Full wwPDB EM Validation Report ⓘ

Nov 4, 2026 – 06:20 PM JST

PDB ID	:	43YC / pdb_000043yc
EMDB ID	:	EMD-82383
Title	:	Cryo-EM structure of AGAP001487 in a nanodisc
Authors	:	Kawaguchi, S.; Hirano, H.; Watanabe, M.; Suzuki, S.; Nishikawa, K.; Fujiyoshi, Y.; Oshima, A.
Deposited on	:	2026-07-21
Resolution	:	3.00 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:

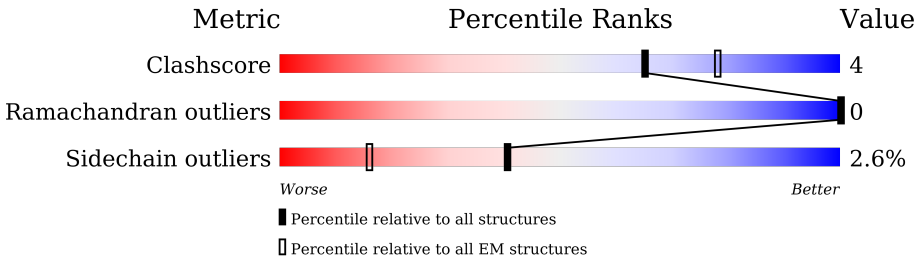
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.2
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

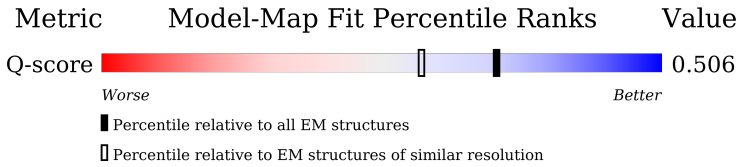
1 Overall quality at a glance

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

The reported resolution of this entry is 3.00 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.





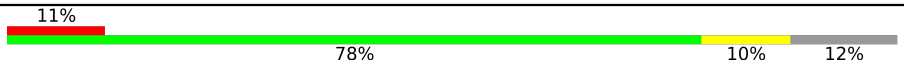
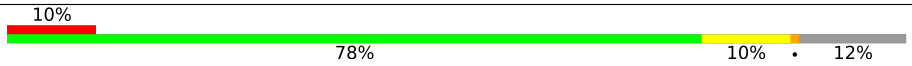
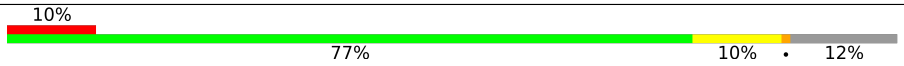
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14081 (2.50 - 3.50)

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	373	11% 78% 10% 12%
1	B	373	11% 77% 11% 12%
1	C	373	10% 77% 11% 12%
1	D	373	9% 78% 10% 12%

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Mol	Chain	Length	Quality of chain
1	E	373	
1	F	373	
1	G	373	

2 Entry composition

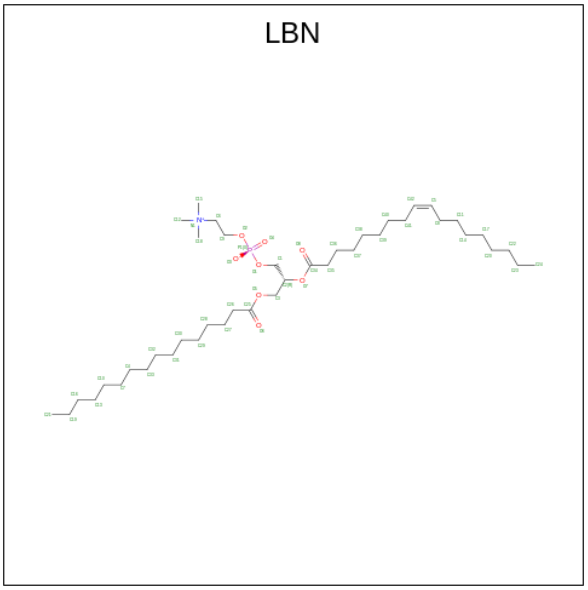
There are 3 unique types of molecules in this entry. The entry contains 20202 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Innexin shaking-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	330	Total 2660	C 1774	N 427	O 440	S 19	0	0
1	B	330	Total 2660	C 1774	N 427	O 440	S 19	0	0
1	D	330	Total 2660	C 1774	N 427	O 440	S 19	0	0
1	C	330	Total 2660	C 1774	N 427	O 440	S 19	0	0
1	E	330	Total 2660	C 1774	N 427	O 440	S 19	0	0
1	G	330	Total 2660	C 1774	N 427	O 440	S 19	0	0
1	F	330	Total 2660	C 1774	N 427	O 440	S 19	0	0

- Molecule 2 is 1-palmitoyl-2-oleoyl-sn-glycero-3-phosphocholine (CCD ID: LBN) (formula: $C_{42}H_{82}NO_8P$).



Mol	Chain	Residues	Atoms	AltConf
2	A	1	Total C O P 40 31 8 1	0
2	A	1	Total C N O P 35 25 1 8 1	0
2	A	1	Total C 12 12	0
2	A	1	Total C 12 12	0
2	A	1	Total C N O P 45 35 1 8 1	0
2	A	1	Total C O P 40 31 8 1	0
2	A	1	Total C O 42 37 5	0
2	A	1	Total C 12 12	0
2	B	1	Total C N O P 35 25 1 8 1	0
2	B	1	Total C 12 12	0
2	B	1	Total C 12 12	0
2	B	1	Total C N O P 45 35 1 8 1	0
2	B	1	Total C O P 40 31 8 1	0
2	B	1	Total C O 42 37 5	0
2	B	1	Total C 12 12	0
2	D	1	Total C N O P 35 25 1 8 1	0
2	D	1	Total C 12 12	0
2	D	1	Total C 12 12	0
2	D	1	Total C N O P 45 35 1 8 1	0
2	D	1	Total C O P 40 31 8 1	0
2	D	1	Total C O 42 37 5	0
2	D	1	Total C 12 12	0

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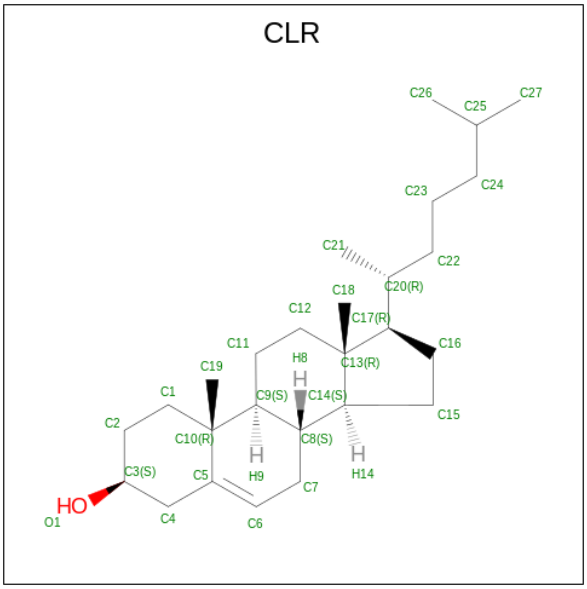
Mol	Chain	Residues	Atoms	AltConf
2	C	1	Total C N O P 45 35 1 8 1	0
2	C	1	Total C O P 40 31 8 1	0
2	C	1	Total C O 42 37 5	0
2	C	1	Total C 12 12	0
2	C	1	Total C N O P 35 25 1 8 1	0
2	C	1	Total C 12 12	0
2	C	1	Total C 12 12	0
2	E	1	Total C N O P 35 25 1 8 1	0
2	E	1	Total C 12 12	0
2	E	1	Total C 12 12	0
2	E	1	Total C N O P 45 35 1 8 1	0
2	E	1	Total C O P 40 31 8 1	0
2	E	1	Total C O 42 37 5	0
2	E	1	Total C 12 12	0
2	G	1	Total C N O P 45 35 1 8 1	0
2	G	1	Total C O 42 37 5	0
2	G	1	Total C 12 12	0
2	G	1	Total C N O P 35 25 1 8 1	0
2	G	1	Total C 12 12	0
2	G	1	Total C 12 12	0
2	F	1	Total C N O P 45 35 1 8 1	0

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Mol	Chain	Residues	Atoms	AltConf
2	F	1	Total C O P 40 31 8 1	0
2	F	1	Total C O 42 37 5	0
2	F	1	Total C 12 12	0
2	F	1	Total C N O P 35 25 1 8 1	0
2	F	1	Total C 12 12	0
2	F	1	Total C 12 12	0

- Molecule 3 is CHOLESTEROL (CCD ID: CLR) (formula: $C_{27}H_{46}O$).



Mol	Chain	Residues	Atoms	AltConf
3	A	1	Total C O 28 27 1	0
3	B	1	Total C O 28 27 1	0
3	D	1	Total C O 28 27 1	0
3	C	1	Total C O 28 27 1	0
3	E	1	Total C O 28 27 1	0

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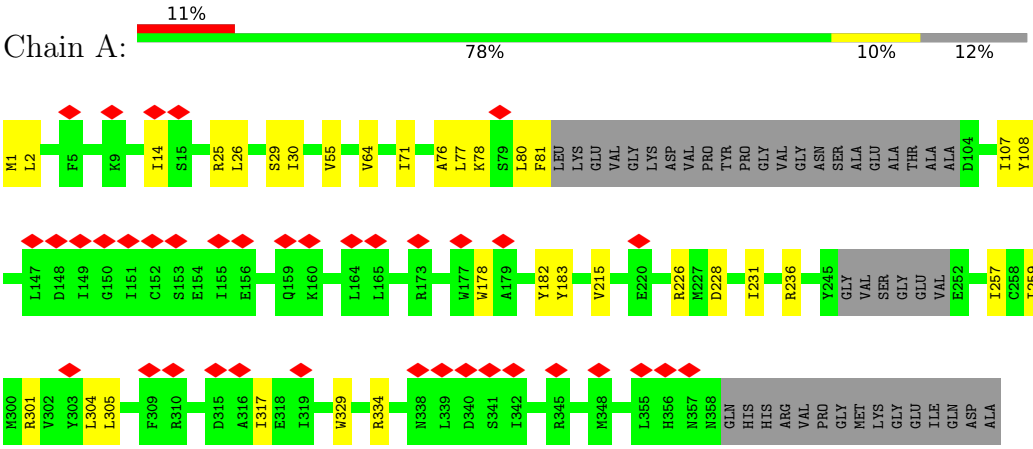
Mol	Chain	Residues	Atoms			AltConf
3	G	1	Total	C	O	0
			28	27	1	
3	F	1	Total	C	O	0
			28	27	1	

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.

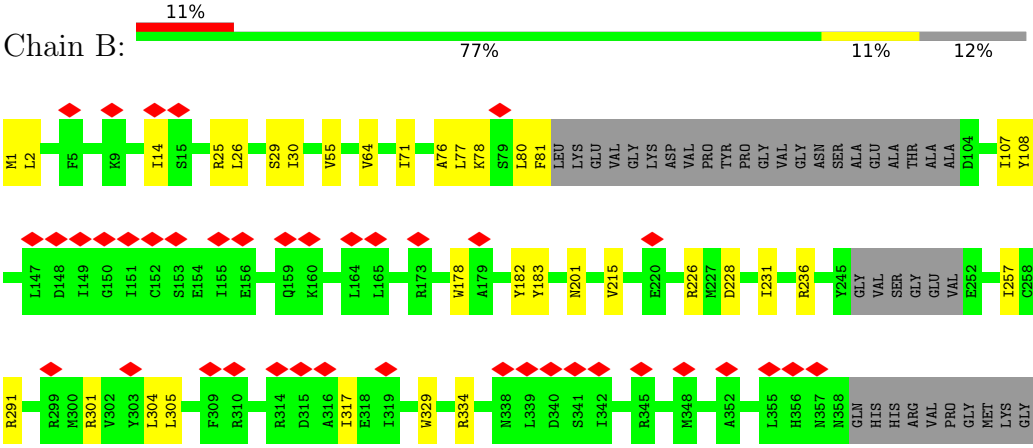
• Molecule 1: Innexin shaking-B

Chain A:



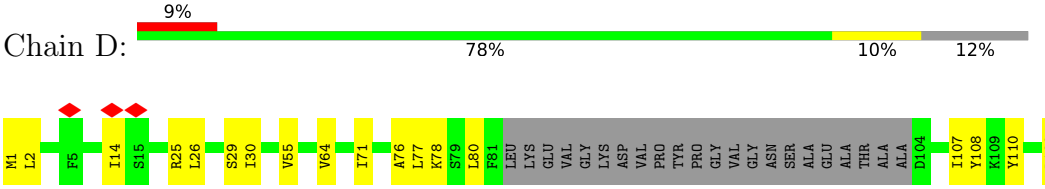
• Molecule 1: Innexin shaking-B

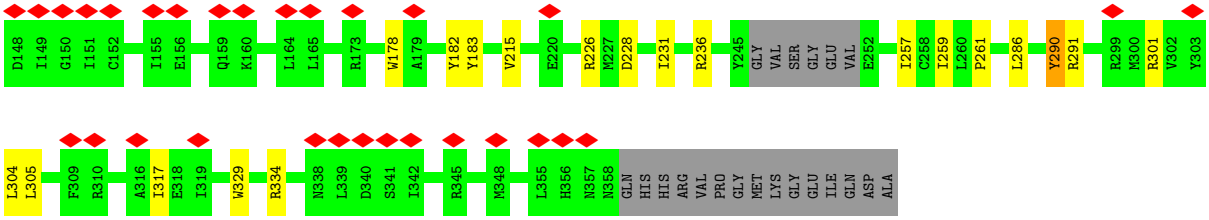
Chain B:



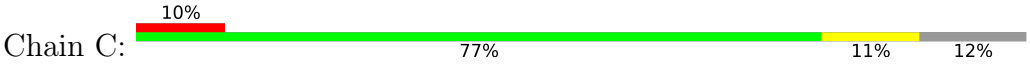
• Molecule 1: Innexin shaking-B

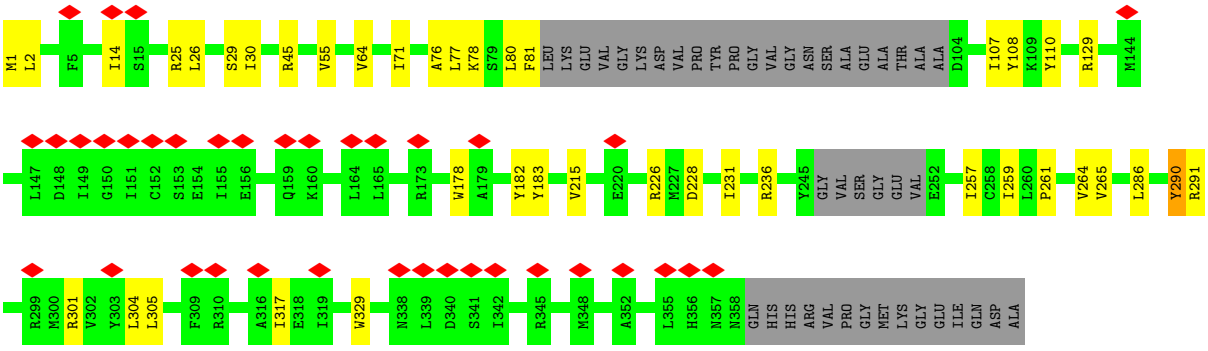
Chain D:



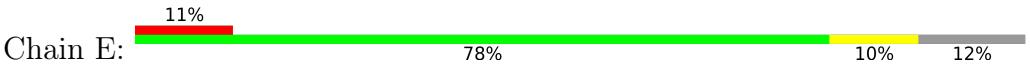


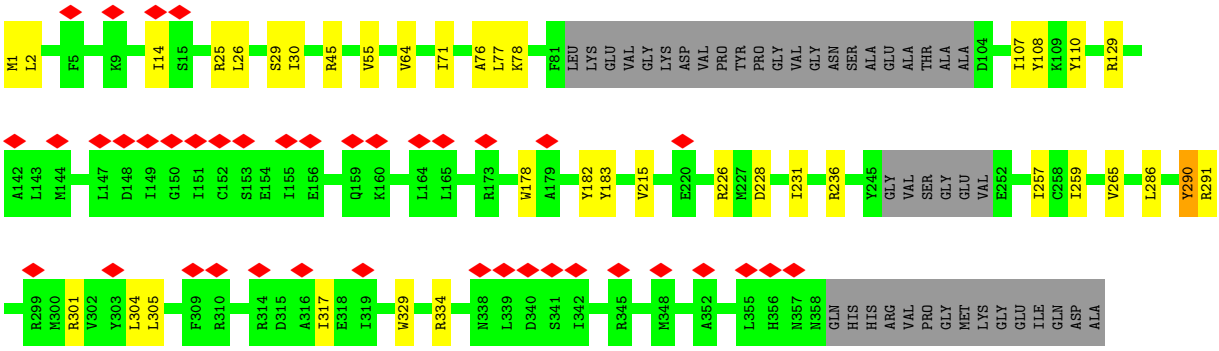
• Molecule 1: Innexin shaking-B



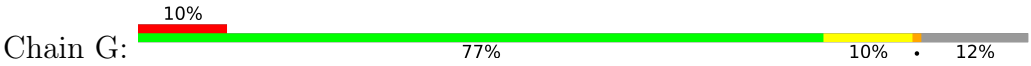


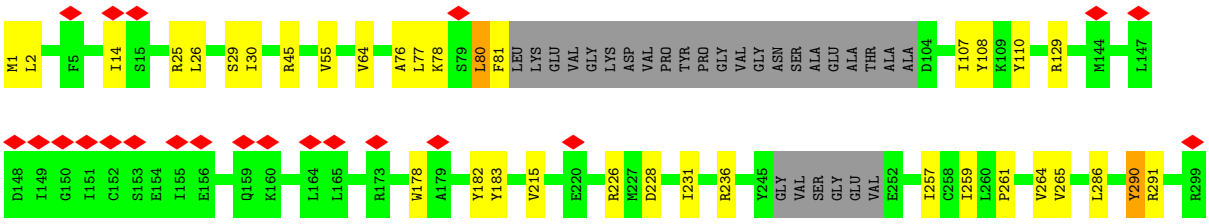
• Molecule 1: Innexin shaking-B

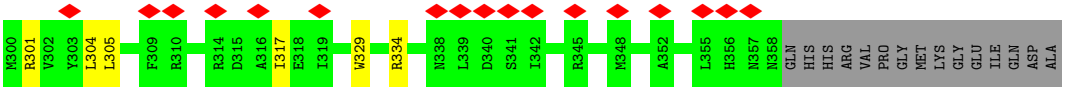




• Molecule 1: Innexin shaking-B



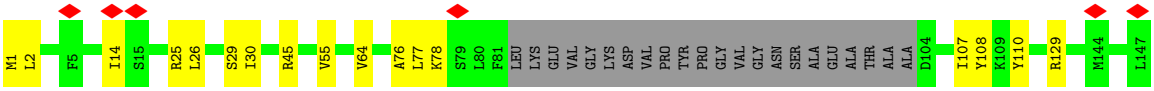


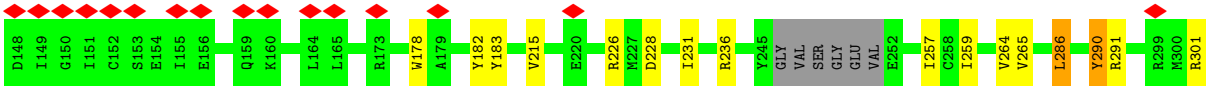


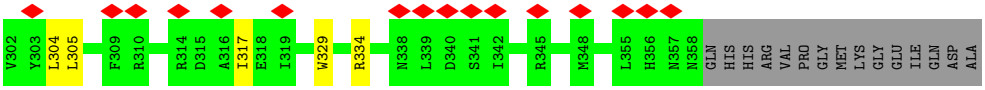
• Molecule 1: Innexin shaking-B

Chain F:









4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	146977	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	JEOL CRYO ARM 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.130	Depositor
Minimum map value	-0.791	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.033	Depositor
Recommended contour level	0.08	Depositor
Map size (Å)	227.52, 227.52, 227.52	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.79, 0.79, 0.79	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LBN, CLR

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	0.13	0/2738	0.28	0/3732
1	B	0.13	0/2738	0.28	0/3732
1	C	0.13	0/2738	0.28	0/3732
1	D	0.13	0/2738	0.28	0/3732
1	E	0.13	0/2738	0.28	0/3732
1	F	0.13	0/2738	0.28	0/3732
1	G	0.13	0/2738	0.28	0/3732
All	All	0.13	0/19166	0.28	0/26124

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	2660	0	2542	28	0
1	B	2660	0	2542	28	0
1	C	2660	0	2542	27	0
1	D	2660	0	2542	27	0
1	E	2660	0	2542	25	0
1	F	2660	0	2542	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	2660	0	2542	26	0
2	A	238	0	0	0	0
2	B	198	0	0	0	0
2	C	198	0	0	0	0
2	D	198	0	0	0	0
2	E	198	0	0	0	0
2	F	198	0	0	0	0
2	G	158	0	0	0	0
3	A	28	0	46	0	0
3	B	28	0	46	0	0
3	C	28	0	46	0	0
3	D	28	0	46	0	0
3	E	28	0	46	0	0
3	F	28	0	46	0	0
3	G	28	0	46	0	0
All	All	20202	0	18116	153	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 4.

All (153) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:LEU:HD11	1:A:257:ILE:HD12	1.69	0.74
1:C:77:LEU:HD11	1:C:257:ILE:HD12	1.68	0.74
1:G:77:LEU:HD11	1:G:257:ILE:HD12	1.69	0.74
1:F:77:LEU:HD11	1:F:257:ILE:HD12	1.68	0.74
1:D:77:LEU:HD11	1:D:257:ILE:HD12	1.69	0.73
1:E:77:LEU:HD11	1:E:257:ILE:HD12	1.69	0.73
1:B:77:LEU:HD11	1:B:257:ILE:HD12	1.68	0.73
1:A:2:LEU:HD21	1:G:129:ARG:HE	1.66	0.60
1:B:76:ALA:HB2	1:B:107:ILE:HG22	1.83	0.60
1:D:14:ILE:HD11	1:E:1:MET:HG3	1.84	0.60
1:E:129:ARG:HE	1:F:2:LEU:HD21	1.66	0.60
1:B:14:ILE:HD11	1:C:1:MET:HG3	1.84	0.60
1:E:14:ILE:HD11	1:F:1:MET:HG3	1.84	0.60
1:G:2:LEU:HD21	1:F:129:ARG:HE	1.67	0.60
1:F:290:TYR:HE1	1:F:304:LEU:HD21	1.66	0.60
1:D:2:LEU:HD21	1:C:129:ARG:HE	1.66	0.59
1:D:1:MET:HG3	1:C:14:ILE:HD11	1.84	0.59
1:A:14:ILE:HD11	1:B:1:MET:HG3	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:ALA:HB2	1:A:107:ILE:HG22	1.84	0.59
1:G:1:MET:HG3	1:F:14:ILE:HD11	1.84	0.59
1:D:290:TYR:HE1	1:D:304:LEU:HD21	1.68	0.59
1:E:290:TYR:HE1	1:E:304:LEU:HD21	1.68	0.59
1:A:1:MET:HG3	1:G:14:ILE:HD11	1.84	0.59
1:A:182:TYR:HE2	1:A:291:ARG:HH12	1.51	0.59
1:G:290:TYR:HE1	1:G:304:LEU:HD21	1.68	0.59
1:F:182:TYR:HE2	1:F:291:ARG:HH12	1.51	0.59
1:D:129:ARG:HE	1:E:2:LEU:HD21	1.67	0.58
1:A:129:ARG:HE	1:B:2:LEU:HD21	1.68	0.58
1:E:182:TYR:HE2	1:E:291:ARG:HH12	1.51	0.58
1:D:182:TYR:HE2	1:D:291:ARG:HH12	1.51	0.58
1:A:290:TYR:HE1	1:A:304:LEU:HD21	1.67	0.58
1:B:129:ARG:HE	1:C:2:LEU:HD21	1.66	0.58
1:C:76:ALA:HB2	1:C:107:ILE:HG22	1.86	0.58
1:E:305:LEU:HD13	1:E:317:ILE:HD12	1.85	0.58
1:B:182:TYR:HE2	1:B:291:ARG:HH12	1.52	0.58
1:G:182:TYR:HE2	1:G:291:ARG:HH12	1.52	0.58
1:F:305:LEU:HD13	1:F:317:ILE:HD12	1.85	0.58
1:D:76:ALA:HB2	1:D:107:ILE:HG22	1.84	0.58
1:D:305:LEU:HD13	1:D:317:ILE:HD12	1.86	0.57
1:B:305:LEU:HD13	1:B:317:ILE:HD12	1.85	0.57
1:C:305:LEU:HD13	1:C:317:ILE:HD12	1.86	0.57
1:F:76:ALA:HB2	1:F:107:ILE:HG22	1.84	0.57
1:C:182:TYR:HE2	1:C:291:ARG:HH12	1.52	0.57
1:A:305:LEU:HD13	1:A:317:ILE:HD12	1.85	0.57
1:G:305:LEU:HD13	1:G:317:ILE:HD12	1.85	0.57
1:B:290:TYR:HE1	1:B:304:LEU:HD21	1.69	0.57
1:C:290:TYR:HE1	1:C:304:LEU:HD21	1.69	0.56
1:E:76:ALA:HB2	1:E:107:ILE:HG22	1.86	0.56
1:G:76:ALA:HB2	1:G:107:ILE:HG22	1.87	0.55
1:E:259:ILE:HD13	1:F:64:VAL:HG13	1.89	0.54
1:G:64:VAL:HG13	1:F:259:ILE:HD13	1.90	0.54
1:A:259:ILE:HD13	1:B:64:VAL:HG13	1.90	0.53
1:B:259:ILE:HD13	1:C:64:VAL:HG13	1.89	0.52
1:D:64:VAL:HG13	1:C:259:ILE:HD13	1.90	0.52
1:D:259:ILE:HD13	1:E:64:VAL:HG13	1.91	0.51
1:E:226:ARG:HD2	1:E:231:ILE:HB	1.93	0.51
1:A:64:VAL:HG13	1:G:259:ILE:HD13	1.93	0.50
1:B:55:VAL:HG22	1:C:64:VAL:HG11	1.94	0.50
1:B:226:ARG:HD2	1:B:231:ILE:HB	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:VAL:HG22	1:B:64:VAL:HG11	1.95	0.49
1:D:55:VAL:HG22	1:E:64:VAL:HG11	1.95	0.48
1:E:26:LEU:HD23	1:E:30:ILE:HG13	1.95	0.48
1:D:26:LEU:HD23	1:D:30:ILE:HG13	1.96	0.48
1:G:64:VAL:HG11	1:F:55:VAL:HG22	1.96	0.48
1:B:26:LEU:HD23	1:B:30:ILE:HG13	1.96	0.48
1:C:290:TYR:CE1	1:C:304:LEU:HD21	2.49	0.48
1:F:26:LEU:HD23	1:F:30:ILE:HG13	1.96	0.48
1:G:26:LEU:HD23	1:G:30:ILE:HG13	1.96	0.47
1:B:228:ASP:O	1:B:231:ILE:HG22	2.15	0.47
1:B:290:TYR:CE1	1:B:304:LEU:HD21	2.49	0.47
1:D:64:VAL:HG11	1:C:55:VAL:HG22	1.96	0.47
1:A:64:VAL:HG11	1:G:55:VAL:HG22	1.97	0.47
1:A:26:LEU:HD23	1:A:30:ILE:HG13	1.97	0.47
1:F:226:ARG:HD2	1:F:231:ILE:HB	1.97	0.47
1:F:290:TYR:CE1	1:F:304:LEU:HD21	2.50	0.46
1:A:226:ARG:HD2	1:A:231:ILE:HB	1.97	0.46
1:D:228:ASP:O	1:D:231:ILE:HG22	2.16	0.46
1:G:228:ASP:O	1:G:231:ILE:HG22	2.16	0.46
1:E:55:VAL:HG22	1:F:64:VAL:HG11	1.98	0.46
1:A:305:LEU:HG	1:A:329:TRP:HE1	1.81	0.46
1:G:305:LEU:HG	1:G:329:TRP:HE1	1.81	0.46
1:F:228:ASP:O	1:F:231:ILE:HG22	2.16	0.46
1:A:228:ASP:O	1:A:231:ILE:HG22	2.15	0.46
1:C:228:ASP:O	1:C:231:ILE:HG22	2.16	0.46
1:B:305:LEU:HG	1:B:329:TRP:HE1	1.81	0.46
1:C:26:LEU:HD23	1:C:30:ILE:HG13	1.98	0.45
1:E:228:ASP:O	1:E:231:ILE:HG22	2.16	0.45
1:E:290:TYR:CE1	1:E:304:LEU:HD21	2.49	0.45
1:G:226:ARG:HD2	1:G:231:ILE:HB	1.99	0.45
1:A:290:TYR:CE1	1:A:304:LEU:HD21	2.49	0.45
1:A:334:ARG:HD3	1:A:334:ARG:HA	1.78	0.45
1:E:305:LEU:HG	1:E:329:TRP:HE1	1.81	0.45
1:B:301:ARG:HB3	1:B:329:TRP:CD1	2.52	0.45
1:D:305:LEU:HG	1:D:329:TRP:HE1	1.82	0.45
1:E:108:TYR:HB3	1:E:110:TYR:CD2	2.52	0.45
1:F:305:LEU:HG	1:F:329:TRP:HE1	1.82	0.45
1:D:226:ARG:HD2	1:D:231:ILE:HB	2.00	0.44
1:D:301:ARG:HB3	1:D:329:TRP:CD1	2.53	0.44
1:F:301:ARG:HB3	1:F:329:TRP:CD1	2.52	0.44
1:C:226:ARG:HD2	1:C:231:ILE:HB	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:305:LEU:HG	1:C:329:TRP:HE1	1.82	0.44
1:C:301:ARG:HB3	1:C:329:TRP:CD1	2.52	0.44
1:D:290:TYR:CE1	1:D:304:LEU:HD21	2.50	0.44
1:E:301:ARG:HB3	1:E:329:TRP:CD1	2.53	0.44
1:A:301:ARG:HB3	1:A:329:TRP:CD1	2.53	0.44
1:A:108:TYR:HB3	1:A:110:TYR:CD2	2.53	0.43
1:B:108:TYR:HB3	1:B:110:TYR:CD2	2.53	0.43
1:G:108:TYR:HB3	1:G:110:TYR:CD2	2.53	0.43
1:G:290:TYR:CE1	1:G:304:LEU:HD21	2.49	0.43
1:G:301:ARG:HB3	1:G:329:TRP:CD1	2.53	0.43
1:F:108:TYR:HB3	1:F:110:TYR:CD2	2.53	0.43
1:B:291:ARG:HA	1:B:291:ARG:HD3	1.88	0.43
1:C:108:TYR:HB3	1:C:110:TYR:CD2	2.53	0.43
1:C:183:TYR:CE1	1:C:291:ARG:HD2	2.53	0.43
1:F:183:TYR:CE1	1:F:291:ARG:HD2	2.54	0.43
1:E:183:TYR:CE1	1:E:291:ARG:HD2	2.54	0.43
1:A:183:TYR:CE1	1:A:291:ARG:HD2	2.54	0.42
1:B:231:ILE:HD12	1:B:231:ILE:HA	1.88	0.42
1:B:261:PRO:HA	1:C:71:ILE:HD11	2.01	0.42
1:D:183:TYR:CE1	1:D:291:ARG:HD2	2.54	0.42
1:G:45:ARG:HH21	1:G:265:VAL:HG21	1.84	0.42
1:D:108:TYR:HB3	1:D:110:TYR:CD2	2.54	0.42
1:B:334:ARG:HD3	1:B:334:ARG:HA	1.78	0.42
1:F:334:ARG:HD3	1:F:334:ARG:HA	1.78	0.42
1:G:80:LEU:HB3	1:G:81:PHE:H	1.62	0.42
1:F:25:ARG:O	1:F:29:SER:HB3	2.20	0.42
1:A:261:PRO:HA	1:B:71:ILE:HD11	2.02	0.42
1:B:183:TYR:CE1	1:B:291:ARG:HD2	2.54	0.42
1:D:25:ARG:O	1:D:29:SER:HB3	2.19	0.42
1:C:25:ARG:O	1:C:29:SER:HB3	2.20	0.42
1:G:25:ARG:O	1:G:29:SER:HB3	2.20	0.42
1:G:183:TYR:CE1	1:G:291:ARG:HD2	2.54	0.41
1:G:334:ARG:HD3	1:G:334:ARG:HA	1.78	0.41
1:B:25:ARG:O	1:B:29:SER:HB3	2.20	0.41
1:D:334:ARG:HA	1:D:334:ARG:HD3	1.78	0.41
1:E:25:ARG:O	1:E:29:SER:HB3	2.20	0.41
1:E:45:ARG:HH21	1:E:265:VAL:HG21	1.85	0.41
1:A:25:ARG:O	1:A:29:SER:HB3	2.19	0.41
1:A:80:LEU:HB3	1:A:81:PHE:H	1.64	0.41
1:A:291:ARG:HA	1:A:291:ARG:HD3	1.89	0.41
1:D:231:ILE:HD12	1:D:231:ILE:HA	1.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:305:LEU:HD23	1:C:305:LEU:HA	1.97	0.40
1:F:45:ARG:HH21	1:F:265:VAL:HG21	1.86	0.40
1:D:291:ARG:HA	1:D:291:ARG:HD3	1.89	0.40
1:C:45:ARG:HH21	1:C:265:VAL:HG21	1.86	0.40
1:A:71:ILE:HD11	1:G:261:PRO:HA	2.03	0.40
1:D:261:PRO:HA	1:E:71:ILE:HD11	2.01	0.40
1:C:80:LEU:HB3	1:C:81:PHE:H	1.63	0.40
1:A:305:LEU:HD23	1:A:305:LEU:HA	1.97	0.40
1:B:80:LEU:HB3	1:B:81:PHE:H	1.65	0.40
1:D:71:ILE:HD11	1:C:261:PRO:HA	2.03	0.40
1:E:334:ARG:HA	1:E:334:ARG:HD3	1.78	0.40
1:F:286:LEU:HD13	1:F:286:LEU:HA	1.94	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	324/373 (87%)	312 (96%)	12 (4%)	0	100	100
1	B	324/373 (87%)	312 (96%)	12 (4%)	0	100	100
1	C	324/373 (87%)	312 (96%)	12 (4%)	0	100	100
1	D	324/373 (87%)	312 (96%)	12 (4%)	0	100	100
1	E	324/373 (87%)	312 (96%)	12 (4%)	0	100	100
1	F	324/373 (87%)	312 (96%)	12 (4%)	0	100	100
1	G	324/373 (87%)	312 (96%)	12 (4%)	0	100	100
All	All	2268/2611 (87%)	2184 (96%)	84 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	270/342 (79%)	264 (98%)	6 (2%)	45	74
1	B	270/342 (79%)	262 (97%)	8 (3%)	36	69
1	C	270/342 (79%)	263 (97%)	7 (3%)	40	72
1	D	270/342 (79%)	263 (97%)	7 (3%)	40	72
1	E	270/342 (79%)	264 (98%)	6 (2%)	45	74
1	F	270/342 (79%)	263 (97%)	7 (3%)	40	72
1	G	270/342 (79%)	262 (97%)	8 (3%)	36	69
All	All	1890/2394 (79%)	1841 (97%)	49 (3%)	41	72

