Full wwPDB EM Validation Report ⓘ

Oct 21, 2026 – 04:56 PM EDT

PDB ID	:	38KG / pdb_000038kg
EMDB ID	:	EMD-78870
Title	:	Connexin-50 Dual-Channel Assembly - Centered
Authors	:	Garrels, C.S.; Reichow, S.L.
Deposited on	:	2026-08-31
Resolution	:	2.88 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:

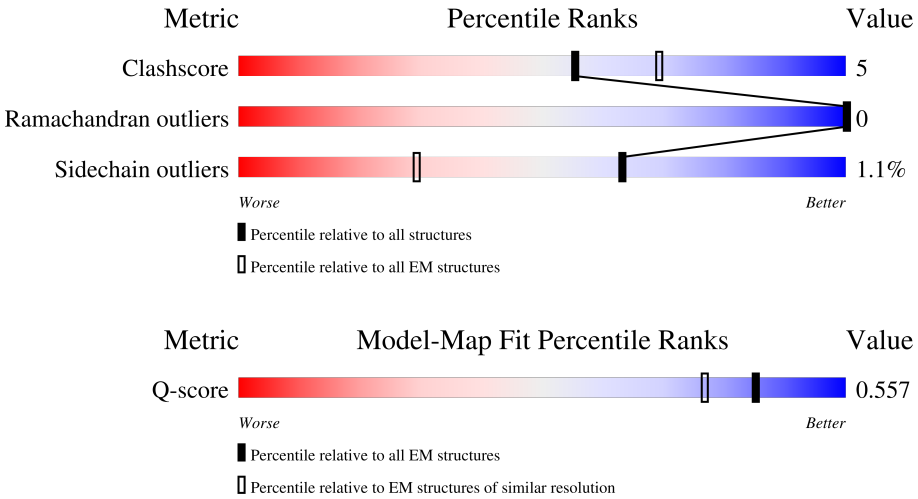
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.2
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data 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 2.88 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	12111 (2.38 - 3.38)

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	440	33% 9% 58%
1	B	440	37% 5% 58%
1	C	440	35% 6% 58%
1	D	440	37% 58%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	E	440	36% 5% 58%
1	F	440	35% 7% 58%
1	G	440	33% 9% 58%
1	H	440	37% 5% 58%
1	I	440	36% 6% 58%
1	J	440	38% 58%
1	K	440	37% 5% 58%
1	L	440	35% 7% 58%
1	M	440	33% 9% 58%
1	N	440	37% 5% 58%
1	O	440	35% 6% 58%
1	P	440	37% 58%
1	Q	440	36% 5% 58%
1	R	440	35% 7% 58%
1	S	440	33% 9% 58%
1	T	440	37% 5% 58%
1	V	440	36% 6% 58%
1	W	440	38% 58%
1	X	440	37% 5% 58%
1	Y	440	35% 7% 58%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 38872 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 Gap junction protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	184	Total	C	N	O	S	0	0
			1490	990	239	252	9		
1	B	184	Total	C	N	O	S	0	0
			1490	990	239	252	9		
1	C	184	Total	C	N	O	S	0	0
			1490	990	239	252	9		
1	D	184	Total	C	N	O	S	0	0
			1490	990	239	252	9		
1	E	184	Total	C	N	O	S	0	0
			1490	990	239	252	9		
1	F	184	Total	C	N	O	S	0	0
			1490	990	239	252	9		
1	G	184	Total	C	N	O	S	0	0
			1490	990	239	252	9		
1	H	184	Total	C	N	O	S	0	0
			1490	990	239	252	9		
1	I	184	Total	C	N	O	S	0	0
			1490	990	239	252	9		
1	J	184	Total	C	N	O	S	0	0
			1490	990	239	252	9		
1	K	184	Total	C	N	O	S	0	0
			1490	990	239	252	9		
1	L	184	Total	C	N	O	S	0	0
			1490	990	239	252	9		
1	M	184	Total	C	N	O	S	0	0
			1490	990	239	252	9		
1	N	184	Total	C	N	O	S	0	0
			1490	990	239	252	9		
1	O	184	Total	C	N	O	S	0	0
			1490	990	239	252	9		
1	P	184	Total	C	N	O	S	0	0
			1490	990	239	252	9		
1	Q	184	Total	C	N	O	S	0	0
			1490	990	239	252	9		

Continued on next page...

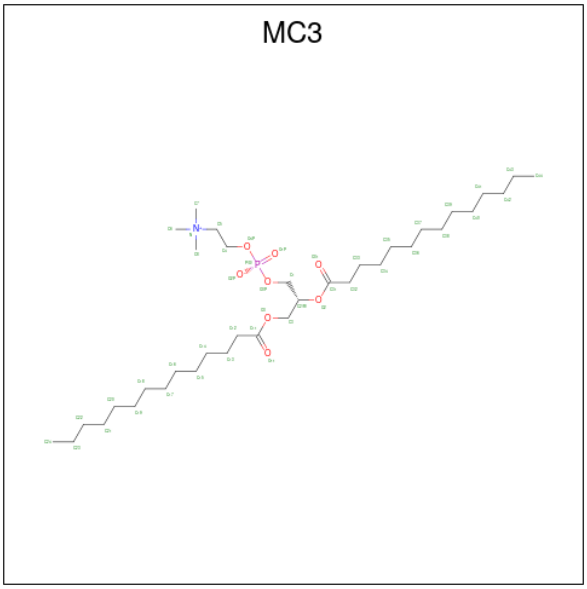
Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
1	R	184	Total	C	N	O	S	0	0
			1490	990	239	252	9		
1	S	184	Total	C	N	O	S	0	0
			1490	990	239	252	9		
1	T	184	Total	C	N	O	S	0	0
			1490	990	239	252	9		
1	V	184	Total	C	N	O	S	0	0
			1490	990	239	252	9		
1	W	184	Total	C	N	O	S	0	0
			1490	990	239	252	9		
1	X	184	Total	C	N	O	S	0	0
			1490	990	239	252	9		
1	Y	184	Total	C	N	O	S	0	0
			1490	990	239	252	9		

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	99	LEU	HIS	conflict	UNP F1MHI7
B	99	LEU	HIS	conflict	UNP F1MHI7
C	99	LEU	HIS	conflict	UNP F1MHI7
D	99	LEU	HIS	conflict	UNP F1MHI7
E	99	LEU	HIS	conflict	UNP F1MHI7
F	99	LEU	HIS	conflict	UNP F1MHI7
G	99	LEU	HIS	conflict	UNP F1MHI7
H	99	LEU	HIS	conflict	UNP F1MHI7
I	99	LEU	HIS	conflict	UNP F1MHI7
J	99	LEU	HIS	conflict	UNP F1MHI7
K	99	LEU	HIS	conflict	UNP F1MHI7
L	99	LEU	HIS	conflict	UNP F1MHI7
M	99	LEU	HIS	conflict	UNP F1MHI7
N	99	LEU	HIS	conflict	UNP F1MHI7
O	99	LEU	HIS	conflict	UNP F1MHI7
P	99	LEU	HIS	conflict	UNP F1MHI7
Q	99	LEU	HIS	conflict	UNP F1MHI7
R	99	LEU	HIS	conflict	UNP F1MHI7
S	99	LEU	HIS	conflict	UNP F1MHI7
T	99	LEU	HIS	conflict	UNP F1MHI7
V	99	LEU	HIS	conflict	UNP F1MHI7
W	99	LEU	HIS	conflict	UNP F1MHI7
X	99	LEU	HIS	conflict	UNP F1MHI7
Y	99	LEU	HIS	conflict	UNP F1MHI7

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



Mol	Chain	Residues	Atoms	AltConf
2	A	1	Total C 10 10	0
2	A	1	Total C N O P 46 36 1 8 1	0
2	A	1	Total C 13 13	0
2	A	1	Total C 13 13	0
2	A	1	Total C O 32 27 5	0
2	A	1	Total C N O P 37 27 1 8 1	0
2	A	1	Total C N O P 25 16 1 7 1	0
2	A	1	Total C 13 13	0
2	B	1	Total C 13 13	0
2	B	1	Total C 13 13	0
2	B	1	Total C N O P 45 35 1 8 1	0
2	B	1	Total C 13 13	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
2	B	1	Total C 13 13	0
2	B	1	Total C 13 13	0
2	C	1	Total C 13 13	0
2	C	1	Total C 13 13	0
2	C	1	Total C 13 13	0
2	C	1	Total C 13 13	0
2	C	1	Total C 13 13	0
2	C	1	Total C 11 11	0
2	C	1	Total C 13 13	0
2	D	1	Total C 13 13	0
2	D	1	Total C 13 13	0
2	D	1	Total C 13 13	0
2	D	1	Total C 13 13	0
2	D	1	Total C 13 13	0
2	D	1	Total C N O P 43 33 1 8 1	0
2	E	1	Total C 13 13	0
2	E	1	Total C 13 13	0
2	E	1	Total C O P 36 27 8 1	0
2	E	1	Total C 13 13	0
2	E	1	Total C 13 13	0
2	E	1	Total C N O P 44 34 1 8 1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
2	F	1	Total C 13 13	0
2	F	1	Total C 13 13	0
2	F	1	Total C 12 12	0
2	F	1	Total C 13 13	0
2	F	1	Total C 13 13	0
2	F	1	Total C O P 16 8 7 1	0
2	F	1	Total C 13 13	0
2	F	1	Total C 13 13	0
2	F	1	Total C O P 8 2 5 1	0
2	G	1	Total C 13 13	0
2	G	1	Total C 10 10	0
2	G	1	Total C N O P 46 36 1 8 1	0
2	G	1	Total C 13 13	0
2	G	1	Total C 13 13	0
2	G	1	Total C O 32 27 5	0
2	G	1	Total C N O P 37 27 1 8 1	0
2	G	1	Total C N O P 25 16 1 7 1	0
2	H	1	Total C 13 13	0
2	H	1	Total C 13 13	0
2	H	1	Total C N O P 45 35 1 8 1	0
2	H	1	Total C 13 13	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
2	H	1	Total C 13 13	0
2	H	1	Total C 13 13	0
2	I	1	Total C 13 13	0
2	I	1	Total C 13 13	0
2	I	1	Total C 13 13	0
2	I	1	Total C 13 13	0
2	I	1	Total C 13 13	0
2	I	1	Total C 11 11	0
2	I	1	Total C 13 13	0
2	J	1	Total C 13 13	0
2	J	1	Total C 13 13	0
2	J	1	Total C 13 13	0
2	J	1	Total C 13 13	0
2	J	1	Total C 13 13	0
2	J	1	Total C N O P 43 33 1 8 1	0
2	K	1	Total C 13 13	0
2	K	1	Total C 13 13	0
2	K	1	Total C O P 36 27 8 1	0
2	K	1	Total C 13 13	0
2	K	1	Total C 13 13	0
2	K	1	Total C N O P 44 34 1 8 1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
2	L	1	Total C O P 8 2 5 1	0
2	L	1	Total C 13 13	0
2	L	1	Total C 13 13	0
2	L	1	Total C 12 12	0
2	L	1	Total C 13 13	0
2	L	1	Total C 13 13	0
2	L	1	Total C O P 16 8 7 1	0
2	L	1	Total C 13 13	0
2	L	1	Total C 13 13	0
2	M	1	Total C 10 10	0
2	M	1	Total C N O P 46 36 1 8 1	0
2	M	1	Total C 13 13	0
2	M	1	Total C 13 13	0
2	M	1	Total C O 32 27 5	0
2	M	1	Total C N O P 37 27 1 8 1	0
2	M	1	Total C N O P 25 16 1 7 1	0
2	M	1	Total C 13 13	0
2	N	1	Total C 13 13	0
2	N	1	Total C 13 13	0
2	N	1	Total C N O P 45 35 1 8 1	0
2	N	1	Total C 13 13	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
2	N	1	Total C 13 13	0
2	N	1	Total C 13 13	0
2	O	1	Total C 13 13	0
2	O	1	Total C 13 13	0
2	O	1	Total C 13 13	0
2	O	1	Total C 13 13	0
2	O	1	Total C 13 13	0
2	O	1	Total C 11 11	0
2	O	1	Total C 13 13	0
2	P	1	Total C 13 13	0
2	P	1	Total C 13 13	0
2	P	1	Total C 13 13	0
2	P	1	Total C 13 13	0
2	P	1	Total C 13 13	0
2	P	1	Total C N O P 43 33 1 8 1	0
2	Q	1	Total C 13 13	0
2	Q	1	Total C 13 13	0
2	Q	1	Total C O P 36 27 8 1	0
2	Q	1	Total C 13 13	0
2	Q	1	Total C 13 13	0
2	Q	1	Total C N O P 44 34 1 8 1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
2	R	1	Total C 13 13	0
2	R	1	Total C 13 13	0
2	R	1	Total C 12 12	0
2	R	1	Total C 13 13	0
2	R	1	Total C 13 13	0
2	R	1	Total C O P 16 8 7 1	0
2	R	1	Total C 13 13	0
2	R	1	Total C 13 13	0
2	R	1	Total C O P 8 2 5 1	0
2	S	1	Total C 13 13	0
2	S	1	Total C 10 10	0
2	S	1	Total C N O P 46 36 1 8 1	0
2	S	1	Total C 13 13	0
2	S	1	Total C 13 13	0
2	S	1	Total C O 32 27 5	0
2	S	1	Total C N O P 37 27 1 8 1	0
2	S	1	Total C N O P 25 16 1 7 1	0
2	T	1	Total C 13 13	0
2	T	1	Total C 13 13	0
2	T	1	Total C N O P 45 35 1 8 1	0
2	T	1	Total C 13 13	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
2	T	1	Total C 13 13	0
2	T	1	Total C 13 13	0
2	V	1	Total C 13 13	0
2	V	1	Total C 13 13	0
2	V	1	Total C 13 13	0
2	V	1	Total C 13 13	0
2	V	1	Total C 13 13	0
2	V	1	Total C 11 11	0
2	V	1	Total C 13 13	0
2	W	1	Total C 13 13	0
2	W	1	Total C 13 13	0
2	W	1	Total C 13 13	0
2	W	1	Total C 13 13	0
2	W	1	Total C 13 13	0
2	W	1	Total C N O P 43 33 1 8 1	0
2	X	1	Total C 13 13	0
2	X	1	Total C 13 13	0
2	X	1	Total C O P 36 27 8 1	0
2	X	1	Total C 13 13	0
2	X	1	Total C 13 13	0
2	X	1	Total C N O P 44 34 1 8 1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
2	Y	1	Total C O P 8 2 5 1	0
2	Y	1	Total C 13 13	0
2	Y	1	Total C 13 13	0
2	Y	1	Total C 12 12	0
2	Y	1	Total C 13 13	0
2	Y	1	Total C 13 13	0
2	Y	1	Total C O P 16 8 7 1	0
2	Y	1	Total C 13 13	0
2	Y	1	Total C 13 13	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	AltConf
3	A	3	Total O 3 3	0
3	B	6	Total O 6 6	0
3	C	10	Total O 10 10	0
3	D	13	Total O 13 13	0
3	E	3	Total O 3 3	0
3	F	1	Total O 1 1	0
3	G	3	Total O 3 3	0
3	H	6	Total O 6 6	0
3	I	10	Total O 10 10	0
3	J	13	Total O 13 13	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
3	K	3	Total O 3 3	0
3	L	1	Total O 1 1	0
3	M	3	Total O 3 3	0
3	N	6	Total O 6 6	0
3	O	10	Total O 10 10	0
3	P	13	Total O 13 13	0
3	Q	3	Total O 3 3	0
3	R	1	Total O 1 1	0
3	S	3	Total O 3 3	0
3	T	6	Total O 6 6	0
3	V	10	Total O 10 10	0
3	W	13	Total O 13 13	0
3	X	3	Total O 3 3	0
3	Y	1	Total O 1 1	0

