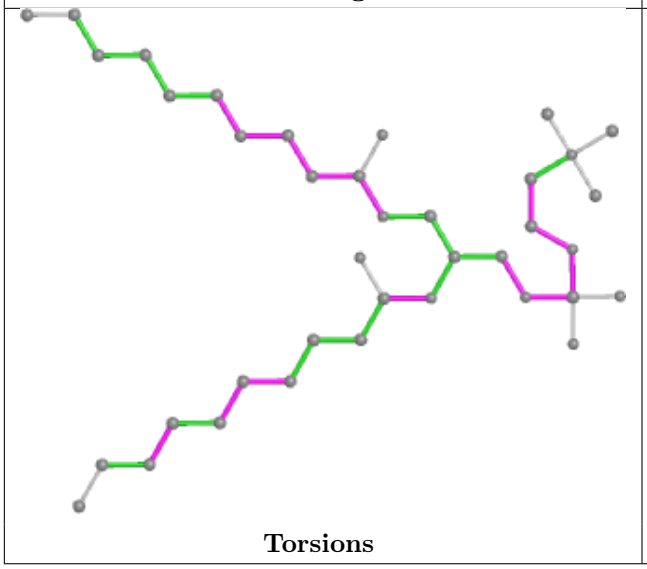
Ligand P1O C 308



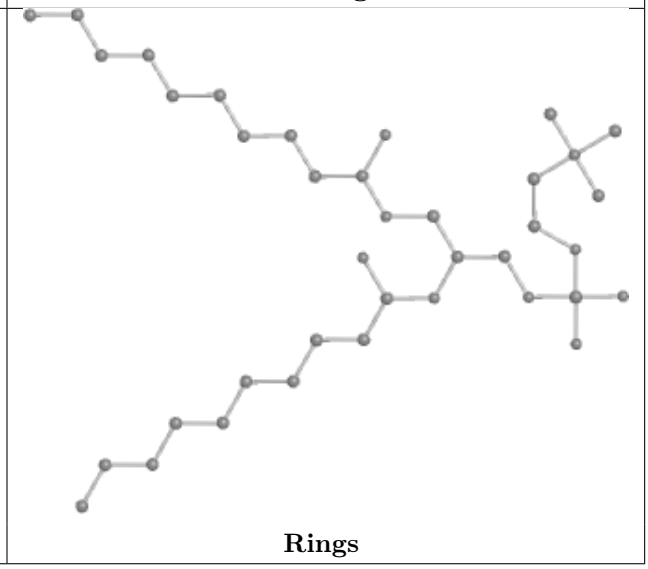
Bond lengths



Bond angles

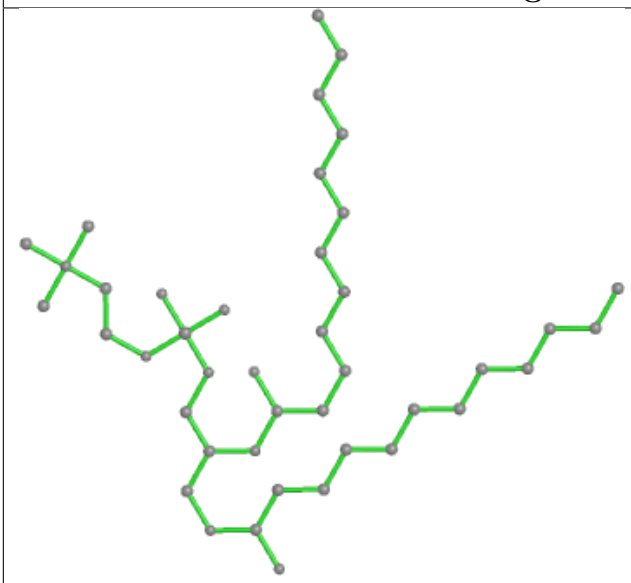


Torsions

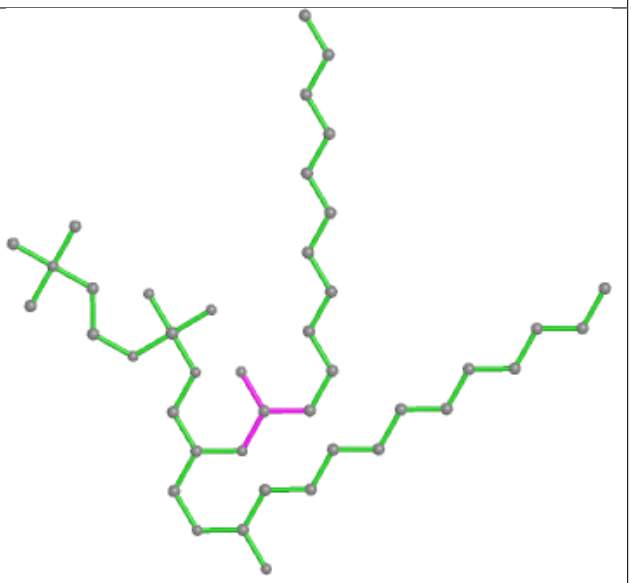


Rings

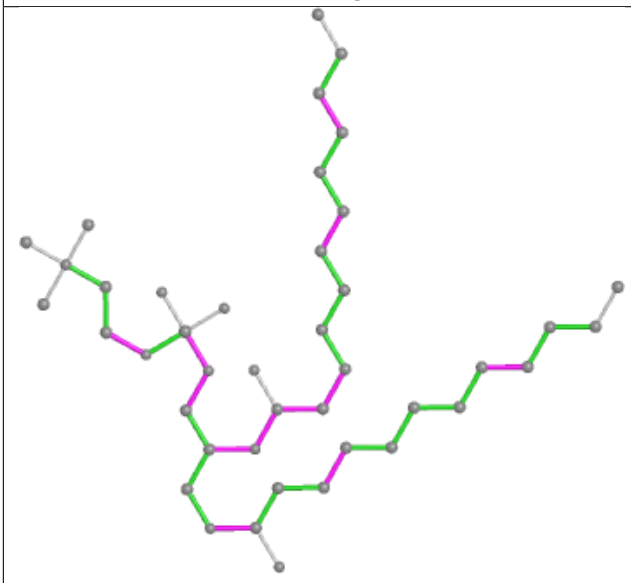
Ligand PLC G 308



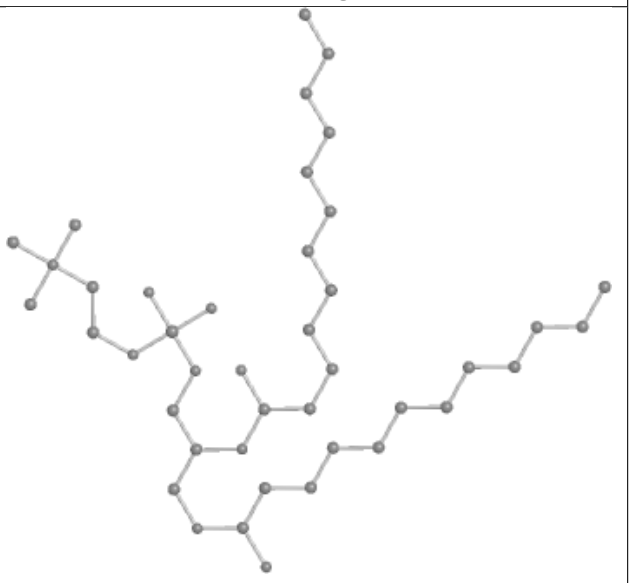
Bond lengths



Bond angles

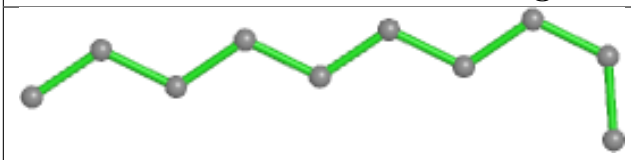


Torsions

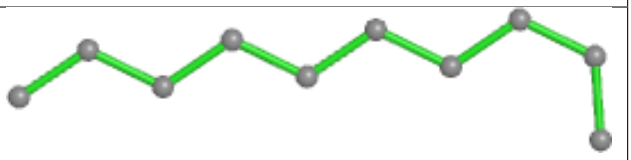