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	78	LYS
1	A	178	TRP
1	A	215	VAL
1	A	236	ARG
1	A	286	LEU
1	A	290	TYR
1	B	78	LYS
1	B	178	TRP
1	B	201	ASN
1	B	215	VAL
1	B	236	ARG
1	B	264	VAL
1	B	286	LEU
1	B	290	TYR
1	D	78	LYS
1	D	80	LEU
1	D	178	TRP
1	D	215	VAL
1	D	236	ARG
1	D	286	LEU

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Mol	Chain	Res	Type
1	D	290	TYR
1	C	78	LYS
1	C	178	TRP
1	C	215	VAL
1	C	236	ARG
1	C	264	VAL
1	C	286	LEU
1	C	290	TYR
1	E	78	LYS
1	E	178	TRP
1	E	215	VAL
1	E	236	ARG
1	E	286	LEU
1	E	290	TYR
1	G	78	LYS
1	G	80	LEU
1	G	178	TRP
1	G	215	VAL
1	G	236	ARG
1	G	264	VAL
1	G	286	LEU
1	G	290	TYR
1	F	78	LYS
1	F	178	TRP
1	F	215	VAL
1	F	236	ARG
1	F	264	VAL
1	F	286	LEU
1	F	290	TYR

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

Mol	Chain	Res	Type
1	B	121	GLN
1	F	121	GLN

5.3.3 RNA

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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

56 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	CLR	D	404	-	31,31,31	0.38	0	48,48,48	0.53	0
2	LBN	B	406	-	39,39,51	0.64	1 (2%)	42,44,59	0.98	2 (4%)
2	LBN	F	503	-	39,39,51	0.64	1 (2%)	42,44,59	0.97	2 (4%)
2	LBN	C	503	-	39,39,51	0.64	1 (2%)	42,44,59	0.98	2 (4%)
2	LBN	E	402	-	11,11,51	0.23	0	10,10,59	0.26	0
2	LBN	B	408	-	11,11,51	0.24	0	10,10,59	0.27	0
2	LBN	E	401	-	34,34,51	0.33	0	38,41,59	0.55	1 (2%)
3	CLR	C	501	-	31,31,31	0.39	0	48,48,48	0.53	0
3	CLR	F	501	-	31,31,31	0.39	0	48,48,48	0.53	0
2	LBN	A	409	-	11,11,51	0.24	0	10,10,59	0.26	0
2	LBN	D	402	-	11,11,51	0.24	0	10,10,59	0.26	0
2	LBN	D	407	-	41,41,51	0.37	0	43,43,59	0.37	0
3	CLR	A	405	-	31,31,31	0.38	0	48,48,48	0.53	0
3	CLR	B	404	-	31,31,31	0.39	0	48,48,48	0.53	0
2	LBN	A	407	-	39,39,51	0.64	1 (2%)	42,44,59	0.97	2 (4%)
2	LBN	E	403	-	11,11,51	0.24	0	10,10,59	0.24	0
2	LBN	A	406	-	44,44,51	0.51	0	50,52,59	0.48	0
2	LBN	G	507	-	11,11,51	0.24	0	10,10,59	0.24	0
2	LBN	D	405	-	44,44,51	0.51	0	50,52,59	0.47	0
2	LBN	E	405	-	44,44,51	0.50	0	50,52,59	0.47	0
2	LBN	A	408	-	41,41,51	0.37	0	43,43,59	0.37	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	LBN	E	406	-	39,39,51	0.64	1 (2%)	42,44,59	0.98	2 (4%)
2	LBN	B	402	-	11,11,51	0.24	0	10,10,59	0.26	0
3	CLR	G	501	-	31,31,31	0.38	0	48,48,48	0.53	0
2	LBN	B	405	-	44,44,51	0.51	0	50,52,59	0.47	0
2	LBN	E	407	-	41,41,51	0.37	0	43,43,59	0.37	0
2	LBN	F	502	-	44,44,51	0.51	0	50,52,59	0.47	0
2	LBN	B	403	-	11,11,51	0.24	0	10,10,59	0.24	0
2	LBN	A	403	-	11,11,51	0.23	0	10,10,59	0.26	0
2	LBN	G	502	-	44,44,51	0.51	0	50,52,59	0.47	0
2	LBN	D	406	-	39,39,51	0.63	1 (2%)	42,44,59	0.97	2 (4%)
2	LBN	C	502	-	44,44,51	0.51	0	50,52,59	0.47	0
2	LBN	E	408	-	11,11,51	0.24	0	10,10,59	0.26	0
2	LBN	F	507	-	11,11,51	0.24	0	10,10,59	0.26	0
2	LBN	C	507	-	11,11,51	0.24	0	10,10,59	0.26	0
2	LBN	C	504	-	41,41,51	0.37	0	43,43,59	0.37	0
2	LBN	G	504	-	11,11,51	0.24	0	10,10,59	0.26	0
2	LBN	F	504	-	41,41,51	0.37	0	43,43,59	0.37	0
2	LBN	D	408	-	11,11,51	0.24	0	10,10,59	0.26	0
2	LBN	A	404	-	11,11,51	0.24	0	10,10,59	0.24	0
2	LBN	F	506	-	34,34,51	0.33	0	38,41,59	0.53	1 (2%)
2	LBN	B	401	-	34,34,51	0.33	0	38,41,59	0.53	1 (2%)
2	LBN	B	407	-	41,41,51	0.36	0	43,43,59	0.37	0
2	LBN	C	506	-	34,34,51	0.34	0	38,41,59	0.53	1 (2%)
2	LBN	C	508	-	11,11,51	0.24	0	10,10,59	0.24	0
2	LBN	A	401	-	39,39,51	0.64	1 (2%)	42,44,59	0.97	2 (4%)
2	LBN	G	506	-	11,11,51	0.24	0	10,10,59	0.26	0
2	LBN	F	508	-	11,11,51	0.24	0	10,10,59	0.24	0
2	LBN	D	403	-	11,11,51	0.24	0	10,10,59	0.24	0
2	LBN	G	503	-	41,41,51	0.36	0	43,43,59	0.37	0
2	LBN	D	401	-	34,34,51	0.34	0	38,41,59	0.55	1 (2%)
2	LBN	F	505	-	11,11,51	0.24	0	10,10,59	0.26	0
2	LBN	C	505	-	11,11,51	0.24	0	10,10,59	0.27	0
2	LBN	G	505	-	34,34,51	0.34	0	38,41,59	0.54	1 (2%)
3	CLR	E	404	-	31,31,31	0.38	0	48,48,48	0.53	0
2	LBN	A	402	-	34,34,51	0.33	0	38,41,59	0.54	1 (2%)

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
3	CLR	D	404	-	-	2/10/68/68	0/4/4/4
2	LBN	B	406	-	-	17/41/41/55	-
2	LBN	F	503	-	-	21/41/41/55	-
2	LBN	C	503	-	-	17/41/41/55	-
2	LBN	E	402	-	-	3/9/9/55	-
2	LBN	B	408	-	-	4/9/9/55	-
2	LBN	E	401	-	-	21/37/37/55	-
3	CLR	C	501	-	-	2/10/68/68	0/4/4/4
3	CLR	F	501	-	-	2/10/68/68	0/4/4/4
2	LBN	A	409	-	-	4/9/9/55	-
2	LBN	D	402	-	-	2/9/9/55	-
2	LBN	D	407	-	-	18/43/43/55	-
3	CLR	A	405	-	-	2/10/68/68	0/4/4/4
3	CLR	B	404	-	-	2/10/68/68	0/4/4/4
2	LBN	A	407	-	-	20/41/41/55	-
2	LBN	E	403	-	-	5/9/9/55	-
2	LBN	A	406	-	-	20/48/48/55	-
2	LBN	G	507	-	-	4/9/9/55	-
2	LBN	D	405	-	-	20/48/48/55	-
2	LBN	E	405	-	-	20/48/48/55	-
2	LBN	A	408	-	-	17/43/43/55	-
2	LBN	E	406	-	-	20/41/41/55	-
2	LBN	B	402	-	-	3/9/9/55	-
3	CLR	G	501	-	-	2/10/68/68	0/4/4/4
2	LBN	B	405	-	-	20/48/48/55	-
2	LBN	E	407	-	-	17/43/43/55	-
2	LBN	F	502	-	-	20/48/48/55	-
2	LBN	B	403	-	-	5/9/9/55	-
2	LBN	A	403	-	-	3/9/9/55	-
2	LBN	G	502	-	-	20/48/48/55	-
2	LBN	D	406	-	-	17/41/41/55	-
2	LBN	C	502	-	-	20/48/48/55	-
2	LBN	E	408	-	-	4/9/9/55	-
2	LBN	F	507	-	-	3/9/9/55	-
2	LBN	C	507	-	-	2/9/9/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	LBN	C	504	-	-	19/43/43/55	-
2	LBN	G	504	-	-	4/9/9/55	-
2	LBN	F	504	-	-	19/43/43/55	-
2	LBN	D	408	-	-	4/9/9/55	-
2	LBN	A	404	-	-	4/9/9/55	-
2	LBN	F	506	-	-	20/37/37/55	-
2	LBN	B	401	-	-	21/37/37/55	-
2	LBN	B	407	-	-	18/43/43/55	-
2	LBN	C	506	-	-	21/37/37/55	-
2	LBN	C	508	-	-	6/9/9/55	-
2	LBN	A	401	-	-	20/41/41/55	-
2	LBN	G	506	-	-	2/9/9/55	-
2	LBN	F	508	-	-	4/9/9/55	-
2	LBN	D	403	-	-	3/9/9/55	-
2	LBN	G	503	-	-	18/43/43/55	-
2	LBN	D	401	-	-	21/37/37/55	-
2	LBN	F	505	-	-	4/9/9/55	-
2	LBN	C	505	-	-	4/9/9/55	-
2	LBN	G	505	-	-	21/37/37/55	-
3	CLR	E	404	-	-	2/10/68/68	0/4/4/4
2	LBN	A	402	-	-	21/37/37/55	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	406	LBN	P1-O2	2.72	1.65	1.54
2	B	406	LBN	P1-O2	2.72	1.65	1.54
2	C	503	LBN	P1-O2	2.71	1.65	1.54
2	F	503	LBN	P1-O2	2.71	1.65	1.54
2	A	407	LBN	P1-O2	2.71	1.65	1.54
2	A	401	LBN	P1-O2	2.70	1.65	1.54
2	D	406	LBN	P1-O2	2.69	1.65	1.54

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	503	LBN	O2-P1-O1	-4.88	93.76	106.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	406	LBN	O2-P1-O1	-4.87	93.79	106.73
2	D	406	LBN	O2-P1-O1	-4.86	93.80	106.73
2	E	406	LBN	O2-P1-O1	-4.85	93.82	106.73
2	F	503	LBN	O2-P1-O1	-4.85	93.82	106.73
2	A	407	LBN	O2-P1-O1	-4.85	93.82	106.73
2	A	401	LBN	O2-P1-O1	-4.84	93.85	106.73
2	E	401	LBN	O7-C34-O8	-2.72	122.10	125.57
2	D	401	LBN	O7-C34-O8	-2.69	122.14	125.57
2	G	505	LBN	O7-C34-O8	-2.67	122.17	125.57
2	A	402	LBN	O7-C34-O8	-2.65	122.19	125.57
2	F	506	LBN	O7-C34-O8	-2.61	122.25	125.57
2	C	506	LBN	O7-C34-O8	-2.56	122.31	125.57
2	B	401	LBN	O7-C34-O8	-2.54	122.33	125.57
2	C	503	LBN	O3-P1-O4	2.27	119.55	110.68
2	E	406	LBN	O3-P1-O4	2.26	119.54	110.68
2	B	406	LBN	O3-P1-O4	2.25	119.51	110.68
2	F	503	LBN	O3-P1-O4	2.25	119.50	110.68
2	A	401	LBN	O3-P1-O4	2.25	119.48	110.68
2	D	406	LBN	O3-P1-O4	2.25	119.47	110.68
2	A	407	LBN	O3-P1-O4	2.24	119.46	110.68

There are no chirality outliers.

All (635) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	LBN	C1-O1-P1-O2
2	A	401	LBN	O8-C34-O7-C2
2	A	402	LBN	C1-O1-P1-O3
2	A	402	LBN	O8-C34-O7-C2
2	A	406	LBN	O1-C1-C2-O7
2	A	406	LBN	C1-O1-P1-O4
2	A	406	LBN	C35-C34-O7-C2
2	A	407	LBN	C1-O1-P1-O2
2	A	407	LBN	C1-O1-P1-O4
2	A	407	LBN	O8-C34-O7-C2
2	A	408	LBN	C35-C34-O7-C2
2	B	401	LBN	C9-O2-P1-O1
2	B	401	LBN	C9-O2-P1-O3
2	B	401	LBN	C9-O2-P1-O4
2	B	401	LBN	N1-C6-C9-O2
2	B	401	LBN	O8-C34-O7-C2
2	B	405	LBN	O1-C1-C2-O7

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Mol	Chain	Res	Type	Atoms
2	B	405	LBN	C1-O1-P1-O4
2	B	405	LBN	C35-C34-O7-C2
2	B	406	LBN	O8-C34-O7-C2
2	B	407	LBN	C35-C34-O7-C2
2	D	401	LBN	C1-O1-P1-O3
2	D	401	LBN	O8-C34-O7-C2
2	D	405	LBN	O1-C1-C2-O7
2	D	405	LBN	C1-O1-P1-O4
2	D	405	LBN	C35-C34-O7-C2
2	D	406	LBN	O8-C34-O7-C2
2	D	407	LBN	C35-C34-O7-C2
2	C	502	LBN	O1-C1-C2-O7
2	C	502	LBN	C1-O1-P1-O4
2	C	502	LBN	C35-C34-O7-C2
2	C	503	LBN	O8-C34-O7-C2
2	C	504	LBN	C35-C34-O7-C2
2	C	506	LBN	C9-O2-P1-O1
2	C	506	LBN	C9-O2-P1-O3
2	C	506	LBN	C9-O2-P1-O4
2	C	506	LBN	N1-C6-C9-O2
2	C	506	LBN	O8-C34-O7-C2
2	E	401	LBN	C1-O1-P1-O3
2	E	401	LBN	O8-C34-O7-C2
2	E	405	LBN	O1-C1-C2-O7
2	E	405	LBN	C1-O1-P1-O4
2	E	405	LBN	C35-C34-O7-C2
2	E	406	LBN	C1-O1-P1-O2
2	E	406	LBN	C1-O1-P1-O3
2	E	406	LBN	C1-O1-P1-O4
2	E	406	LBN	O8-C34-O7-C2
2	E	407	LBN	C35-C34-O7-C2
2	G	502	LBN	O1-C1-C2-O7
2	G	502	LBN	C1-O1-P1-O4
2	G	502	LBN	C35-C34-O7-C2
2	G	503	LBN	C35-C34-O7-C2
2	G	505	LBN	C1-O1-P1-O2
2	G	505	LBN	C1-O1-P1-O3
2	G	505	LBN	O8-C34-O7-C2
2	F	502	LBN	O1-C1-C2-O7
2	F	502	LBN	C1-O1-P1-O4
2	F	502	LBN	C35-C34-O7-C2
2	F	503	LBN	C1-O1-P1-O2

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Mol	Chain	Res	Type	Atoms
2	F	503	LBN	C1-O1-P1-O3
2	F	503	LBN	C1-O1-P1-O4
2	F	503	LBN	O8-C34-O7-C2
2	F	504	LBN	C35-C34-O7-C2
2	F	506	LBN	O8-C34-O7-C2
2	C	506	LBN	O6-C25-O5-C3
2	C	506	LBN	C26-C25-O5-C3
2	A	408	LBN	O6-C25-O5-C3
2	B	401	LBN	O6-C25-O5-C3
2	B	407	LBN	O6-C25-O5-C3
2	D	407	LBN	O6-C25-O5-C3
2	C	504	LBN	O6-C25-O5-C3
2	E	407	LBN	O6-C25-O5-C3
2	G	503	LBN	O6-C25-O5-C3
2	F	504	LBN	O6-C25-O5-C3
2	A	406	LBN	O8-C34-O7-C2
2	A	408	LBN	O8-C34-O7-C2
2	B	405	LBN	O8-C34-O7-C2
2	B	407	LBN	O8-C34-O7-C2
2	D	405	LBN	O8-C34-O7-C2
2	D	407	LBN	O8-C34-O7-C2
2	C	502	LBN	O8-C34-O7-C2
2	C	504	LBN	O8-C34-O7-C2
2	E	405	LBN	O8-C34-O7-C2
2	E	407	LBN	O8-C34-O7-C2
2	G	502	LBN	O8-C34-O7-C2
2	G	503	LBN	O8-C34-O7-C2
2	F	502	LBN	O8-C34-O7-C2
2	F	504	LBN	O8-C34-O7-C2
2	A	408	LBN	C26-C25-O5-C3
2	B	401	LBN	C26-C25-O5-C3
2	B	407	LBN	C26-C25-O5-C3
2	D	407	LBN	C26-C25-O5-C3
2	C	504	LBN	C26-C25-O5-C3
2	E	407	LBN	C26-C25-O5-C3
2	G	503	LBN	C26-C25-O5-C3
2	F	504	LBN	C26-C25-O5-C3
2	A	401	LBN	C35-C34-O7-C2
2	A	407	LBN	C35-C34-O7-C2
2	B	406	LBN	C35-C34-O7-C2
2	D	406	LBN	C35-C34-O7-C2
2	C	503	LBN	C35-C34-O7-C2

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Mol	Chain	Res	Type	Atoms
2	E	406	LBN	C35-C34-O7-C2
2	F	503	LBN	C35-C34-O7-C2
2	G	505	LBN	O6-C25-O5-C3
2	A	402	LBN	C26-C25-O5-C3
2	D	401	LBN	C26-C25-O5-C3
2	E	401	LBN	C26-C25-O5-C3
2	G	505	LBN	C26-C25-O5-C3
2	F	503	LBN	C26-C25-O5-C3
2	A	402	LBN	O6-C25-O5-C3
2	D	401	LBN	O6-C25-O5-C3
2	A	401	LBN	C26-C25-O5-C3
2	A	407	LBN	C26-C25-O5-C3
2	E	406	LBN	C26-C25-O5-C3
2	E	401	LBN	O6-C25-O5-C3
2	B	401	LBN	C30-C31-C32-C33
2	C	506	LBN	C30-C31-C32-C33
2	E	406	LBN	O6-C25-O5-C3
2	F	503	LBN	O6-C25-O5-C3
2	A	407	LBN	O6-C25-O5-C3
2	C	503	LBN	C26-C25-O5-C3
2	F	506	LBN	C30-C31-C32-C33
2	A	401	LBN	O6-C25-O5-C3
2	C	503	LBN	O6-C25-O5-C3
2	A	402	LBN	C9-C6-N1-C12
2	D	401	LBN	C9-C6-N1-C12
2	E	401	LBN	C9-C6-N1-C12
2	G	505	LBN	C9-C6-N1-C12
2	B	406	LBN	C26-C25-O5-C3
2	D	406	LBN	C26-C25-O5-C3
3	D	404	CLR	C22-C23-C24-C25
3	A	405	CLR	C22-C23-C24-C25
3	B	404	CLR	C22-C23-C24-C25
3	G	501	CLR	C22-C23-C24-C25
3	F	501	CLR	C22-C23-C24-C25
2	B	407	LBN	O7-C2-C3-O5
2	D	407	LBN	O7-C2-C3-O5
2	G	503	LBN	O7-C2-C3-O5
2	F	504	LBN	O7-C2-C3-O5
2	B	406	LBN	O6-C25-O5-C3
2	D	406	LBN	O6-C25-O5-C3
3	E	404	CLR	C22-C23-C24-C25
2	F	506	LBN	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
3	C	501	CLR	C22-C23-C24-C25
2	B	401	LBN	C25-C26-C27-C28
2	F	503	LBN	C39-C40-C41-C42
3	A	405	CLR	C20-C22-C23-C24
2	E	401	LBN	C9-C6-N1-C15
2	C	506	LBN	C25-C26-C27-C28
3	B	404	CLR	C20-C22-C23-C24
3	D	404	CLR	C20-C22-C23-C24
3	G	501	CLR	C20-C22-C23-C24
3	F	501	CLR	C20-C22-C23-C24
3	E	404	CLR	C20-C22-C23-C24
2	A	407	LBN	C39-C40-C41-C42
2	D	406	LBN	C39-C40-C41-C42
2	G	503	LBN	C31-C32-C33-C4
3	C	501	CLR	C20-C22-C23-C24
2	A	402	LBN	C1-O1-P1-O2
2	A	406	LBN	C1-O1-P1-O2
2	B	405	LBN	C1-O1-P1-O2
2	D	401	LBN	C1-O1-P1-O2
2	D	405	LBN	C1-O1-P1-O2
2	C	502	LBN	C1-O1-P1-O2
2	E	401	LBN	C1-O1-P1-O2
2	E	405	LBN	C1-O1-P1-O2
2	G	502	LBN	C1-O1-P1-O2
2	F	502	LBN	C1-O1-P1-O2
2	F	506	LBN	C1-O1-P1-O2
2	C	504	LBN	C31-C32-C33-C4
2	A	402	LBN	C30-C31-C32-C33
2	D	401	LBN	C30-C31-C32-C33
2	A	402	LBN	C9-C6-N1-C18
2	B	401	LBN	C9-C6-N1-C12
2	D	401	LBN	C9-C6-N1-C18
2	C	506	LBN	C9-C6-N1-C12
2	G	505	LBN	C9-C6-N1-C15
2	G	505	LBN	C9-C6-N1-C18
2	F	506	LBN	C9-C6-N1-C12
2	F	506	LBN	C9-C6-N1-C18
2	G	505	LBN	C30-C31-C32-C33
2	D	407	LBN	C31-C32-C33-C4
2	D	406	LBN	C38-C39-C40-C41
2	F	503	LBN	C38-C39-C40-C41
2	F	504	LBN	C31-C32-C33-C4

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Mol	Chain	Res	Type	Atoms
2	A	408	LBN	C8-C11-C14-C17
2	A	407	LBN	C38-C39-C40-C41
2	B	406	LBN	C38-C39-C40-C41
2	A	401	LBN	C38-C39-C40-C41
2	C	503	LBN	C32-C33-C4-C7
2	E	406	LBN	C38-C39-C40-C41
2	A	408	LBN	O7-C2-C3-O5
2	D	405	LBN	C28-C29-C30-C31
2	F	506	LBN	C26-C27-C28-C29
2	A	401	LBN	C32-C33-C4-C7
2	B	405	LBN	C28-C29-C30-C31
2	D	406	LBN	C32-C33-C4-C7
2	C	502	LBN	C28-C29-C30-C31
2	C	503	LBN	C38-C39-C40-C41
2	C	506	LBN	C28-C29-C30-C31
2	E	405	LBN	C28-C29-C30-C31
2	G	502	LBN	C28-C29-C30-C31
2	F	502	LBN	C28-C29-C30-C31
2	F	503	LBN	C32-C33-C4-C7
2	A	406	LBN	C28-C29-C30-C31
2	B	401	LBN	C28-C29-C30-C31
2	B	406	LBN	C36-C37-C38-C39
2	C	504	LBN	C7-C10-C13-C16
2	C	502	LBN	C39-C40-C41-C42
2	G	503	LBN	C39-C40-C41-C42
2	E	405	LBN	C25-C26-C27-C28
2	A	402	LBN	C7-C10-C13-C16
2	A	407	LBN	C32-C33-C4-C7
2	A	408	LBN	C37-C38-C39-C40
2	B	406	LBN	C32-C33-C4-C7
2	D	401	LBN	C7-C10-C13-C16
2	D	405	LBN	C32-C33-C4-C7
2	D	407	LBN	C37-C38-C39-C40
2	C	504	LBN	C37-C38-C39-C40
2	E	406	LBN	C32-C33-C4-C7
2	E	407	LBN	C37-C38-C39-C40
2	G	502	LBN	C32-C33-C4-C7
2	F	502	LBN	C32-C33-C4-C7
2	F	504	LBN	C7-C10-C13-C16
2	F	504	LBN	C37-C38-C39-C40
2	F	506	LBN	C7-C10-C13-C16
2	F	506	LBN	C28-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
2	A	402	LBN	C9-C6-N1-C15
2	B	401	LBN	C9-C6-N1-C15
2	B	401	LBN	C9-C6-N1-C18
2	D	401	LBN	C9-C6-N1-C15
2	C	506	LBN	C9-C6-N1-C18
2	E	401	LBN	C9-C6-N1-C18
2	F	506	LBN	C9-C6-N1-C15
2	B	407	LBN	C37-C38-C39-C40
2	D	405	LBN	C35-C36-C37-C38
2	G	503	LBN	C7-C10-C13-C16
2	A	408	LBN	C7-C10-C13-C16
2	D	407	LBN	C7-C10-C13-C16
2	C	502	LBN	C35-C36-C37-C38
2	E	401	LBN	C7-C10-C13-C16
2	E	406	LBN	C36-C37-C38-C39
2	D	405	LBN	C25-C26-C27-C28
2	A	401	LBN	C36-C37-C38-C39
2	B	406	LBN	C37-C38-C39-C40
2	G	502	LBN	C35-C36-C37-C38
2	G	503	LBN	C37-C38-C39-C40
2	G	505	LBN	C7-C10-C13-C16
2	F	502	LBN	C35-C36-C37-C38
2	A	401	LBN	C37-C38-C39-C40
2	C	502	LBN	C32-C33-C4-C7
2	E	405	LBN	C32-C33-C4-C7
2	E	407	LBN	C7-C10-C13-C16
2	A	408	LBN	C31-C32-C33-C4
2	B	405	LBN	C35-C36-C37-C38
2	C	503	LBN	C36-C37-C38-C39
2	A	406	LBN	C35-C36-C37-C38
2	B	405	LBN	C32-C33-C4-C7
2	B	407	LBN	C7-C10-C13-C16
2	E	405	LBN	C35-C36-C37-C38
2	A	406	LBN	C39-C40-C41-C42
2	B	405	LBN	C39-C40-C41-C42
2	B	407	LBN	C39-C40-C41-C42
2	D	407	LBN	C39-C40-C41-C42
2	G	502	LBN	C39-C40-C41-C42
2	F	503	LBN	C36-C37-C38-C39
2	B	405	LBN	C25-C26-C27-C28
2	A	406	LBN	C32-C33-C4-C7
2	E	401	LBN	C29-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
2	E	406	LBN	C37-C38-C39-C40
2	A	402	LBN	C29-C30-C31-C32
2	A	407	LBN	C36-C37-C38-C39
2	D	401	LBN	C29-C30-C31-C32
2	C	506	LBN	C7-C10-C13-C16
2	G	505	LBN	C29-C30-C31-C32
2	C	506	LBN	C9-C6-N1-C15
2	A	406	LBN	C25-C26-C27-C28
2	C	502	LBN	C25-C26-C27-C28
2	G	502	LBN	C25-C26-C27-C28
2	F	502	LBN	C25-C26-C27-C28
2	C	503	LBN	C37-C38-C39-C40
2	E	401	LBN	C30-C31-C32-C33
2	F	504	LBN	C27-C28-C29-C30
2	A	408	LBN	C36-C37-C38-C39
2	C	504	LBN	C27-C28-C29-C30
2	A	408	LBN	C39-C40-C41-C42
2	D	405	LBN	C39-C40-C41-C42
2	C	504	LBN	C39-C40-C41-C42
2	E	407	LBN	C39-C40-C41-C42
2	F	504	LBN	C39-C40-C41-C42
2	A	408	LBN	C27-C28-C29-C30
2	D	407	LBN	C27-C28-C29-C30
2	E	407	LBN	C31-C32-C33-C4
2	G	503	LBN	C27-C28-C29-C30
2	B	407	LBN	C28-C29-C30-C31
2	E	407	LBN	C27-C28-C29-C30
2	B	407	LBN	C31-C32-C33-C4
2	B	407	LBN	C27-C28-C29-C30
2	G	503	LBN	C28-C29-C30-C31
2	G	502	LBN	C26-C27-C28-C29
2	F	502	LBN	C26-C27-C28-C29
2	C	504	LBN	O7-C2-C3-O5
2	E	407	LBN	O7-C2-C3-O5
2	A	406	LBN	C13-C10-C7-C4
2	B	405	LBN	C13-C10-C7-C4
2	D	407	LBN	C28-C29-C30-C31
2	C	502	LBN	C26-C27-C28-C29
2	D	405	LBN	C13-C10-C7-C4
2	E	405	LBN	C38-C39-C40-C41
2	E	407	LBN	C28-C29-C30-C31
2	C	503	LBN	C39-C40-C41-C42