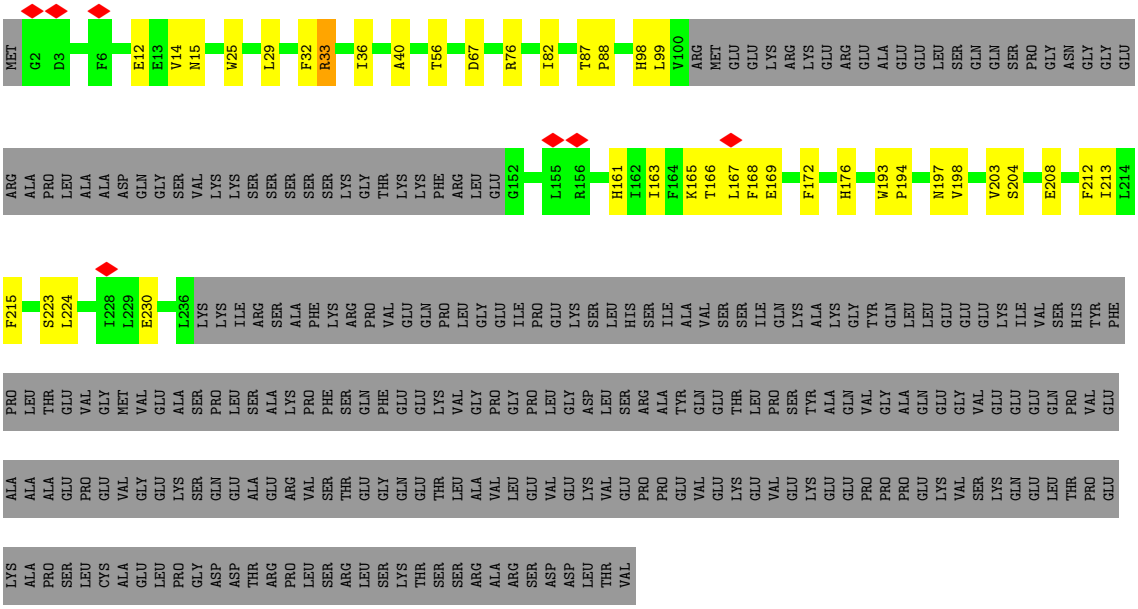
3 Residue-property plots (i)

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

• Molecule 1: Gap junction protein

Chain A:

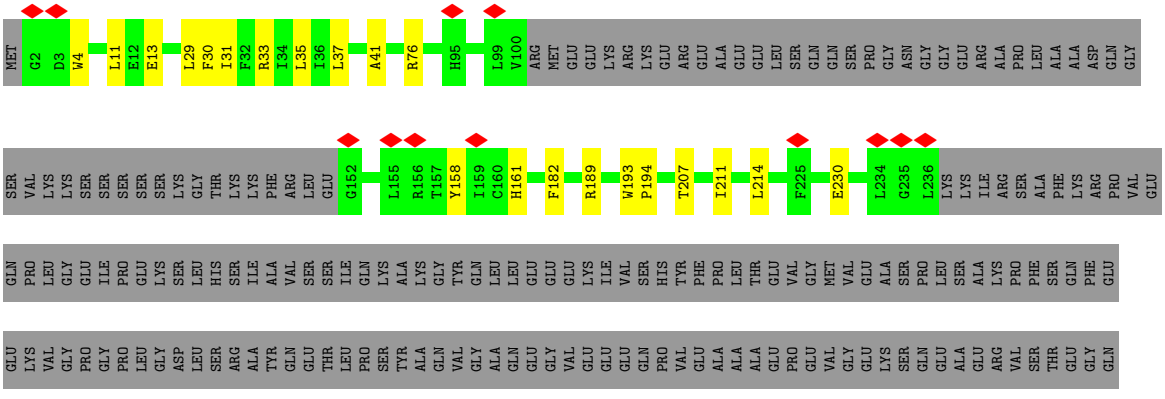


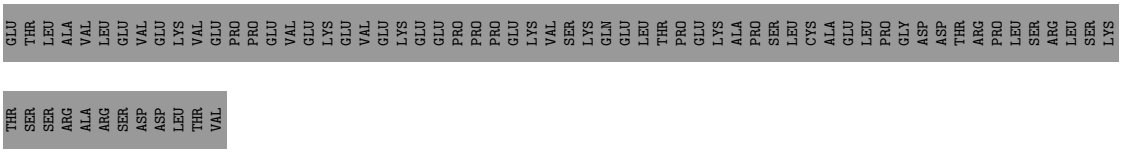


• Molecule 1: Gap junction protein

Chain B:



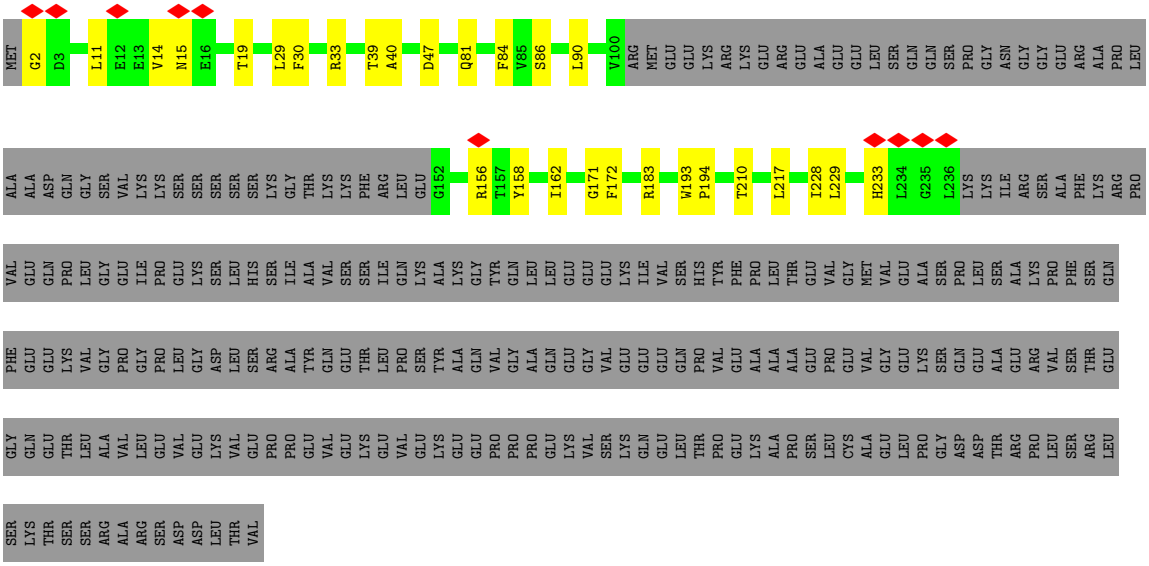




• Molecule 1: Gap junction protein

Chain C:

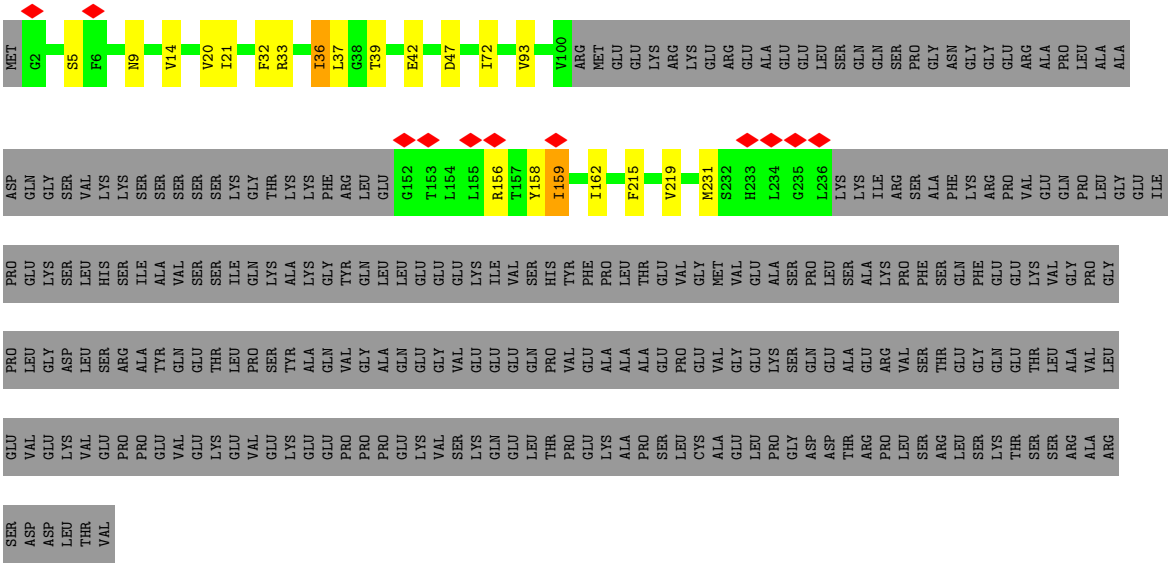




• Molecule 1: Gap junction protein

Chain D:

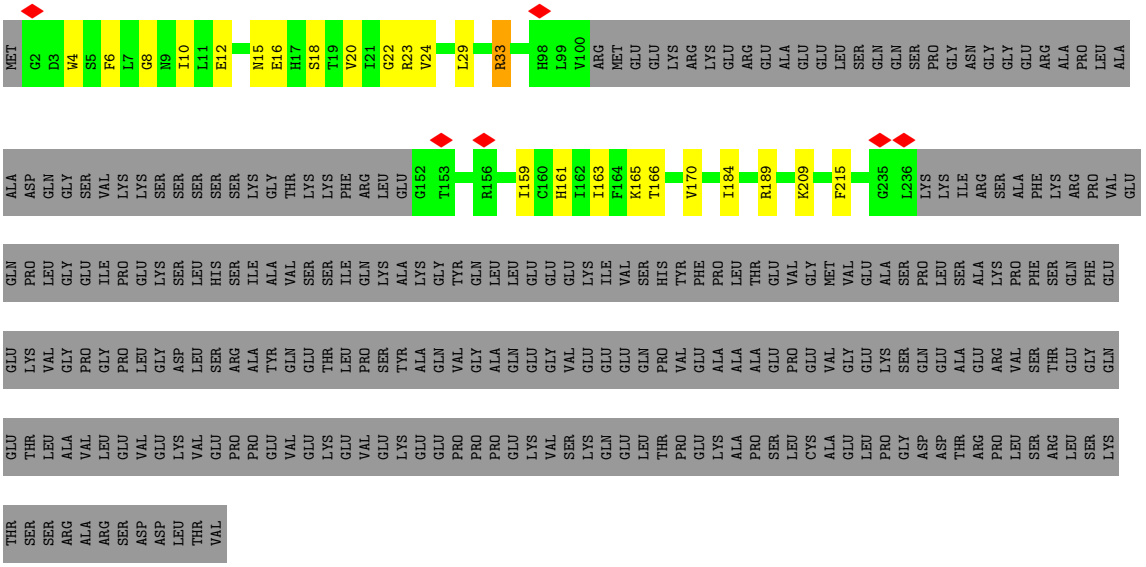




• Molecule 1: Gap junction protein

Chain E:

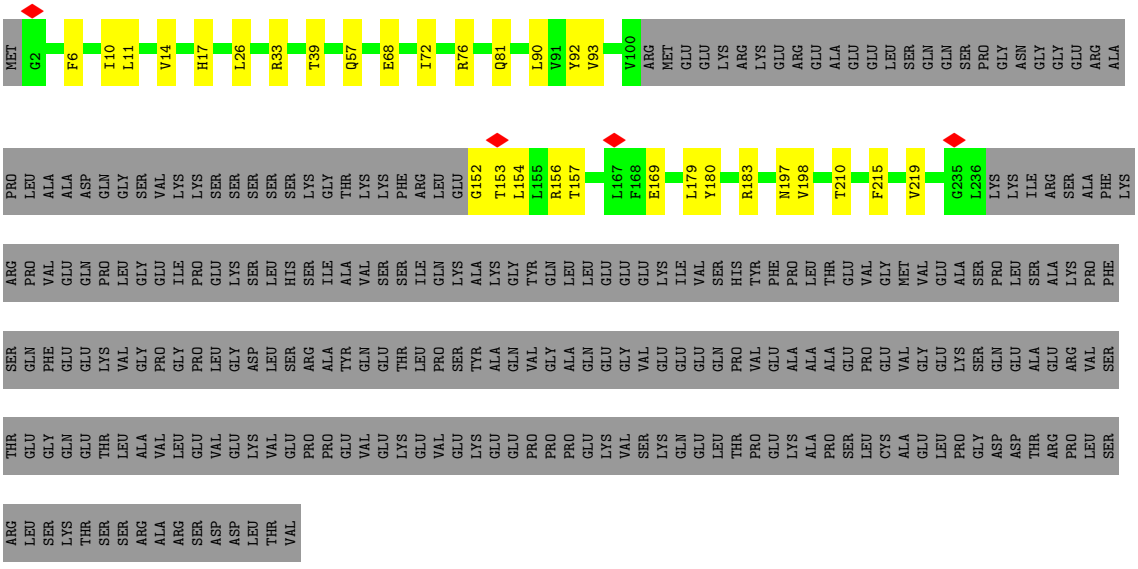




• Molecule 1: Gap junction protein

Chain F:

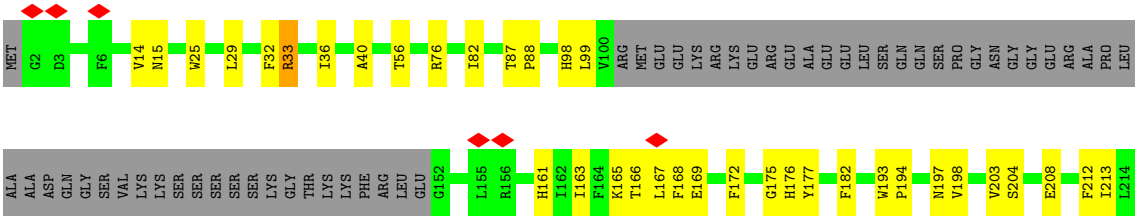


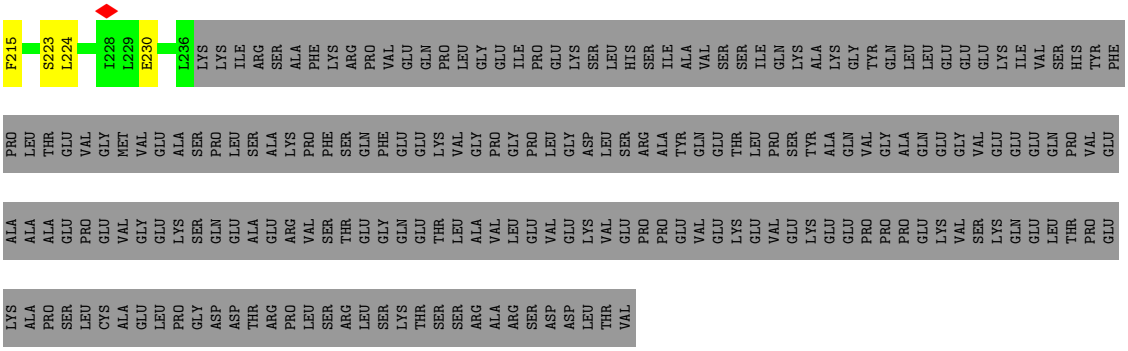


• Molecule 1: Gap junction protein

Chain G:



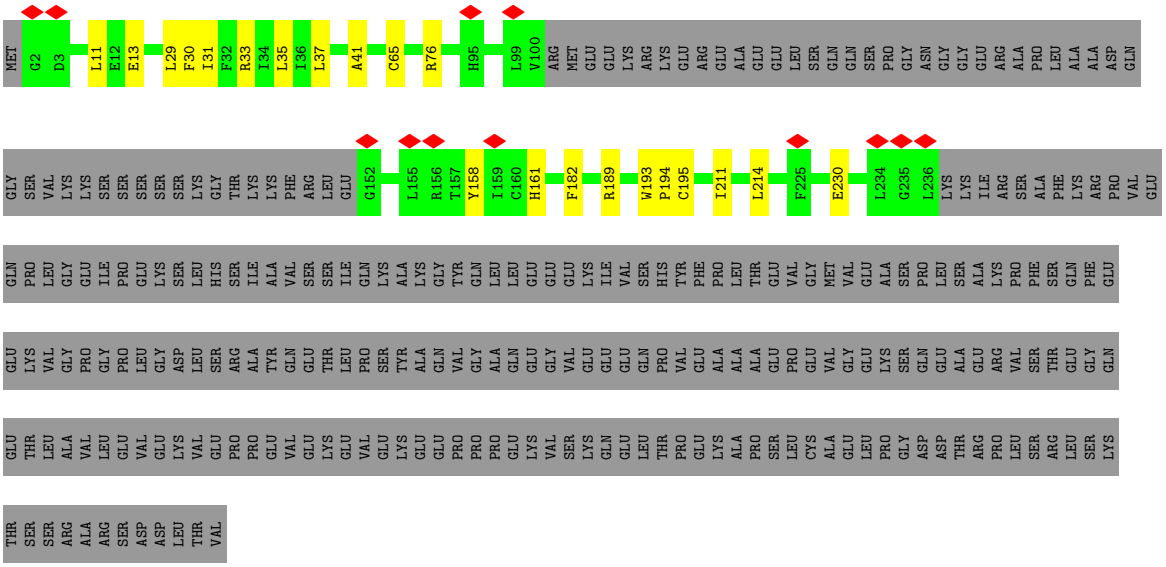




• Molecule 1: Gap junction protein

Chain H:

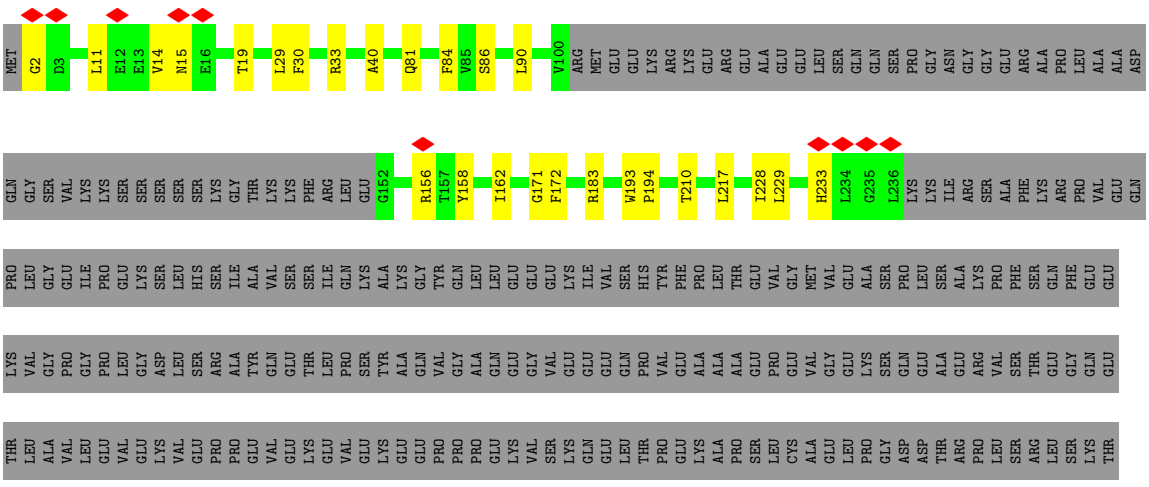




• Molecule 1: Gap junction protein

Chain I:



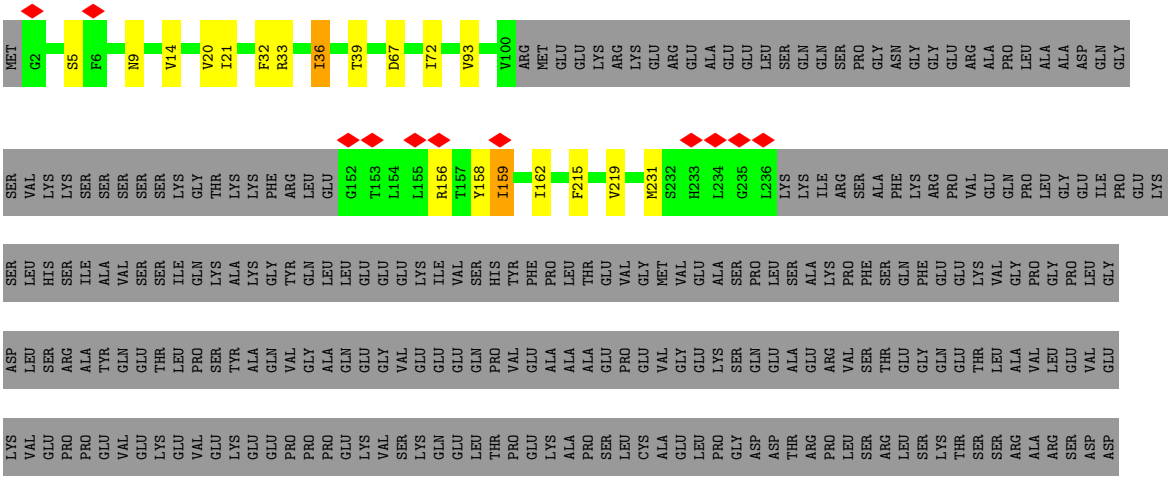




• Molecule 1: Gap junction protein

Chain J:

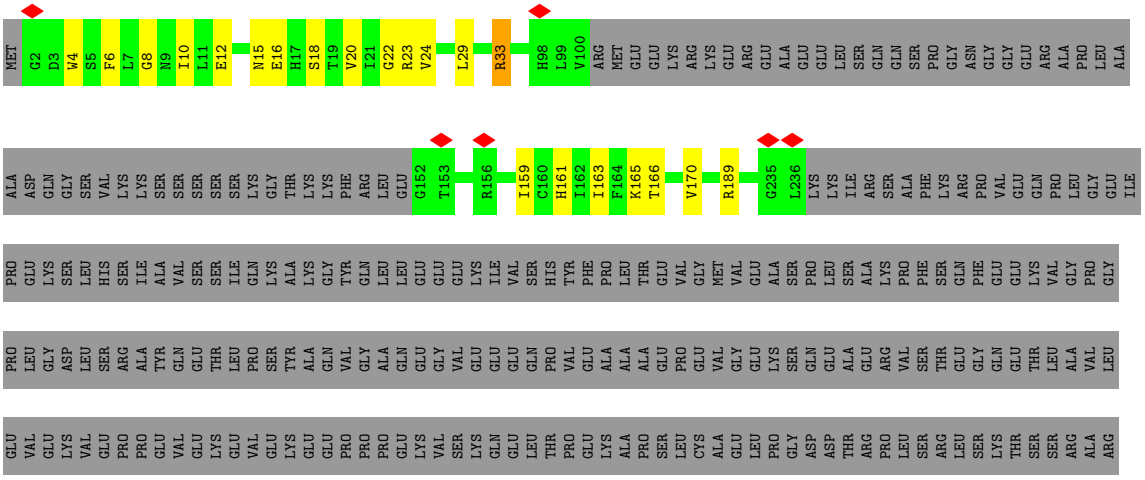




• Molecule 1: Gap junction protein

Chain K:

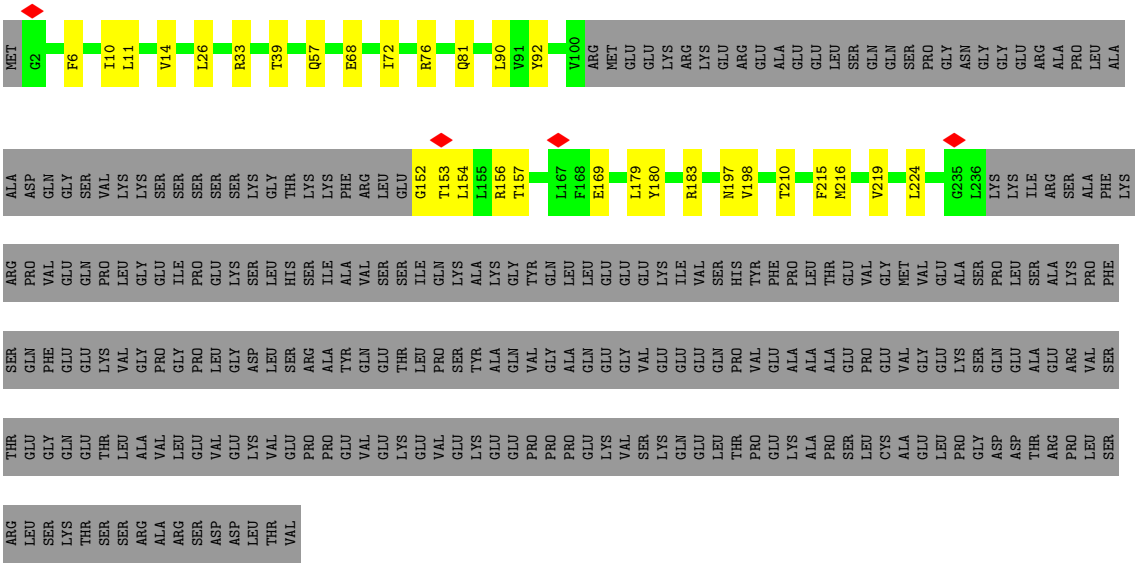




• Molecule 1: Gap junction protein

Chain L:

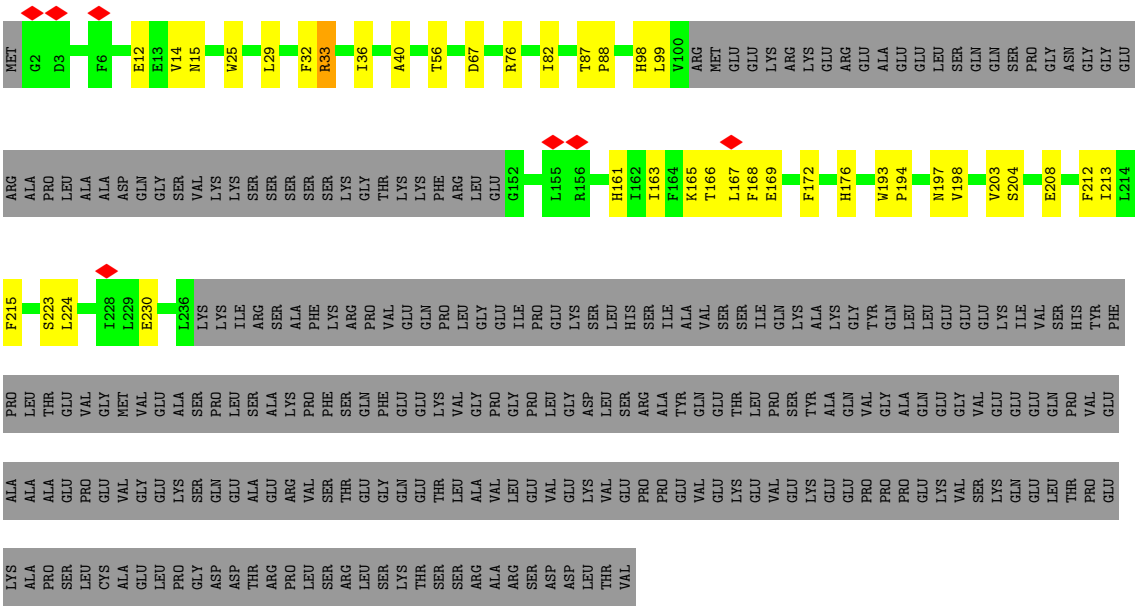




• Molecule 1: Gap junction protein

Chain M:

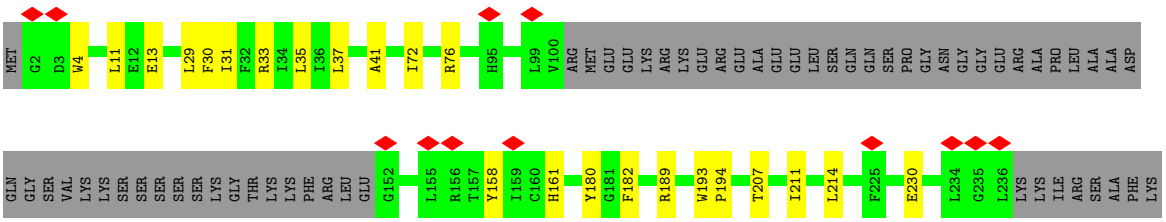


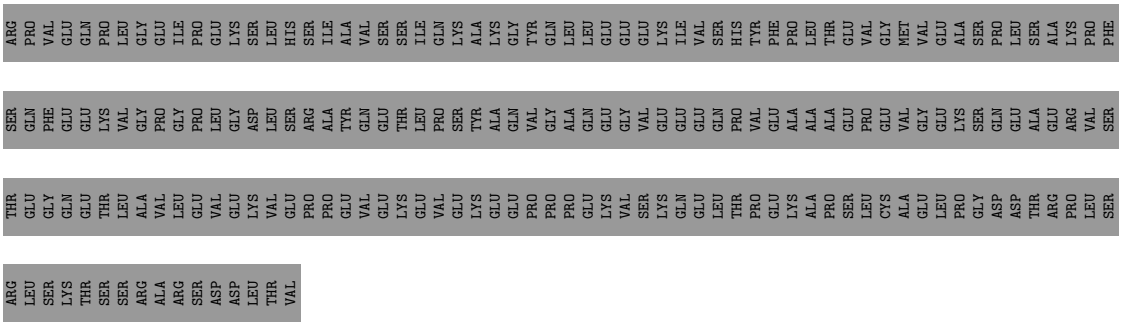


• Molecule 1: Gap junction protein

Chain N:



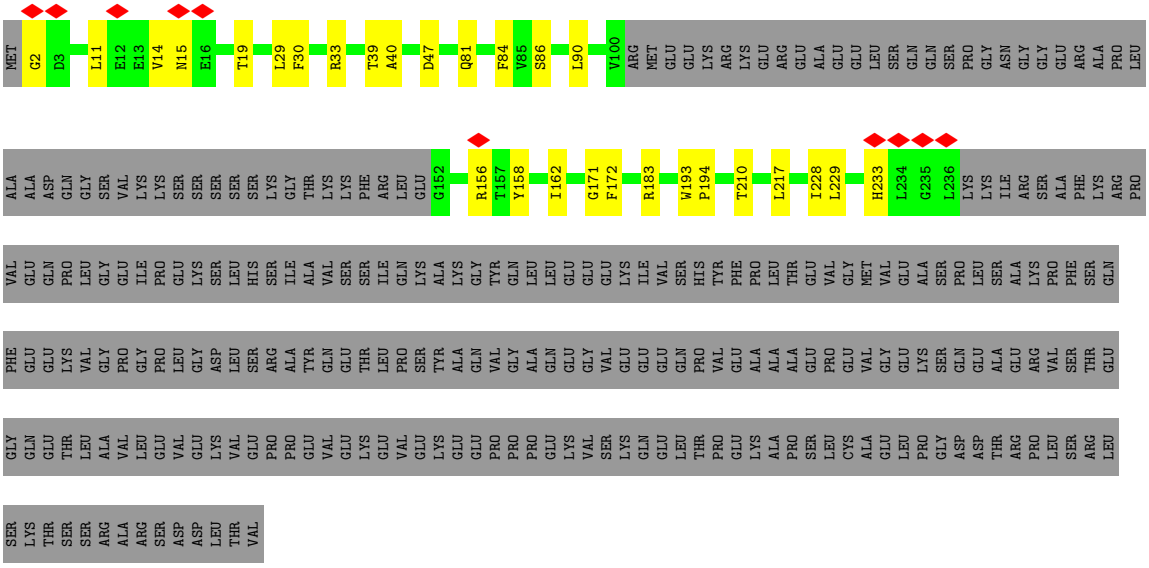




• Molecule 1: Gap junction protein

Chain O:

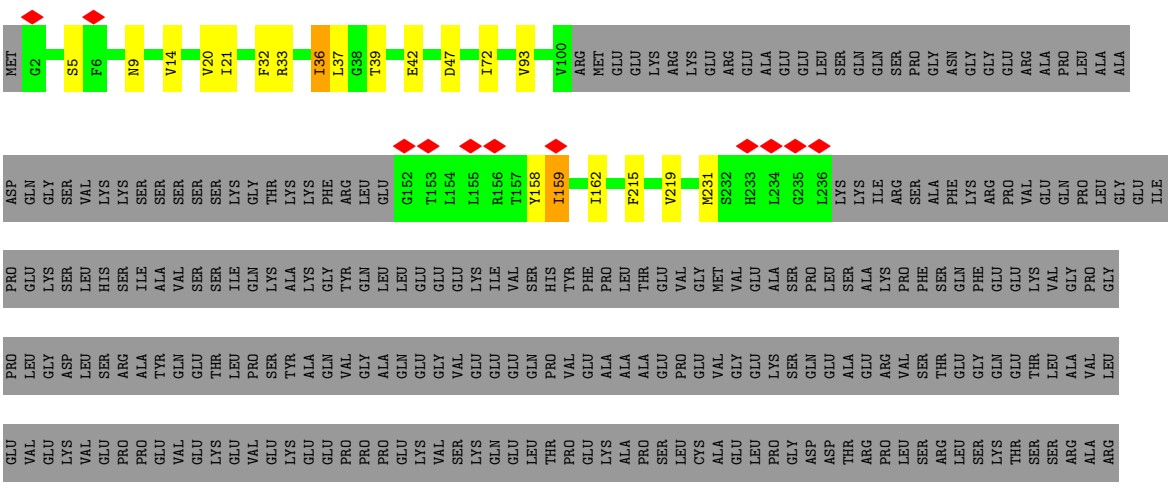




• Molecule 1: Gap junction protein

Chain P:



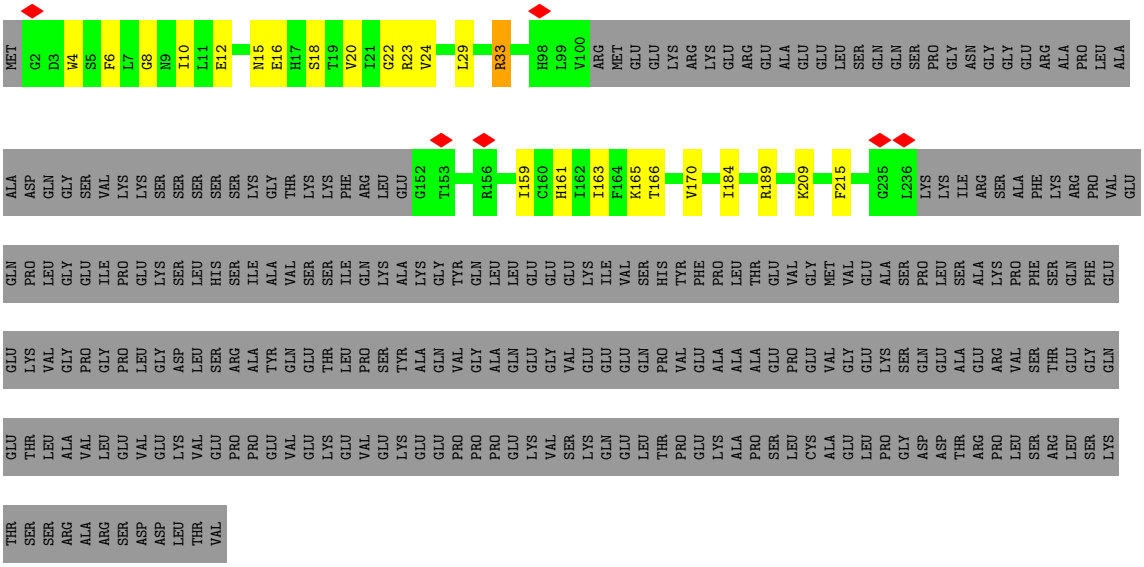




• Molecule 1: Gap junction protein

Chain Q:

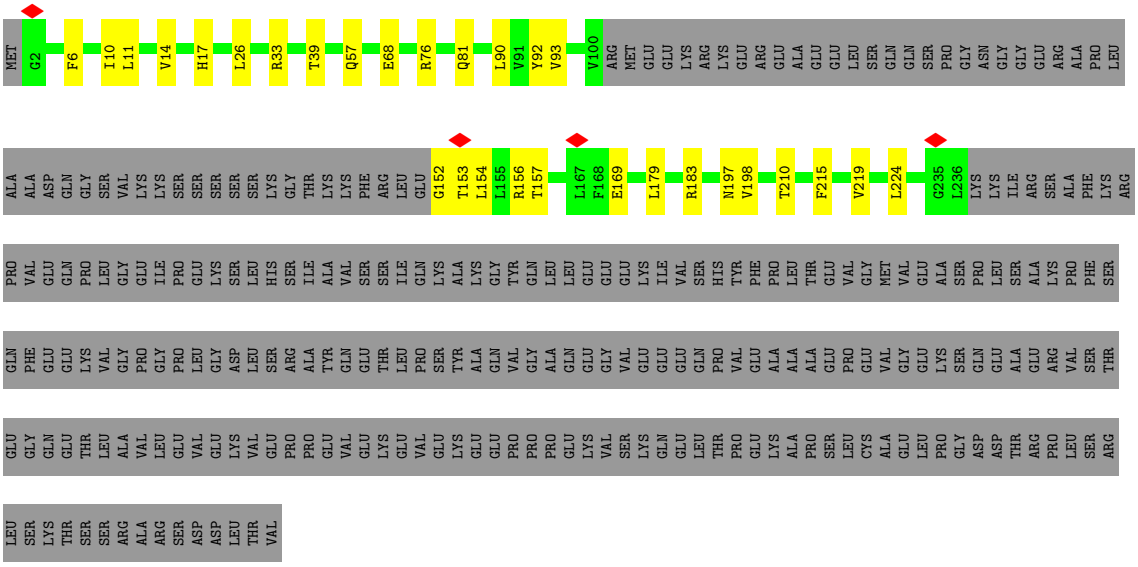




• Molecule 1: Gap junction protein

Chain R:

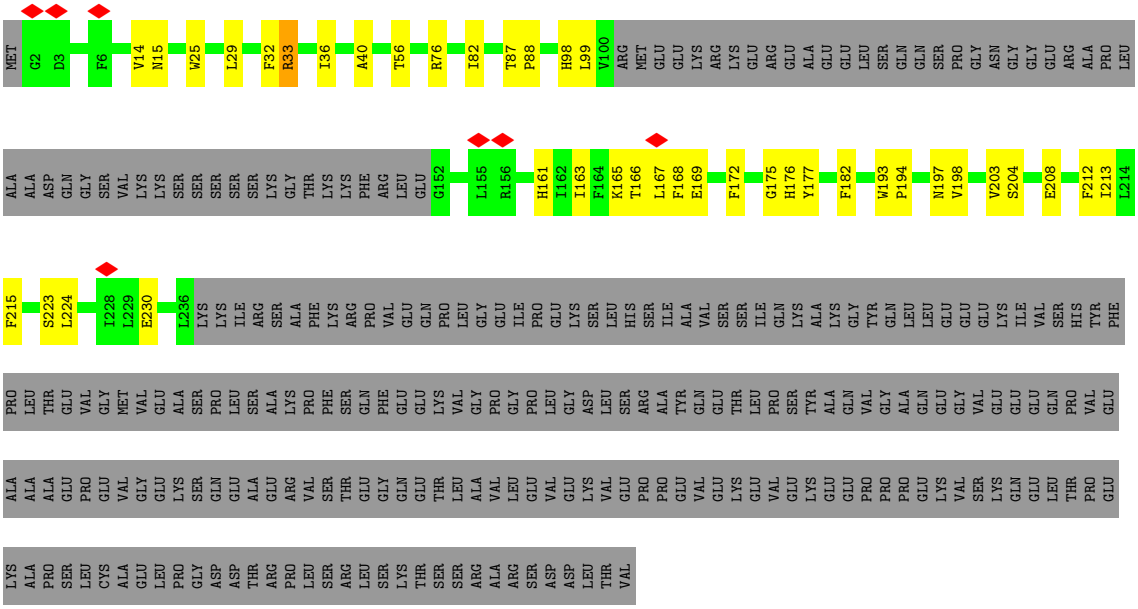




• Molecule 1: Gap junction protein

Chain S:

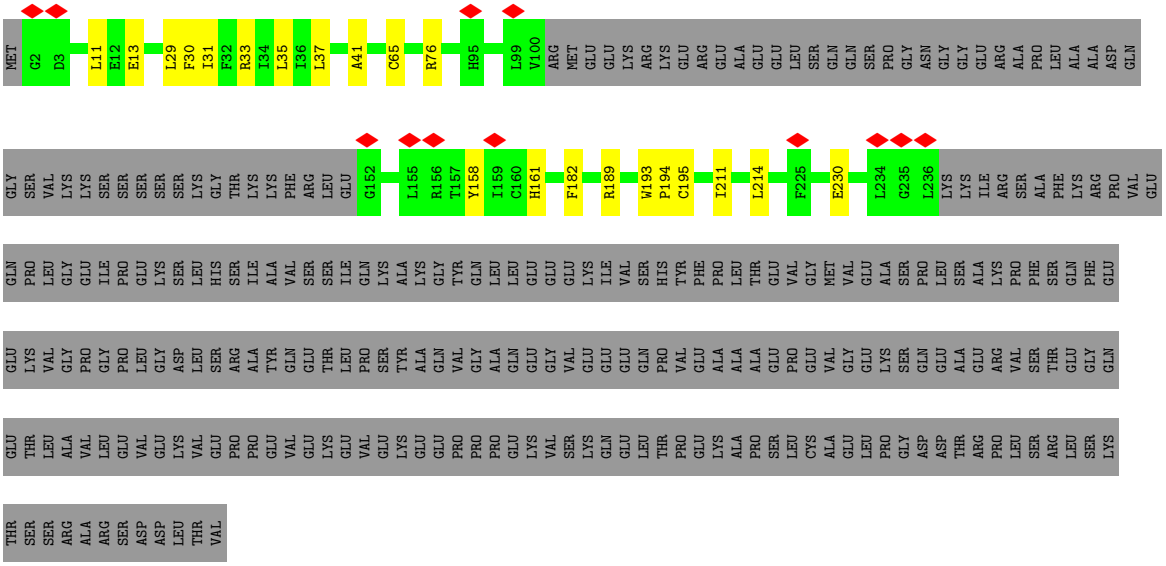




• Molecule 1: Gap junction protein

Chain T:

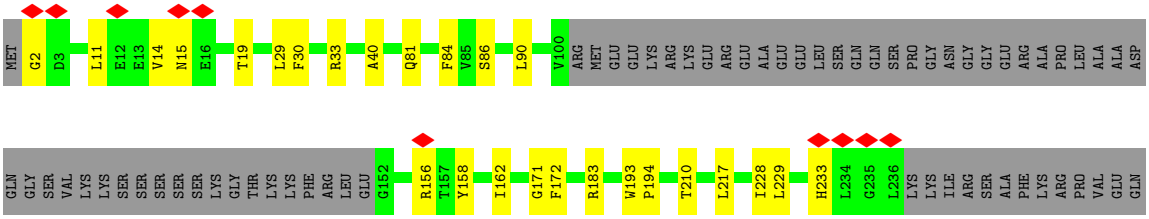


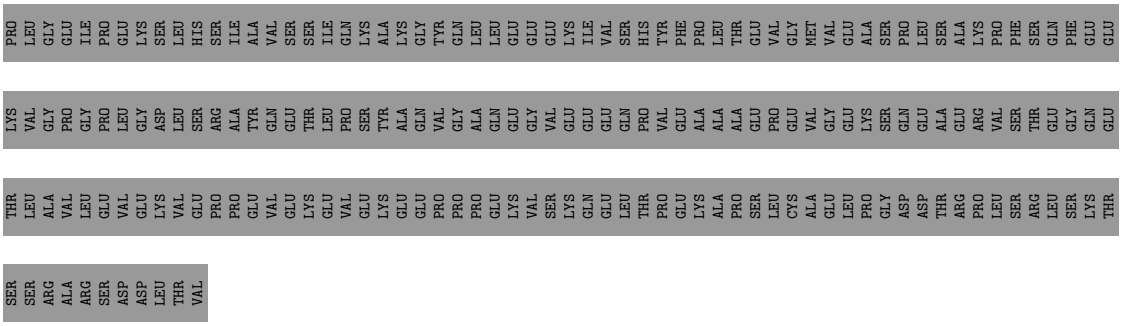


• Molecule 1: Gap junction protein

Chain V:



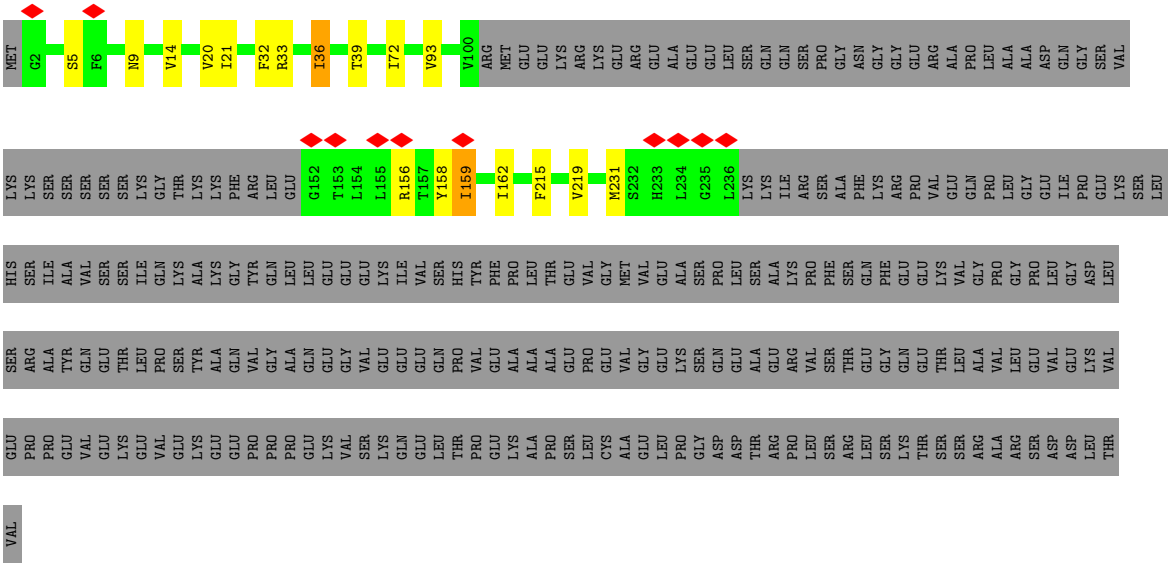




• Molecule 1: Gap junction protein

Chain W:

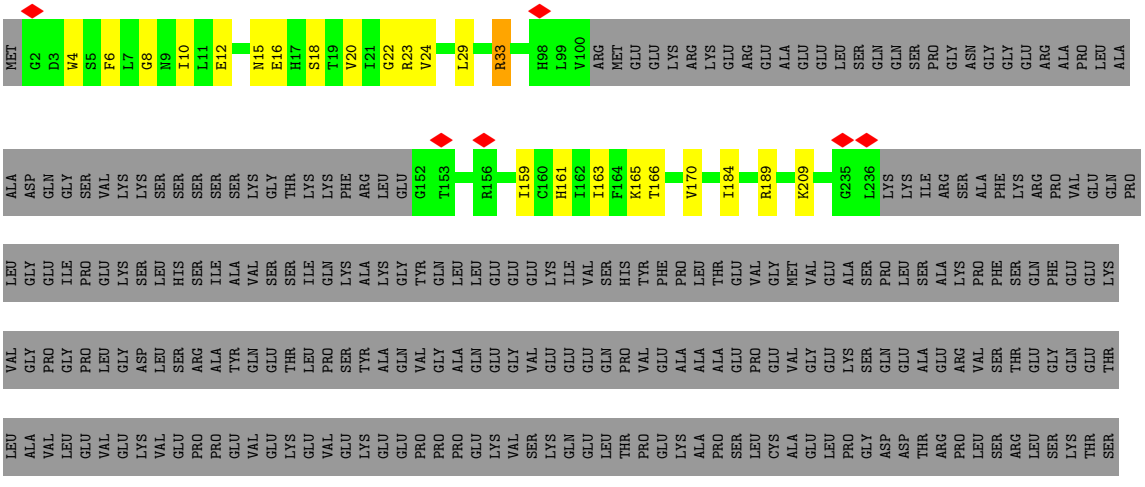




• Molecule 1: Gap junction protein

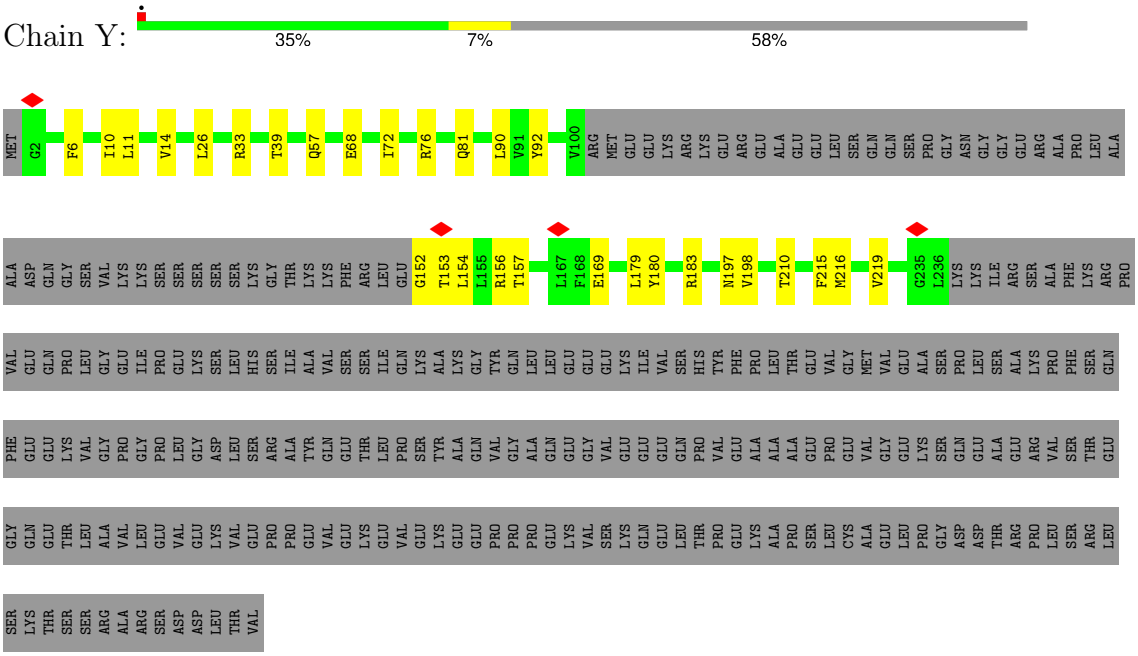
Chain X:







• Molecule 1: Gap junction protein



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, D2	Depositor
Number of particles used	64687	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOCONTINUUM (6k x 4k)	Depositor
Maximum map value	4.540	Depositor
Minimum map value	-2.617	Depositor
Average map value	0.015	Depositor
Map value standard deviation	0.110	Depositor
Recommended contour level	0.65	Depositor
Map size (Å)	358.56, 358.56, 358.56	wwPDB
Map dimensions	432, 432, 432	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83, 0.83, 0.83	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.83	0/1534	1.09	0/2092
1	B	0.71	0/1534	0.94	0/2092
1	C	0.65	0/1534	0.82	0/2092
1	D	0.67	0/1534	0.82	0/2092
1	E	0.78	0/1534	0.97	0/2092
1	F	0.68	0/1534	0.89	0/2092
1	G	0.83	0/1534	1.09	0/2092
1	H	0.71	0/1534	0.94	0/2092
1	I	0.65	0/1534	0.82	0/2092
1	J	0.67	0/1534	0.82	0/2092
1	K	0.78	0/1534	0.97	0/2092
1	L	0.68	0/1534	0.89	0/2092
1	M	0.83	0/1534	1.09	0/2092
1	N	0.71	0/1534	0.94	0/2092
1	O	0.65	0/1534	0.82	0/2092
1	P	0.67	0/1534	0.82	0/2092
1	Q	0.78	0/1534	0.97	0/2092
1	R	0.68	0/1534	0.89	0/2092
1	S	0.83	0/1534	1.09	0/2092
1	T	0.71	0/1534	0.94	0/2092
1	V	0.65	0/1534	0.82	0/2092
1	W	0.67	0/1534	0.82	0/2092
1	X	0.78	0/1534	0.97	0/2092
1	Y	0.68	0/1534	0.89	0/2092
All	All	0.72	0/36816	0.93	0/50208

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	1
1	C	0	1
1	D	0	1
1	E	0	2
1	F	0	1
1	G	0	2
1	H	0	1
1	I	0	1
1	J	0	1
1	K	0	2
1	L	0	1
1	M	0	2
1	N	0	1
1	O	0	1
1	P	0	1
1	Q	0	2
1	R	0	1
1	S	0	2
1	T	0	1
1	V	0	1
1	W	0	1
1	X	0	2
1	Y	0	1
All	All	0	32

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (32) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	33	ARG	Sidechain
1	A	76	ARG	Sidechain
1	B	189	ARG	Sidechain
1	C	156	ARG	Sidechain
1	D	33	ARG	Sidechain
1	E	189	ARG	Sidechain
1	E	33	ARG	Sidechain
1	F	33	ARG	Sidechain
1	G	33	ARG	Sidechain
1	G	76	ARG	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	H	189	ARG	Sidechain
1	I	156	ARG	Sidechain
1	J	33	ARG	Sidechain
1	K	189	ARG	Sidechain
1	K	33	ARG	Sidechain
1	L	33	ARG	Sidechain
1	M	33	ARG	Sidechain
1	M	76	ARG	Sidechain
1	N	189	ARG	Sidechain
1	O	156	ARG	Sidechain
1	P	33	ARG	Sidechain
1	Q	189	ARG	Sidechain
1	Q	33	ARG	Sidechain
1	R	33	ARG	Sidechain
1	S	33	ARG	Sidechain
1	S	76	ARG	Sidechain
1	T	189	ARG	Sidechain
1	V	156	ARG	Sidechain
1	W	33	ARG	Sidechain
1	X	189	ARG	Sidechain
1	X	33	ARG	Sidechain
1	Y	33	ARG	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1490	0	1480	28	0
1	B	1490	0	1480	11	0
1	C	1490	0	1480	19	0
1	D	1490	0	1480	10	0
1	E	1490	0	1480	14	0
1	F	1490	0	1480	20	0
1	G	1490	0	1480	28	0
1	H	1490	0	1480	10	0
1	I	1490	0	1480	17	0
1	J	1490	0	1480	9	0
1	K	1490	0	1480	12	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L	1490	0	1480	21	0
1	M	1490	0	1480	28	0
1	N	1490	0	1480	12	0
1	O	1490	0	1480	19	0
1	P	1490	0	1480	9	0
1	Q	1490	0	1480	14	0
1	R	1490	0	1480	20	0
1	S	1490	0	1480	28	0
1	T	1490	0	1480	10	0
1	V	1490	0	1480	17	0
1	W	1490	0	1480	8	0
1	X	1490	0	1480	13	0
1	Y	1490	0	1480	20	0
2	A	189	0	292	7	0
2	B	110	0	192	4	0
2	C	89	0	171	2	0
2	D	108	0	188	0	0
2	E	132	0	210	3	0
2	F	114	0	182	2	0
2	G	189	0	292	8	0
2	H	110	0	192	3	0
2	I	89	0	171	2	0
2	J	108	0	188	2	0
2	K	132	0	210	3	0
2	L	114	0	182	2	0
2	M	189	0	292	7	0
2	N	110	0	192	5	0
2	O	89	0	171	2	0
2	P	108	0	188	0	0
2	Q	132	0	210	2	0
2	R	114	0	182	2	0
2	S	189	0	292	8	0
2	T	110	0	192	3	0
2	V	89	0	171	2	0
2	W	108	0	188	3	0
2	X	132	0	210	3	0
2	Y	114	0	182	2	0
3	A	3	0	0	0	0
3	B	6	0	0	0	0
3	C	10	0	0	0	0
3	D	13	0	0	0	0
3	E	3	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	1	0	0	0	0
3	G	3	0	0	0	0
3	H	6	0	0	0	0
3	I	10	0	0	0	0
3	J	13	0	0	1	0
3	K	3	0	0	0	0
3	L	1	0	0	0	0
3	M	3	0	0	0	0
3	N	6	0	0	0	0
3	O	10	0	0	0	0
3	P	13	0	0	0	0
3	Q	3	0	0	0	0
3	R	1	0	0	0	0
3	S	3	0	0	0	0
3	T	6	0	0	0	0
3	V	10	0	0	0	0
3	W	13	0	0	0	0
3	X	3	0	0	0	0
3	Y	1	0	0	0	0
All	All	38872	0	40460	398	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 5.