Rings

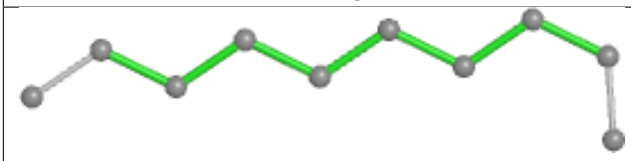
Ligand D10 J 305



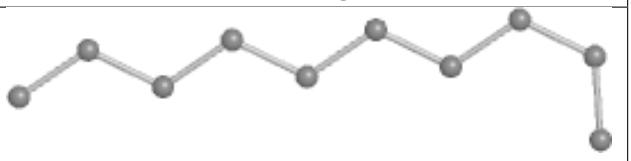
Bond lengths



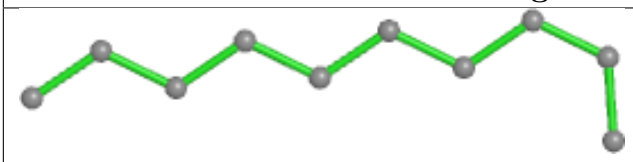
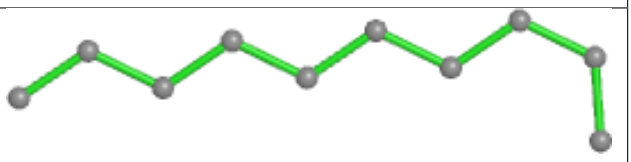
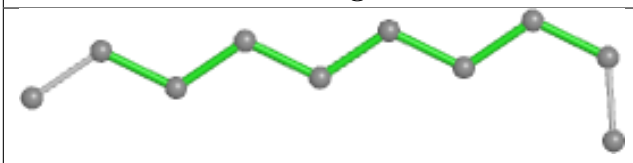
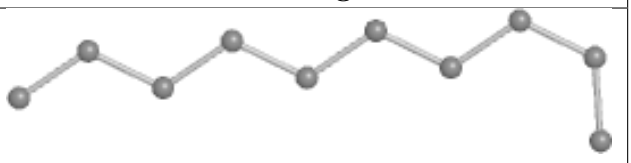
Bond angles

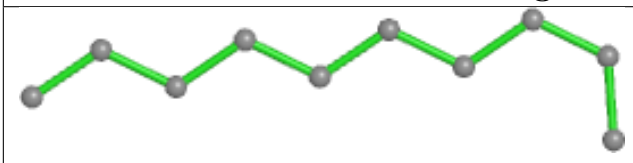
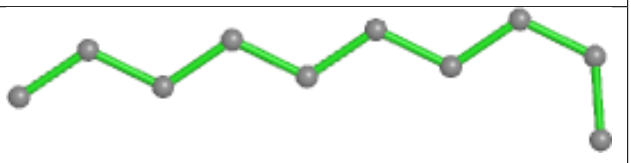
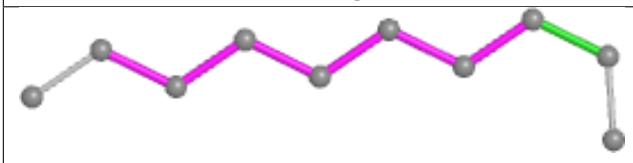
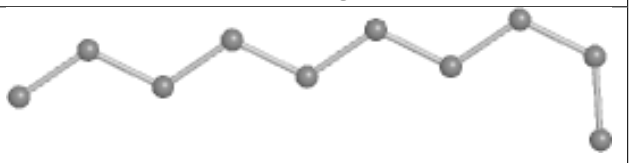