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Mol	Chain	Res	Type	Atoms
2	E	405	LBN	C39-C40-C41-C42
2	F	502	LBN	C39-C40-C41-C42
2	B	405	LBN	C26-C27-C28-C29
2	C	502	LBN	C13-C10-C7-C4
2	A	406	LBN	C26-C27-C28-C29
2	G	502	LBN	C13-C10-C7-C4
2	A	403	LBN	C37-C38-C39-C40
2	F	502	LBN	C13-C10-C7-C4
2	D	405	LBN	C26-C27-C28-C29
2	C	504	LBN	C35-C36-C37-C38
2	G	503	LBN	C35-C36-C37-C38
2	G	506	LBN	C37-C38-C39-C40
2	F	504	LBN	C28-C29-C30-C31
2	A	406	LBN	O1-C1-C2-C3
2	B	405	LBN	O1-C1-C2-C3
2	D	405	LBN	O1-C1-C2-C3
2	C	502	LBN	O1-C1-C2-C3
2	E	405	LBN	O1-C1-C2-C3
2	G	502	LBN	O1-C1-C2-C3
2	F	502	LBN	O1-C1-C2-C3
2	A	407	LBN	C37-C38-C39-C40
2	E	405	LBN	C26-C27-C28-C29
2	F	502	LBN	C38-C39-C40-C41
2	B	402	LBN	C37-C38-C39-C40
2	D	405	LBN	C38-C39-C40-C41
2	F	507	LBN	C37-C38-C39-C40
2	C	504	LBN	C28-C29-C30-C31
2	E	402	LBN	C37-C38-C39-C40
2	E	405	LBN	C13-C10-C7-C4
2	E	407	LBN	C8-C11-C14-C17
2	A	408	LBN	C28-C29-C30-C31
2	C	507	LBN	C37-C38-C39-C40
2	E	406	LBN	C39-C40-C41-C42
2	B	407	LBN	C35-C36-C37-C38
2	C	502	LBN	C38-C39-C40-C41
2	D	406	LBN	C36-C37-C38-C39
2	G	502	LBN	C38-C39-C40-C41
2	F	503	LBN	C37-C38-C39-C40
2	B	407	LBN	C1-C2-C3-O5
2	D	407	LBN	C1-C2-C3-O5
2	E	405	LBN	C33-C4-C7-C10
2	G	503	LBN	C1-C2-C3-O5

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Mol	Chain	Res	Type	Atoms
2	F	504	LBN	C1-C2-C3-O5
2	D	402	LBN	C37-C38-C39-C40
2	D	407	LBN	C8-C11-C14-C17
2	A	406	LBN	C38-C39-C40-C41
2	D	407	LBN	C35-C36-C37-C38
2	E	407	LBN	C36-C37-C38-C39
2	F	504	LBN	C8-C11-C14-C17
2	B	405	LBN	C38-C39-C40-C41
2	D	406	LBN	C37-C38-C39-C40
2	A	406	LBN	C33-C4-C7-C10
2	G	502	LBN	C33-C4-C7-C10
2	F	504	LBN	C35-C36-C37-C38
2	G	503	LBN	C8-C11-C14-C17
2	B	405	LBN	C33-C4-C7-C10
2	A	407	LBN	C10-C13-C16-C19
2	E	406	LBN	C13-C10-C7-C4
2	B	406	LBN	C10-C13-C16-C19
2	D	406	LBN	C13-C10-C7-C4
2	D	407	LBN	C36-C37-C38-C39
2	E	407	LBN	C35-C36-C37-C38
2	D	405	LBN	C7-C10-C13-C16
2	C	503	LBN	C13-C10-C7-C4
2	F	502	LBN	C33-C4-C7-C10
2	B	407	LBN	C8-C11-C14-C17
2	D	401	LBN	C28-C29-C30-C31
2	A	402	LBN	C13-C16-C19-C21
2	D	407	LBN	C26-C27-C28-C29
2	F	504	LBN	C36-C37-C38-C39
2	F	502	LBN	C7-C10-C13-C16
2	F	504	LBN	C26-C27-C28-C29
2	B	407	LBN	C26-C27-C28-C29
2	F	506	LBN	C13-C16-C19-C21
2	A	402	LBN	O1-C1-C2-C3
2	D	401	LBN	O1-C1-C2-C3
2	E	401	LBN	O1-C1-C2-C3
2	G	505	LBN	O1-C1-C2-C3
2	A	408	LBN	C26-C27-C28-C29
2	A	401	LBN	C13-C10-C7-C4
2	C	504	LBN	C8-C11-C14-C17
2	C	502	LBN	C33-C4-C7-C10
2	C	504	LBN	C26-C27-C28-C29
2	D	405	LBN	C33-C4-C7-C10

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Mol	Chain	Res	Type	Atoms
2	D	406	LBN	C10-C13-C16-C19
2	A	403	LBN	C14-C11-C8-C5
2	B	402	LBN	C14-C11-C8-C5
2	D	402	LBN	C14-C11-C8-C5
2	C	507	LBN	C14-C11-C8-C5
2	E	406	LBN	C10-C13-C16-C19
2	G	506	LBN	C14-C11-C8-C5
2	G	503	LBN	C26-C27-C28-C29
2	F	503	LBN	C13-C10-C7-C4
2	F	503	LBN	C10-C13-C16-C19
2	A	401	LBN	C10-C13-C16-C19
2	E	407	LBN	C26-C27-C28-C29
2	C	502	LBN	C7-C10-C13-C16
2	F	506	LBN	C29-C30-C31-C32
2	G	502	LBN	C7-C10-C13-C16
2	C	504	LBN	C1-C2-C3-O5
2	E	407	LBN	C1-C2-C3-O5
2	B	401	LBN	C32-C33-C4-C7
2	B	401	LBN	C7-C10-C13-C16
2	G	505	LBN	C13-C16-C19-C21
2	C	503	LBN	C10-C13-C16-C19
2	C	503	LBN	C25-C26-C27-C28
2	G	503	LBN	C36-C37-C38-C39
2	F	506	LBN	C32-C33-C4-C7
2	F	503	LBN	C25-C26-C27-C28
2	D	401	LBN	C13-C16-C19-C21
2	C	508	LBN	C35-C36-C37-C38
2	E	401	LBN	C13-C16-C19-C21
2	D	401	LBN	C32-C33-C4-C7
2	E	403	LBN	C35-C36-C37-C38
2	F	502	LBN	C27-C28-C29-C30
2	C	506	LBN	O7-C2-C3-O5
2	B	401	LBN	C26-C27-C28-C29
2	D	403	LBN	C35-C36-C37-C38
2	A	408	LBN	C35-C36-C37-C38
2	B	406	LBN	C13-C10-C7-C4
2	G	502	LBN	C27-C28-C29-C30
2	F	508	LBN	C35-C36-C37-C38
2	A	404	LBN	C35-C36-C37-C38
2	C	502	LBN	C27-C28-C29-C30
2	D	406	LBN	C42-C5-C8-C11
2	C	503	LBN	C42-C5-C8-C11

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Mol	Chain	Res	Type	Atoms
2	A	407	LBN	C13-C10-C7-C4
2	B	403	LBN	C35-C36-C37-C38
2	D	406	LBN	C30-C31-C32-C33
2	A	402	LBN	C28-C29-C30-C31
2	C	506	LBN	C32-C33-C4-C7
2	B	406	LBN	C30-C31-C32-C33
2	A	407	LBN	C1-O1-P1-O3
2	C	506	LBN	C13-C16-C19-C21
2	A	407	LBN	C30-C31-C32-C33
2	E	406	LBN	C30-C31-C32-C33
2	E	405	LBN	C7-C10-C13-C16
2	G	507	LBN	C35-C36-C37-C38
2	A	401	LBN	C39-C40-C41-C42
2	A	408	LBN	C1-C2-C3-O5
2	G	505	LBN	C2-C1-O1-P1
2	C	506	LBN	C27-C28-C29-C30
2	B	405	LBN	C7-C10-C13-C16
2	E	401	LBN	C32-C33-C4-C7
2	B	405	LBN	C27-C28-C29-C30
2	B	407	LBN	C36-C37-C38-C39
2	A	401	LBN	C30-C31-C32-C33
2	A	406	LBN	C27-C28-C29-C30
2	C	504	LBN	C36-C37-C38-C39
2	C	503	LBN	C28-C29-C30-C31
2	C	503	LBN	C30-C31-C32-C33
2	G	505	LBN	C32-C33-C4-C7
2	A	402	LBN	C2-C1-O1-P1
2	D	401	LBN	C2-C1-O1-P1
2	E	401	LBN	C2-C1-O1-P1
2	F	506	LBN	C2-C1-O1-P1
2	A	402	LBN	C1-O1-P1-O4
2	A	406	LBN	C1-O1-P1-O3
2	B	405	LBN	C1-O1-P1-O3
2	D	401	LBN	C1-O1-P1-O4
2	D	405	LBN	C1-O1-P1-O3
2	C	502	LBN	C1-O1-P1-O3
2	E	401	LBN	C1-O1-P1-O4
2	E	405	LBN	C1-O1-P1-O3
2	G	502	LBN	C1-O1-P1-O3
2	G	505	LBN	C1-O1-P1-O4
2	F	502	LBN	C1-O1-P1-O3
2	F	506	LBN	C1-O1-P1-O3

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Mol	Chain	Res	Type	Atoms
2	F	506	LBN	C1-O1-P1-O4
2	A	401	LBN	C25-C26-C27-C28
2	F	506	LBN	O1-C1-C2-C3
2	A	402	LBN	C32-C33-C4-C7
2	A	407	LBN	C26-C27-C28-C29
2	D	405	LBN	C27-C28-C29-C30
2	F	503	LBN	C30-C31-C32-C33
2	A	401	LBN	C28-C29-C30-C31
2	A	402	LBN	O1-C1-C2-O7
2	D	401	LBN	O1-C1-C2-O7
2	D	406	LBN	C25-C26-C27-C28
2	E	401	LBN	O1-C1-C2-O7
2	B	406	LBN	C26-C27-C28-C29
2	B	406	LBN	C25-C26-C27-C28
2	D	408	LBN	C37-C38-C39-C40
2	B	401	LBN	C27-C28-C29-C30
2	E	406	LBN	C25-C26-C27-C28
2	A	402	LBN	N1-C6-C9-O2
2	B	401	LBN	C1-C2-C3-O5
2	D	401	LBN	N1-C6-C9-O2
2	C	506	LBN	C1-C2-C3-O5
2	E	401	LBN	N1-C6-C9-O2
2	G	505	LBN	N1-C6-C9-O2
2	F	506	LBN	N1-C6-C9-O2
2	E	406	LBN	C33-C4-C7-C10
2	E	405	LBN	C27-C28-C29-C30
2	C	505	LBN	C37-C38-C39-C40
2	A	406	LBN	C7-C10-C13-C16
2	B	406	LBN	C33-C4-C7-C10
2	G	504	LBN	C37-C38-C39-C40
2	A	409	LBN	C37-C38-C39-C40
2	F	505	LBN	C37-C38-C39-C40
2	A	407	LBN	C25-C26-C27-C28
2	C	503	LBN	C33-C4-C7-C10
2	F	503	LBN	C33-C4-C7-C10
2	G	505	LBN	C28-C29-C30-C31
2	A	407	LBN	C33-C4-C7-C10
2	A	401	LBN	C33-C4-C7-C10
2	F	503	LBN	C28-C29-C30-C31
2	D	405	LBN	C36-C37-C38-C39
2	B	408	LBN	C37-C38-C39-C40
2	G	505	LBN	O1-C1-C2-O7

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Mol	Chain	Res	Type	Atoms
2	E	408	LBN	C37-C38-C39-C40
2	F	508	LBN	C42-C5-C8-C11
2	B	401	LBN	O7-C2-C3-O5
2	A	402	LBN	C9-O2-P1-O1
2	A	406	LBN	C9-O2-P1-O1
2	B	405	LBN	C9-O2-P1-O1
2	D	401	LBN	C9-O2-P1-O1
2	D	405	LBN	C9-O2-P1-O1
2	C	502	LBN	C9-O2-P1-O1
2	E	401	LBN	C9-O2-P1-O1
2	E	405	LBN	C9-O2-P1-O1
2	G	502	LBN	C9-O2-P1-O1
2	G	505	LBN	C9-O2-P1-O1
2	F	502	LBN	C9-O2-P1-O1
2	F	506	LBN	C9-O2-P1-O1
2	A	401	LBN	C42-C5-C8-C11
2	A	407	LBN	C42-C5-C8-C11
2	B	406	LBN	C42-C5-C8-C11
2	E	406	LBN	C42-C5-C8-C11
2	F	503	LBN	C42-C5-C8-C11
2	D	406	LBN	C33-C4-C7-C10
2	E	401	LBN	C28-C29-C30-C31
2	E	408	LBN	C36-C37-C38-C39
2	E	406	LBN	C28-C29-C30-C31
2	B	403	LBN	C42-C5-C8-C11
2	A	401	LBN	C26-C27-C28-C29
2	F	505	LBN	C36-C37-C38-C39
2	B	401	LBN	C29-C30-C31-C32
2	A	409	LBN	C38-C39-C40-C41
2	C	505	LBN	C36-C37-C38-C39
2	B	406	LBN	C39-C40-C41-C42
2	E	403	LBN	C42-C5-C8-C11
2	G	507	LBN	C42-C5-C8-C11
2	A	409	LBN	C36-C37-C38-C39
2	D	406	LBN	C26-C27-C28-C29
2	A	404	LBN	C14-C11-C8-C5
2	B	403	LBN	C14-C11-C8-C5
2	B	407	LBN	C20-C22-C23-C24
2	D	403	LBN	C14-C11-C8-C5
2	C	508	LBN	C14-C11-C8-C5
2	E	402	LBN	C14-C11-C8-C5
2	E	403	LBN	C14-C11-C8-C5

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Mol	Chain	Res	Type	Atoms
2	G	507	LBN	C14-C11-C8-C5
2	F	507	LBN	C14-C11-C8-C5
2	F	508	LBN	C14-C11-C8-C5
2	C	506	LBN	C29-C30-C31-C32
2	E	407	LBN	C20-C22-C23-C24
2	E	406	LBN	C26-C27-C28-C29
2	A	404	LBN	C42-C5-C8-C11
2	D	403	LBN	C42-C5-C8-C11
2	C	508	LBN	C42-C5-C8-C11
2	D	406	LBN	C28-C29-C30-C31
2	F	502	LBN	C36-C37-C38-C39
2	G	504	LBN	C36-C37-C38-C39
2	E	408	LBN	C38-C39-C40-C41
2	C	502	LBN	C36-C37-C38-C39
2	G	504	LBN	C38-C39-C40-C41
2	G	502	LBN	C36-C37-C38-C39
2	F	504	LBN	C20-C22-C23-C24
2	D	408	LBN	C38-C39-C40-C41
2	F	503	LBN	O7-C2-C3-O5
2	A	408	LBN	C20-C22-C23-C24
2	D	407	LBN	C20-C22-C23-C24
2	C	504	LBN	C20-C22-C23-C24
2	C	505	LBN	C38-C39-C40-C41
2	G	503	LBN	C20-C22-C23-C24
2	D	408	LBN	C36-C37-C38-C39
2	G	507	LBN	C36-C37-C38-C39
2	B	408	LBN	C36-C37-C38-C39
2	E	405	LBN	C36-C37-C38-C39
2	B	408	LBN	C38-C39-C40-C41
2	F	505	LBN	C38-C39-C40-C41
2	F	503	LBN	C26-C27-C28-C29
2	B	408	LBN	C42-C5-C8-C11
2	G	504	LBN	C42-C5-C8-C11
2	A	409	LBN	C42-C5-C8-C11
2	F	505	LBN	C42-C5-C8-C11
2	A	401	LBN	C1-O1-P1-O3
2	B	405	LBN	C36-C37-C38-C39
2	A	403	LBN	C39-C40-C41-C42
2	D	408	LBN	C42-C5-C8-C11
2	C	505	LBN	C42-C5-C8-C11
2	E	408	LBN	C42-C5-C8-C11
2	C	503	LBN	C26-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
2	A	406	LBN	C36-C37-C38-C39
2	B	401	LBN	C13-C16-C19-C21
2	E	402	LBN	C39-C40-C41-C42
2	F	507	LBN	C39-C40-C41-C42
2	A	401	LBN	C1-O1-P1-O4
2	C	504	LBN	C29-C30-C31-C32
2	A	404	LBN	C36-C37-C38-C39
2	F	508	LBN	C36-C37-C38-C39
2	G	503	LBN	C29-C30-C31-C32
2	B	403	LBN	C36-C37-C38-C39
2	A	407	LBN	C28-C29-C30-C31
2	C	504	LBN	C17-C20-C22-C23
2	F	504	LBN	C17-C20-C22-C23
2	C	508	LBN	C36-C37-C38-C39
2	F	504	LBN	C29-C30-C31-C32
2	B	402	LBN	C39-C40-C41-C42
2	B	403	LBN	C39-C40-C41-C42
2	B	407	LBN	C17-C20-C22-C23
2	C	506	LBN	C26-C27-C28-C29
2	A	402	LBN	C9-O2-P1-O4
2	D	401	LBN	C9-O2-P1-O4
2	E	401	LBN	C9-O2-P1-O4
2	G	505	LBN	C9-O2-P1-O4
2	B	406	LBN	O1-C1-C2-C3
2	F	506	LBN	O5-C25-C26-C27
2	E	403	LBN	C38-C39-C40-C41
2	C	508	LBN	C38-C39-C40-C41
2	D	407	LBN	C17-C20-C22-C23
2	C	508	LBN	C39-C40-C41-C42
2	E	403	LBN	C36-C37-C38-C39

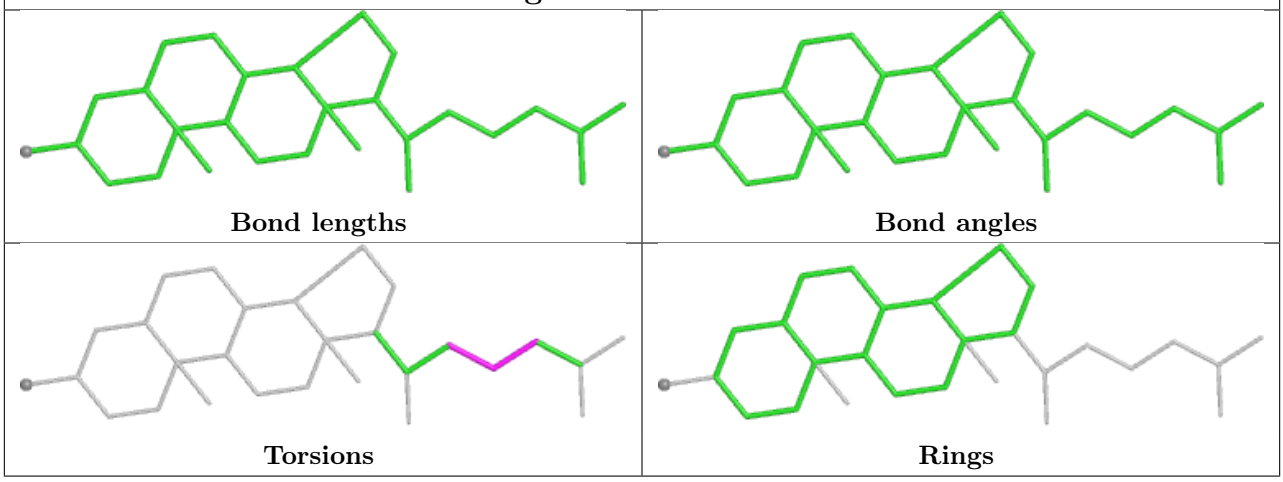
There are no ring outliers.

No monomer is involved in short contacts.

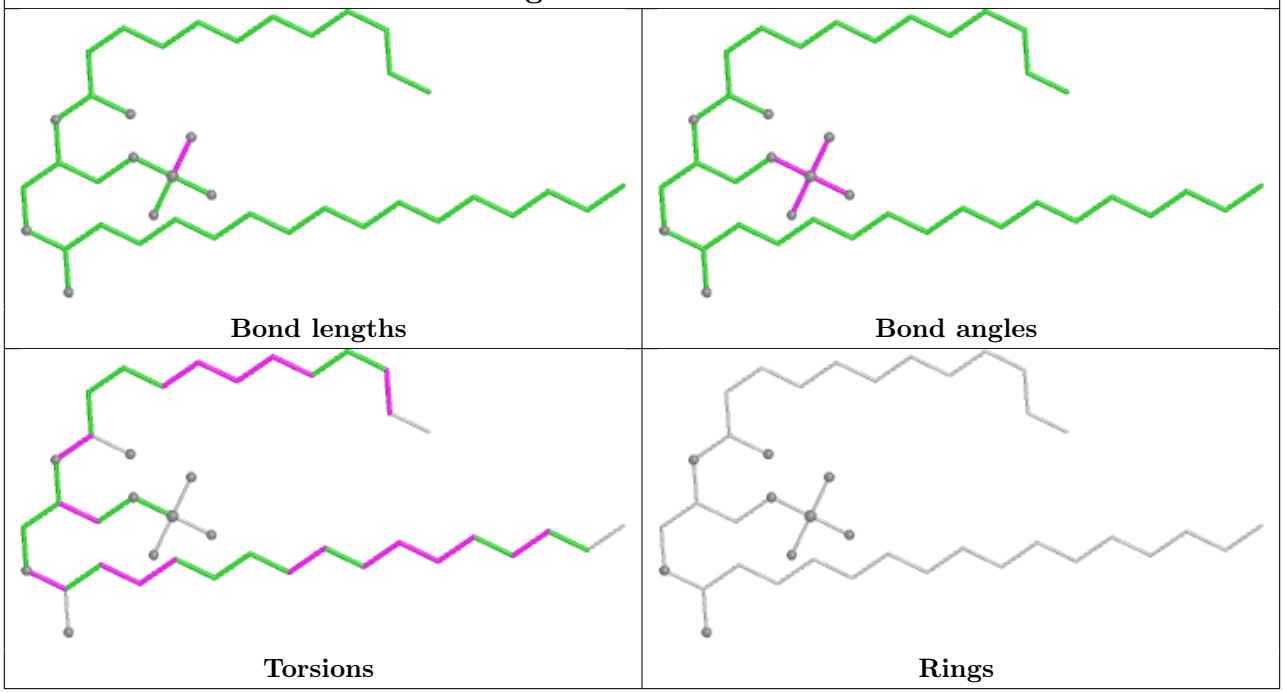
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

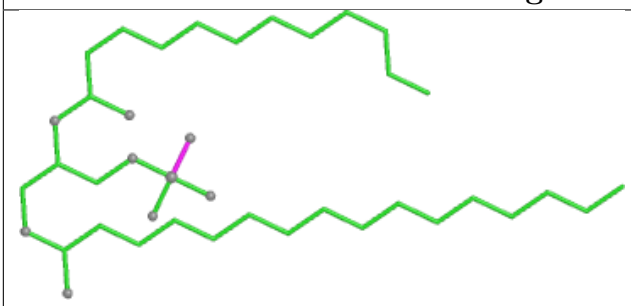
Ligand CLR D 404



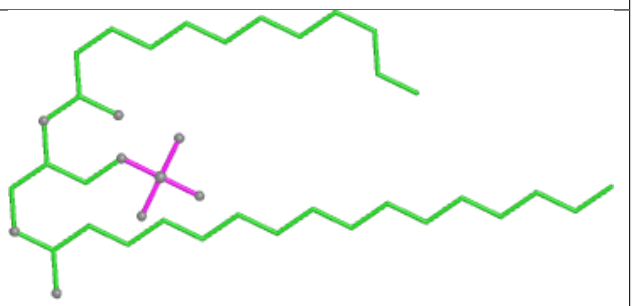
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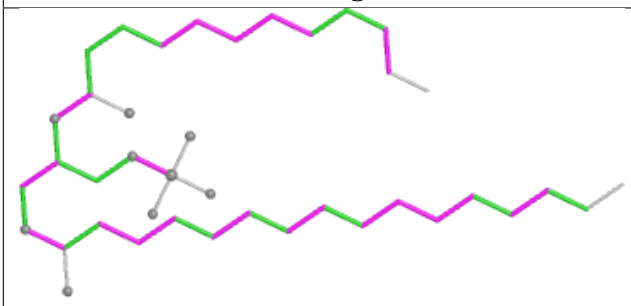
Ligand LBN F 503



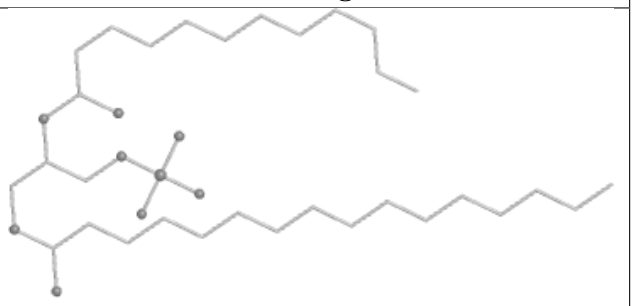
Bond lengths



Bond angles

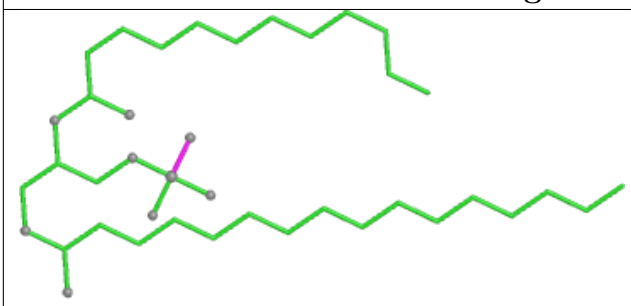


Torsions

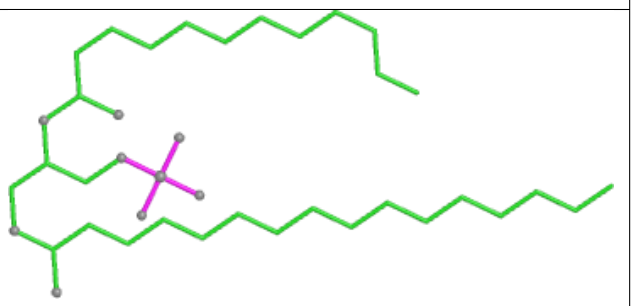


Rings

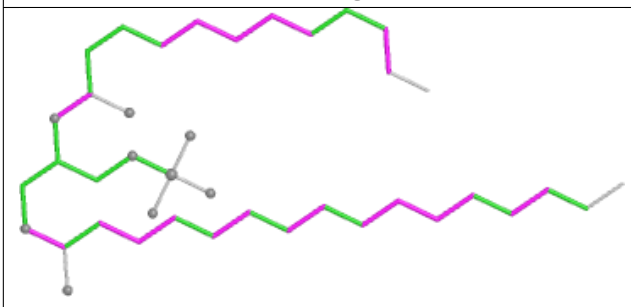
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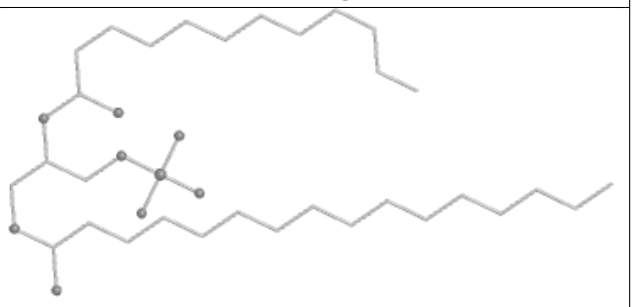
Bond lengths



Bond angles

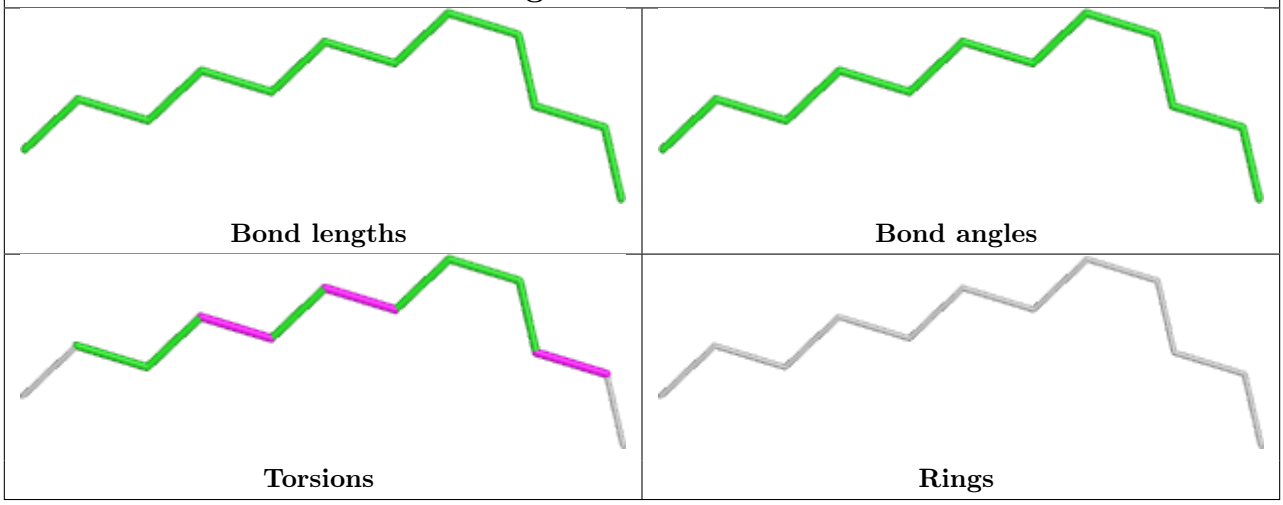


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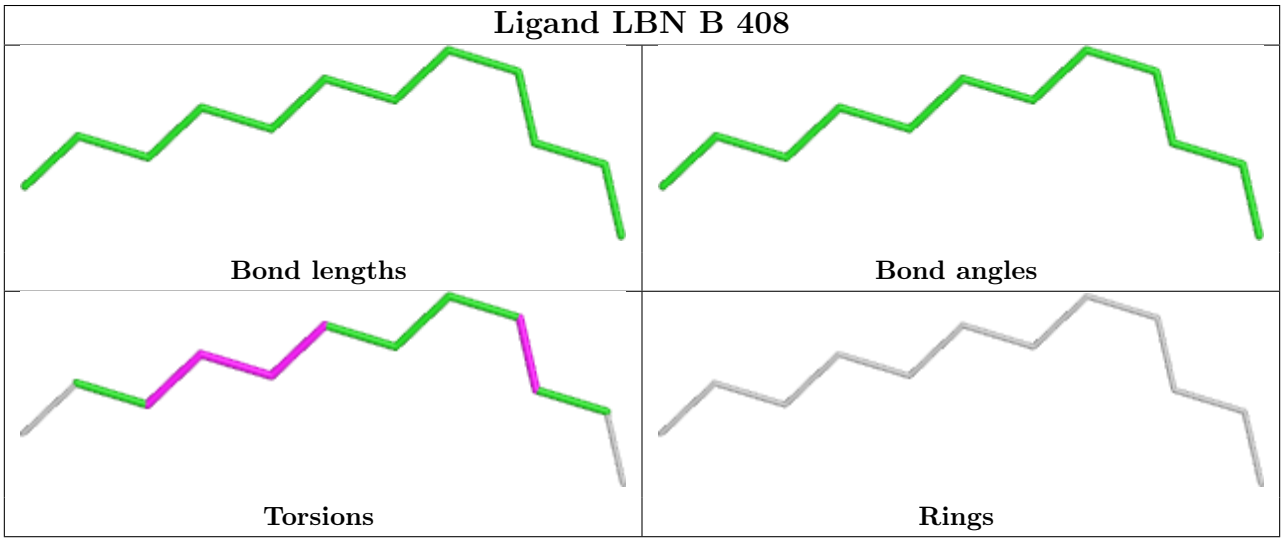