All (398) 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:K:12:GLU:HA	1:K:15:ASN:HD22	1.61	0.65
1:X:12:GLU:HA	1:X:15:ASN:HD22	1.61	0.65
1:Q:12:GLU:HA	1:Q:15:ASN:HD22	1.61	0.65
1:E:12:GLU:HA	1:E:15:ASN:HD22	1.61	0.65
1:K:16:GLU:HA	1:K:23:ARG:HH21	1.64	0.63
1:X:16:GLU:HA	1:X:23:ARG:HH21	1.64	0.63
1:E:16:GLU:HA	1:E:23:ARG:HH21	1.64	0.63
1:Q:16:GLU:HA	1:Q:23:ARG:HH21	1.64	0.62
1:O:81:GLN:HG3	1:O:172:PHE:CD2	2.35	0.62
1:C:81:GLN:HG3	1:C:172:PHE:CD2	2.35	0.62
1:I:81:GLN:HG3	1:I:172:PHE:CD2	2.35	0.61
1:V:81:GLN:HG3	1:V:172:PHE:CD2	2.35	0.60
1:K:6:PHE:O	1:K:10:ILE:HG13	2.02	0.59
1:X:6:PHE:O	1:X:10:ILE:HG13	2.02	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:6:PHE:O	1:E:10:ILE:HG13	2.02	0.58
1:Q:6:PHE:O	1:Q:10:ILE:HG13	2.02	0.58
1:F:14:VAL:HG13	1:F:26:LEU:HD11	1.86	0.57
1:R:14:VAL:HG13	1:R:26:LEU:HD11	1.86	0.57
1:Y:14:VAL:HG13	1:Y:26:LEU:HD11	1.86	0.57
1:L:14:VAL:HG13	1:L:26:LEU:HD11	1.86	0.57
1:F:198:VAL:HB	1:M:197:ASN:HD22	1.72	0.54
1:A:197:ASN:HD22	1:R:198:VAL:HB	1.72	0.54
1:L:198:VAL:HB	1:S:197:ASN:HD22	1.72	0.54
1:G:197:ASN:HD22	1:Y:198:VAL:HB	1.72	0.54
1:I:81:GLN:HG3	1:I:172:PHE:CG	2.43	0.54
1:V:81:GLN:HG3	1:V:172:PHE:CG	2.43	0.54
1:O:81:GLN:HG3	1:O:172:PHE:CG	2.43	0.53
1:C:81:GLN:HG3	1:C:172:PHE:CG	2.43	0.53
1:G:198:VAL:HG12	1:Y:197:ASN:ND2	2.24	0.53
1:L:197:ASN:ND2	1:S:198:VAL:HG12	2.24	0.53
1:F:197:ASN:ND2	1:M:198:VAL:HG12	2.24	0.53
1:A:198:VAL:HG12	1:R:197:ASN:ND2	2.24	0.53
1:N:182:PHE:HB3	1:N:214:LEU:HD21	1.92	0.52
1:B:182:PHE:HB3	1:B:214:LEU:HD21	1.92	0.52
1:H:182:PHE:HB3	1:H:214:LEU:HD21	1.92	0.52
1:T:182:PHE:HB3	1:T:214:LEU:HD21	1.92	0.52
1:O:47:ASP:OD1	1:O:47:ASP:N	2.44	0.50
1:S:88:PRO:HB2	1:S:161:HIS:HB2	1.94	0.49
1:G:88:PRO:HB2	1:G:161:HIS:HB2	1.94	0.49
1:B:158:TYR:HA	1:B:161:HIS:HB3	1.95	0.48
1:M:88:PRO:HB2	1:M:161:HIS:HB2	1.94	0.48
1:A:88:PRO:HB2	1:A:161:HIS:HB2	1.94	0.48
1:N:158:TYR:HA	1:N:161:HIS:HB3	1.95	0.48
1:K:29:LEU:HA	1:K:33:ARG:HG3	1.96	0.47
1:X:29:LEU:HA	1:X:33:ARG:HG3	1.96	0.47
2:A:505:MC3:H341	2:A:505:MC3:H152	1.97	0.47
1:H:158:TYR:HA	1:H:161:HIS:HB3	1.95	0.47
2:M:505:MC3:H341	2:M:505:MC3:H152	1.97	0.47
1:G:172:PHE:CD1	2:G:503:MC3:H401	2.50	0.47
1:L:152:GLY:O	1:L:153:THR:C	2.57	0.47
1:L:156:ARG:NH1	2:L:501:MC3:O4P	2.48	0.47
1:S:172:PHE:CD1	2:S:503:MC3:H401	2.50	0.47
1:T:158:TYR:HA	1:T:161:HIS:HB3	1.95	0.47
1:Y:152:GLY:O	1:Y:153:THR:C	2.57	0.47
1:Y:156:ARG:NH1	2:Y:501:MC3:O4P	2.48	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:506:MC3:H62	2:K:506:MC3:H41	1.72	0.47
1:C:84:PHE:HB2	1:C:172:PHE:CZ	2.50	0.47
1:F:156:ARG:NH1	2:F:509:MC3:O4P	2.48	0.47
1:I:84:PHE:HB2	1:I:172:PHE:CZ	2.50	0.47
1:V:84:PHE:HB2	1:V:172:PHE:CZ	2.50	0.47
2:N:503:MC3:H341	2:N:503:MC3:H371	1.78	0.46
1:O:84:PHE:HB2	1:O:172:PHE:CZ	2.50	0.46
1:R:156:ARG:NH1	2:R:509:MC3:O4P	2.48	0.46
1:I:11:LEU:HB2	1:I:30:PHE:HZ	1.81	0.46
1:V:11:LEU:HB2	1:V:30:PHE:HZ	1.81	0.46
1:C:19:THR:HB	1:C:233:HIS:HE1	1.80	0.46
1:E:29:LEU:HA	1:E:33:ARG:HG3	1.96	0.46
1:H:193:TRP:CG	1:H:194:PRO:HA	2.51	0.46
1:Q:29:LEU:HA	1:Q:33:ARG:HG3	1.96	0.46
1:A:172:PHE:CD1	2:A:502:MC3:H401	2.50	0.46
1:G:40:ALA:HB1	1:L:76:ARG:HG3	1.98	0.46
1:M:172:PHE:CD1	2:M:502:MC3:H401	2.50	0.46
1:S:40:ALA:HB1	1:Y:76:ARG:HG3	1.98	0.46
2:X:506:MC3:H62	2:X:506:MC3:H41	1.72	0.46
2:B:503:MC3:H341	2:B:503:MC3:H371	1.78	0.46
1:O:19:THR:HB	1:O:233:HIS:HE1	1.80	0.46
1:T:193:TRP:CG	1:T:194:PRO:HA	2.51	0.46
2:G:506:MC3:H341	2:G:506:MC3:H152	1.97	0.46
1:R:152:GLY:O	1:R:153:THR:C	2.57	0.46
2:S:506:MC3:H341	2:S:506:MC3:H152	1.97	0.46
1:A:215:PHE:HA	2:A:505:MC3:H412	1.98	0.46
1:F:152:GLY:O	1:F:153:THR:C	2.57	0.46
1:M:215:PHE:HA	2:M:505:MC3:H412	1.98	0.46
1:S:215:PHE:HA	2:S:506:MC3:H412	1.98	0.46
1:C:11:LEU:HB2	1:C:30:PHE:HZ	1.81	0.46
1:G:215:PHE:HA	2:G:506:MC3:H412	1.98	0.46
1:O:11:LEU:HB2	1:O:30:PHE:HZ	1.81	0.46
1:A:40:ALA:HB1	1:F:76:ARG:HG3	1.98	0.45
1:N:193:TRP:CG	1:N:194:PRO:HA	2.51	0.45
1:B:193:TRP:CG	1:B:194:PRO:HA	2.51	0.45
1:D:5:SER:O	1:D:9:ASN:ND2	2.49	0.45
1:M:40:ALA:HB1	1:R:76:ARG:HG3	1.98	0.45
1:G:25:TRP:HE1	1:G:223:SER:HB2	1.81	0.45
1:H:29:LEU:HA	1:H:33:ARG:HG3	1.97	0.45
1:M:98:HIS:O	1:M:99:LEU:C	2.59	0.45
1:P:5:SER:O	1:P:9:ASN:ND2	2.49	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:25:TRP:HE1	1:S:223:SER:HB2	1.81	0.45
1:G:176:HIS:HE1	1:G:213:ILE:HG23	1.82	0.45
1:M:25:TRP:HE1	1:M:223:SER:HB2	1.81	0.45
1:S:98:HIS:O	1:S:99:LEU:C	2.59	0.45
1:S:176:HIS:HE1	1:S:213:ILE:HG23	1.82	0.45
1:T:29:LEU:HA	1:T:33:ARG:HG3	1.97	0.45
1:A:98:HIS:O	1:A:99:LEU:C	2.59	0.45
1:D:159:ILE:HD12	1:D:159:ILE:HA	1.88	0.45
1:E:159:ILE:O	1:E:163:ILE:HG12	2.17	0.45
1:G:98:HIS:O	1:G:99:LEU:C	2.59	0.45
1:K:29:LEU:O	1:K:33:ARG:HB2	2.16	0.45
1:Q:29:LEU:O	1:Q:33:ARG:HB2	2.16	0.45
1:X:29:LEU:O	1:X:33:ARG:HB2	2.16	0.45
1:A:25:TRP:HE1	1:A:223:SER:HB2	1.81	0.45
1:I:183:ARG:HA	1:I:210:THR:HG23	1.99	0.45
1:Q:159:ILE:O	1:Q:163:ILE:HG12	2.17	0.45
1:V:183:ARG:HA	1:V:210:THR:HG23	1.99	0.45
1:E:29:LEU:O	1:E:33:ARG:HB2	2.16	0.45
1:B:29:LEU:HA	1:B:33:ARG:HG3	1.97	0.45
1:F:6:PHE:O	1:F:10:ILE:HG13	2.17	0.45
1:O:228:ILE:O	1:O:229:LEU:C	2.59	0.45
1:R:6:PHE:O	1:R:10:ILE:HG13	2.17	0.45
1:V:19:THR:HB	1:V:233:HIS:HE1	1.80	0.45
1:E:161:HIS:CE1	1:E:165:LYS:HD3	2.52	0.45
1:I:19:THR:HB	1:I:233:HIS:HE1	1.80	0.45
1:N:29:LEU:HA	1:N:33:ARG:HG3	1.97	0.45
1:Q:161:HIS:CE1	1:Q:165:LYS:HD3	2.52	0.45
1:C:228:ILE:O	1:C:229:LEU:C	2.59	0.45
1:G:163:ILE:O	1:G:167:LEU:HG	2.17	0.45
1:C:183:ARG:HA	1:C:210:THR:HG23	1.99	0.44
1:F:72:ILE:O	1:F:180:TYR:OH	2.26	0.44
1:O:183:ARG:HA	1:O:210:THR:HG23	1.99	0.44
1:P:159:ILE:HD12	1:P:159:ILE:HA	1.88	0.44
1:S:163:ILE:O	1:S:167:LEU:HG	2.17	0.44
1:Y:6:PHE:O	1:Y:10:ILE:HG13	2.17	0.44
1:L:6:PHE:O	1:L:10:ILE:HG13	2.17	0.44
1:M:161:HIS:O	1:M:165:LYS:N	2.45	0.44
1:D:158:TYR:O	1:D:162:ILE:HG13	2.18	0.44
1:P:158:TYR:O	1:P:162:ILE:HG13	2.18	0.44
1:X:159:ILE:O	1:X:163:ILE:HG12	2.17	0.44
1:J:158:TYR:O	1:J:162:ILE:HG13	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:193:TRP:CG	1:M:194:PRO:HA	2.53	0.44
1:S:193:TRP:CG	1:S:194:PRO:HA	2.53	0.44
1:W:158:TYR:O	1:W:162:ILE:HG13	2.18	0.44
1:A:32:PHE:HA	1:A:36:ILE:HG13	2.00	0.44
1:A:161:HIS:O	1:A:165:LYS:N	2.45	0.44
1:A:176:HIS:HE1	1:A:213:ILE:HG23	1.82	0.44
1:A:193:TRP:CG	1:A:194:PRO:HA	2.53	0.44
1:C:14:VAL:O	1:C:15:ASN:C	2.61	0.44
1:G:193:TRP:CG	1:G:194:PRO:HA	2.53	0.44
1:H:11:LEU:HB2	1:H:30:PHE:HZ	1.82	0.44
1:I:14:VAL:O	1:I:15:ASN:C	2.61	0.44
1:K:8:GLY:O	1:K:12:GLU:HG2	2.18	0.44
1:K:159:ILE:O	1:K:163:ILE:HG12	2.17	0.44
1:O:14:VAL:O	1:O:15:ASN:C	2.61	0.44
1:V:14:VAL:O	1:V:15:ASN:C	2.61	0.44
1:X:8:GLY:O	1:X:12:GLU:HG2	2.18	0.44
1:C:217:LEU:HD21	2:C:504:MC3:H391	2.00	0.44
1:J:5:SER:O	1:J:9:ASN:ND2	2.49	0.44
1:K:4:TRP:CZ2	1:L:39:THR:HG21	2.53	0.44
1:M:32:PHE:HA	1:M:36:ILE:HG13	2.00	0.44
1:N:11:LEU:HB2	1:N:30:PHE:HZ	1.82	0.44
1:O:217:LEU:HD21	2:O:504:MC3:H391	2.00	0.44
1:X:4:TRP:CZ2	1:Y:39:THR:HG21	2.53	0.44
1:A:87:THR:N	1:A:88:PRO:HD2	2.33	0.44
1:B:11:LEU:HB2	1:B:30:PHE:HZ	1.82	0.44
1:C:86:SER:O	1:C:90:LEU:HG	2.18	0.44
1:M:87:THR:N	1:M:88:PRO:HD2	2.33	0.44
1:M:176:HIS:HE1	1:M:213:ILE:HG23	1.82	0.44
1:T:11:LEU:HB2	1:T:30:PHE:HZ	1.82	0.44
1:A:29:LEU:HD11	1:A:82:ILE:HG23	1.99	0.44
2:E:506:MC3:H41	2:E:506:MC3:H62	1.72	0.44
1:O:86:SER:O	1:O:90:LEU:HG	2.18	0.44
1:W:5:SER:O	1:W:9:ASN:ND2	2.49	0.44
2:B:503:MC3:H391	2:B:503:MC3:H361	1.68	0.44
1:F:10:ILE:HG21	1:F:90:LEU:HD22	2.00	0.44
1:G:29:LEU:HD11	1:G:82:ILE:HG23	1.99	0.44
1:M:29:LEU:HD11	1:M:82:ILE:HG23	1.99	0.44
1:M:163:ILE:O	1:M:167:LEU:HG	2.17	0.44
1:Q:4:TRP:CZ2	1:R:39:THR:HG21	2.53	0.44
1:R:10:ILE:HG21	1:R:90:LEU:HD22	2.00	0.44
1:S:29:LEU:HD11	1:S:82:ILE:HG23	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:ILE:O	1:A:167:LEU:HG	2.17	0.43
1:E:4:TRP:CZ2	1:F:39:THR:HG21	2.53	0.43
1:I:217:LEU:HD21	2:I:504:MC3:H391	2.00	0.43
1:V:217:LEU:HD21	2:V:504:MC3:H391	2.00	0.43
1:I:29:LEU:O	1:I:33:ARG:HB2	2.18	0.43
1:K:161:HIS:CE1	1:K:165:LYS:HD3	2.52	0.43
1:L:154:LEU:HA	1:L:157:THR:HG22	2.00	0.43
2:N:503:MC3:H391	2:N:503:MC3:H361	1.68	0.43
1:V:2:GLY:HA3	1:W:39:THR:HG22	1.99	0.43
1:G:87:THR:N	1:G:88:PRO:HD2	2.33	0.43
1:H:37:LEU:HD12	1:H:41:ALA:HB3	2.01	0.43
1:T:37:LEU:HD12	1:T:41:ALA:HB3	2.01	0.43
1:V:29:LEU:O	1:V:33:ARG:HB2	2.18	0.43
1:Y:154:LEU:HA	1:Y:157:THR:HG22	2.00	0.43
1:A:176:HIS:CE1	1:A:213:ILE:HG23	2.53	0.43
1:E:8:GLY:O	1:E:12:GLU:HG2	2.18	0.43
1:M:176:HIS:CE1	1:M:213:ILE:HG23	2.53	0.43
1:X:161:HIS:CE1	1:X:165:LYS:HD3	2.52	0.43
1:Y:92:TYR:HD1	1:Y:157:THR:HG23	1.84	0.43
1:F:92:TYR:HD1	1:F:157:THR:HG23	1.84	0.43
1:I:2:GLY:HA3	1:J:39:THR:HG22	1.99	0.43
1:I:86:SER:O	1:I:90:LEU:HG	2.18	0.43
1:L:92:TYR:HD1	1:L:157:THR:HG23	1.84	0.43
1:O:29:LEU:O	1:O:33:ARG:HB2	2.18	0.43
1:Q:8:GLY:O	1:Q:12:GLU:HG2	2.18	0.43
1:R:92:TYR:HD1	1:R:157:THR:HG23	1.84	0.43
1:C:2:GLY:HA3	1:D:39:THR:HG22	1.99	0.43
1:C:29:LEU:O	1:C:33:ARG:HB2	2.18	0.43
1:F:154:LEU:HA	1:F:157:THR:HG22	2.00	0.43
1:O:2:GLY:HA3	1:P:39:THR:HG22	1.99	0.43
1:R:154:LEU:HA	1:R:157:THR:HG22	2.00	0.43
1:S:87:THR:N	1:S:88:PRO:HD2	2.33	0.43
1:S:161:HIS:O	1:S:165:LYS:N	2.45	0.43
1:V:11:LEU:HA	1:V:14:VAL:HG12	2.00	0.43
1:V:86:SER:O	1:V:90:LEU:HG	2.18	0.43
1:I:11:LEU:HA	1:I:14:VAL:HG12	2.00	0.43
2:E:506:MC3:H172	2:E:506:MC3:H372	2.01	0.43
1:G:32:PHE:HA	1:G:36:ILE:HG13	2.00	0.43
1:G:161:HIS:O	1:G:165:LYS:N	2.45	0.43
2:H:503:MC3:H391	2:H:503:MC3:H361	1.68	0.43
1:H:31:ILE:O	1:H:35:LEU:HB3	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:506:MC3:H172	2:Q:506:MC3:H372	2.01	0.43
1:T:31:ILE:O	1:T:35:LEU:HB3	2.19	0.43
1:V:228:ILE:O	1:V:229:LEU:C	2.59	0.43
1:G:56:THR:O	1:Y:57:GLN:NE2	2.52	0.43
1:L:57:GLN:NE2	1:S:56:THR:O	2.52	0.43
1:S:32:PHE:HA	1:S:36:ILE:HG13	2.00	0.43
1:X:18:SER:HB3	1:X:22:GLY:HA3	2.01	0.43
1:B:37:LEU:HD12	1:B:41:ALA:HB3	2.01	0.42
1:J:159:ILE:HD12	1:J:159:ILE:HA	1.88	0.42
1:K:18:SER:HB3	1:K:22:GLY:HA3	2.01	0.42
2:T:503:MC3:H361	2:T:503:MC3:H391	1.68	0.42
1:N:37:LEU:HD12	1:N:41:ALA:HB3	2.01	0.42
1:S:176:HIS:CE1	1:S:213:ILE:HG23	2.53	0.42
1:G:176:HIS:CE1	1:G:213:ILE:HG23	2.53	0.42
1:I:228:ILE:O	1:I:229:LEU:C	2.59	0.42
2:J:506:MC3:H361	2:J:506:MC3:H392	1.87	0.42
1:V:158:TYR:O	1:V:162:ILE:HG13	2.19	0.42
1:F:215:PHE:O	1:F:219:VAL:HG23	2.19	0.42
1:I:158:TYR:O	1:I:162:ILE:HG13	2.19	0.42
1:L:10:ILE:HG21	1:L:90:LEU:HD22	2.00	0.42
1:M:166:THR:C	1:M:168:PHE:N	2.77	0.42
1:R:215:PHE:O	1:R:219:VAL:HG23	2.19	0.42
1:Y:10:ILE:HG21	1:Y:90:LEU:HD22	2.00	0.42
1:A:166:THR:C	1:A:168:PHE:N	2.77	0.42
1:N:211:ILE:HG12	2:N:503:MC3:H132	2.02	0.42
2:N:503:MC3:H172	2:N:503:MC3:H141	1.85	0.42
1:O:11:LEU:HA	1:O:14:VAL:HG12	2.00	0.42
1:W:159:ILE:HD12	1:W:159:ILE:HA	1.88	0.42
1:B:211:ILE:HG12	2:B:503:MC3:H132	2.02	0.42
1:C:11:LEU:HA	1:C:14:VAL:HG12	2.00	0.42
1:C:158:TYR:O	1:C:162:ILE:HG13	2.19	0.42
2:L:506:MC3:H341	2:L:508:MC3:H442	2.02	0.42
1:P:215:PHE:O	1:P:219:VAL:HG23	2.19	0.42
1:S:169:GLU:HB2	1:S:224:LEU:HD21	2.01	0.42
1:A:56:THR:O	1:R:57:GLN:NE2	2.52	0.42
1:A:169:GLU:HB2	1:A:224:LEU:HD21	2.01	0.42
1:A:208:GLU:O	1:A:212:PHE:HD1	2.02	0.42
1:B:31:ILE:O	1:B:35:LEU:HB3	2.19	0.42
1:G:169:GLU:HB2	1:G:224:LEU:HD21	2.01	0.42
1:L:198:VAL:HB	1:S:197:ASN:ND2	2.35	0.42
1:N:31:ILE:O	1:N:35:LEU:HB3	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:158:TYR:O	1:O:162:ILE:HG13	2.19	0.42
1:V:171:GLY:HA2	2:V:506:MC3:H431	2.01	0.42
1:D:215:PHE:O	1:D:219:VAL:HG23	2.19	0.42
1:F:57:GLN:NE2	1:M:56:THR:O	2.52	0.42
1:G:197:ASN:ND2	1:Y:198:VAL:HB	2.35	0.42
1:G:208:GLU:O	1:G:212:PHE:HD1	2.02	0.42
1:H:211:ILE:HG12	2:H:503:MC3:H132	2.02	0.42
1:M:169:GLU:HB2	1:M:224:LEU:HD21	2.01	0.42
1:M:208:GLU:O	1:M:212:PHE:HD1	2.02	0.42
2:W:506:MC3:H361	2:W:506:MC3:H392	1.87	0.42
2:Y:506:MC3:H341	2:Y:508:MC3:H442	2.02	0.42
2:H:503:MC3:H73	2:H:503:MC3:H41	1.74	0.42
1:I:171:GLY:HA2	2:I:506:MC3:H431	2.01	0.42
1:S:208:GLU:O	1:S:212:PHE:HD1	2.02	0.42
1:F:81:GLN:NE2	1:F:169:GLU:OE2	2.53	0.42
2:K:506:MC3:H372	2:K:506:MC3:H172	2.01	0.42
1:R:81:GLN:NE2	1:R:169:GLU:OE2	2.53	0.42
1:T:211:ILE:HG12	2:T:503:MC3:H132	2.02	0.42
2:X:506:MC3:H172	2:X:506:MC3:H372	2.01	0.42
1:Y:72:ILE:O	1:Y:180:TYR:OH	2.26	0.42
1:L:81:GLN:NE2	1:L:169:GLU:OE2	2.53	0.41
1:R:17:HIS:ND1	1:R:93:VAL:HG23	2.35	0.41
1:Y:81:GLN:NE2	1:Y:169:GLU:OE2	2.53	0.41
1:E:18:SER:HB3	1:E:22:GLY:HA3	2.01	0.41
1:F:17:HIS:ND1	1:F:93:VAL:HG23	2.35	0.41
1:J:215:PHE:O	1:J:219:VAL:HG23	2.19	0.41
1:L:183:ARG:HA	1:L:210:THR:OG1	2.20	0.41
1:W:215:PHE:O	1:W:219:VAL:HG23	2.19	0.41
1:Y:183:ARG:HA	1:Y:210:THR:OG1	2.20	0.41
1:C:171:GLY:HA2	2:C:506:MC3:H431	2.01	0.41
1:E:20:VAL:O	1:E:24:VAL:HG23	2.21	0.41
1:F:197:ASN:ND2	1:M:198:VAL:CG1	2.83	0.41
1:K:20:VAL:O	1:K:24:VAL:HG23	2.21	0.41
1:L:215:PHE:O	1:L:219:VAL:HG23	2.19	0.41
2:N:503:MC3:H32	2:N:503:MC3:H121	1.74	0.41
1:Q:18:SER:HB3	1:Q:22:GLY:HA3	2.01	0.41
1:Q:20:VAL:O	1:Q:24:VAL:HG23	2.21	0.41
1:X:20:VAL:O	1:X:24:VAL:HG23	2.21	0.41
1:A:198:VAL:CG1	1:R:197:ASN:ND2	2.83	0.41
1:B:76:ARG:HG3	1:C:40:ALA:HB1	2.02	0.41
1:C:193:TRP:CG	1:C:194:PRO:HA	2.56	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:72:ILE:O	1:N:180:TYR:OH	2.37	0.41
1:O:193:TRP:CG	1:O:194:PRO:HA	2.56	0.41
1:Q:184:ILE:HD12	1:Q:209:LYS:HB3	2.03	0.41
1:S:166:THR:C	1:S:168:PHE:N	2.77	0.41
1:C:47:ASP:OD1	1:C:47:ASP:N	2.44	0.41
1:E:184:ILE:HD12	1:E:209:LYS:HB3	2.03	0.41
1:G:166:THR:C	1:G:168:PHE:N	2.77	0.41
1:L:72:ILE:O	1:L:180:TYR:OH	2.26	0.41
1:M:203:VAL:HG12	1:M:204:SER:N	2.35	0.41
1:N:76:ARG:HG3	1:O:40:ALA:HB1	2.02	0.41
1:O:171:GLY:HA2	2:O:506:MC3:H431	2.01	0.41
1:Y:215:PHE:O	1:Y:219:VAL:HG23	2.19	0.41
1:A:203:VAL:HG12	1:A:204:SER:N	2.35	0.41
1:G:168:PHE:CD1	2:G:503:MC3:H443	2.56	0.41
2:T:503:MC3:H73	2:T:503:MC3:H41	1.74	0.41
1:V:193:TRP:CG	1:V:194:PRO:HA	2.56	0.41
1:A:198:VAL:HG12	1:R:197:ASN:HD22	1.86	0.41
2:A:503:MC3:H332	2:G:501:MC3:H442	2.03	0.41
1:F:197:ASN:HD22	1:M:198:VAL:HG12	1.86	0.41
1:I:193:TRP:CG	1:I:194:PRO:HA	2.56	0.41
2:M:503:MC3:H332	2:S:501:MC3:H442	2.03	0.41
1:S:168:PHE:CD1	2:S:503:MC3:H443	2.56	0.41
1:A:168:PHE:CD1	2:A:502:MC3:H443	2.56	0.41
1:D:20:VAL:HG13	1:D:21:ILE:N	2.36	0.41
2:F:505:MC3:H341	2:F:507:MC3:H442	2.02	0.41
1:G:198:VAL:CG1	1:Y:197:ASN:ND2	2.83	0.41
1:M:14:VAL:O	1:M:15:ASN:C	2.63	0.41
1:M:168:PHE:CD1	2:M:502:MC3:H443	2.56	0.41
1:P:20:VAL:HG13	1:P:21:ILE:N	2.36	0.41
1:A:14:VAL:O	1:A:15:ASN:C	2.63	0.41
2:B:503:MC3:H32	2:B:503:MC3:H121	1.74	0.41
1:D:32:PHE:HA	1:D:36:ILE:HG13	2.02	0.41
1:E:215:PHE:HD1	2:E:502:MC3:H431	1.86	0.41
1:F:11:LEU:HA	1:F:14:VAL:HG12	2.02	0.41
1:F:183:ARG:HA	1:F:210:THR:OG1	2.20	0.41
1:G:29:LEU:HA	1:G:33:ARG:HG3	2.03	0.41
1:G:177:TYR:HB2	1:G:182:PHE:CE2	2.56	0.41
2:J:501:MC3:H401	2:J:502:MC3:H391	2.03	0.41
1:L:197:ASN:ND2	1:S:198:VAL:CG1	2.83	0.41
1:M:67:ASP:OD2	1:N:207:THR:OG1	2.33	0.41
1:N:4:TRP:CZ2	1:O:39:THR:HG21	2.56	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:215:PHE:HD1	2:Q:502:MC3:H431	1.86	0.41
1:R:183:ARG:HA	1:R:210:THR:OG1	2.20	0.41
2:R:505:MC3:H341	2:R:507:MC3:H442	2.02	0.41
1:S:29:LEU:HA	1:S:33:ARG:HG3	2.03	0.41
1:B:4:TRP:CZ2	1:C:39:THR:HG21	2.56	0.41
1:E:166:THR:O	1:E:170:VAL:HG23	2.21	0.41
1:J:32:PHE:HA	1:J:36:ILE:HG13	2.02	0.41
1:J:67:ASP:OD1	3:J:601:HOH:O	2.22	0.41
1:K:166:THR:O	1:K:170:VAL:HG23	2.21	0.41
1:L:11:LEU:HA	1:L:14:VAL:HG12	2.02	0.41
2:M:503:MC3:H371	2:M:505:MC3:H382	2.03	0.41
1:P:32:PHE:HA	1:P:36:ILE:HG13	2.02	0.41
1:R:11:LEU:HA	1:R:14:VAL:HG12	2.02	0.41
1:S:177:TYR:HB2	1:S:182:PHE:CE2	2.56	0.41
2:W:501:MC3:H401	2:W:502:MC3:H391	2.03	0.41
2:W:506:MC3:H83	2:W:506:MC3:H41	1.89	0.41
1:X:166:THR:O	1:X:170:VAL:HG23	2.22	0.41
1:A:67:ASP:OD2	1:B:207:THR:OG1	2.33	0.40
2:A:503:MC3:H371	2:A:505:MC3:H382	2.03	0.40
1:D:37:LEU:O	1:D:42:GLU:HG2	2.21	0.40
1:H:76:ARG:HG3	1:I:40:ALA:HB1	2.02	0.40
1:P:37:LEU:O	1:P:42:GLU:HG2	2.21	0.40
1:Q:166:THR:O	1:Q:170:VAL:HG23	2.21	0.40
1:S:14:VAL:O	1:S:15:ASN:C	2.63	0.40
2:S:504:MC3:H371	2:S:506:MC3:H382	2.03	0.40
1:T:76:ARG:HG3	1:V:40:ALA:HB1	2.02	0.40
1:Y:11:LEU:HA	1:Y:14:VAL:HG12	2.02	0.40
1:G:203:VAL:HG12	1:G:204:SER:N	2.35	0.40
2:G:504:MC3:H371	2:G:506:MC3:H382	2.03	0.40
1:J:20:VAL:HG13	1:J:21:ILE:N	2.36	0.40
1:W:32:PHE:HA	1:W:36:ILE:HG13	2.02	0.40
1:A:29:LEU:HA	1:A:33:ARG:HG3	2.03	0.40
2:A:508:MC3:H442	2:G:504:MC3:H332	2.03	0.40
1:D:47:ASP:OD1	1:D:47:ASP:N	2.54	0.40
1:G:14:VAL:O	1:G:15:ASN:C	2.63	0.40
1:H:65:CYS:SG	1:H:195:CYS:SG	3.20	0.40
2:K:505:MC3:H402	2:K:506:MC3:H391	2.04	0.40
2:M:508:MC3:H442	2:S:504:MC3:H332	2.03	0.40
1:T:65:CYS:SG	1:T:195:CYS:SG	3.20	0.40
1:W:20:VAL:HG13	1:W:21:ILE:N	2.36	0.40
2:X:505:MC3:H402	2:X:506:MC3:H391	2.04	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:215:PHE:HD2	1:Y:216:MET:HE2	1.87	0.40
1:A:12:GLU:OE1	1:A:12:GLU:C	2.65	0.40
1:G:175:GLY:CA	2:G:503:MC3:H362	2.52	0.40
1:M:12:GLU:OE1	1:M:12:GLU:C	2.65	0.40
1:M:29:LEU:HA	1:M:33:ARG:HG3	2.03	0.40
1:R:224:LEU:HD23	1:R:224:LEU:HA	1.96	0.40
1:S:203:VAL:HG12	1:S:204:SER:N	2.35	0.40
1:W:156:ARG:O	1:W:159:ILE:HG22	2.21	0.40
1:D:156:ARG:O	1:D:159:ILE:HG22	2.21	0.40
1:J:156:ARG:O	1:J:159:ILE:HG22	2.21	0.40
1:L:215:PHE:HD2	1:L:216:MET:HE2	1.87	0.40
1:L:224:LEU:HD23	1:L:224:LEU:HA	1.95	0.40
1:P:47:ASP:OD1	1:P:47:ASP:N	2.54	0.40
1:S:175:GLY:CA	2:S:503:MC3:H362	2.52	0.40
1:X:184:ILE:HD12	1:X:209:LYS:HB3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	180/440 (41%)	168 (93%)	12 (7%)	0	100	100
1	B	180/440 (41%)	175 (97%)	5 (3%)	0	100	100
1	C	180/440 (41%)	174 (97%)	6 (3%)	0	100	100
1	D	180/440 (41%)	175 (97%)	5 (3%)	0	100	100
1	E	180/440 (41%)	175 (97%)	5 (3%)	0	100	100
1	F	180/440 (41%)	173 (96%)	7 (4%)	0	100	100
1	G	180/440 (41%)	168 (93%)	12 (7%)	0	100	100
1	H	180/440 (41%)	175 (97%)	5 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	I	180/440 (41%)	174 (97%)	6 (3%)	0	100	100
1	J	180/440 (41%)	175 (97%)	5 (3%)	0	100	100
1	K	180/440 (41%)	175 (97%)	5 (3%)	0	100	100
1	L	180/440 (41%)	173 (96%)	7 (4%)	0	100	100
1	M	180/440 (41%)	168 (93%)	12 (7%)	0	100	100
1	N	180/440 (41%)	175 (97%)	5 (3%)	0	100	100
1	O	180/440 (41%)	174 (97%)	6 (3%)	0	100	100
1	P	180/440 (41%)	175 (97%)	5 (3%)	0	100	100
1	Q	180/440 (41%)	175 (97%)	5 (3%)	0	100	100
1	R	180/440 (41%)	173 (96%)	7 (4%)	0	100	100
1	S	180/440 (41%)	168 (93%)	12 (7%)	0	100	100
1	T	180/440 (41%)	175 (97%)	5 (3%)	0	100	100
1	V	180/440 (41%)	174 (97%)	6 (3%)	0	100	100
1	W	180/440 (41%)	175 (97%)	5 (3%)	0	100	100
1	X	180/440 (41%)	175 (97%)	5 (3%)	0	100	100
1	Y	180/440 (41%)	173 (96%)	7 (4%)	0	100	100
All	All	4320/10560 (41%)	4160 (96%)	160 (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	167/387 (43%)	166 (99%)	1 (1%)	78	92
1	B	167/387 (43%)	165 (99%)	2 (1%)	63	84
1	C	167/387 (43%)	167 (100%)	0	100	100
1	D	167/387 (43%)	161 (96%)	6 (4%)	31	63
1	E	167/387 (43%)	167 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	F	167/387 (43%)	165 (99%)	2 (1%)	63 84
1	G	167/387 (43%)	166 (99%)	1 (1%)	78 92
1	H	167/387 (43%)	165 (99%)	2 (1%)	63 84
1	I	167/387 (43%)	167 (100%)	0	100 100
1	J	167/387 (43%)	161 (96%)	6 (4%)	31 63
1	K	167/387 (43%)	167 (100%)	0	100 100
1	L	167/387 (43%)	165 (99%)	2 (1%)	63 84
1	M	167/387 (43%)	166 (99%)	1 (1%)	78 92
1	N	167/387 (43%)	165 (99%)	2 (1%)	63 84
1	O	167/387 (43%)	167 (100%)	0	100 100
1	P	167/387 (43%)	161 (96%)	6 (4%)	31 63
1	Q	167/387 (43%)	167 (100%)	0	100 100
1	R	167/387 (43%)	165 (99%)	2 (1%)	63 84
1	S	167/387 (43%)	166 (99%)	1 (1%)	78 92
1	T	167/387 (43%)	165 (99%)	2 (1%)	63 84
1	V	167/387 (43%)	167 (100%)	0	100 100
1	W	167/387 (43%)	161 (96%)	6 (4%)	31 63
1	X	167/387 (43%)	167 (100%)	0	100 100
1	Y	167/387 (43%)	165 (99%)	2 (1%)	63 84
All	All	4008/9288 (43%)	3964 (99%)	44 (1%)	63 86