Torsions



Rings

Ligand D10 E 503	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand D10 J 307	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

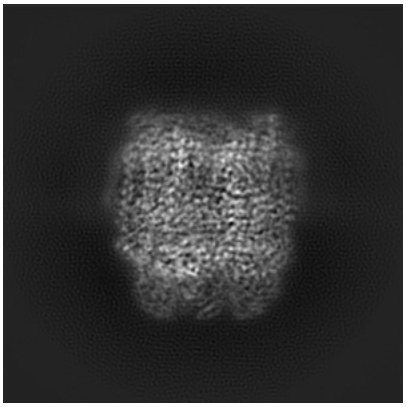
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-24827. These allow visual inspection of the internal detail of the map and identification of artifacts.

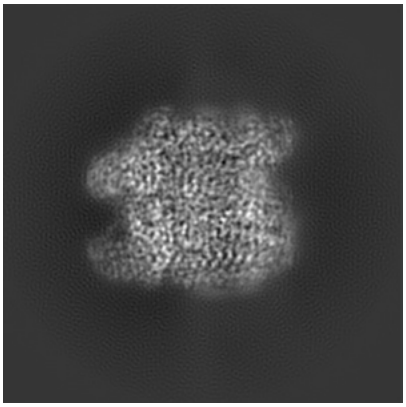
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

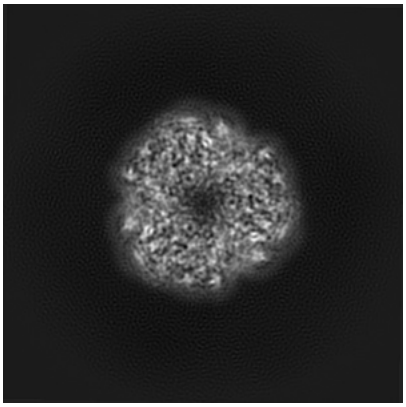
6.1.1 Primary map



X



Y

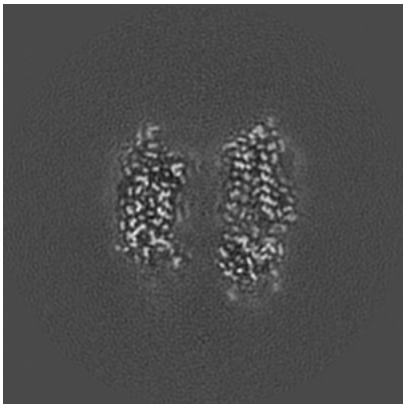


Z

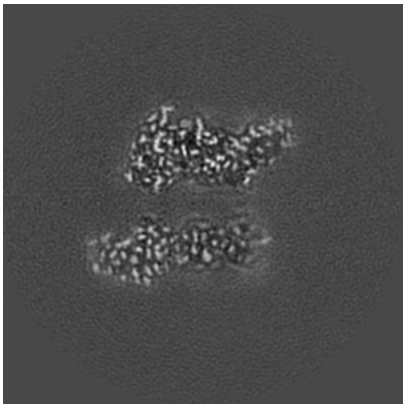
The images above show the map projected in three orthogonal directions.

6.2 Central slices

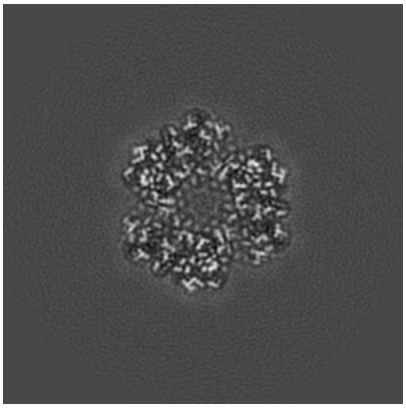
6.2.1 Primary map



X Index: 216



Y Index: 216

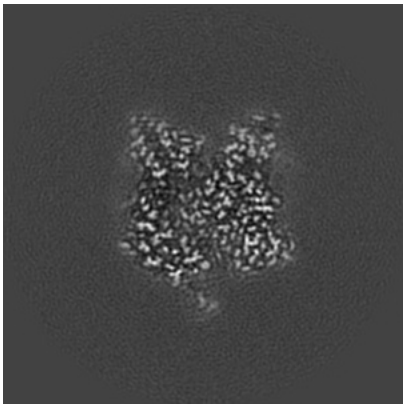


Z Index: 216

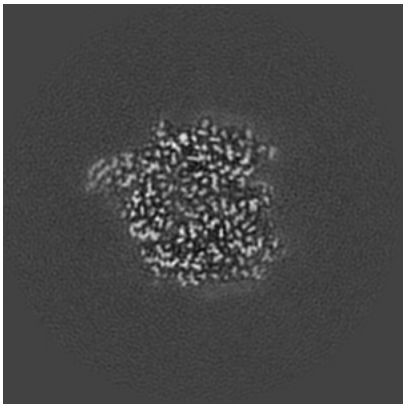
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