Rings

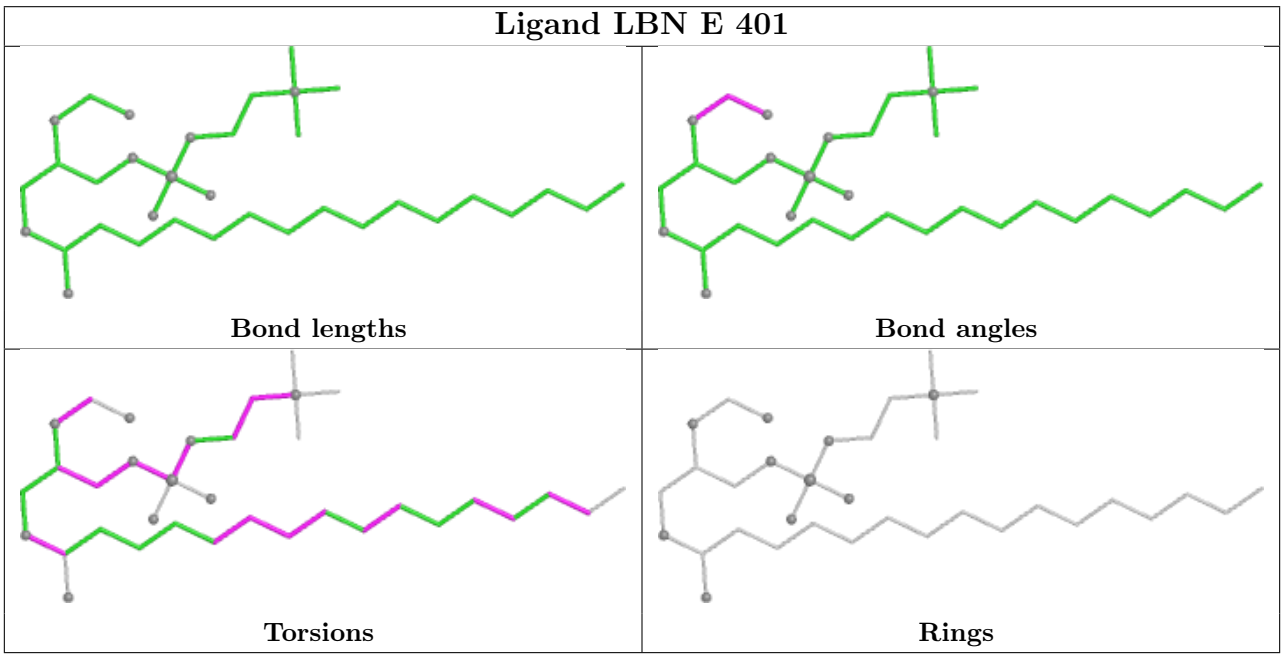
Ligand LBN E 402



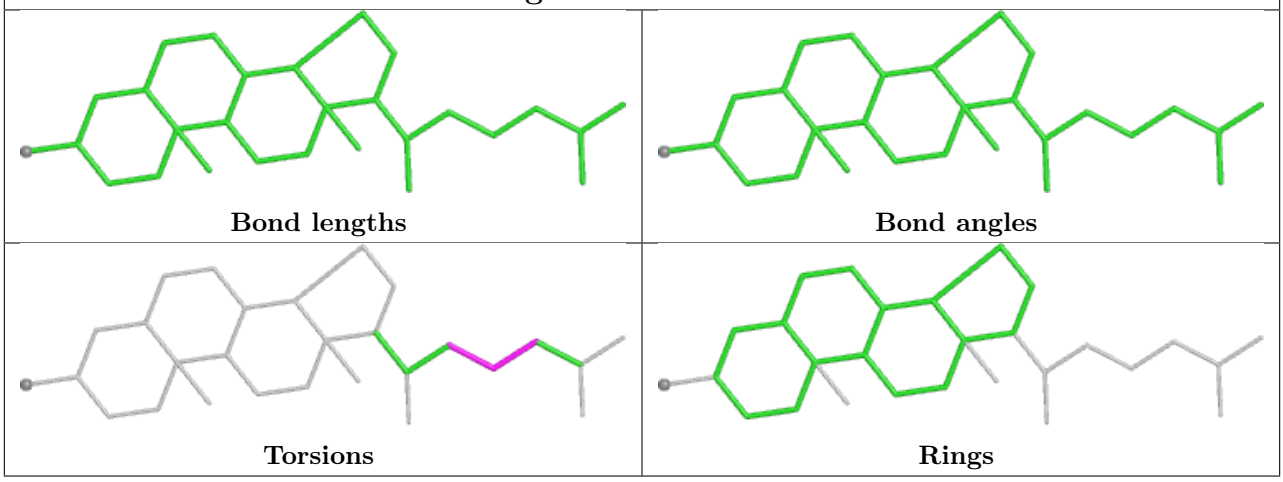
Ligand LBN B 408



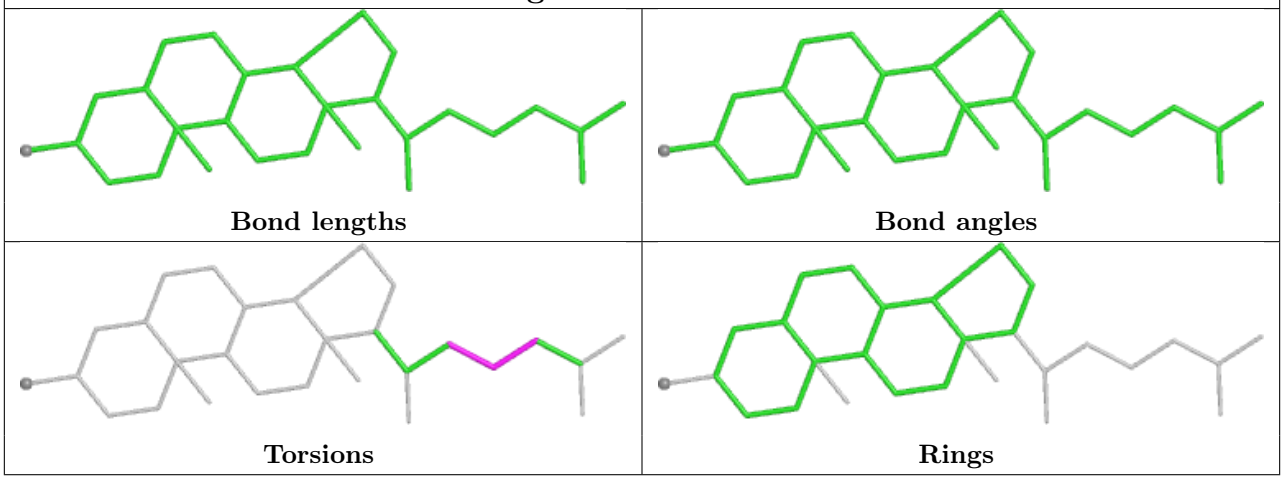
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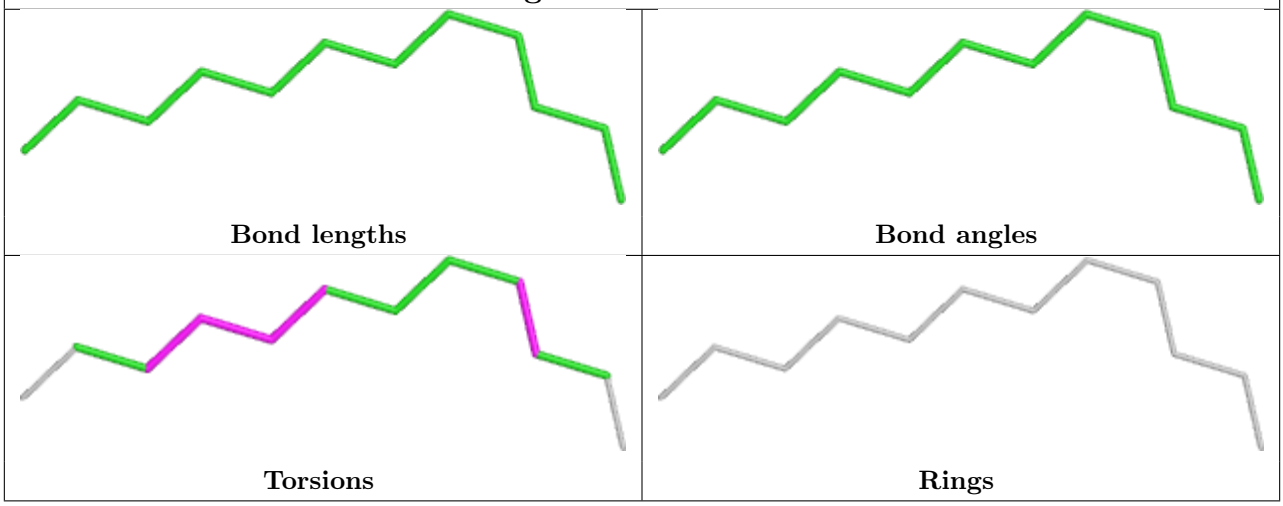
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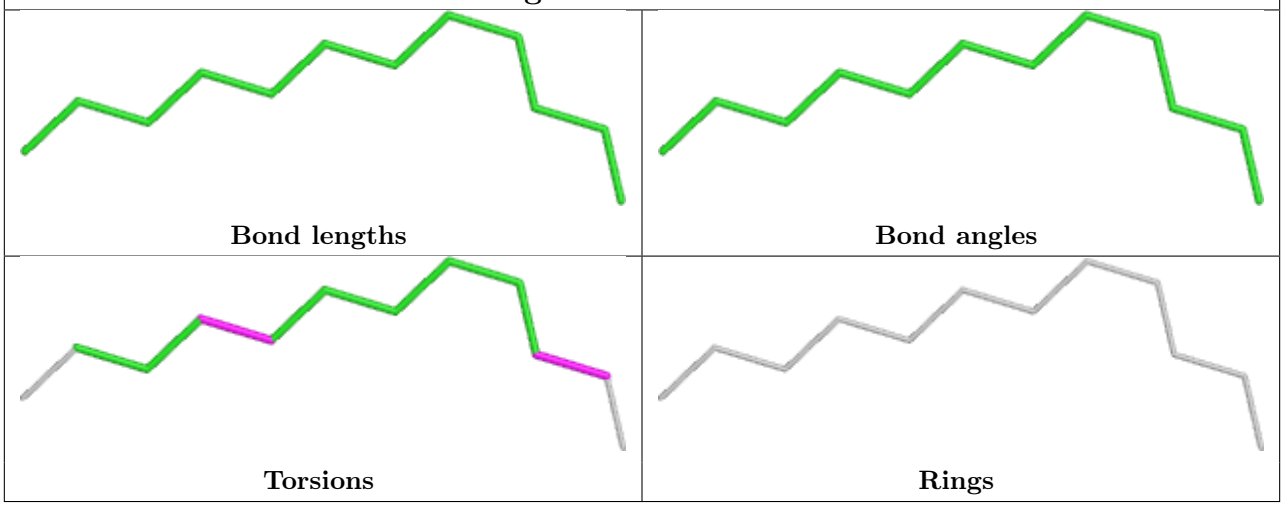
Ligand CLR F 501



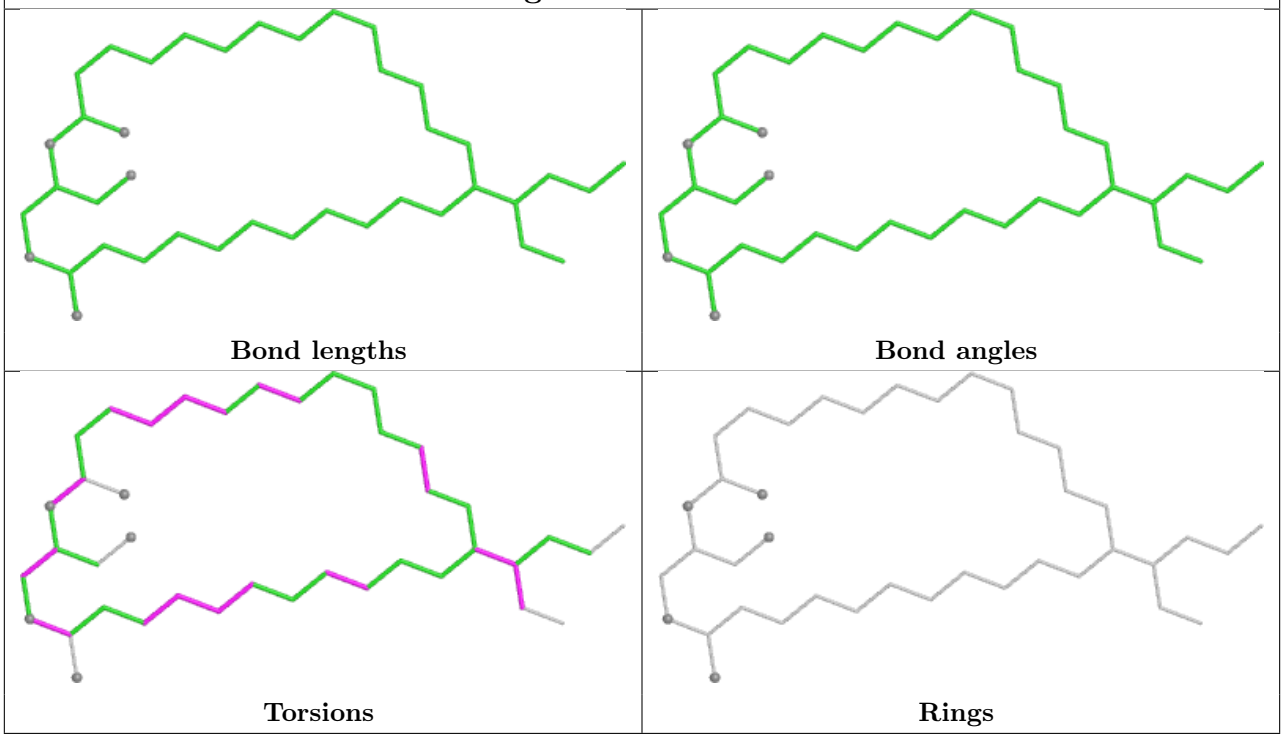
Ligand LBN A 409



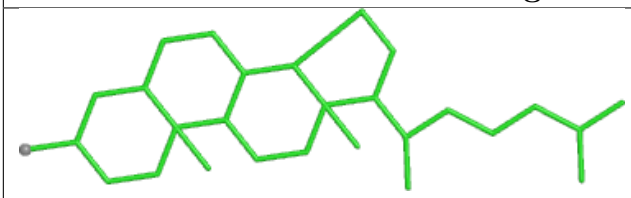
Ligand LBN D 402



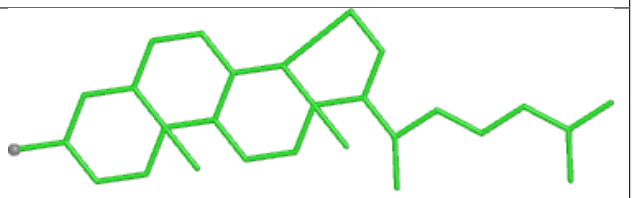
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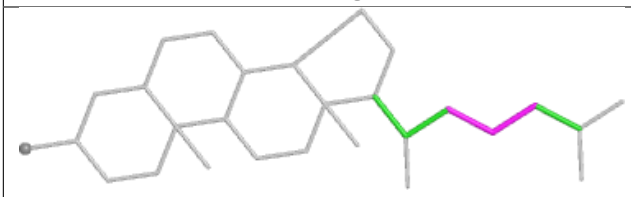
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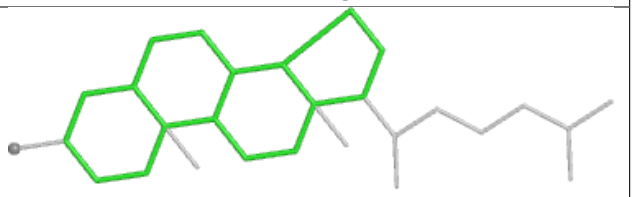
Bond lengths



Bond angles

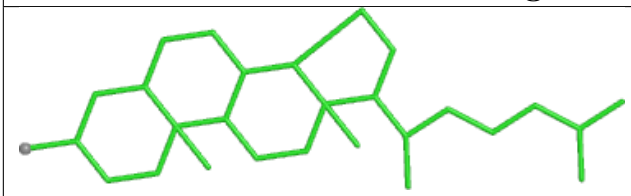


Torsions

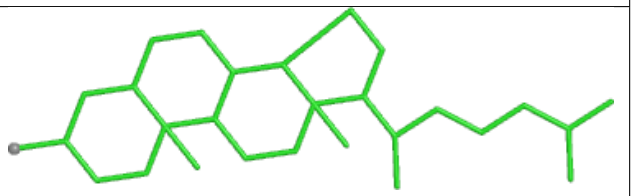


Rings

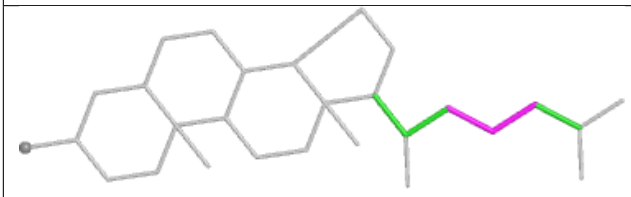
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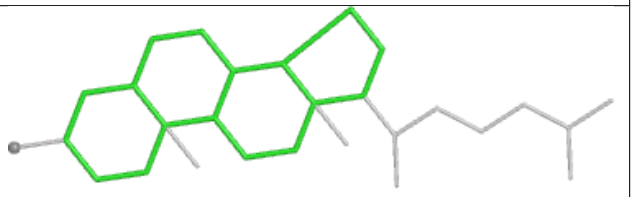
Bond lengths



Bond angles

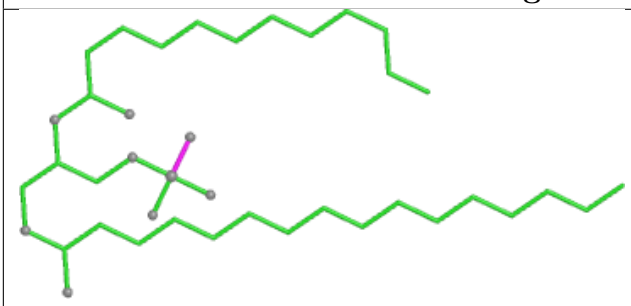


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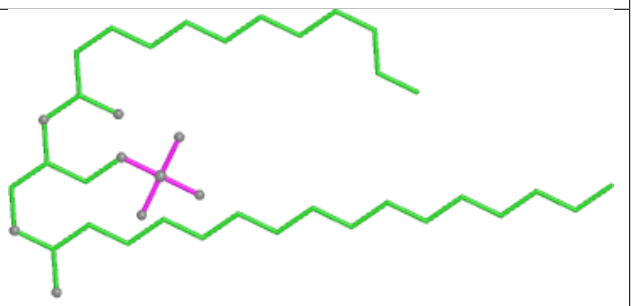


Rings

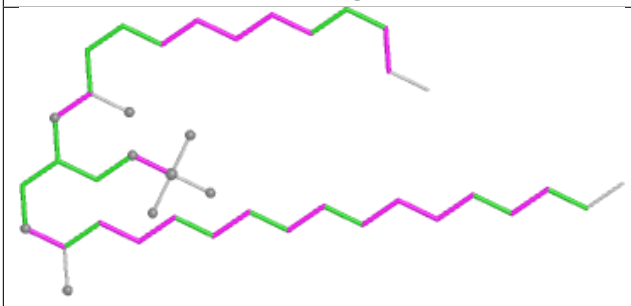
Ligand LBN A 407



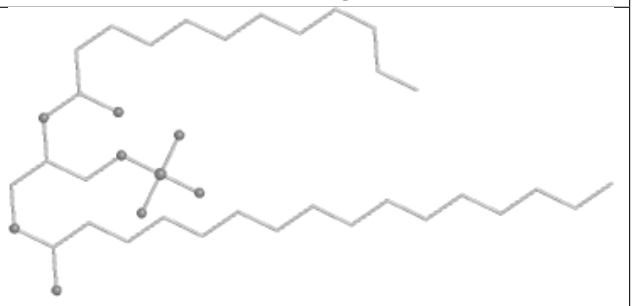
Bond lengths



Bond angles

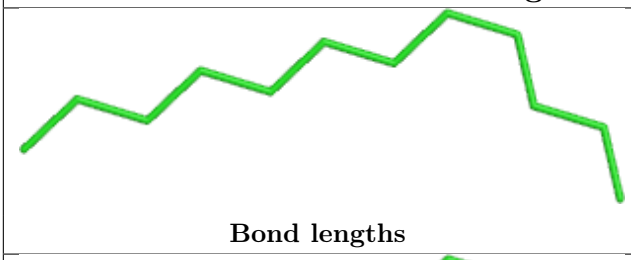


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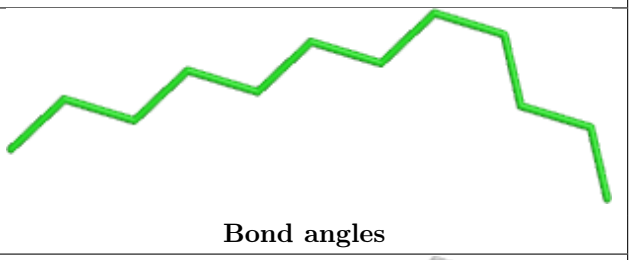


Rings

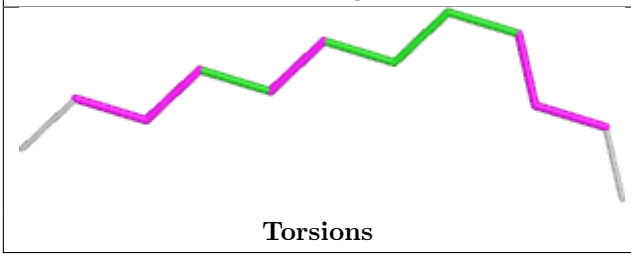
Ligand LBN E 403



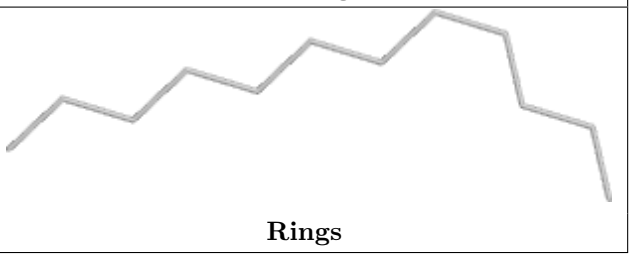
Bond lengths



Bond angles

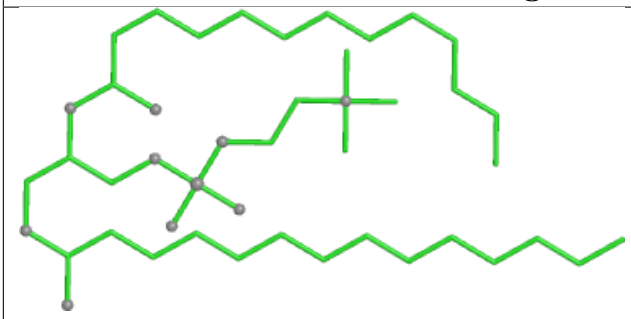


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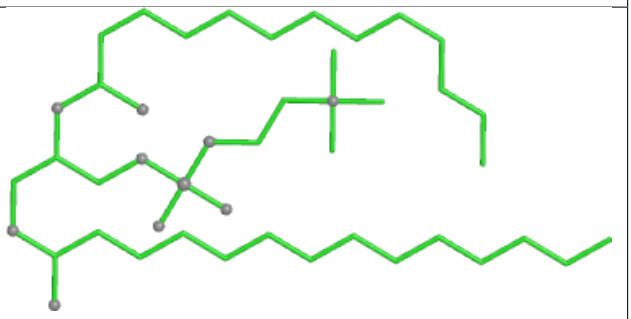


Rings

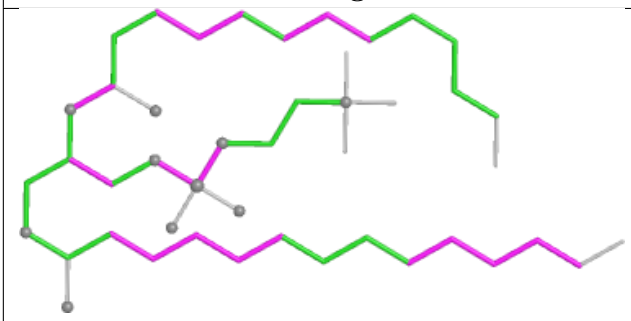
Ligand LBN A 406



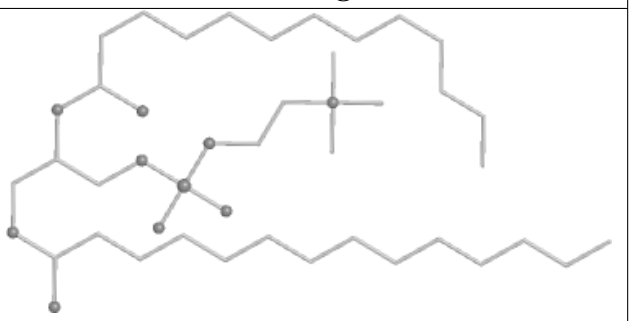
Bond lengths



Bond angles

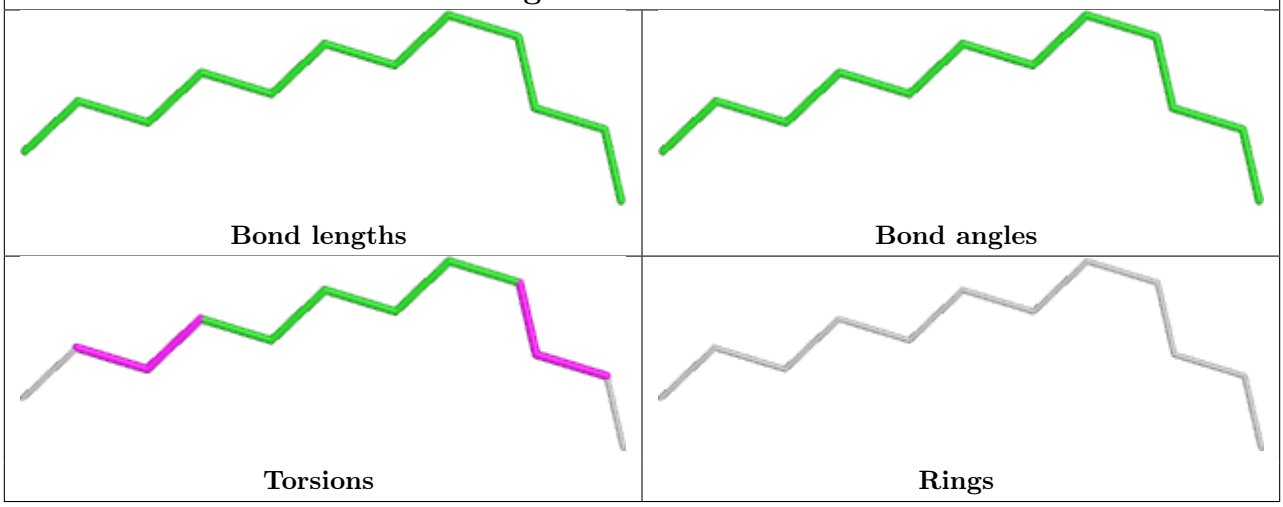


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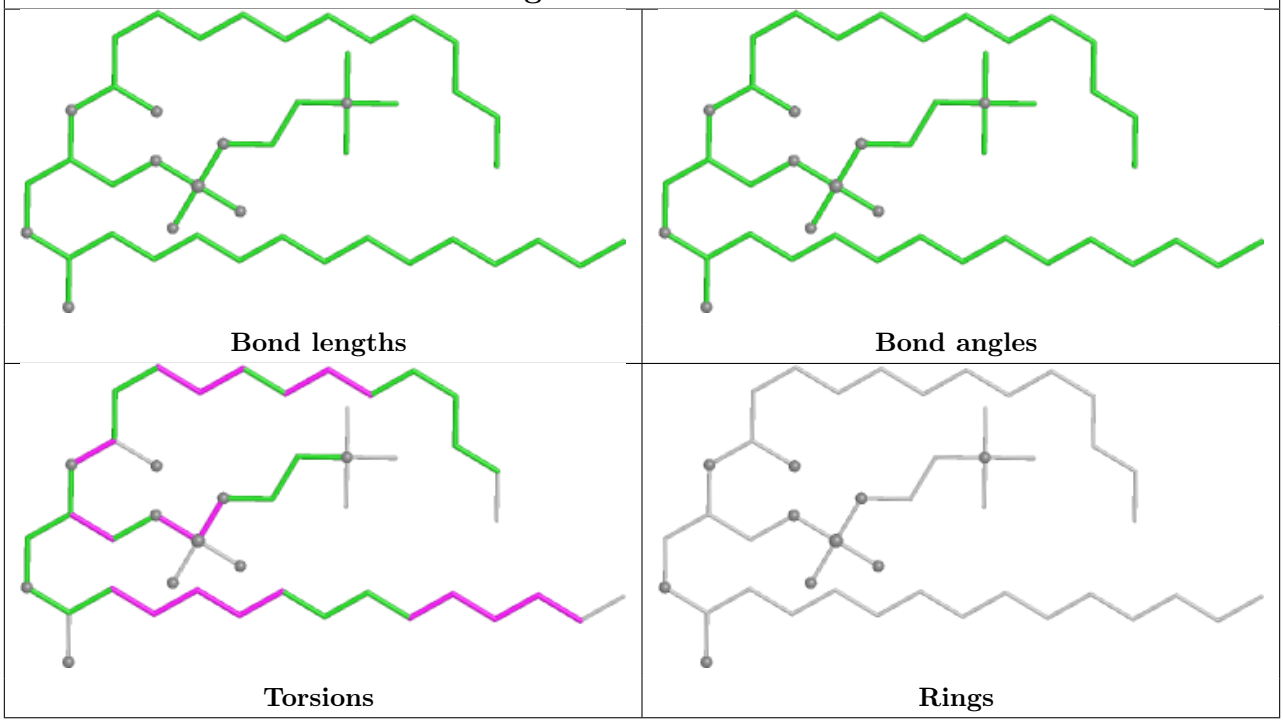