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	230	GLU
1	B	13	GLU
1	B	230	GLU
1	D	14	VAL
1	D	36	ILE
1	D	72	ILE
1	D	93	VAL
1	D	159	ILE
1	D	231	MET
1	F	68	GLU
1	F	179	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	230	GLU
1	H	13	GLU
1	H	230	GLU
1	J	14	VAL
1	J	36	ILE
1	J	72	ILE
1	J	93	VAL
1	J	159	ILE
1	J	231	MET
1	L	68	GLU
1	L	179	LEU
1	M	230	GLU
1	N	13	GLU
1	N	230	GLU
1	P	14	VAL
1	P	36	ILE
1	P	72	ILE
1	P	93	VAL
1	P	159	ILE
1	P	231	MET
1	R	68	GLU
1	R	179	LEU
1	S	230	GLU
1	T	13	GLU
1	T	230	GLU
1	W	14	VAL
1	W	36	ILE
1	W	72	ILE
1	W	93	VAL
1	W	159	ILE
1	W	231	MET
1	Y	68	GLU
1	Y	179	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (98) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	49	GLN
1	A	176	HIS
1	B	49	GLN
1	B	58	GLN
1	B	74	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	227	ASN
1	C	176	HIS
1	C	233	HIS
1	D	17	HIS
1	D	58	GLN
1	D	74	HIS
1	D	95	HIS
1	D	176	HIS
1	D	233	HIS
1	E	9	ASN
1	E	15	ASN
1	E	49	GLN
1	E	98	HIS
1	E	161	HIS
1	F	15	ASN
1	F	57	GLN
1	F	74	HIS
1	F	98	HIS
1	F	197	ASN
1	F	233	HIS
1	G	49	GLN
1	G	161	HIS
1	G	176	HIS
1	H	49	GLN
1	H	58	GLN
1	H	74	HIS
1	H	227	ASN
1	I	9	ASN
1	I	95	HIS
1	I	176	HIS
1	I	233	HIS
1	J	17	HIS
1	J	58	GLN
1	J	74	HIS
1	J	95	HIS
1	J	176	HIS
1	J	233	HIS
1	K	9	ASN
1	K	15	ASN
1	K	49	GLN
1	K	98	HIS
1	L	74	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L	98	HIS
1	L	197	ASN
1	L	233	HIS
1	M	49	GLN
1	M	176	HIS
1	N	49	GLN
1	N	58	GLN
1	N	74	HIS
1	N	227	ASN
1	O	176	HIS
1	O	233	HIS
1	P	17	HIS
1	P	58	GLN
1	P	74	HIS
1	P	95	HIS
1	P	176	HIS
1	P	233	HIS
1	Q	9	ASN
1	Q	15	ASN
1	Q	49	GLN
1	Q	98	HIS
1	Q	161	HIS
1	R	57	GLN
1	R	74	HIS
1	R	98	HIS
1	R	197	ASN
1	S	49	GLN
1	S	161	HIS
1	S	176	HIS
1	T	49	GLN
1	T	58	GLN
1	T	74	HIS
1	T	227	ASN
1	V	9	ASN
1	V	95	HIS
1	V	176	HIS
1	V	233	HIS
1	W	17	HIS
1	W	58	GLN
1	W	74	HIS
1	W	95	HIS
1	W	176	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	W	233	HIS
1	X	9	ASN
1	X	15	ASN
1	X	49	GLN
1	X	98	HIS
1	Y	74	HIS
1	Y	98	HIS
1	Y	197	ASN
1	Y	233	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