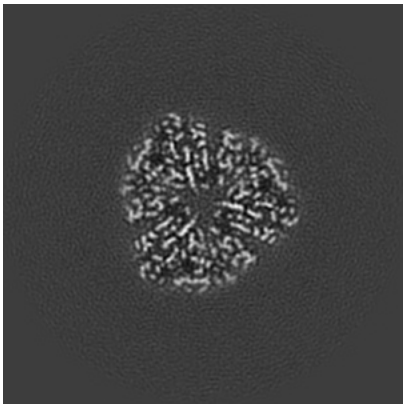
6.3.1 Primary map



X Index: 179



Y Index: 253

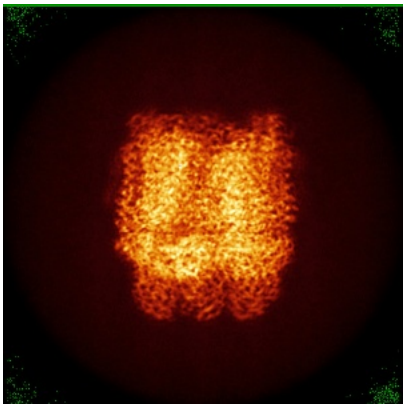


Z Index: 167

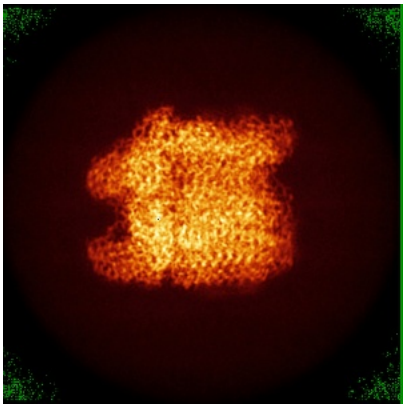
The images above show the largest variance slices of the map in three orthogonal directions.

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

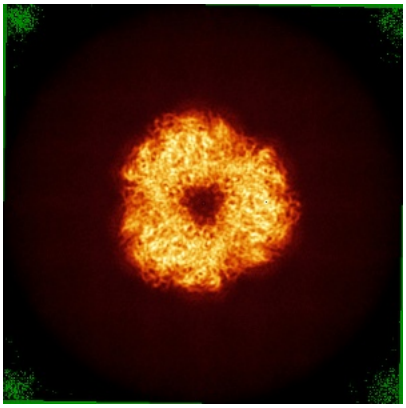
6.4.1 Primary map



X



Y

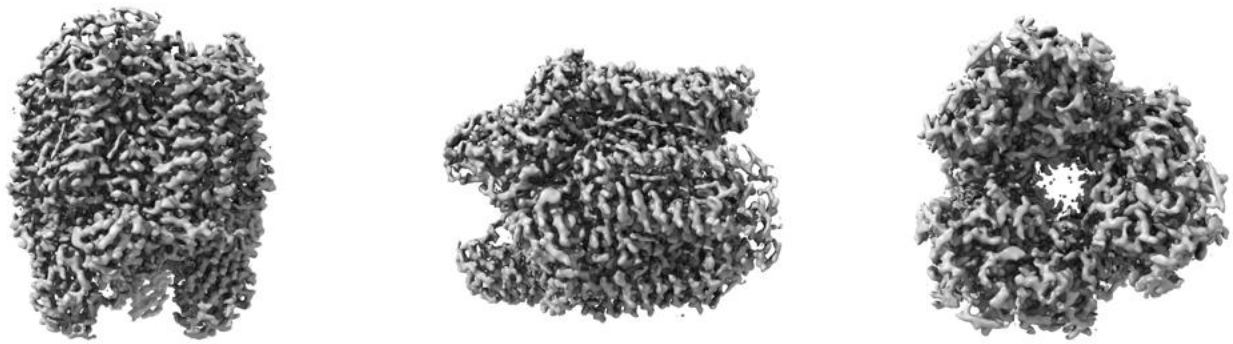


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0229. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

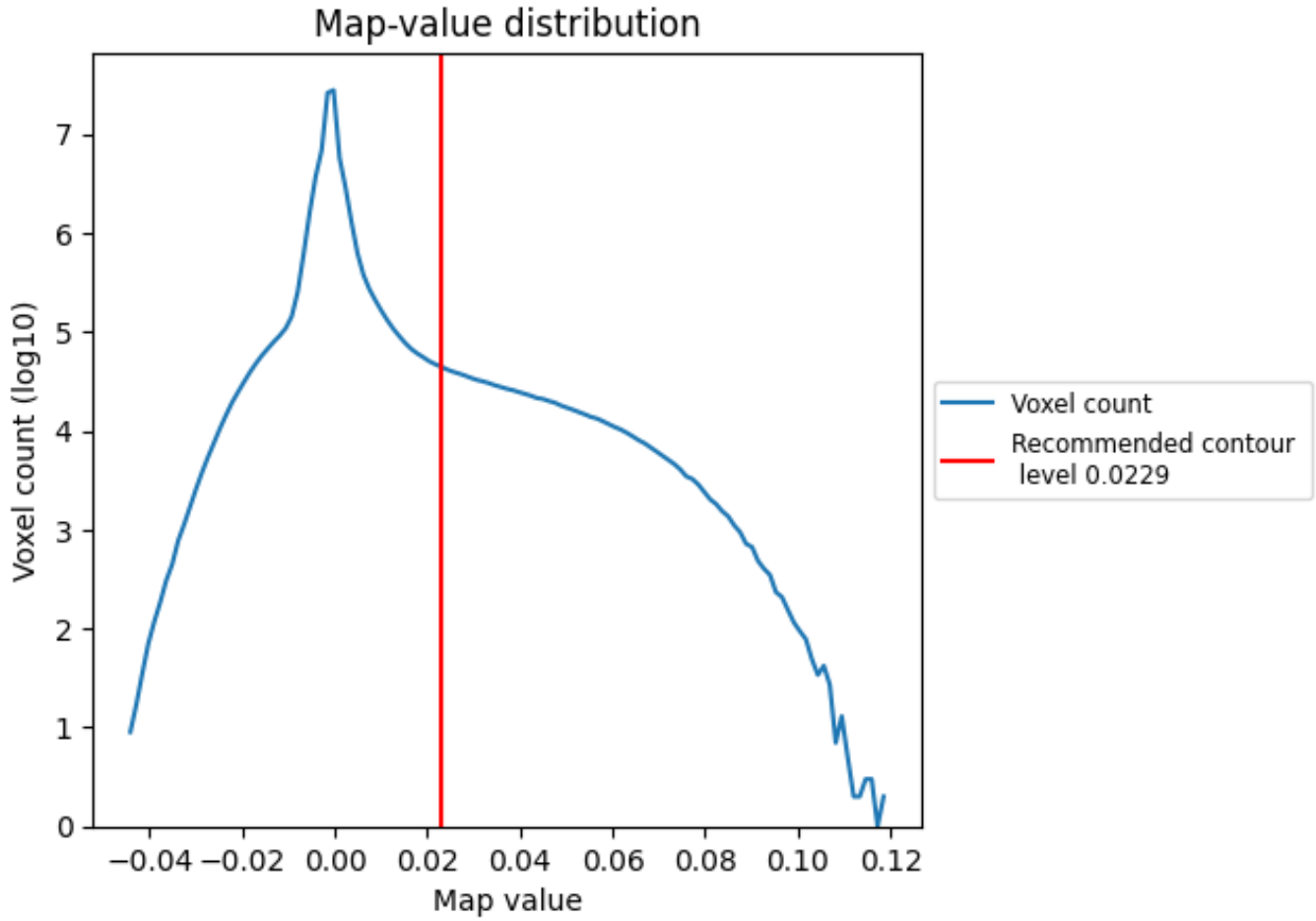
6.6 Mask visualisation (i)