Rings

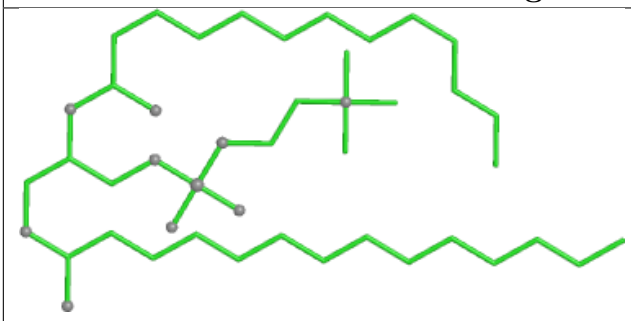
Ligand LBN G 507



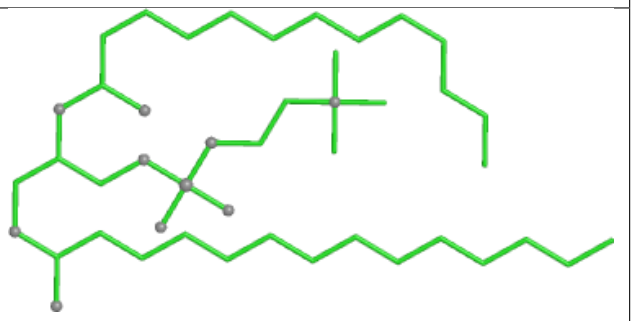
Ligand LBN D 405



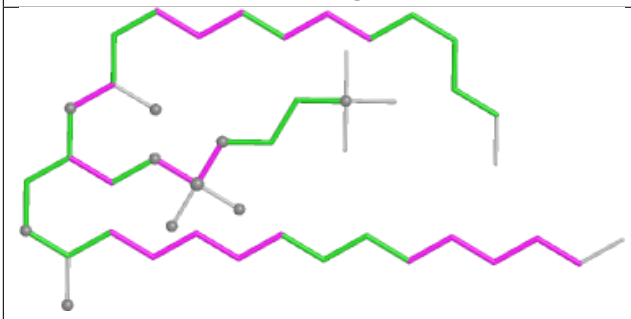
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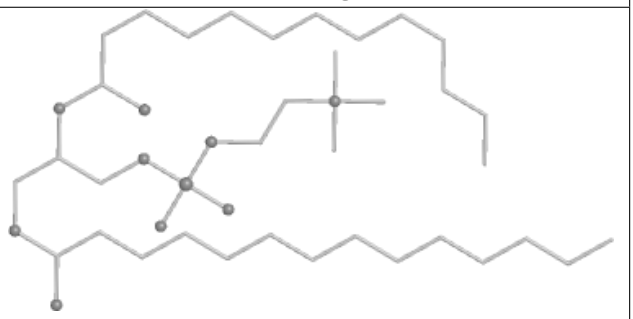
Bond lengths



Bond angles

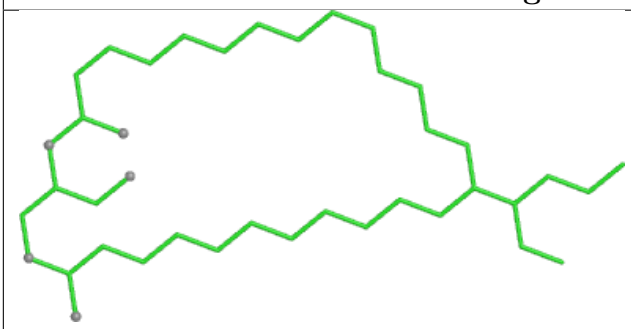


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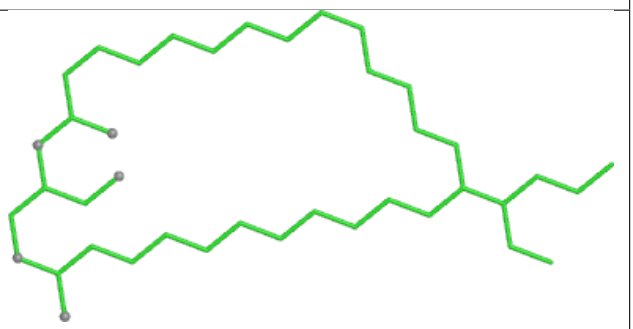


Rings

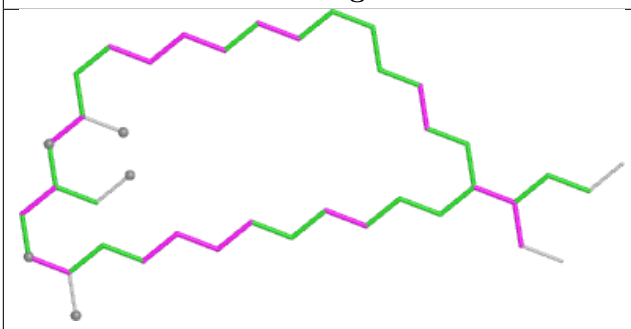
Ligand LBN A 408



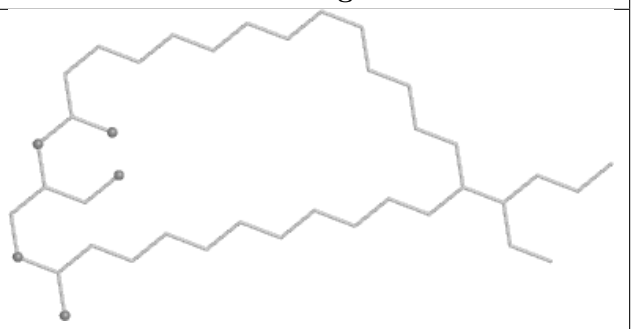
Bond lengths



Bond angles

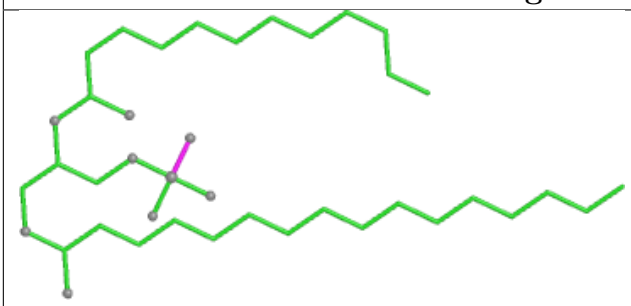


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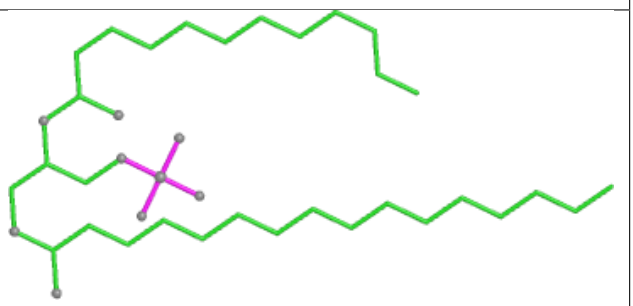


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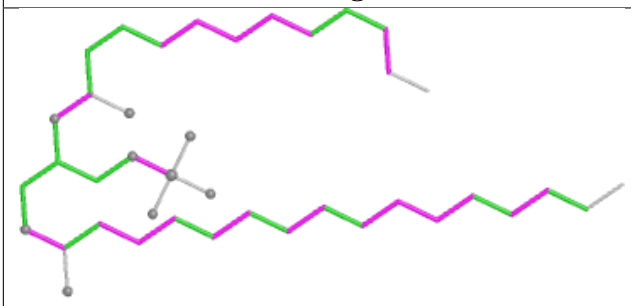
Ligand LBN E 406



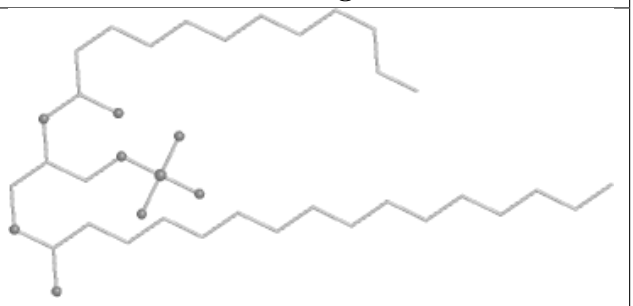
Bond lengths



Bond angles

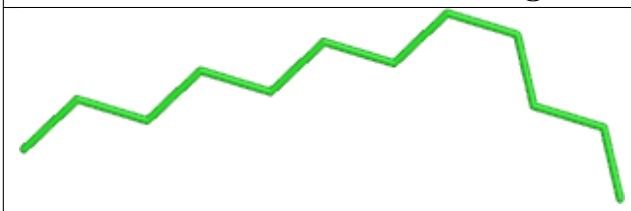


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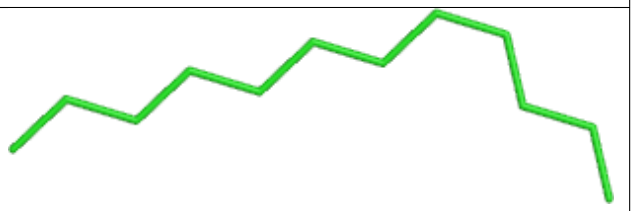


Rings

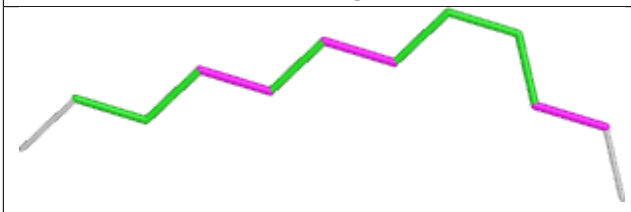
Ligand LBN B 402



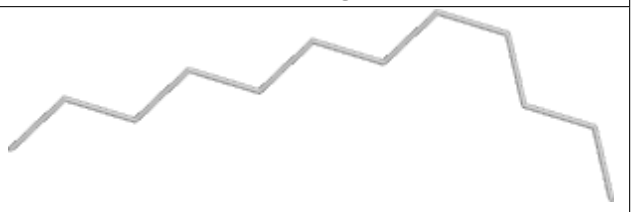
Bond lengths



Bond angles

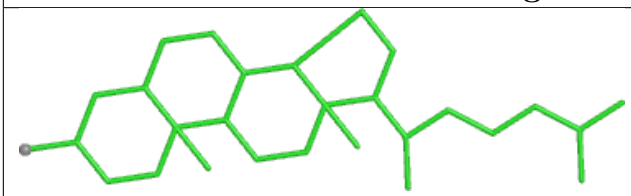


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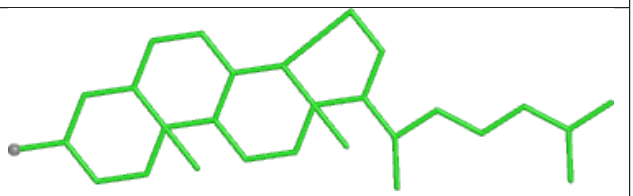


Rings

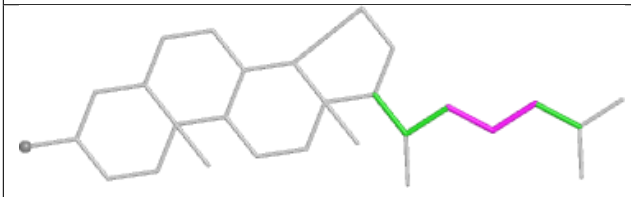
Ligand CLR G 501



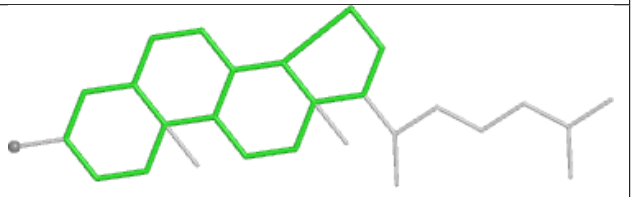
Bond lengths



Bond angles

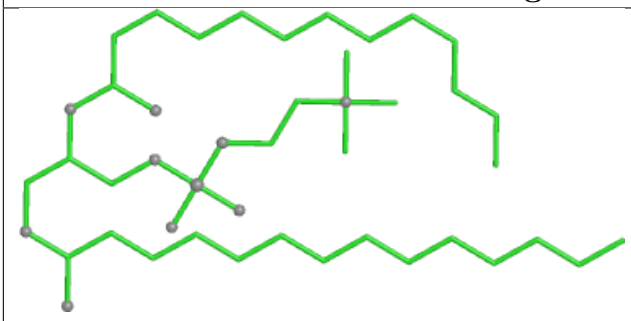


Torsions

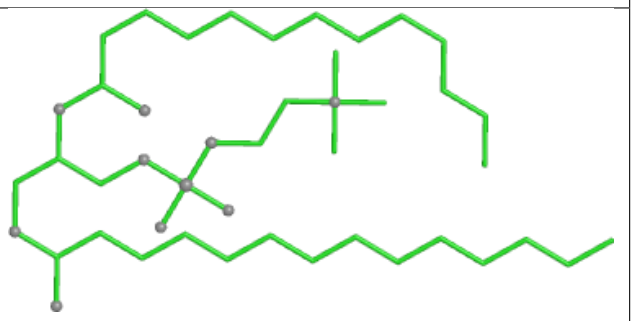


Rings

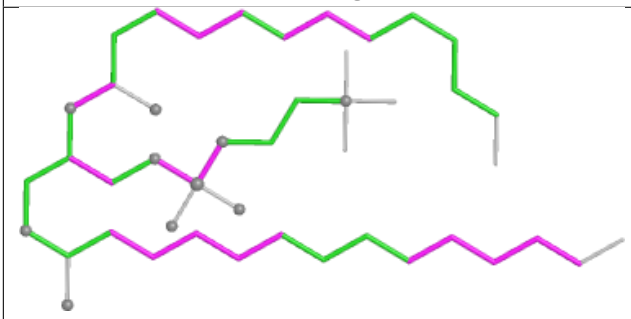
Ligand LBN B 405



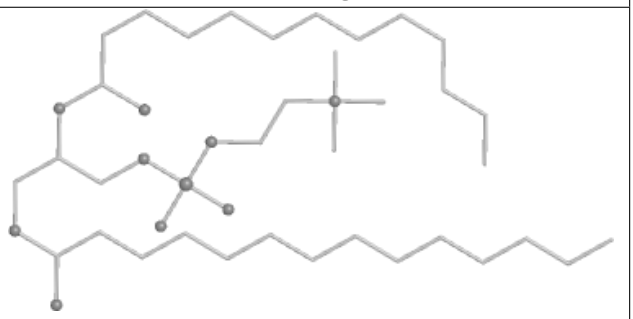
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Bond angles

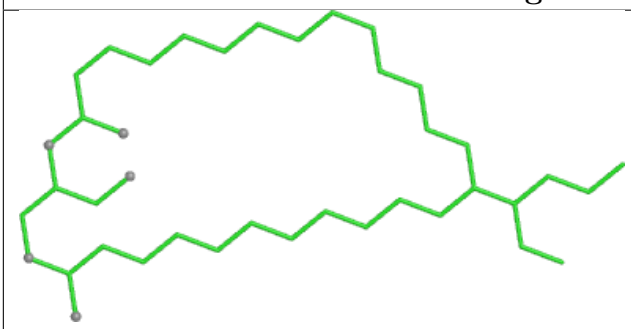


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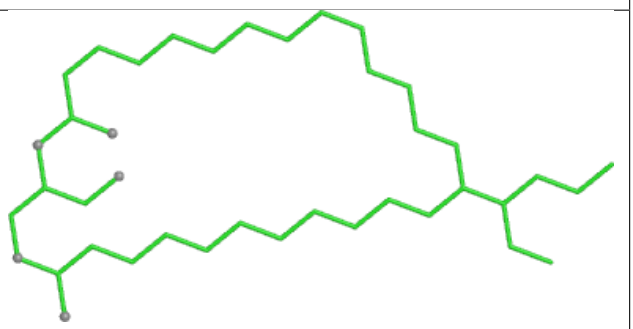


Rings

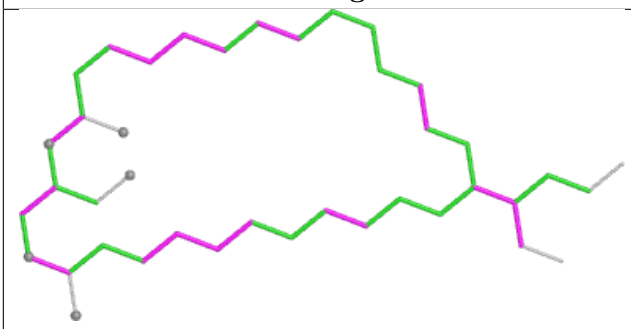
Ligand LBN E 407



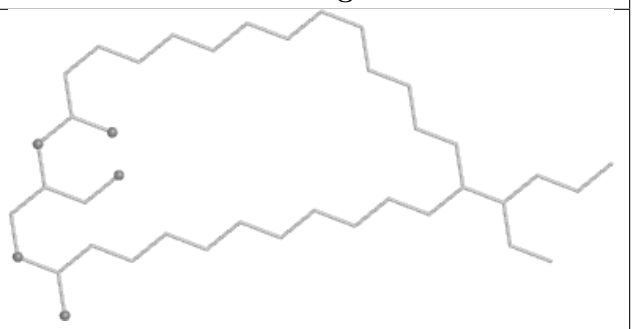
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Bond angles

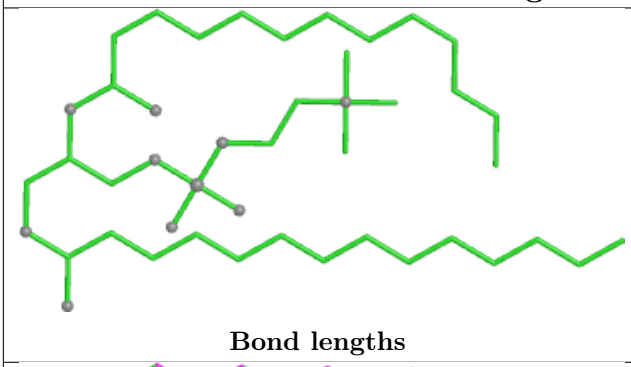


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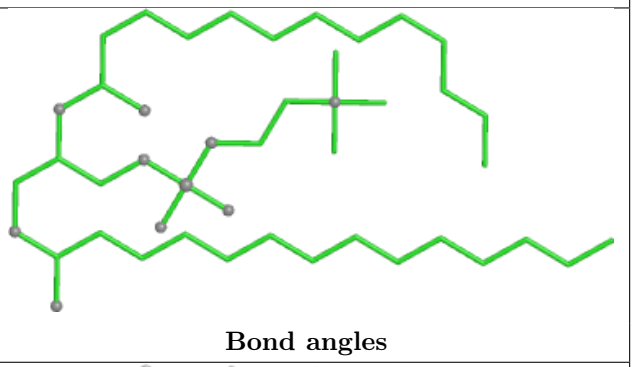


Rings

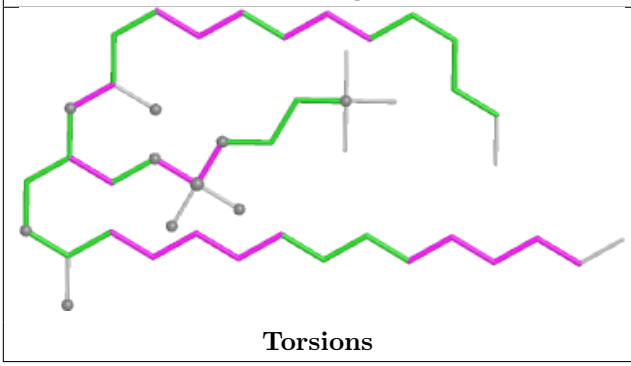
Ligand LBN F 502



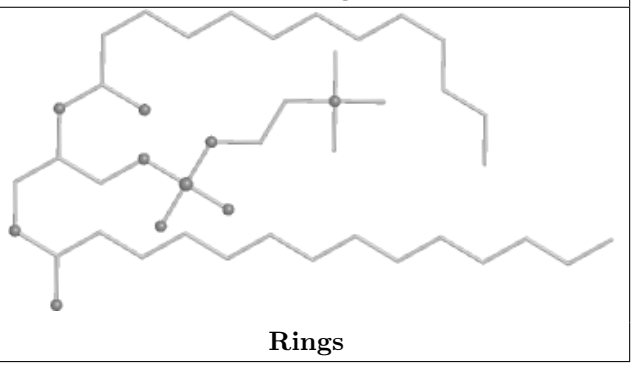
Bond lengths



Bond angles

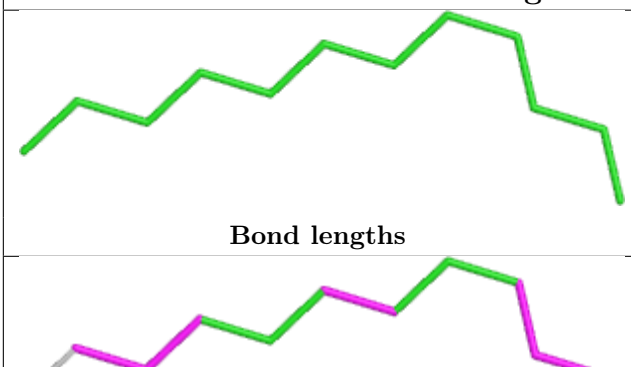


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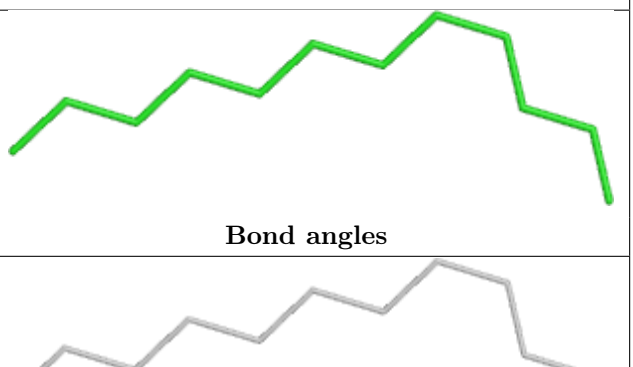


Rings

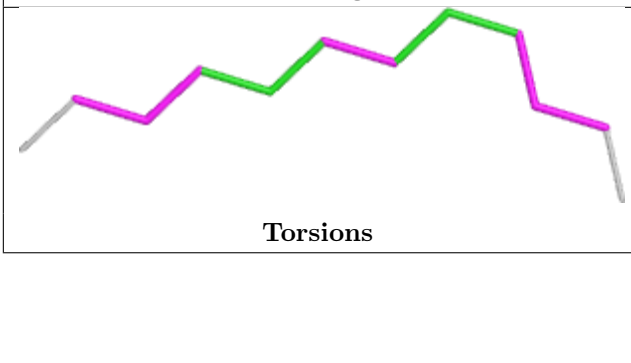
Ligand LBN B 403



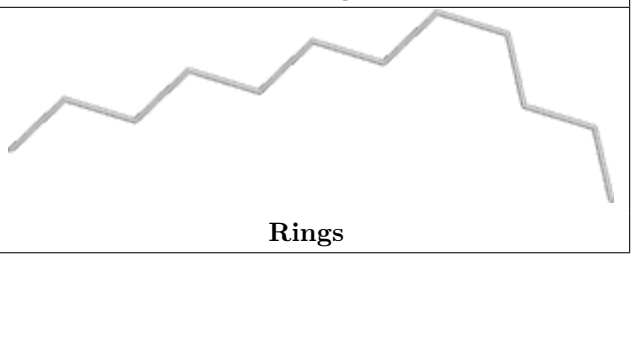
Bond lengths



Bond angles

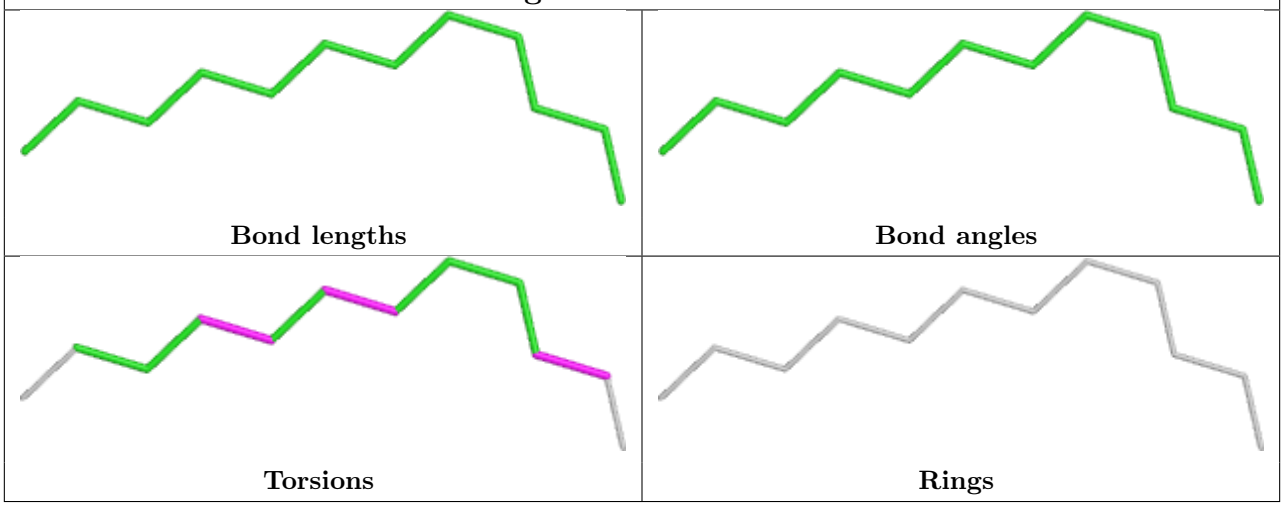


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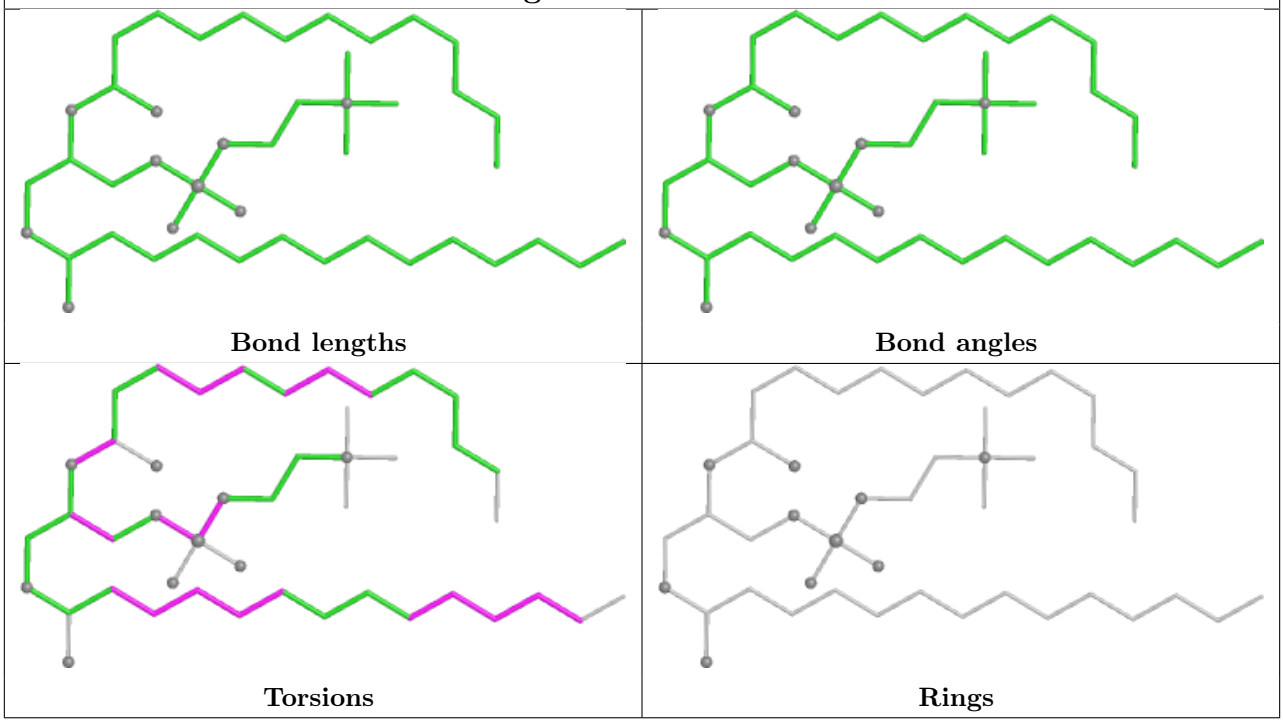


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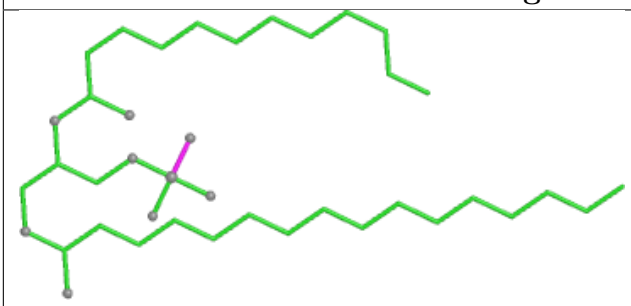
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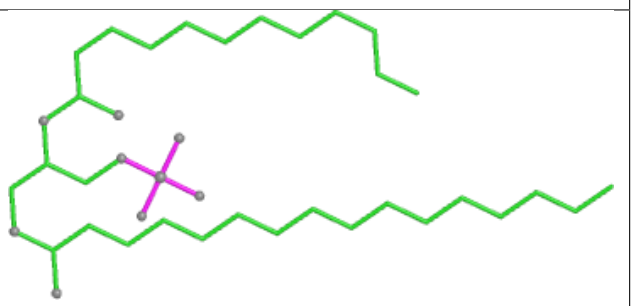
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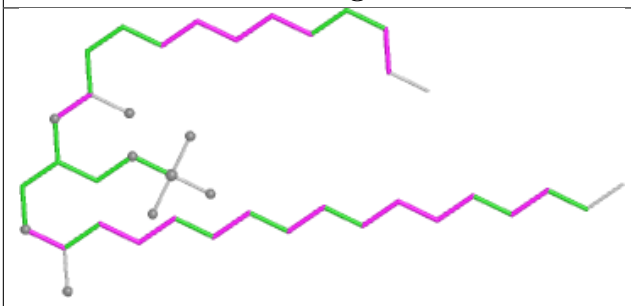
Ligand LBN D 406



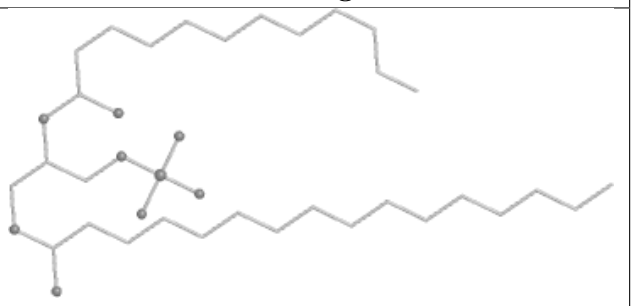
Bond lengths



Bond angles

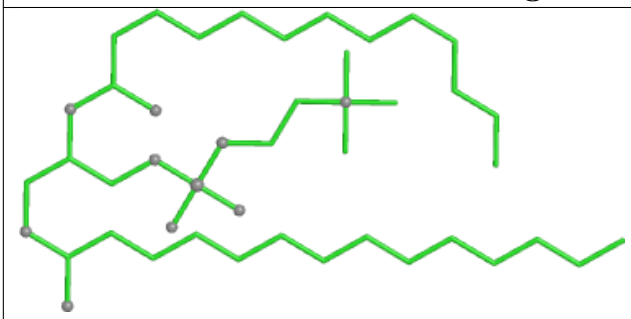


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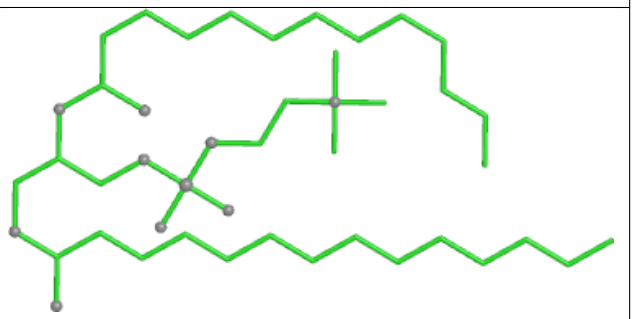