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

7 Map analysis

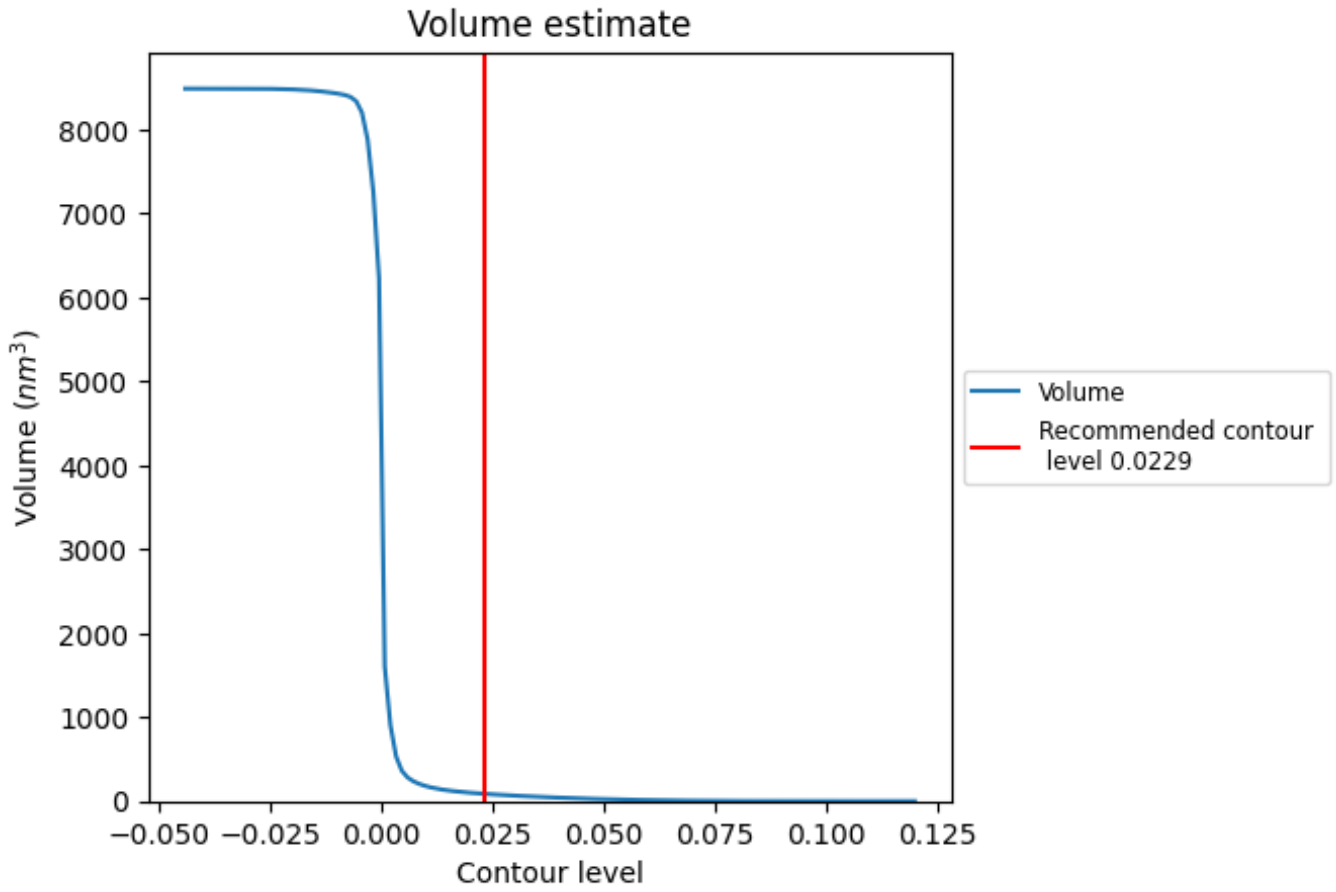
This section contains the results of statistical analysis of the map.

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.

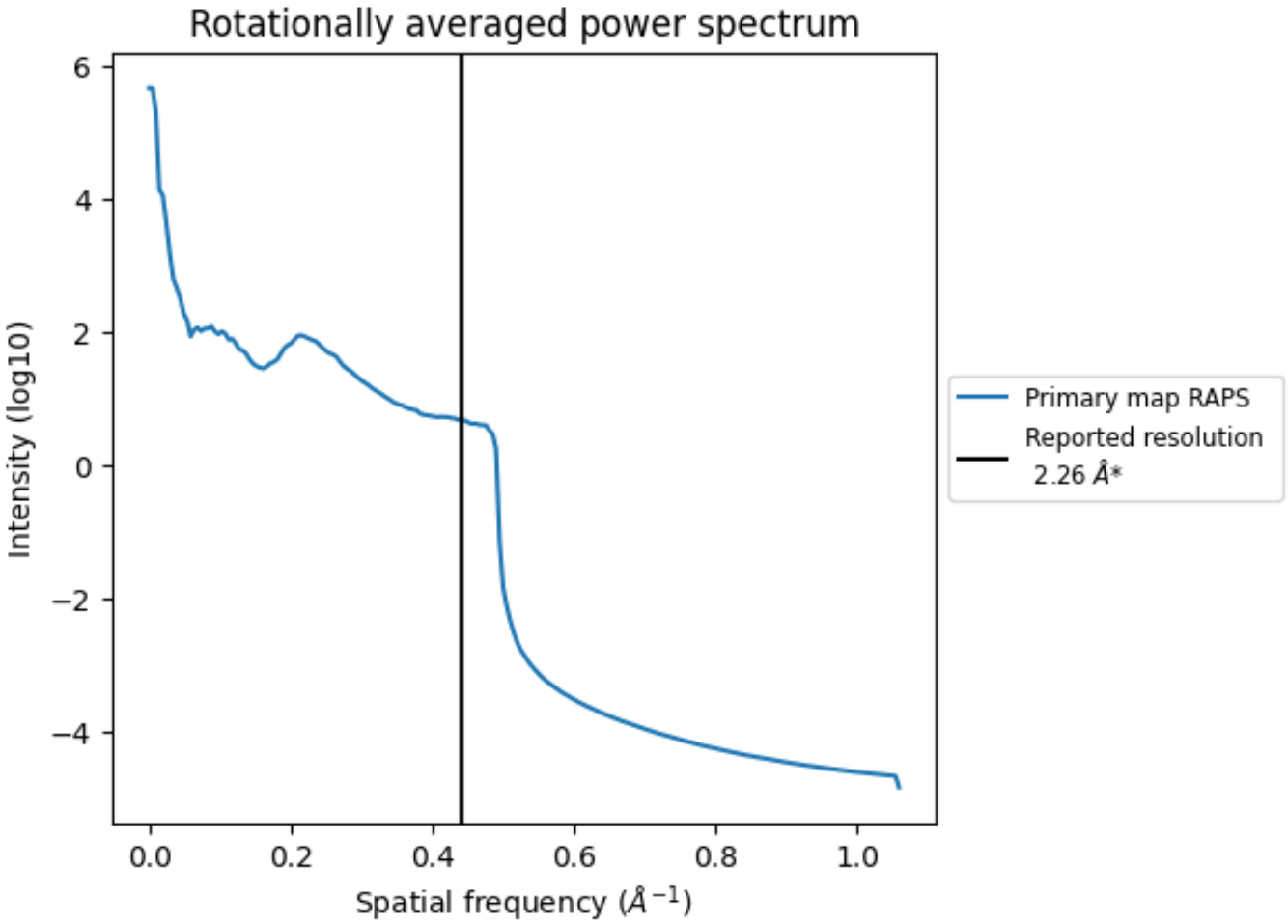
7.2 Volume estimate



The volume at the recommended contour level is 88 nm^3; this corresponds to an approximate mass of 80 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)