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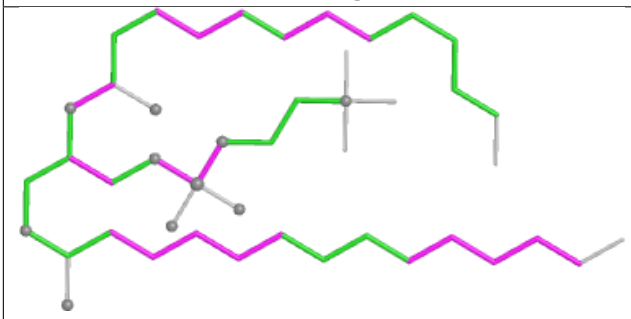
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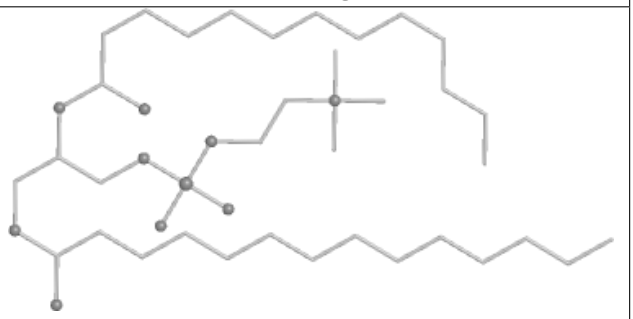
Bond lengths



Bond angles

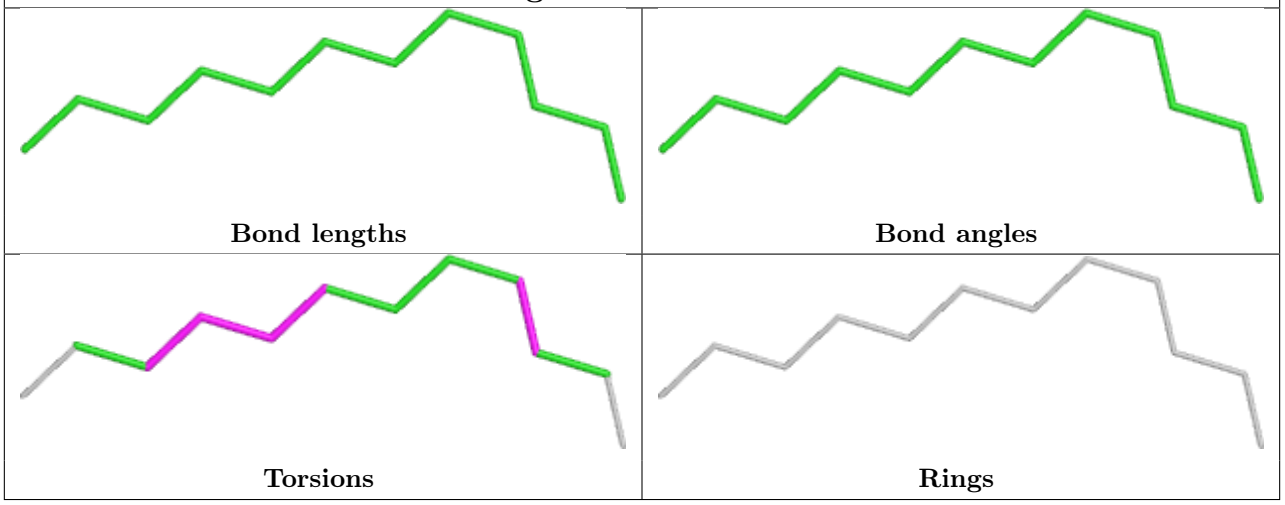


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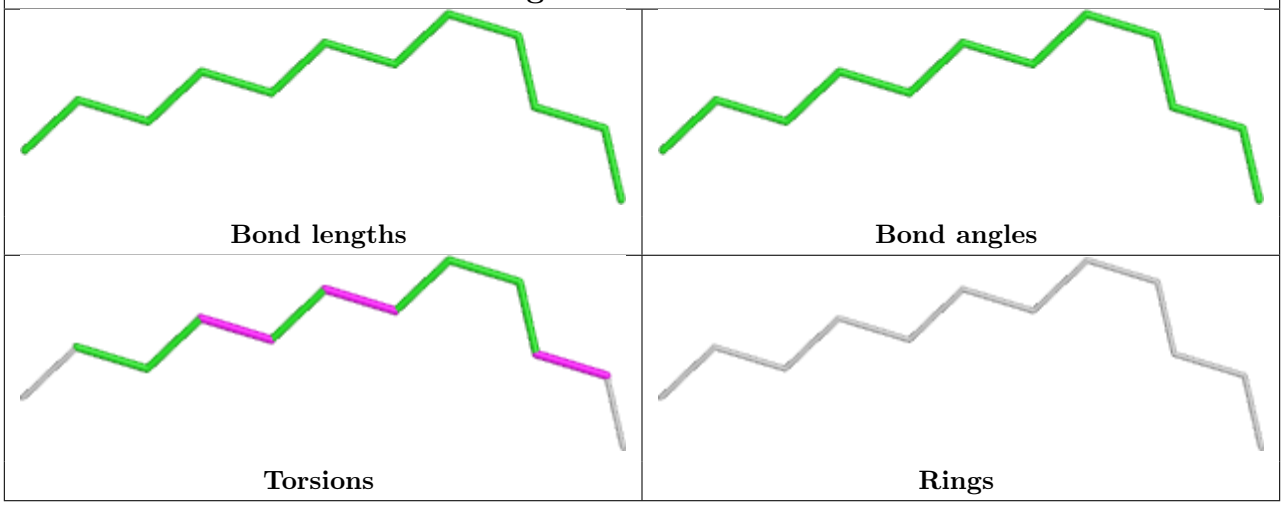


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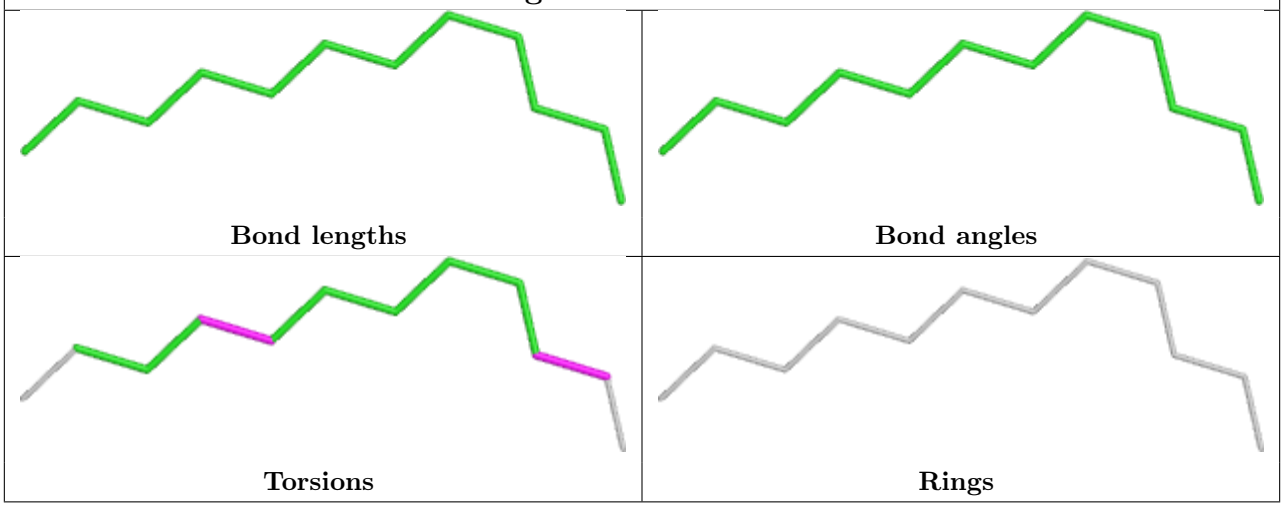
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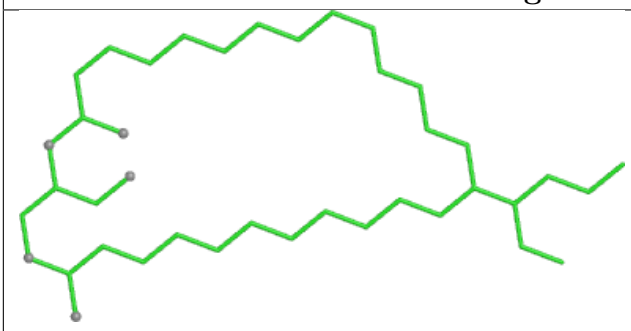
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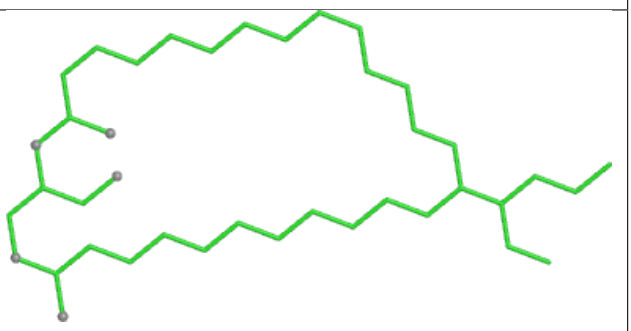
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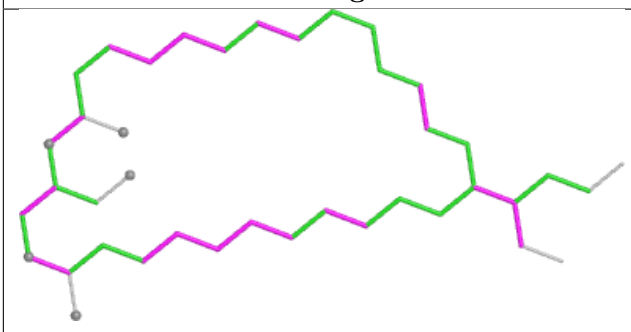
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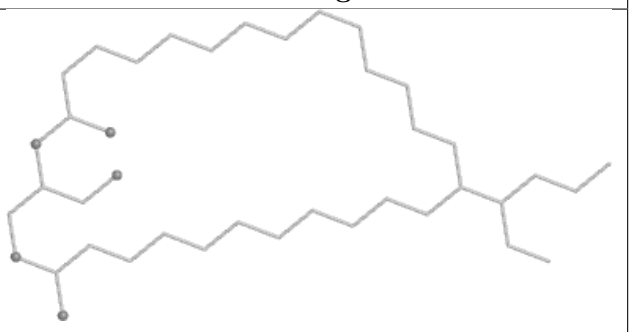
Bond lengths



Bond angles



Torsions



Rings

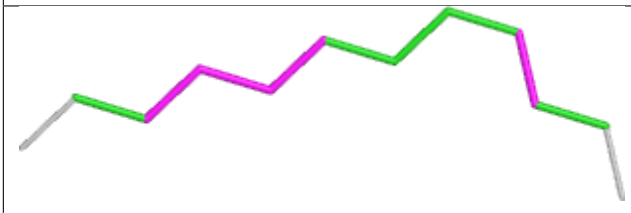
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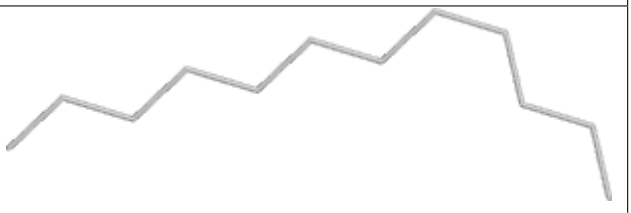
Bond lengths



Bond angles

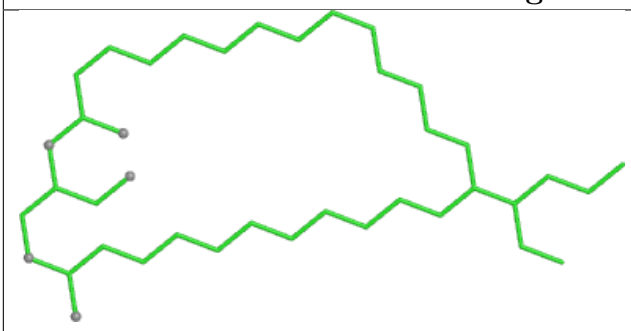


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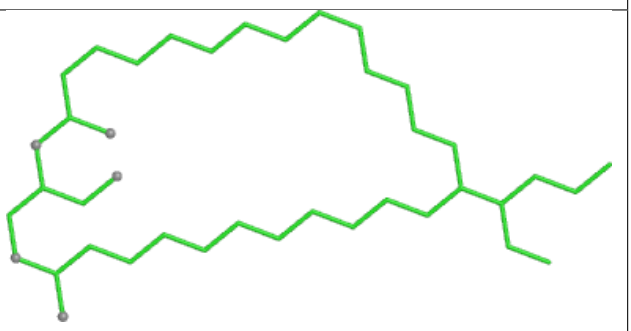


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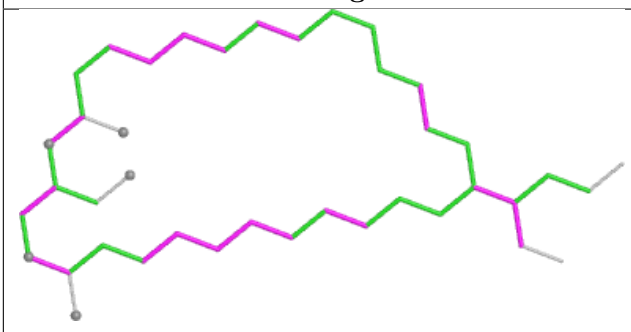
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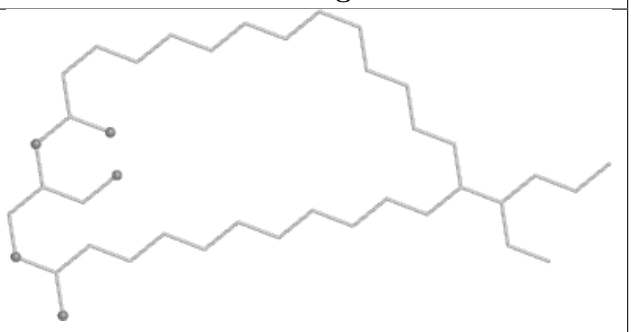
Bond lengths



Bond angles

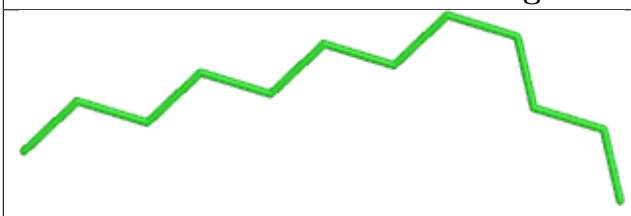


Torsions



Rings

Ligand LBN D 408



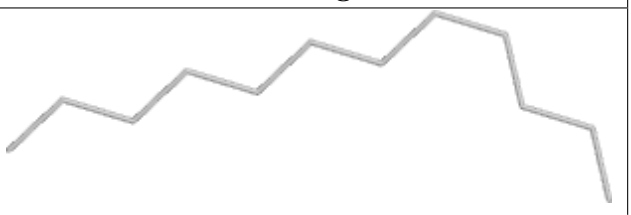
Bond lengths



Bond angles

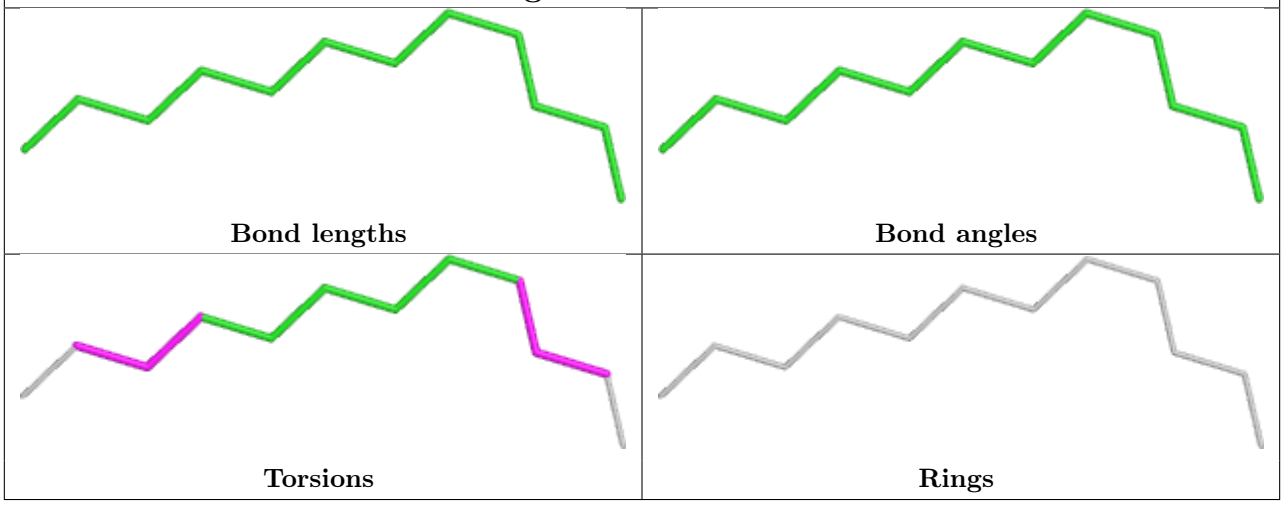


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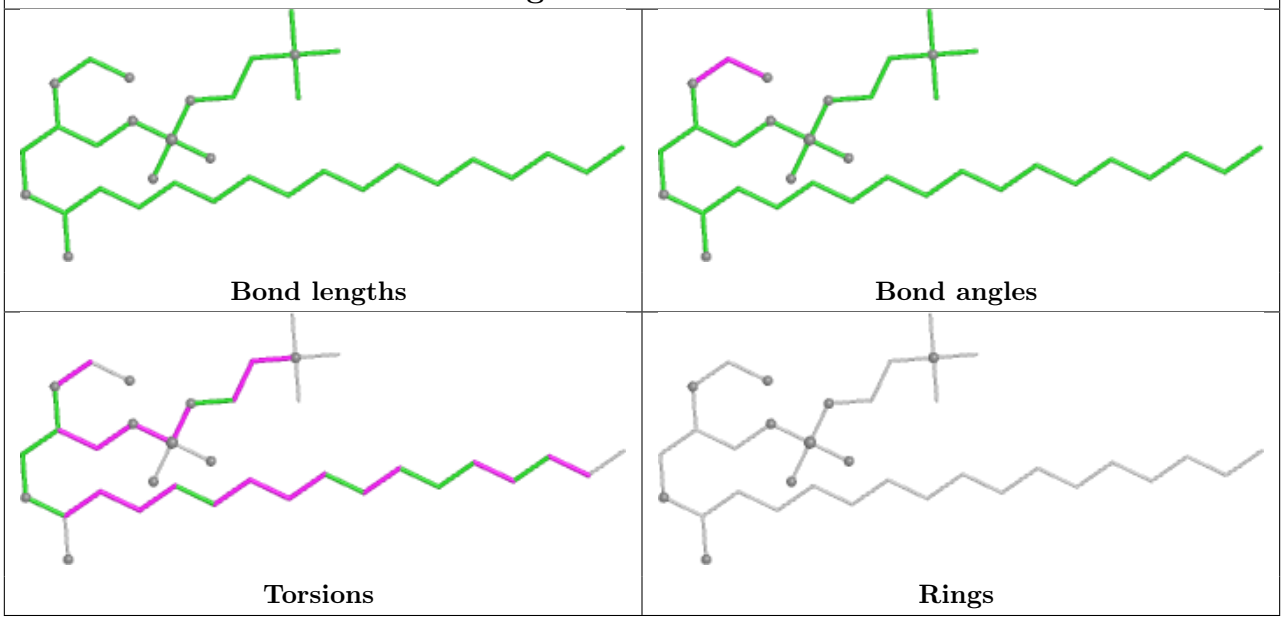


Rings

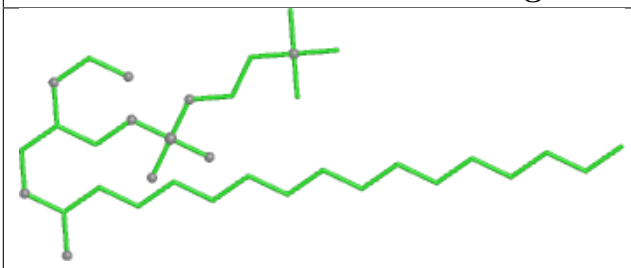
Ligand LBN A 404



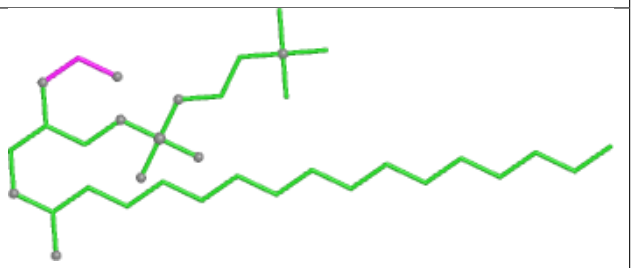
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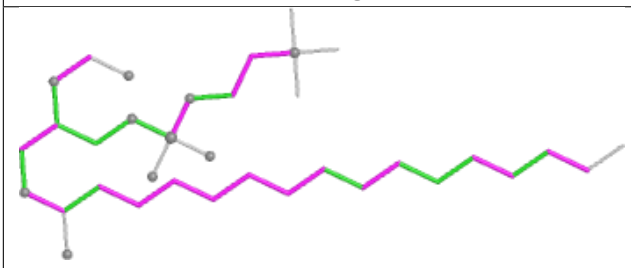
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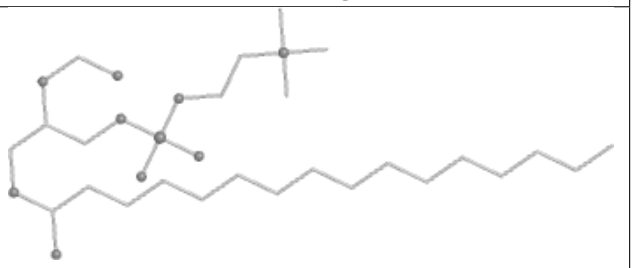
Bond lengths



Bond angles

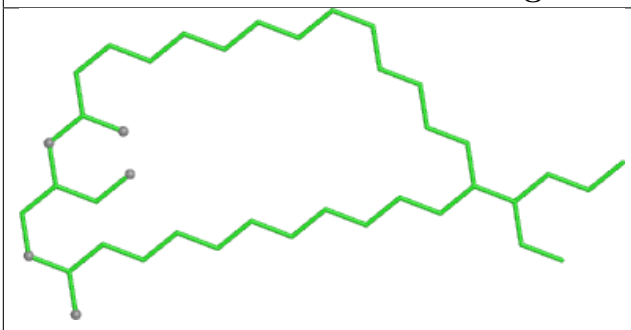


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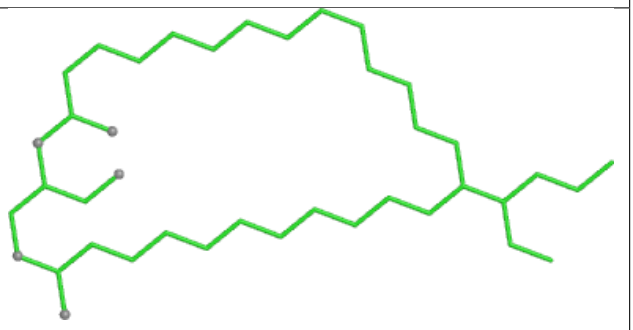


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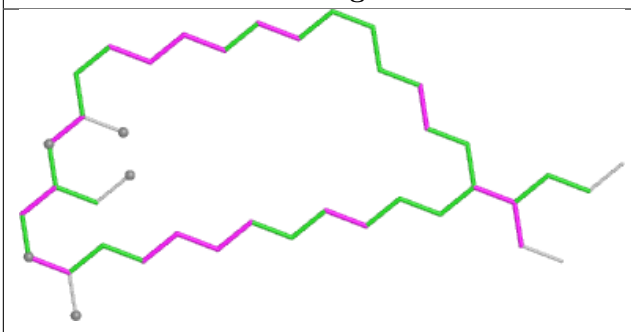
Ligand LBN B 407



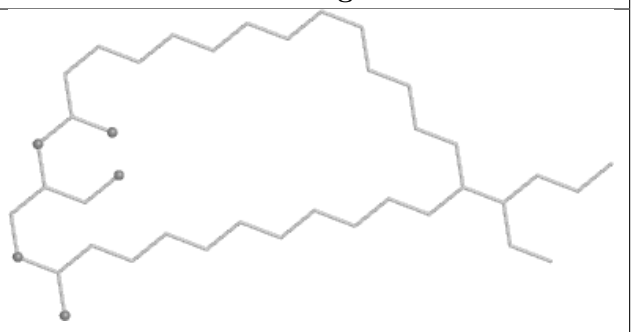
Bond lengths



Bond angles

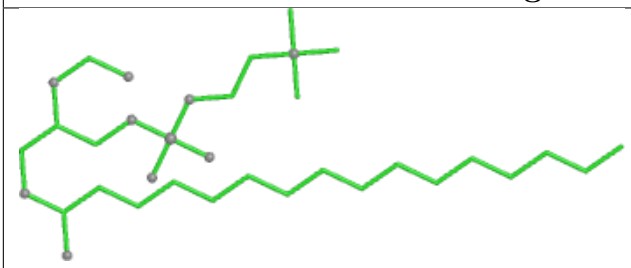


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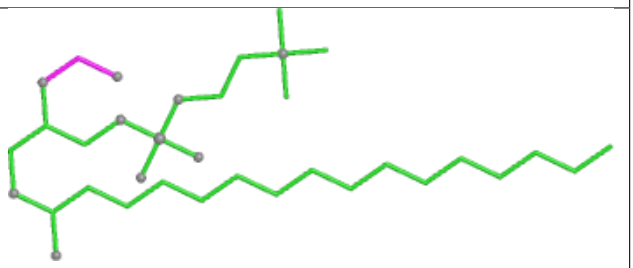


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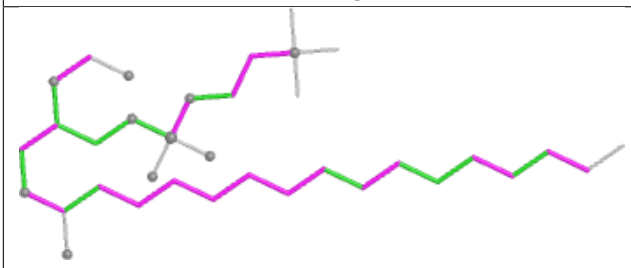
Ligand LBN C 506



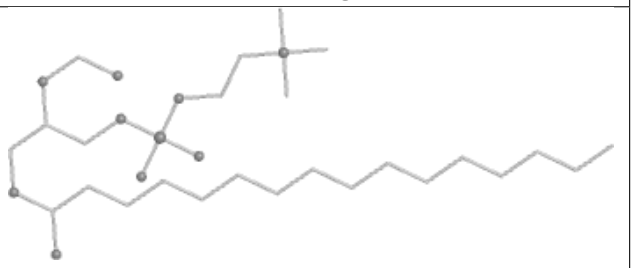
Bond lengths



Bond angles



Torsions



Rings

Ligand LBN C 508



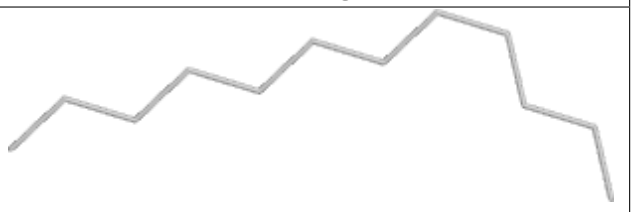
Bond lengths



Bond angles

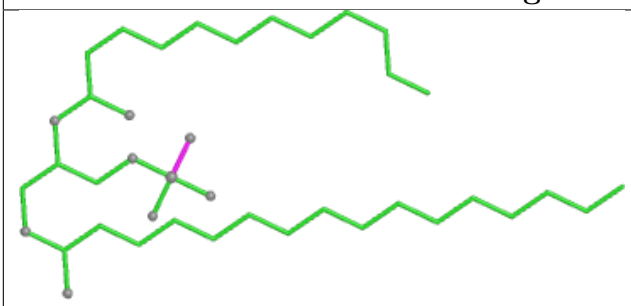


Torsions

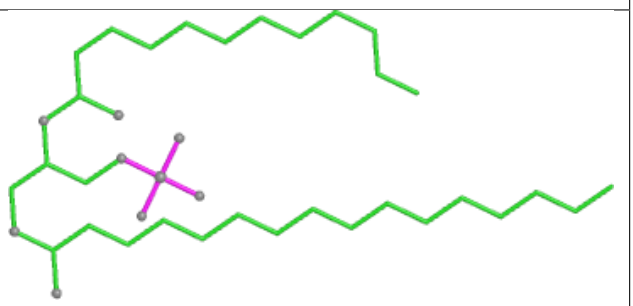


Rings

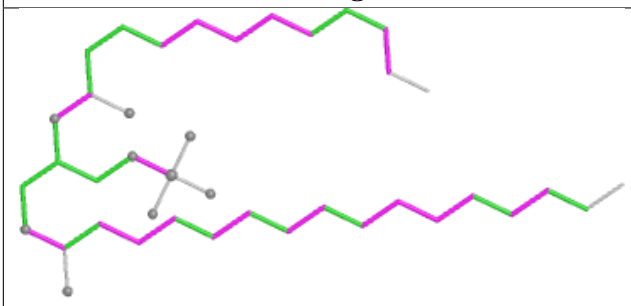
Ligand LBN A 401



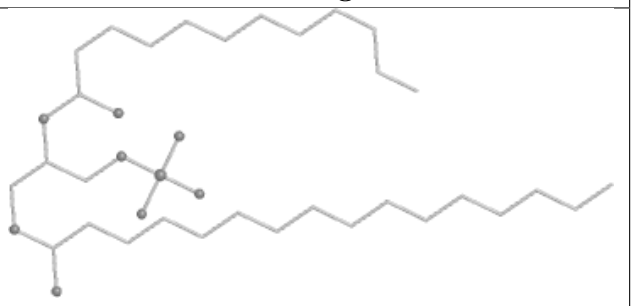
Bond lengths



Bond angles

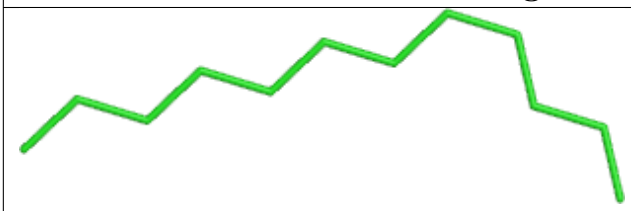


Torsions

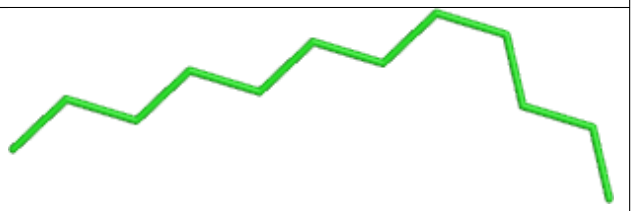


Rings

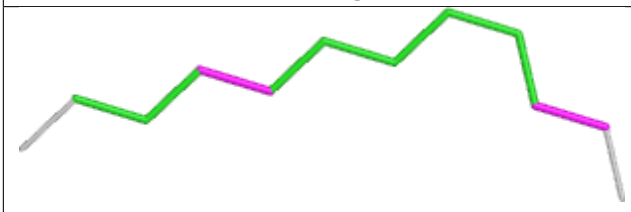
Ligand LBN G 506



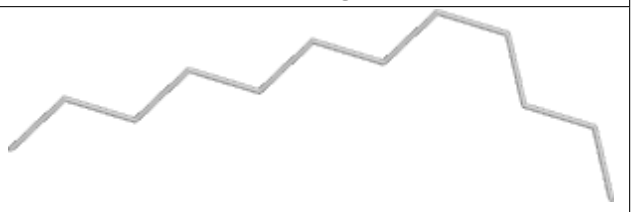
Bond lengths



Bond angles

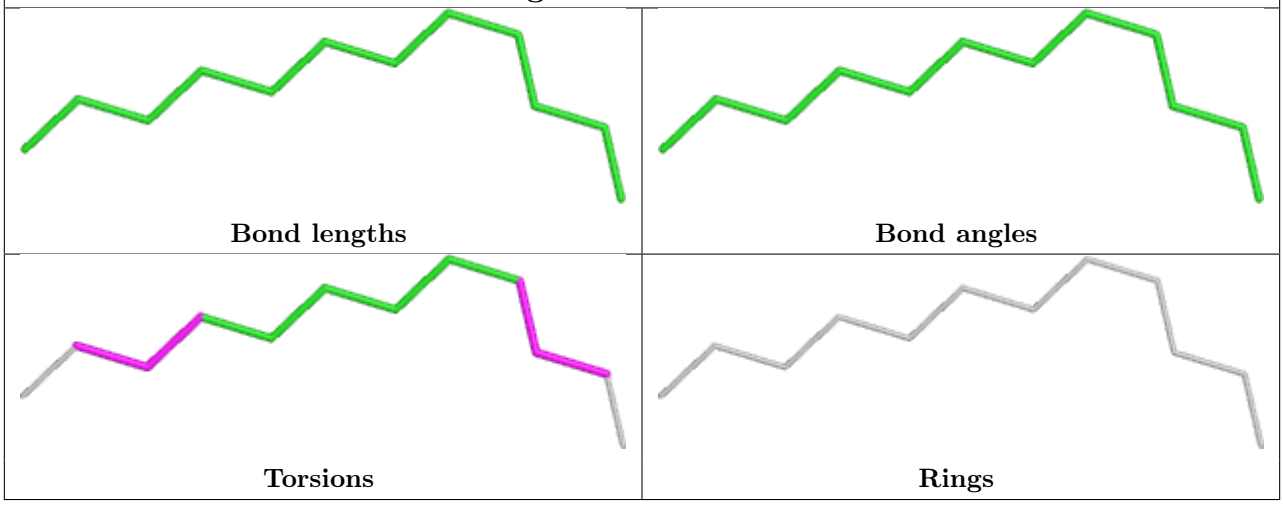


Torsions

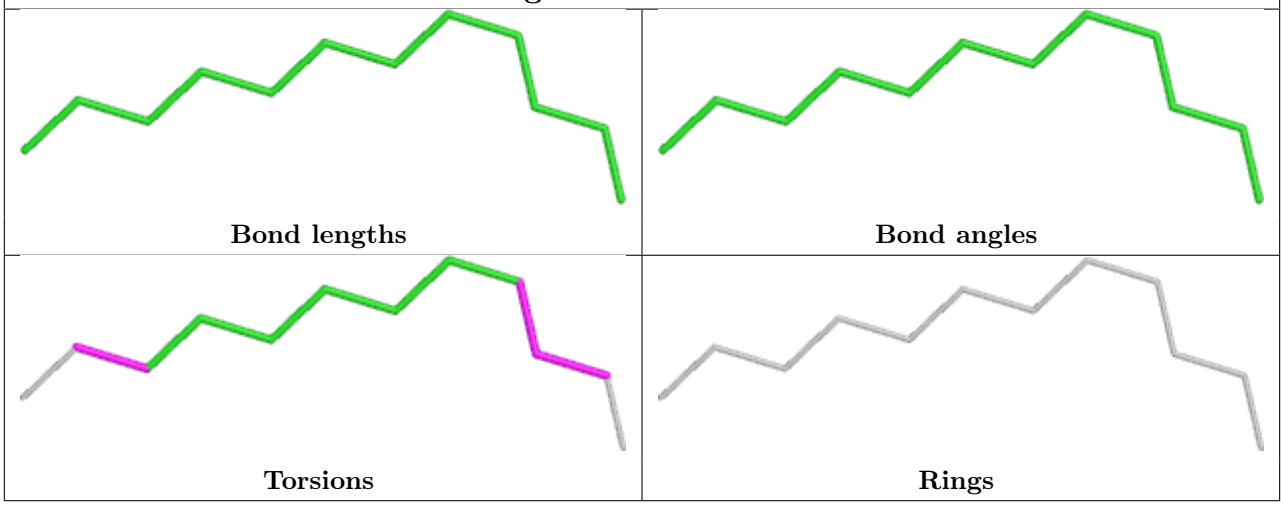


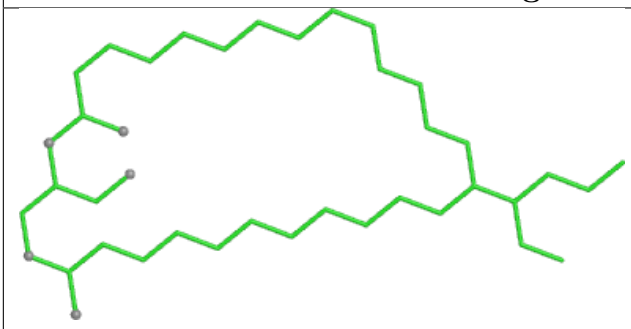
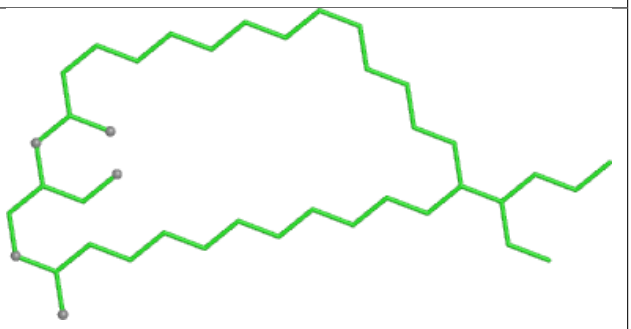
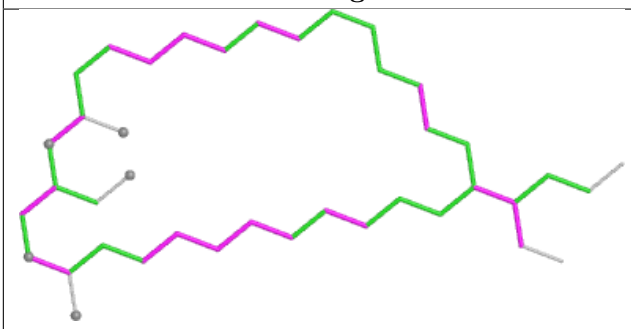
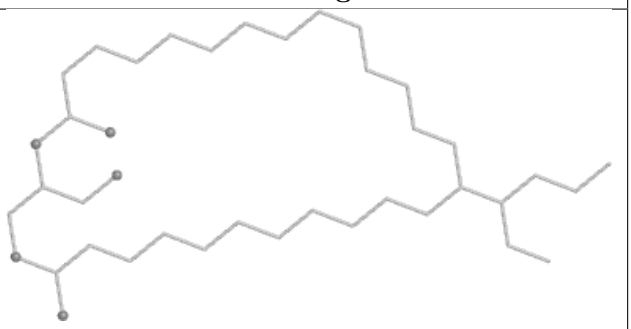
Rings

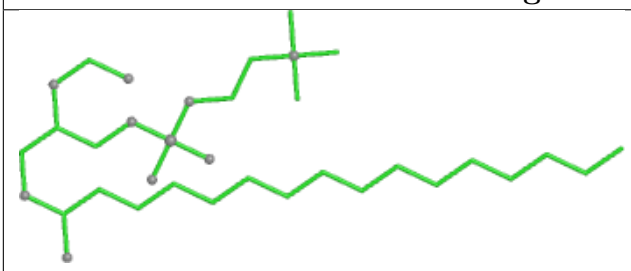
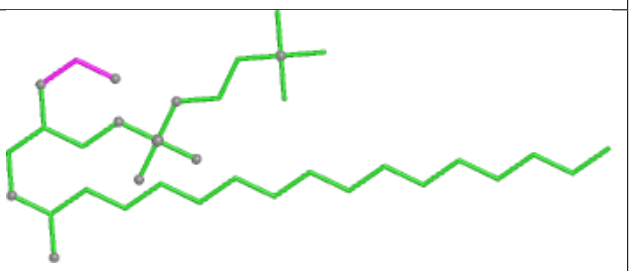
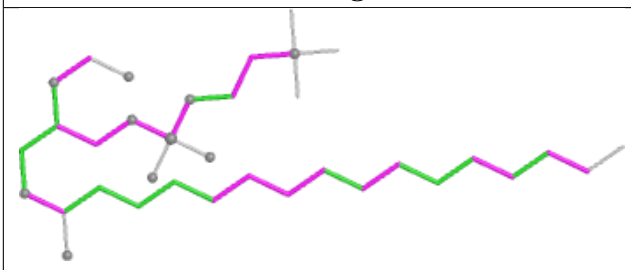
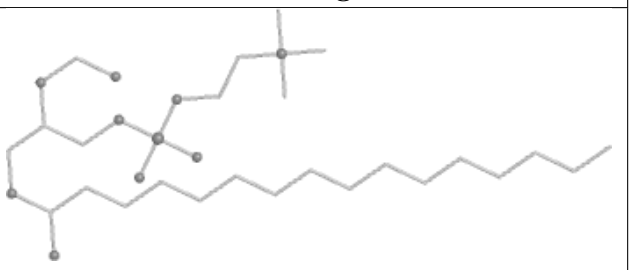
Ligand LBN F 508



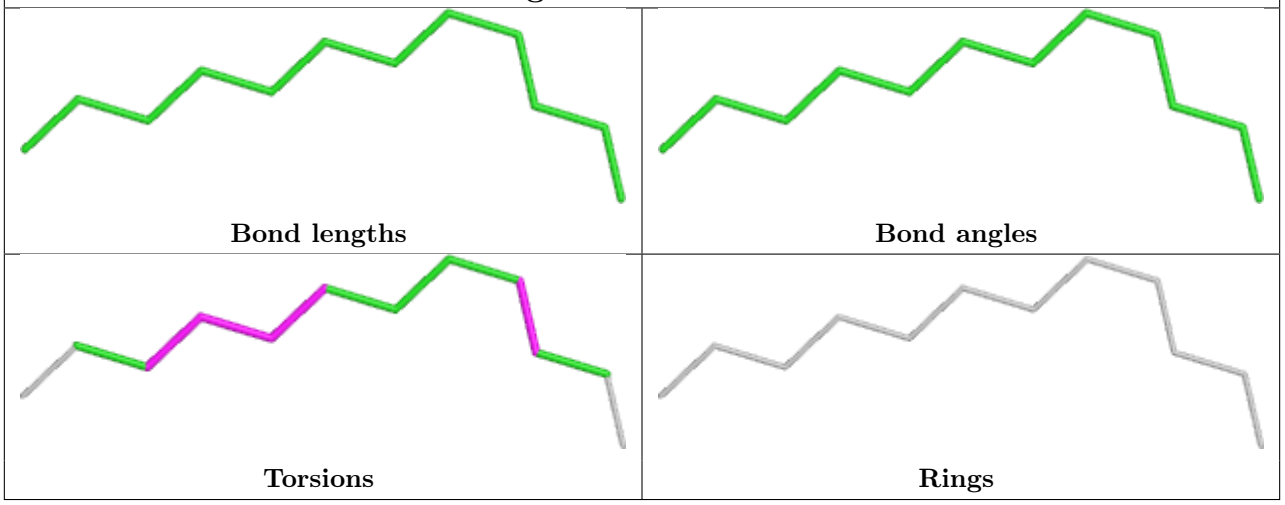
Ligand LBN D 403



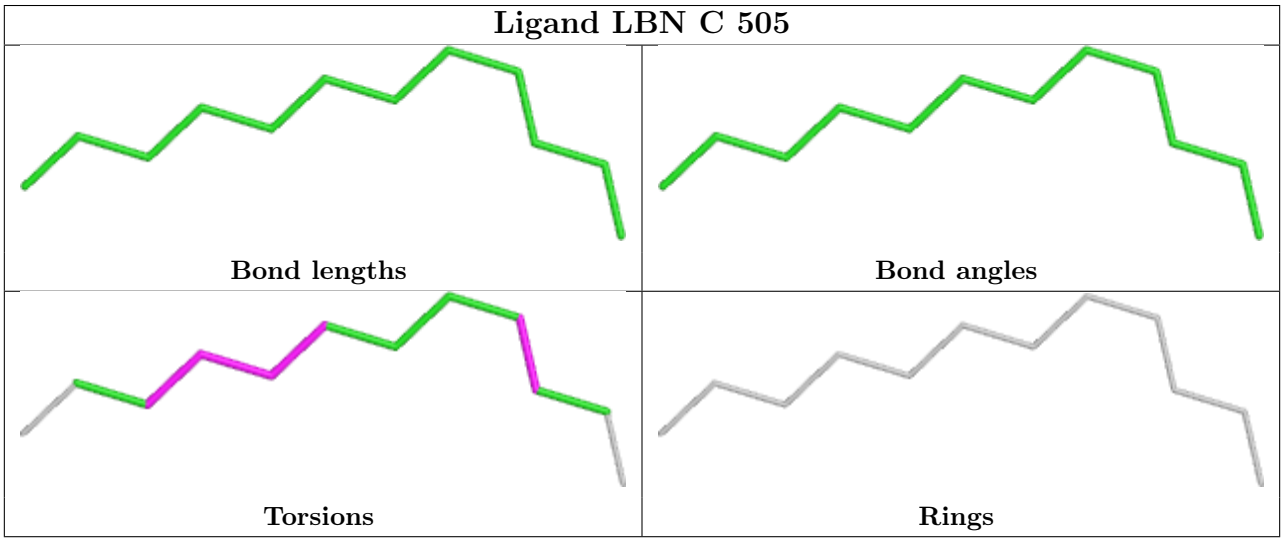
Ligand LBN G 503	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LBN D 401	
 Bond lengths	 Bond angles
 Torsions	 Rings

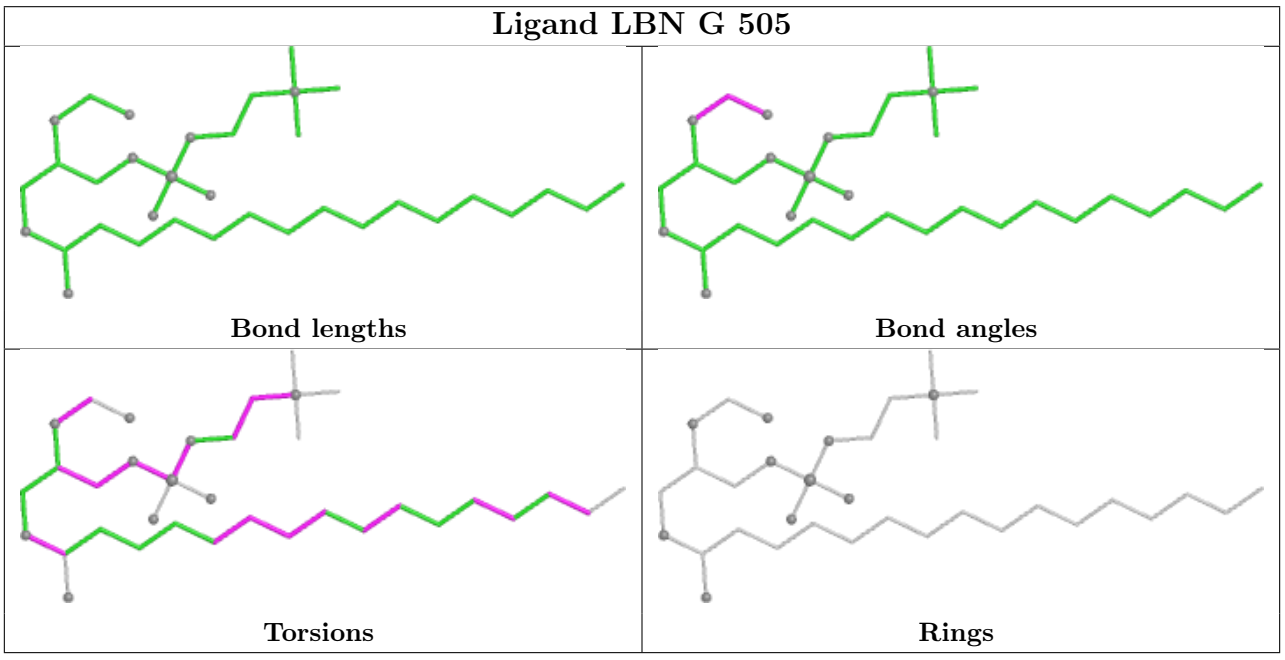
Ligand LBN F 505



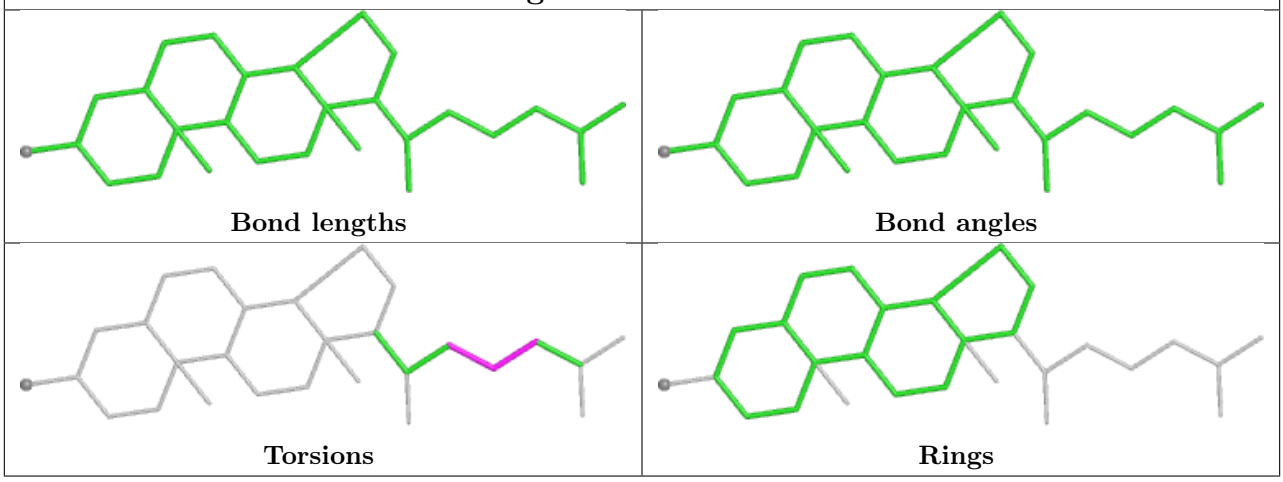
Ligand LBN C 505



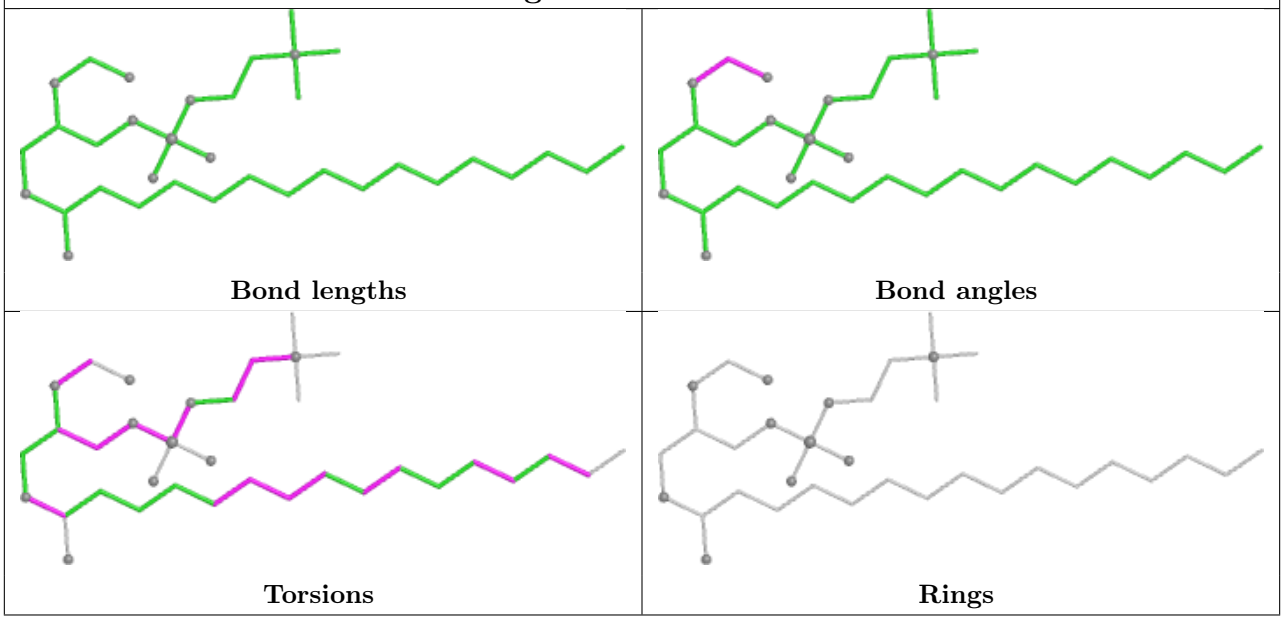
Ligand LBN G 505



Ligand CLR E 404



Ligand LBN A 402



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

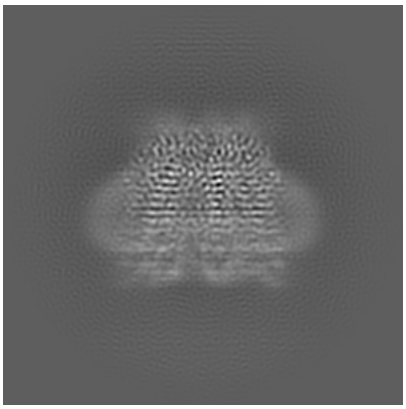
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-82383. These allow visual inspection of the internal detail of the map and identification of artifacts.

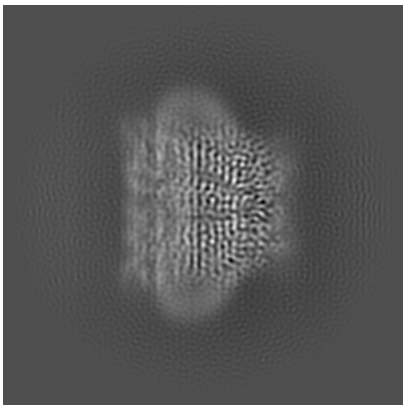
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

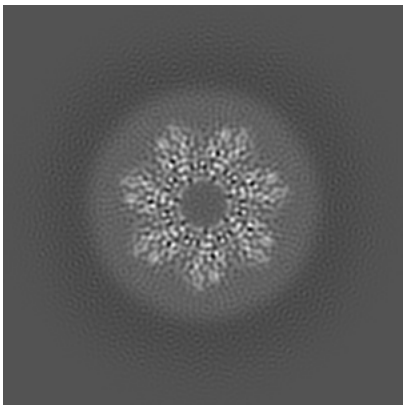
6.1.1 Primary map



X

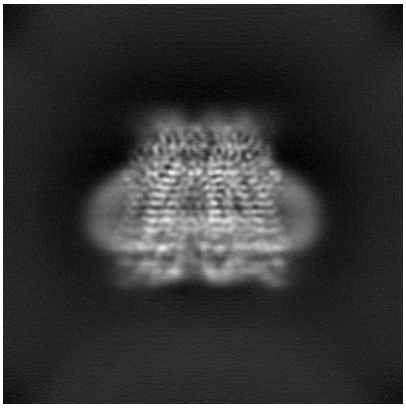


Y

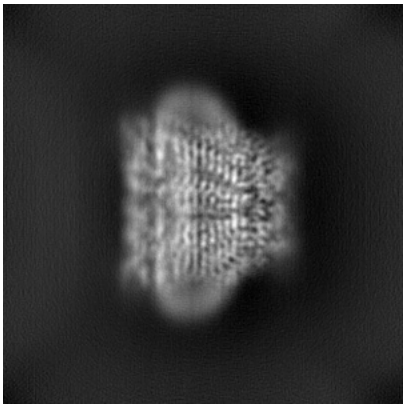


Z

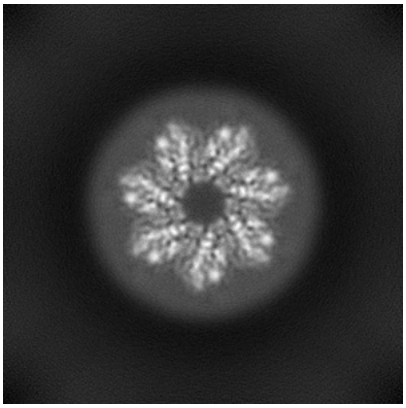
6.1.2 Raw map



X



Y

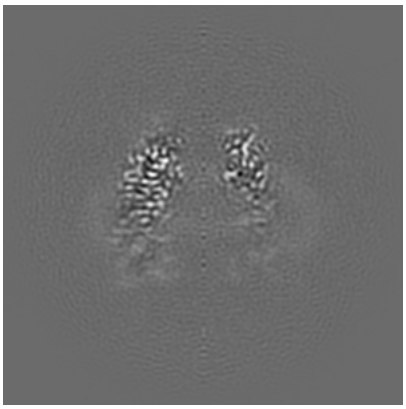


Z

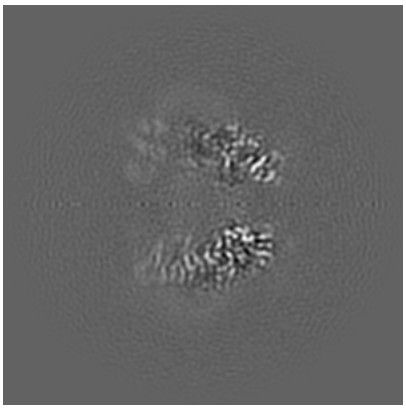
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

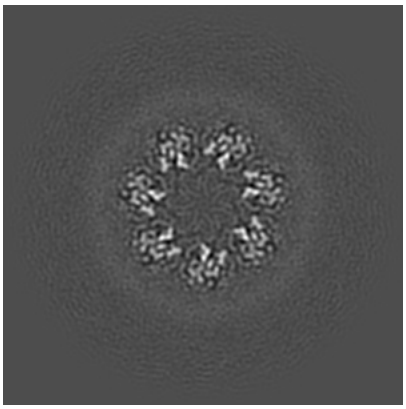
6.2.1 Primary map



X Index: 144

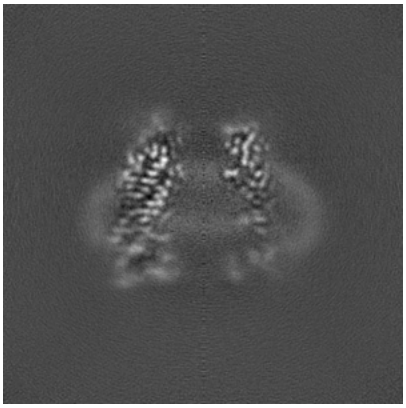


Y Index: 144

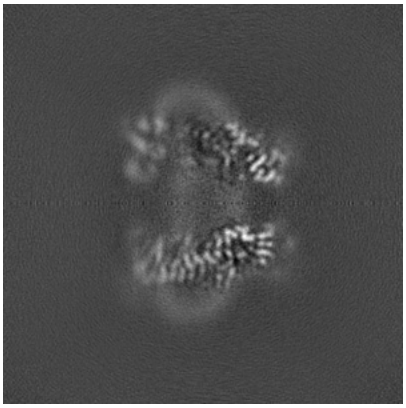


Z Index: 144

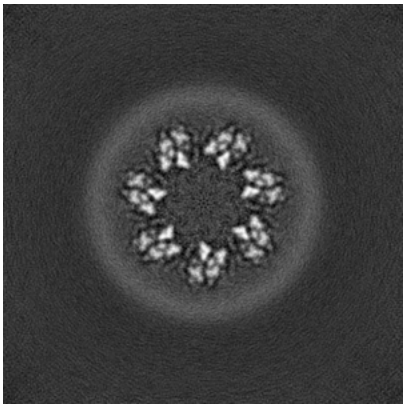
6.2.2 Raw map



X Index: 144



Y Index: 144

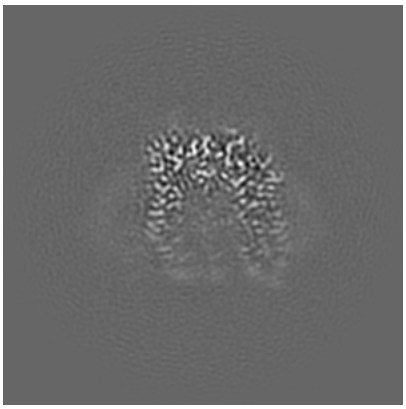


Z Index: 144

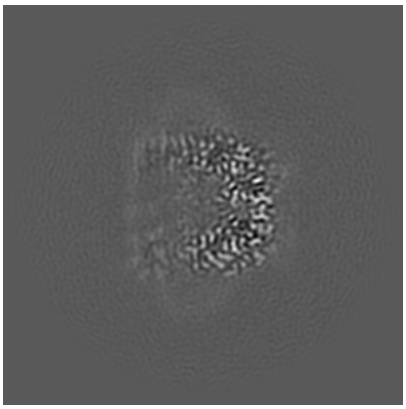
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

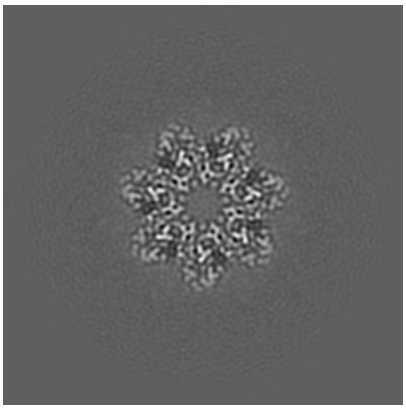
6.3.1 Primary map



X Index: 121

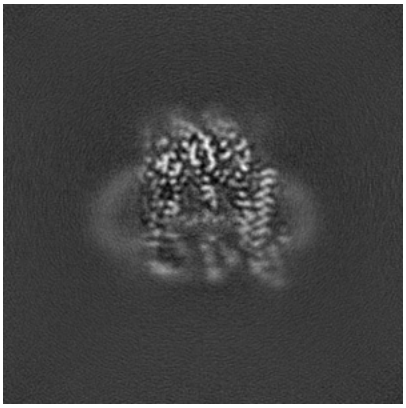


Y Index: 121

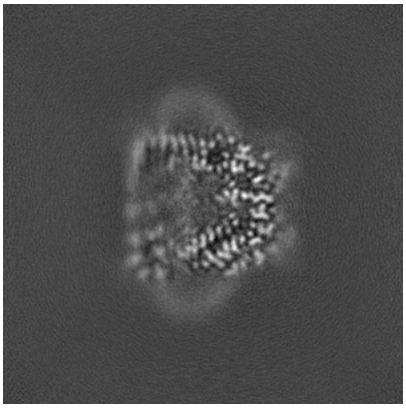


Z Index: 166

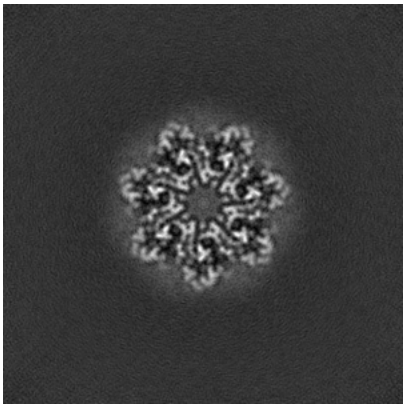
6.3.2 Raw map



X Index: 115



Y Index: 121

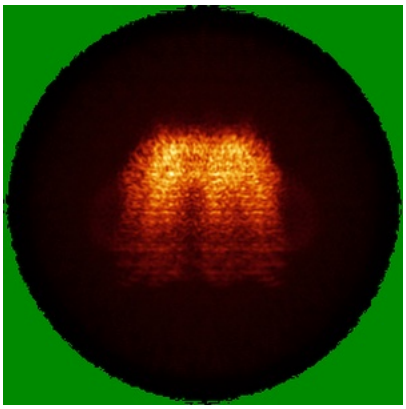


Z Index: 166

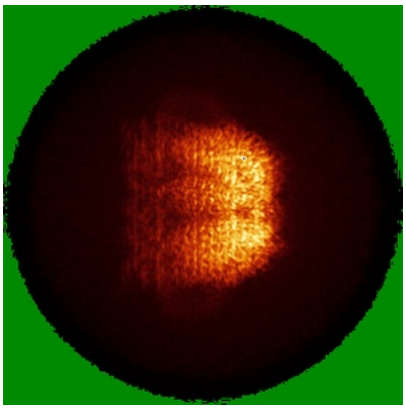
The images above show the largest variance slices of the map in three orthogonal directions.