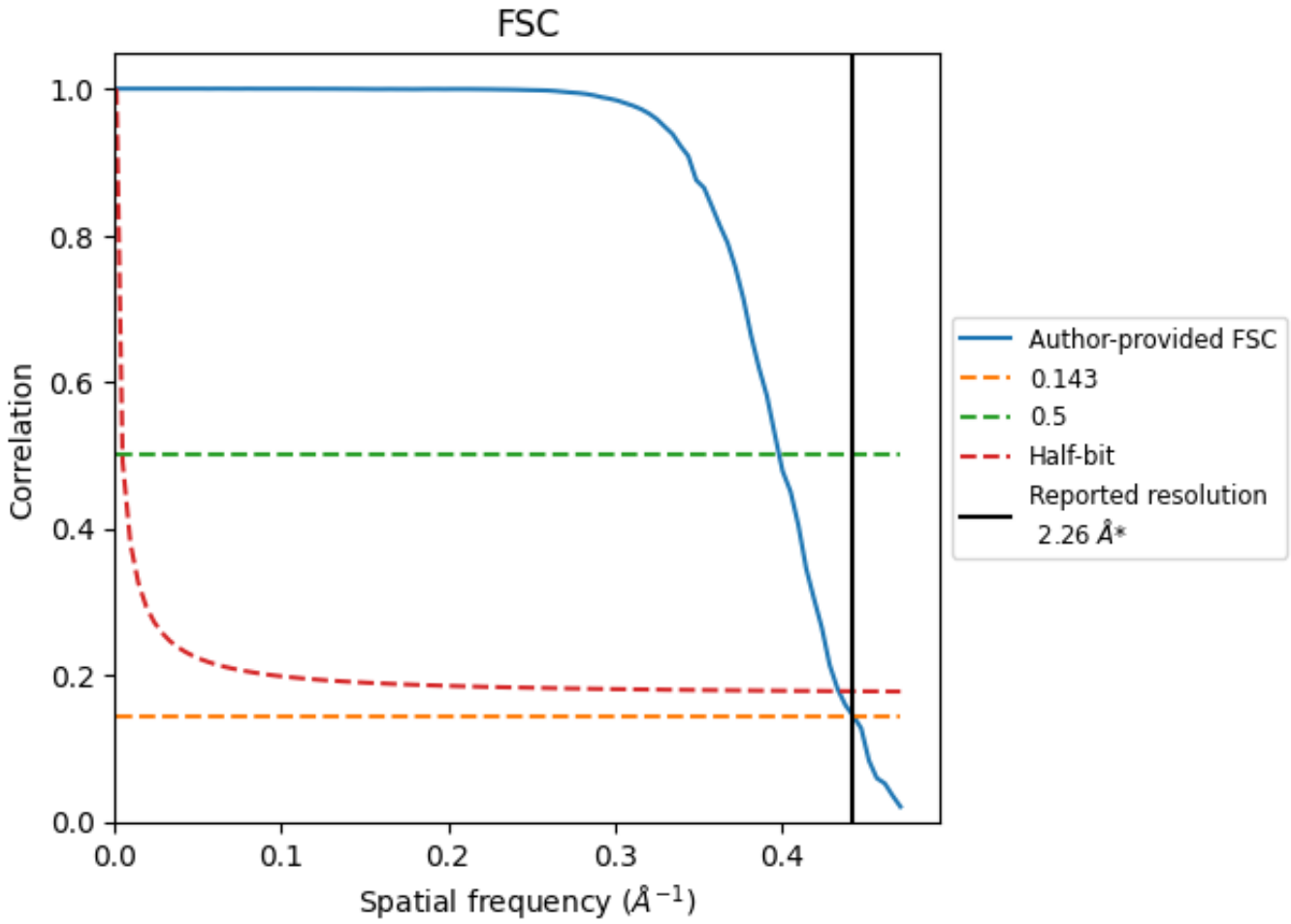


*Reported resolution corresponds to spatial frequency of 0.442 Å^{-1}

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 0.442 Å^{-1}

8.2 Resolution estimates (i)

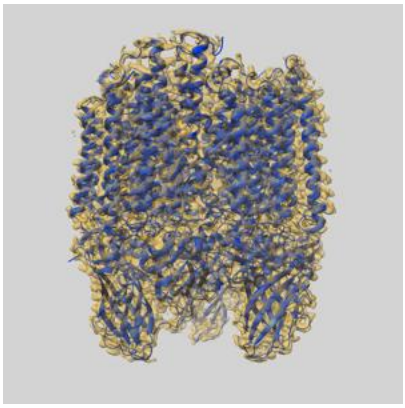
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.26	-	-
Author-provided FSC curve	2.25	2.51	2.30
Unmasked-calculated*	-	-	-

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

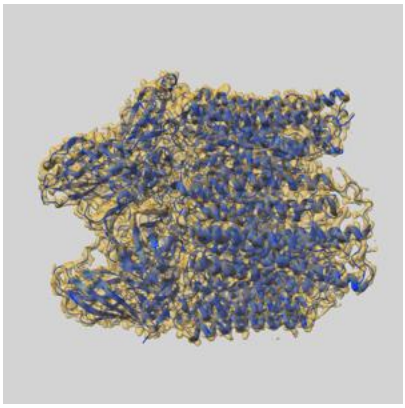
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-24827 and PDB model 7S4I. Per-residue inclusion information can be found in section 3 on page 11.

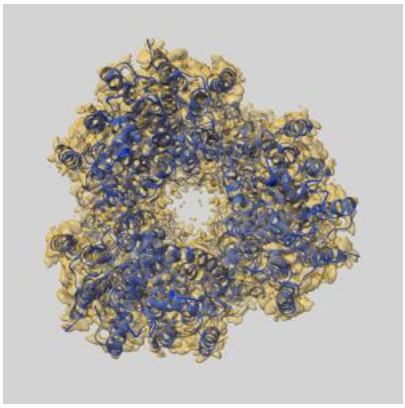
9.1 Map-model overlay



X



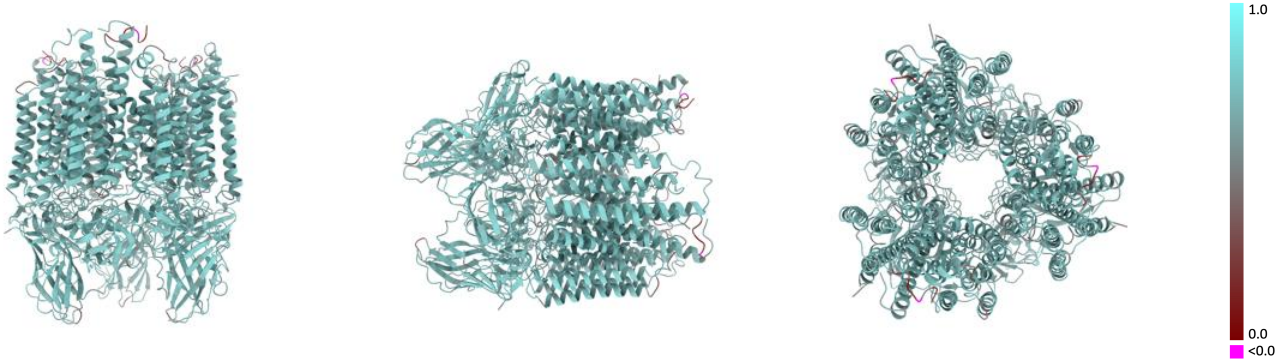
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0229 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.

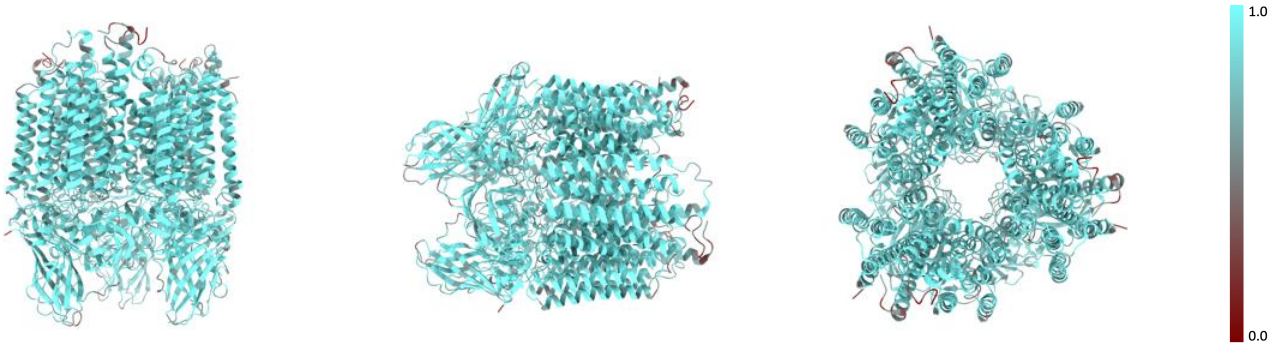
9.2 Q-score mapped to coordinate model



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.

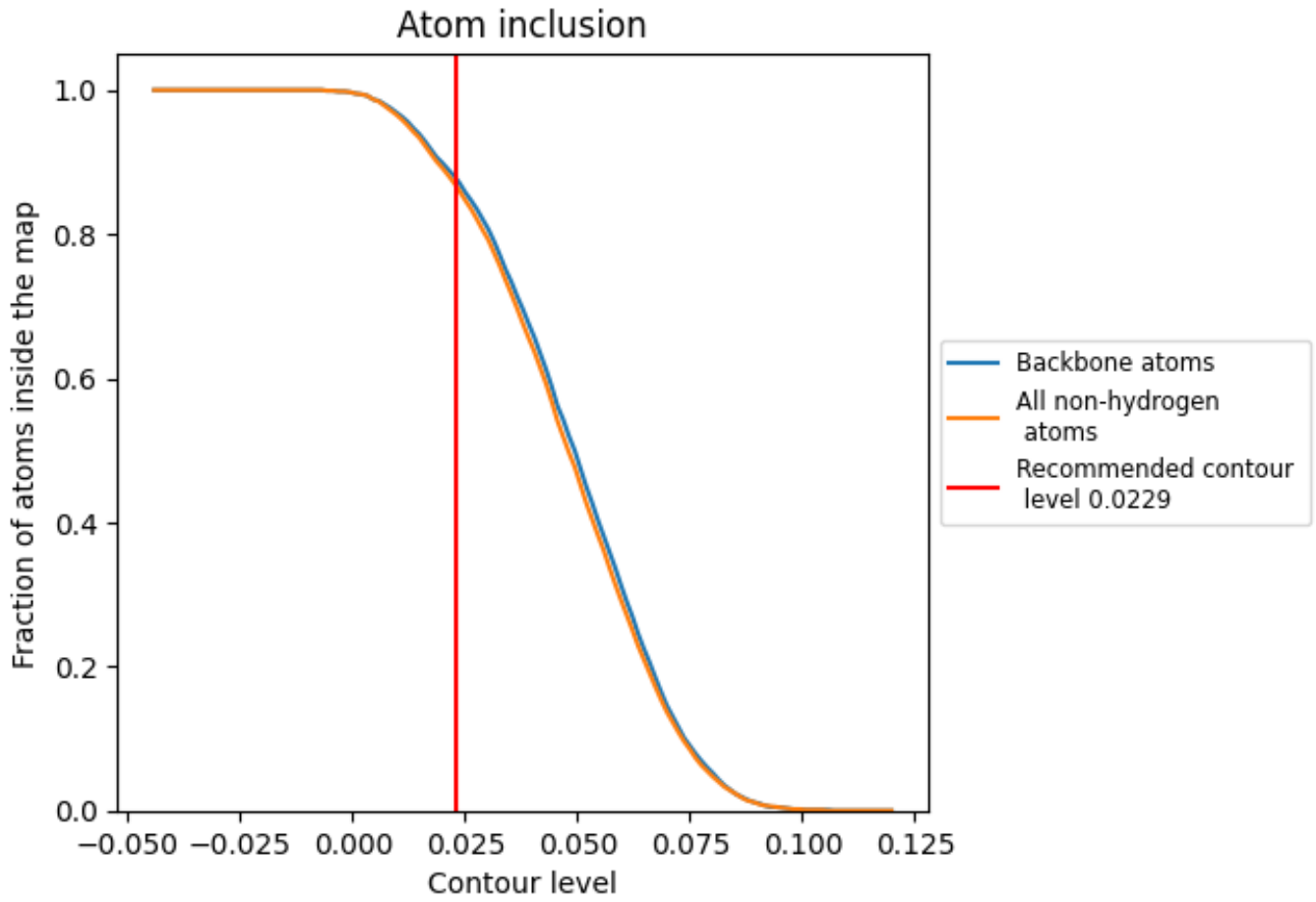
9.3 Atom inclusion mapped to coordinate model



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 (0.0229).

9.4 Atom inclusion (i)



At the recommended contour level, 88% of all backbone atoms, 87% 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 (0.0229) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8680	0.6790
A	0.8910	0.6950
B	0.8820	0.6890
C	0.8100	0.6460
E	0.8920	0.6950
F	0.8840	0.6880
G	0.8090	0.6470
I	0.8910	0.6960
J	0.8830	0.6890
K	0.8100	0.6460