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

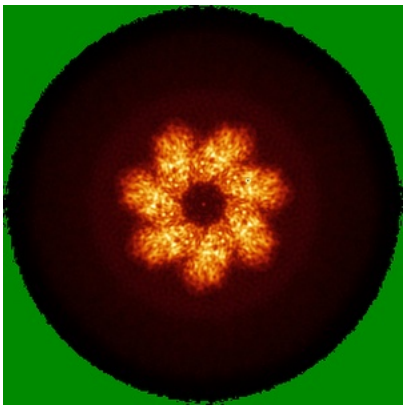
6.4.1 Primary map



X

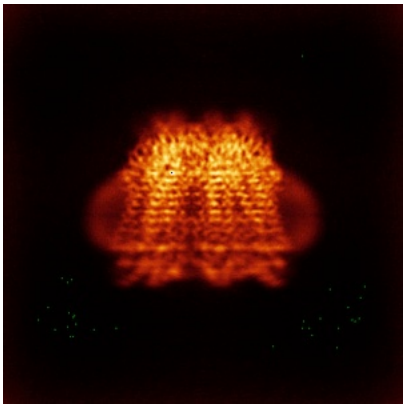


Y

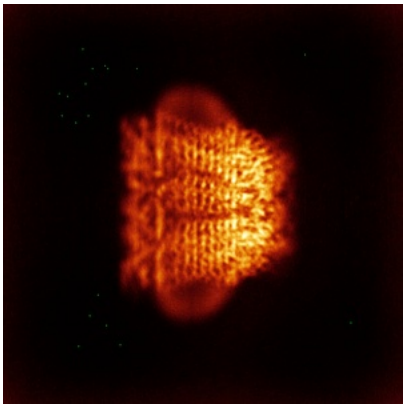


Z

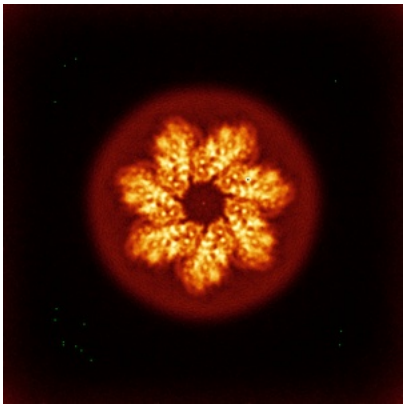
6.4.2 Raw map



X



Y

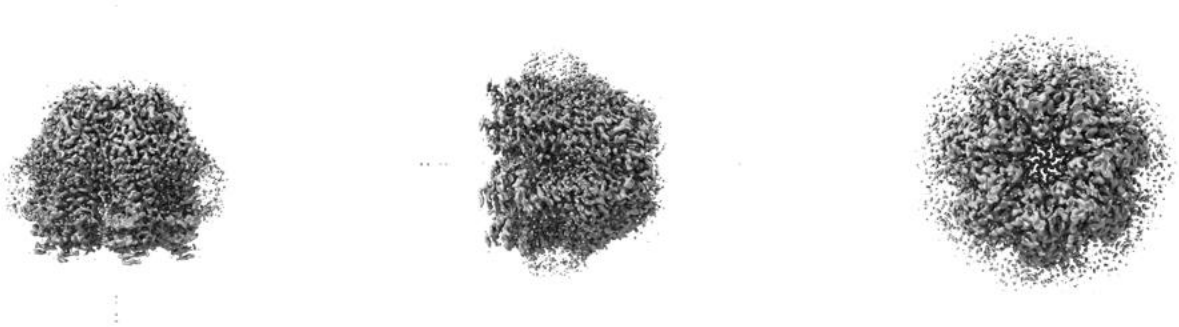


Z

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)

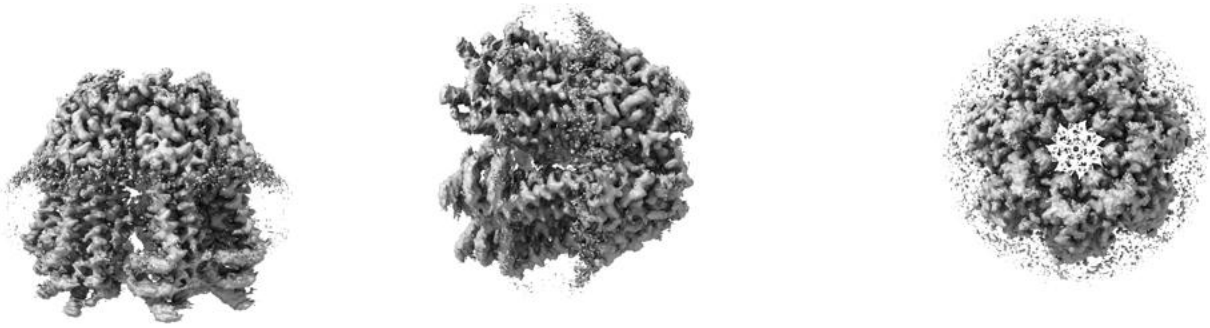
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.08. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

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

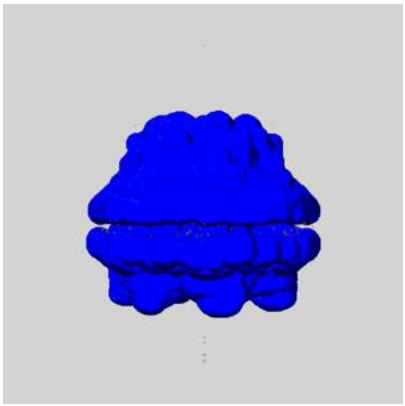
6.6 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

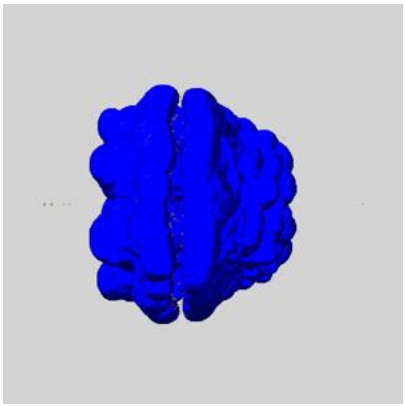
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

6.6.1 emd_82383_msk_1.map (i)



X



Y

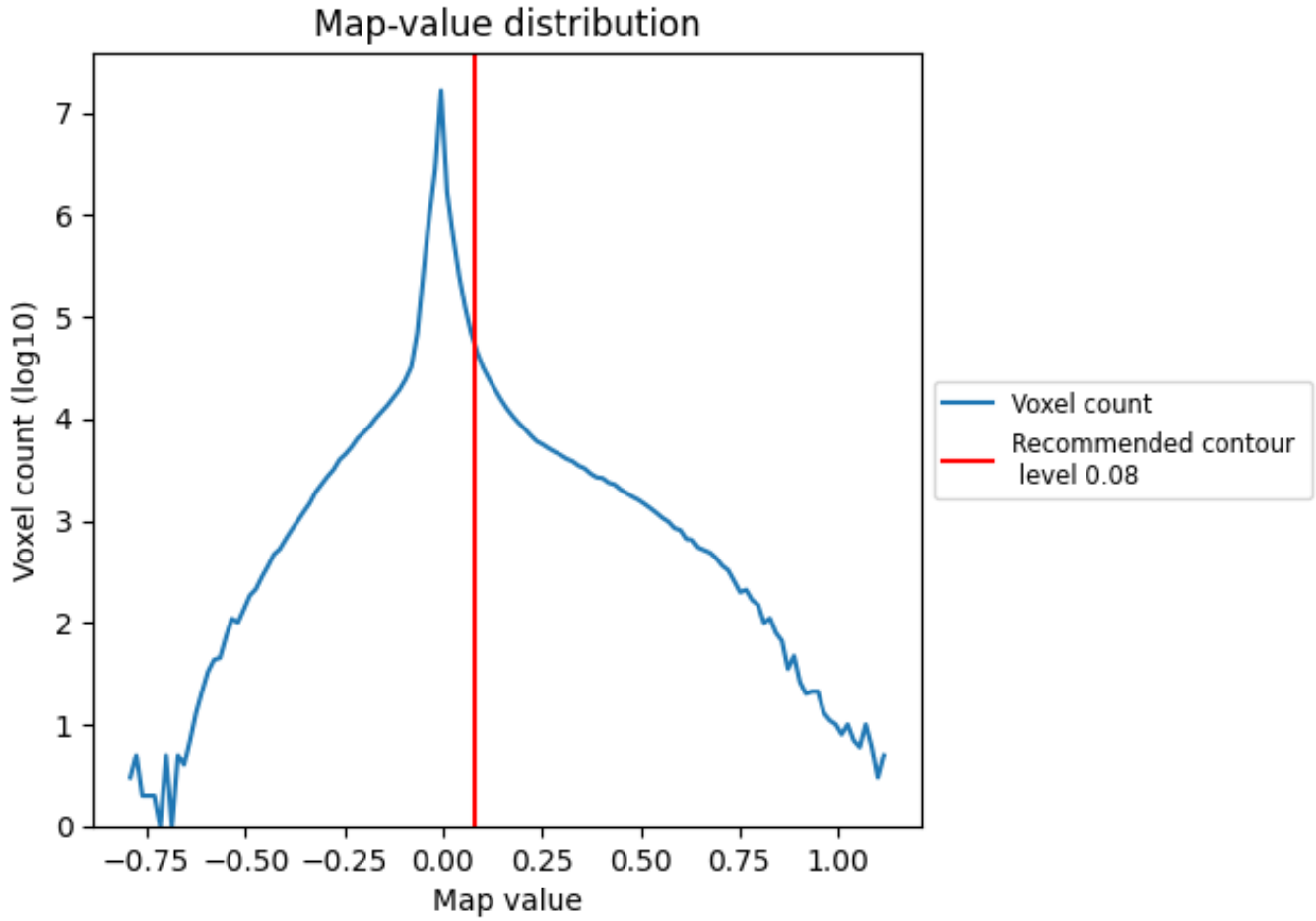


Z

7 Map analysis

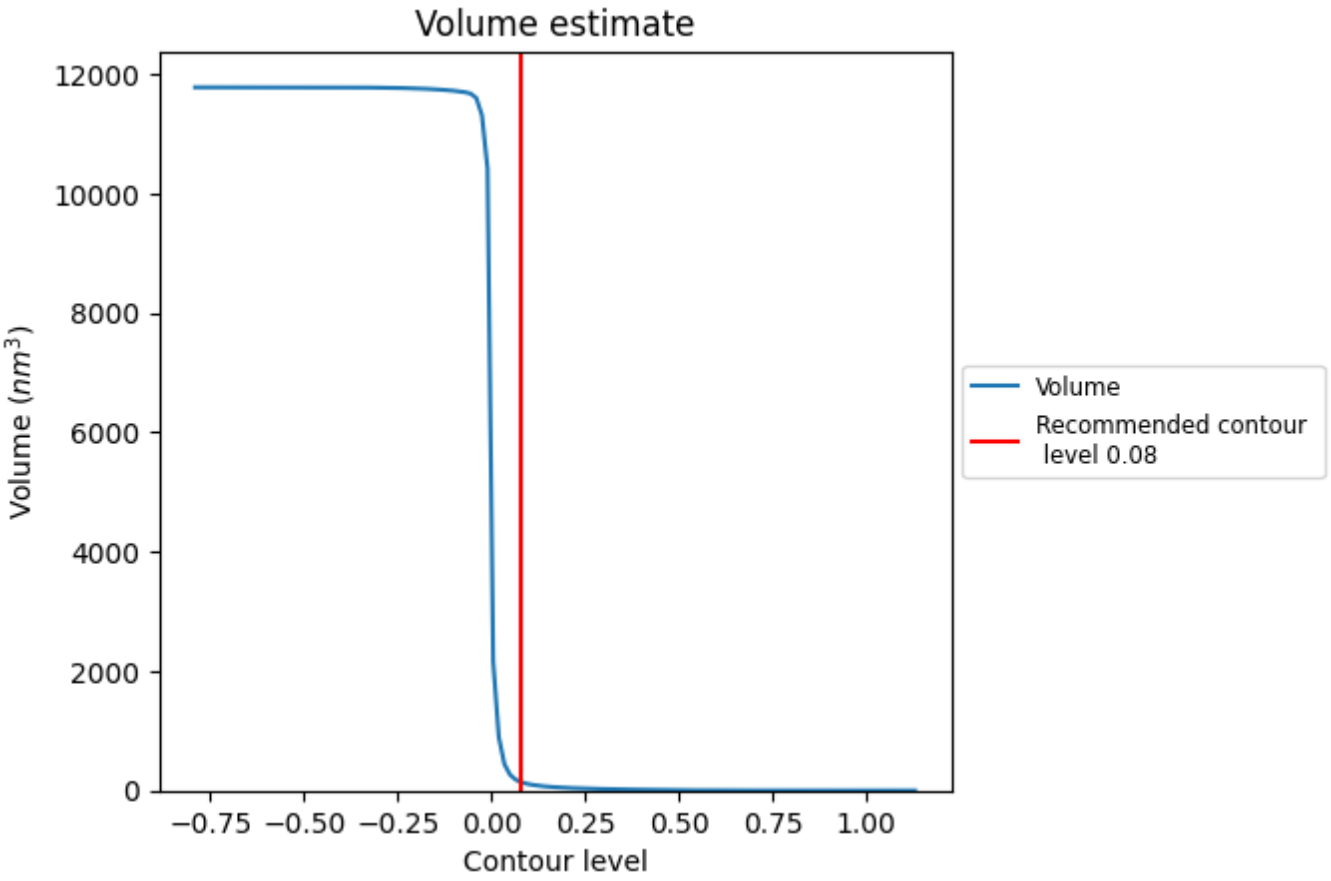
This section contains the results of statistical analysis of the map.

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.

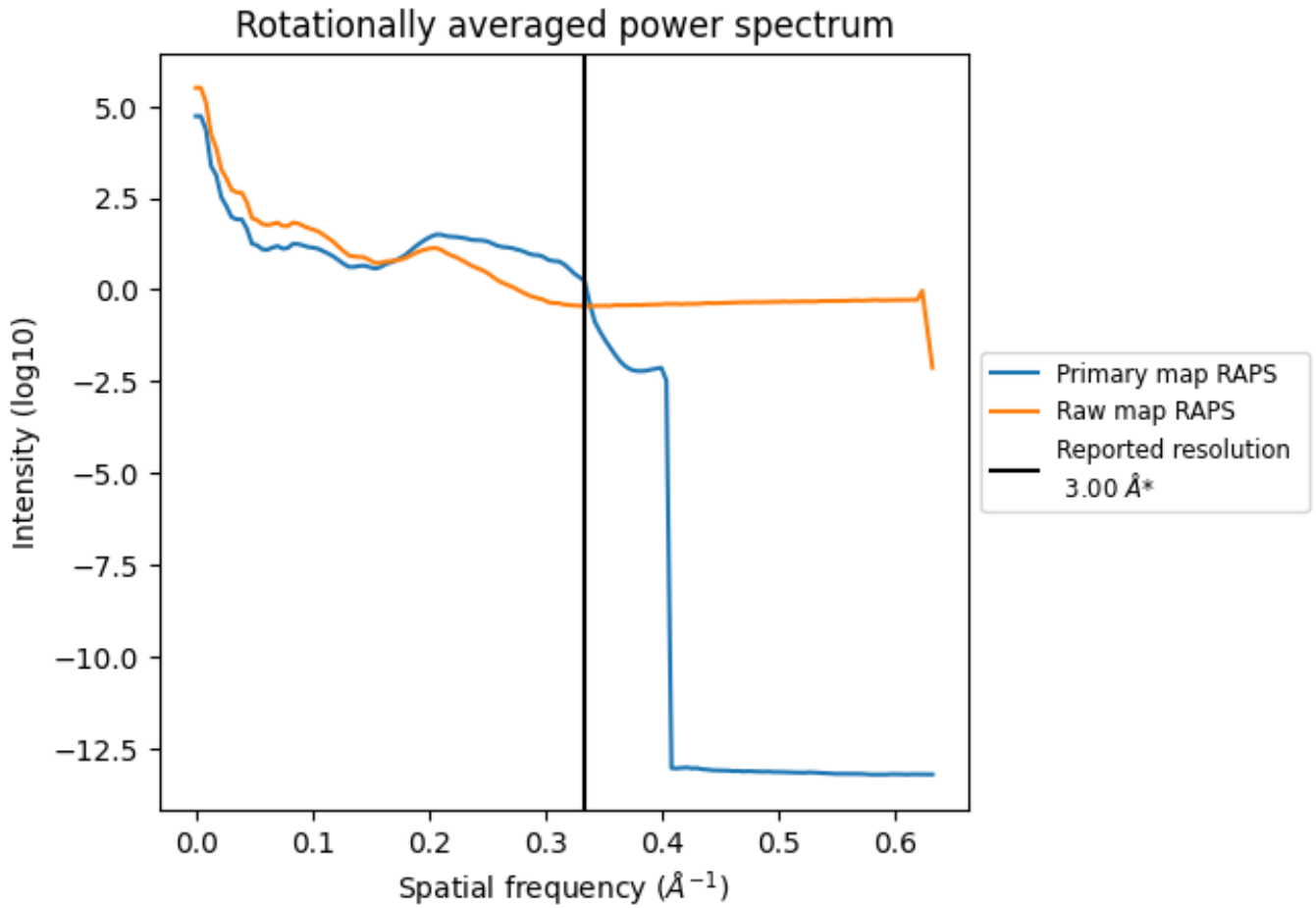
7.2 Volume estimate



The volume at the recommended contour level is 139 nm^3; this corresponds to an approximate mass of 125 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)

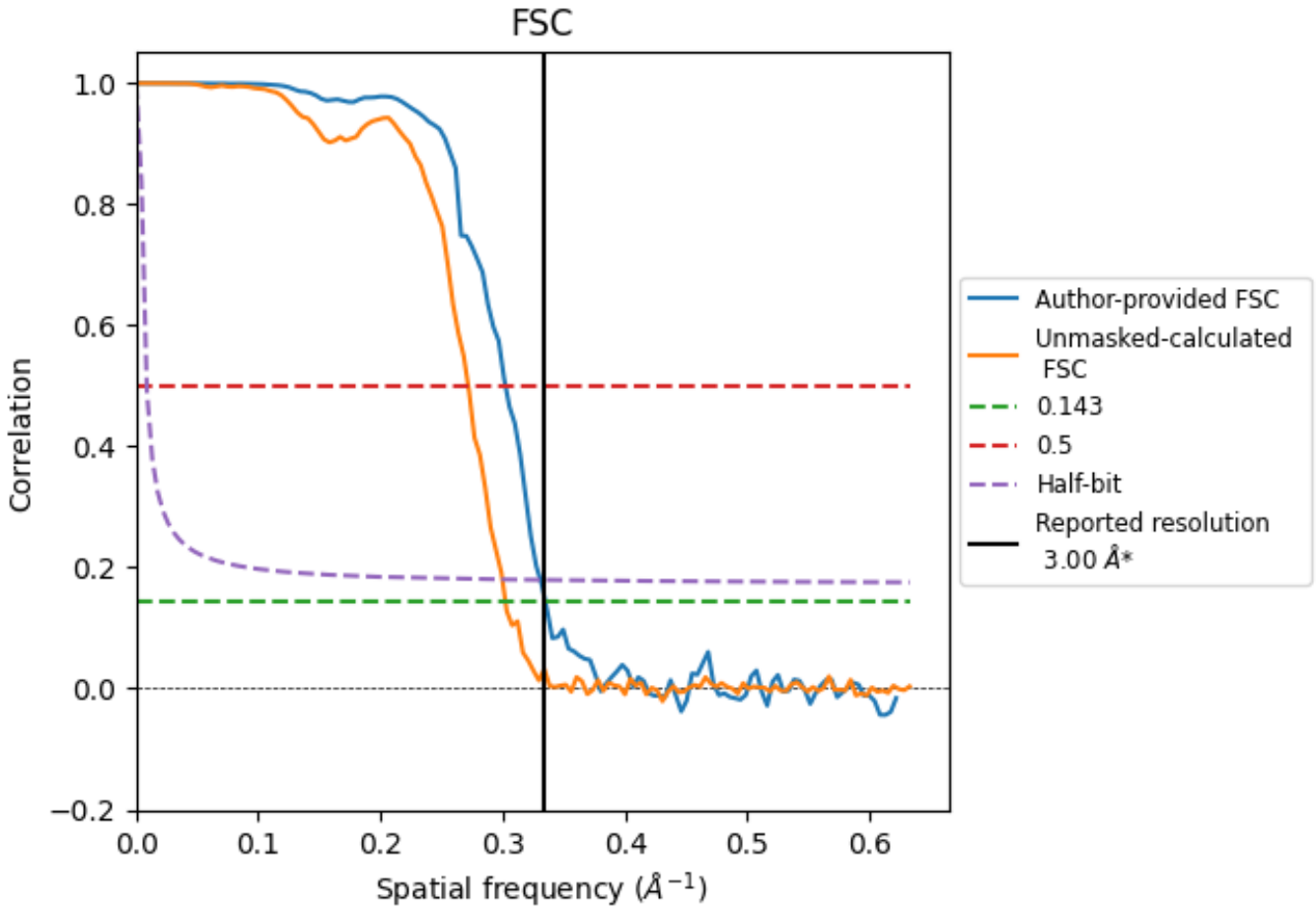


*Reported resolution corresponds to spatial frequency of 0.333 $Å^{-1}$

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 0.333 Å^{-1}

8.2 Resolution estimates (i)

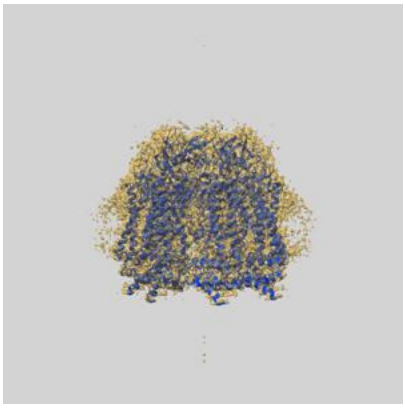
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	2.99	3.31	3.02
Unmasked-calculated*	3.31	3.68	3.34

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.31 differs from the reported value 3.0 by more than 10 %

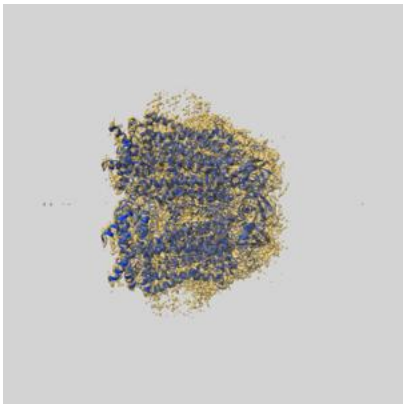
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-82383 and PDB model 43YC. Per-residue inclusion information can be found in section 3 on page 9.

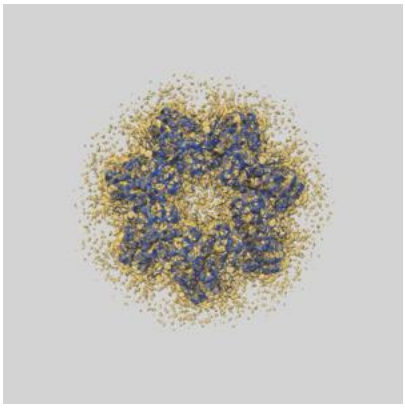
9.1 Map-model overlay



X



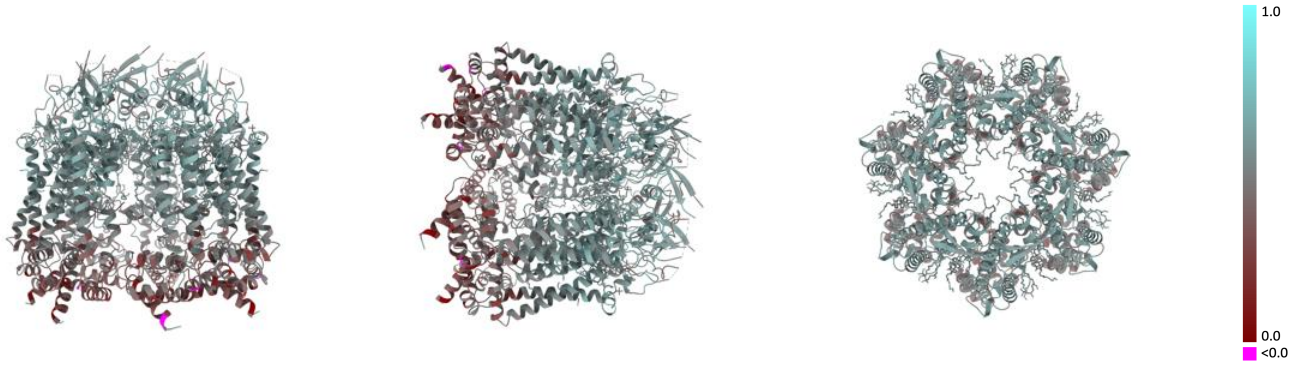
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.08 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

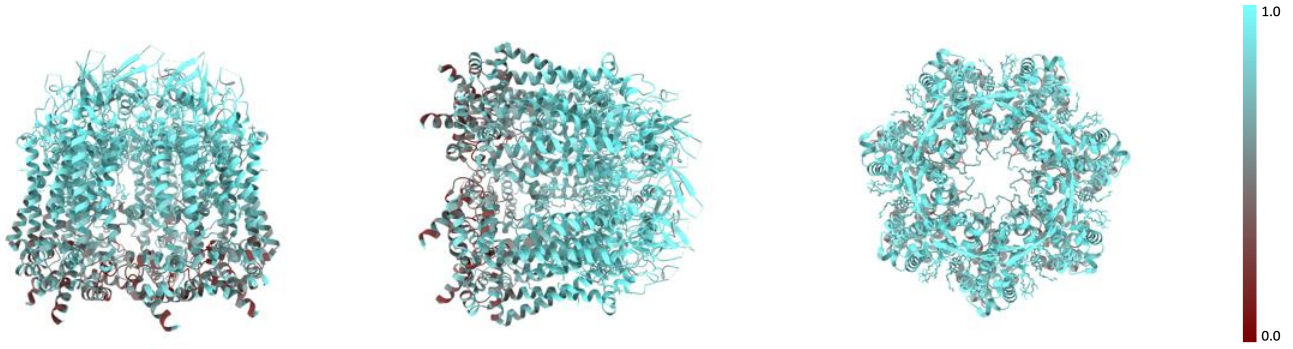
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

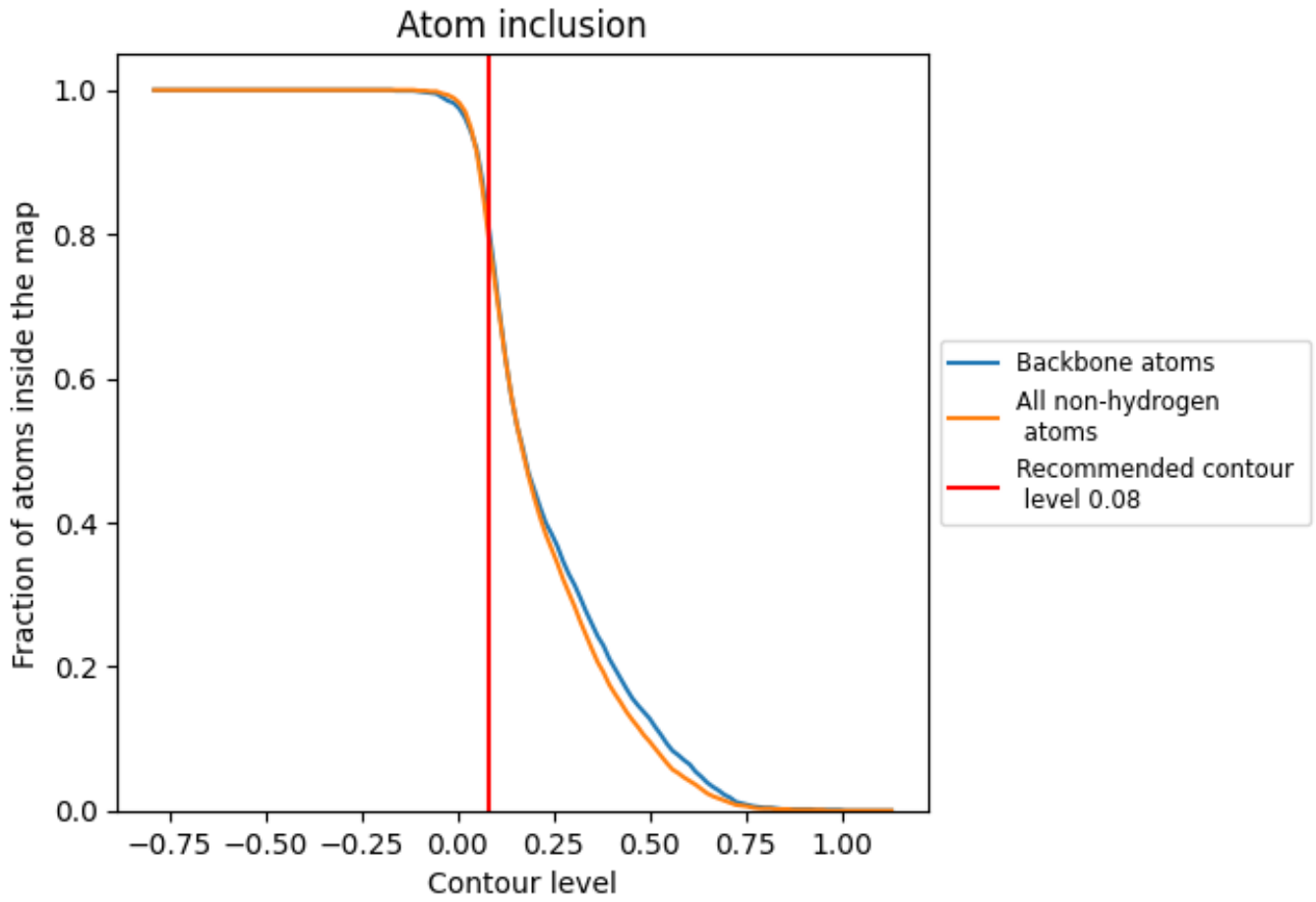
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.08).

9.4 Atom inclusion (i)



At the recommended contour level, 81% of all backbone atoms, 80% 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 (0.08) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7970	0.5060
A	0.7970	0.5070
B	0.7950	0.5050
C	0.7960	0.5060
D	0.7980	0.5050
E	0.7960	0.5060
F	0.8000	0.5060
G	0.7940	0.5060