168 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	MC3	G	501	-	12,12,45	0.18	0	11,11,53	0.38	0
2	MC3	F	502	-	12,12,45	0.21	0	11,11,53	0.24	0
2	MC3	A	504	-	12,12,45	0.77	0	11,11,53	0.47	0
2	MC3	P	506	-	42,42,45	0.54	0	48,50,53	0.48	0
2	MC3	R	509	-	7,7,45	0.81	0	9,9,53	0.99	1 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	MC3	Q	503	-	35,35,45	0.68	1 (2%)	38,40,53	1.14	3 (7%)
2	MC3	A	508	-	12,12,45	0.18	0	11,11,53	0.37	0
2	MC3	O	502	-	12,12,45	0.21	0	11,11,53	0.24	0
2	MC3	V	502	-	12,12,45	0.21	0	11,11,53	0.24	0
2	MC3	C	502	-	12,12,45	0.21	0	11,11,53	0.24	0
2	MC3	H	502	-	12,12,45	0.19	0	11,11,53	0.11	0
2	MC3	X	504	-	12,12,45	0.27	0	11,11,53	0.17	0
2	MC3	B	503	-	44,44,45	0.44	0	50,52,53	0.34	0
2	MC3	L	502	-	12,12,45	0.20	0	11,11,53	0.28	0
2	MC3	C	506	-	10,10,45	0.50	0	9,9,53	0.40	0
2	MC3	D	505	-	12,12,45	0.16	0	11,11,53	0.33	0
2	MC3	C	505	-	12,12,45	0.19	0	11,11,53	0.35	0
2	MC3	L	507	-	15,15,45	0.75	1 (6%)	17,19,53	0.84	0
2	MC3	T	506	-	12,12,45	0.18	0	11,11,53	0.30	0
2	MC3	Y	508	-	12,12,45	0.20	0	11,11,53	0.25	0
2	MC3	P	502	-	12,12,45	0.22	0	11,11,53	0.23	0
2	MC3	T	504	-	12,12,45	0.21	0	11,11,53	0.24	0
2	MC3	Y	506	-	12,12,45	0.18	0	11,11,53	0.27	0
2	MC3	L	505	-	12,12,45	0.22	0	11,11,53	0.24	0
2	MC3	B	502	-	12,12,45	0.19	0	11,11,53	0.12	0
2	MC3	G	506	-	31,31,45	0.31	0	33,33,53	0.26	0
2	MC3	V	504	-	12,12,45	0.23	0	11,11,53	0.22	0
2	MC3	C	504	-	12,12,45	0.23	0	11,11,53	0.22	0
2	MC3	K	505	-	12,12,45	0.20	0	11,11,53	0.26	0
2	MC3	M	507	-	24,24,45	0.39	0	29,31,53	0.49	0
2	MC3	D	502	-	12,12,45	0.22	0	11,11,53	0.23	0
2	MC3	L	509	-	12,12,45	0.21	0	11,11,53	0.26	0
2	MC3	N	502	-	12,12,45	0.19	0	11,11,53	0.12	0
2	MC3	L	501	-	7,7,45	0.82	0	9,9,53	0.99	1 (11%)
2	MC3	M	501	-	9,9,45	0.19	0	8,8,53	0.12	0
2	MC3	V	501	-	12,12,45	0.20	0	11,11,53	0.09	0
2	MC3	Q	504	-	12,12,45	0.27	0	11,11,53	0.17	0
2	MC3	P	501	-	12,12,45	0.23	0	11,11,53	0.12	0
2	MC3	G	503	-	45,45,45	0.54	0	51,53,53	0.53	0
2	MC3	D	506	-	42,42,45	0.54	0	48,50,53	0.48	0
2	MC3	Y	509	-	12,12,45	0.21	0	11,11,53	0.26	0
2	MC3	R	504	-	12,12,45	0.22	0	11,11,53	0.24	0
2	MC3	E	504	-	12,12,45	0.27	0	11,11,53	0.17	0
2	MC3	L	506	-	12,12,45	0.18	0	11,11,53	0.27	0
2	MC3	M	503	-	12,12,45	0.20	0	11,11,53	0.26	0
2	MC3	V	503	-	12,12,45	0.37	0	11,11,53	0.24	0
2	MC3	V	507	-	12,12,45	0.19	0	11,11,53	0.24	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	MC3	K	506	-	43,43,45	0.42	0	49,51,53	0.34	0
2	MC3	F	505	-	12,12,45	0.18	0	11,11,53	0.27	0
2	MC3	T	502	-	12,12,45	0.19	0	11,11,53	0.12	0
2	MC3	I	505	-	12,12,45	0.18	0	11,11,53	0.35	0
2	MC3	I	506	-	10,10,45	0.50	0	9,9,53	0.40	0
2	MC3	M	505	-	31,31,45	0.31	0	33,33,53	0.26	0
2	MC3	M	506	-	36,36,45	0.46	0	42,44,53	0.52	0
2	MC3	R	508	-	12,12,45	0.21	0	11,11,53	0.26	0
2	MC3	E	503	-	35,35,45	0.68	1 (2%)	38,40,53	1.14	3 (7%)
2	MC3	W	504	-	12,12,45	0.22	0	11,11,53	0.22	0
2	MC3	A	506	-	36,36,45	0.46	0	42,44,53	0.52	0
2	MC3	F	506	-	15,15,45	0.75	1 (6%)	17,19,53	0.84	0
2	MC3	A	503	-	12,12,45	0.20	0	11,11,53	0.26	0
2	MC3	B	504	-	12,12,45	0.21	0	11,11,53	0.24	0
2	MC3	K	503	-	35,35,45	0.68	1 (2%)	38,40,53	1.14	3 (7%)
2	MC3	B	505	-	12,12,45	0.22	0	11,11,53	0.18	0
2	MC3	K	504	-	12,12,45	0.27	0	11,11,53	0.17	0
2	MC3	B	506	-	12,12,45	0.18	0	11,11,53	0.30	0
2	MC3	N	505	-	12,12,45	0.22	0	11,11,53	0.18	0
2	MC3	C	503	-	12,12,45	0.37	0	11,11,53	0.23	0
2	MC3	G	504	-	12,12,45	0.20	0	11,11,53	0.26	0
2	MC3	W	501	-	12,12,45	0.23	0	11,11,53	0.12	0
2	MC3	G	508	-	24,24,45	0.39	0	29,31,53	0.49	0
2	MC3	G	507	-	36,36,45	0.46	0	42,44,53	0.52	0
2	MC3	N	501	-	12,12,45	0.22	0	11,11,53	0.14	0
2	MC3	C	501	-	12,12,45	0.20	0	11,11,53	0.08	0
2	MC3	W	503	-	12,12,45	0.16	0	11,11,53	0.12	0
2	MC3	Y	503	-	12,12,45	0.21	0	11,11,53	0.24	0
2	MC3	H	504	-	12,12,45	0.21	0	11,11,53	0.24	0
2	MC3	J	501	-	12,12,45	0.23	0	11,11,53	0.12	0
2	MC3	Y	501	-	7,7,45	0.82	0	9,9,53	0.99	1 (11%)
2	MC3	J	504	-	12,12,45	0.22	0	11,11,53	0.22	0
2	MC3	X	506	-	43,43,45	0.42	0	49,51,53	0.35	0
2	MC3	K	501	-	12,12,45	0.21	0	11,11,53	0.24	0
2	MC3	F	503	-	11,11,45	0.32	0	10,10,53	0.27	0
2	MC3	X	503	-	35,35,45	0.68	1 (2%)	38,40,53	1.14	3 (7%)
2	MC3	S	502	-	9,9,45	0.19	0	8,8,53	0.12	0
2	MC3	F	504	-	12,12,45	0.22	0	11,11,53	0.24	0
2	MC3	O	503	-	12,12,45	0.37	0	11,11,53	0.23	0
2	MC3	N	506	-	12,12,45	0.18	0	11,11,53	0.30	0
2	MC3	G	505	-	12,12,45	0.77	0	11,11,53	0.47	0
2	MC3	E	506	-	43,43,45	0.42	0	49,51,53	0.34	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	MC3	A	502	-	45,45,45	0.54	0	51,53,53	0.53	0
2	MC3	L	503	-	12,12,45	0.21	0	11,11,53	0.24	0
2	MC3	R	501	-	12,12,45	0.20	0	11,11,53	0.28	0
2	MC3	I	504	-	12,12,45	0.23	0	11,11,53	0.22	0
2	MC3	S	507	-	36,36,45	0.46	0	42,44,53	0.52	0
2	MC3	Y	502	-	12,12,45	0.20	0	11,11,53	0.28	0
2	MC3	S	506	-	31,31,45	0.31	0	33,33,53	0.26	0
2	MC3	H	503	-	44,44,45	0.44	0	50,52,53	0.34	0
2	MC3	X	502	-	12,12,45	0.31	0	11,11,53	0.14	0
2	MC3	G	502	-	9,9,45	0.19	0	8,8,53	0.12	0
2	MC3	J	505	-	12,12,45	0.16	0	11,11,53	0.33	0
2	MC3	O	507	-	12,12,45	0.19	0	11,11,53	0.24	0
2	MC3	R	502	-	12,12,45	0.21	0	11,11,53	0.24	0
2	MC3	L	508	-	12,12,45	0.20	0	11,11,53	0.25	0
2	MC3	C	507	-	12,12,45	0.19	0	11,11,53	0.24	0
2	MC3	F	501	-	12,12,45	0.20	0	11,11,53	0.28	0
2	MC3	O	506	-	10,10,45	0.50	0	9,9,53	0.40	0
2	MC3	O	504	-	12,12,45	0.23	0	11,11,53	0.22	0
2	MC3	F	508	-	12,12,45	0.21	0	11,11,53	0.26	0
2	MC3	D	504	-	12,12,45	0.22	0	11,11,53	0.22	0
2	MC3	J	502	-	12,12,45	0.22	0	11,11,53	0.23	0
2	MC3	N	504	-	12,12,45	0.21	0	11,11,53	0.24	0
2	MC3	Y	507	-	15,15,45	0.75	1 (6%)	17,19,53	0.84	0
2	MC3	A	501	-	9,9,45	0.19	0	8,8,53	0.12	0
2	MC3	S	508	-	24,24,45	0.39	0	29,31,53	0.49	0
2	MC3	J	506	-	42,42,45	0.54	0	48,50,53	0.48	0
2	MC3	R	506	-	15,15,45	0.75	1 (6%)	17,19,53	0.84	0
2	MC3	I	503	-	12,12,45	0.37	0	11,11,53	0.24	0
2	MC3	N	503	-	44,44,45	0.44	0	50,52,53	0.34	0
2	MC3	Q	505	-	12,12,45	0.20	0	11,11,53	0.26	0
2	MC3	W	505	-	12,12,45	0.16	0	11,11,53	0.33	0
2	MC3	W	506	-	42,42,45	0.54	0	48,50,53	0.48	0
2	MC3	Q	501	-	12,12,45	0.21	0	11,11,53	0.24	0
2	MC3	V	505	-	12,12,45	0.19	0	11,11,53	0.35	0
2	MC3	Y	504	-	11,11,45	0.32	0	10,10,53	0.27	0
2	MC3	O	501	-	12,12,45	0.20	0	11,11,53	0.08	0
2	MC3	B	501	-	12,12,45	0.22	0	11,11,53	0.14	0
2	MC3	H	501	-	12,12,45	0.22	0	11,11,53	0.14	0
2	MC3	M	504	-	12,12,45	0.77	0	11,11,53	0.47	0
2	MC3	X	505	-	12,12,45	0.20	0	11,11,53	0.26	0
2	MC3	V	506	-	10,10,45	0.50	0	9,9,53	0.40	0
2	MC3	E	502	-	12,12,45	0.31	0	11,11,53	0.14	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	MC3	X	501	-	12,12,45	0.21	0	11,11,53	0.24	0
2	MC3	S	505	-	12,12,45	0.77	0	11,11,53	0.47	0
2	MC3	S	504	-	12,12,45	0.20	0	11,11,53	0.26	0
2	MC3	Q	506	-	43,43,45	0.42	0	49,51,53	0.34	0
2	MC3	K	502	-	12,12,45	0.31	0	11,11,53	0.14	0
2	MC3	H	505	-	12,12,45	0.22	0	11,11,53	0.18	0
2	MC3	H	506	-	12,12,45	0.18	0	11,11,53	0.30	0
2	MC3	J	503	-	12,12,45	0.16	0	11,11,53	0.12	0
2	MC3	L	504	-	11,11,45	0.32	0	10,10,53	0.26	0
2	MC3	P	505	-	12,12,45	0.16	0	11,11,53	0.33	0
2	MC3	Q	502	-	12,12,45	0.31	0	11,11,53	0.14	0
2	MC3	R	503	-	11,11,45	0.32	0	10,10,53	0.27	0
2	MC3	T	501	-	12,12,45	0.22	0	11,11,53	0.14	0
2	MC3	T	505	-	12,12,45	0.22	0	11,11,53	0.18	0
2	MC3	F	509	-	7,7,45	0.82	0	9,9,53	0.99	1 (11%)
2	MC3	E	505	-	12,12,45	0.20	0	11,11,53	0.26	0
2	MC3	E	501	-	12,12,45	0.21	0	11,11,53	0.24	0
2	MC3	A	507	-	24,24,45	0.39	0	29,31,53	0.49	0
2	MC3	I	502	-	12,12,45	0.21	0	11,11,53	0.24	0
2	MC3	T	503	-	44,44,45	0.44	0	50,52,53	0.34	0
2	MC3	W	502	-	12,12,45	0.22	0	11,11,53	0.23	0
2	MC3	M	508	-	12,12,45	0.18	0	11,11,53	0.37	0
2	MC3	P	503	-	12,12,45	0.17	0	11,11,53	0.12	0
2	MC3	F	507	-	12,12,45	0.20	0	11,11,53	0.25	0
2	MC3	P	504	-	12,12,45	0.22	0	11,11,53	0.22	0
2	MC3	A	505	-	31,31,45	0.31	0	33,33,53	0.26	0
2	MC3	O	505	-	12,12,45	0.19	0	11,11,53	0.35	0
2	MC3	D	501	-	12,12,45	0.23	0	11,11,53	0.12	0
2	MC3	I	507	-	12,12,45	0.19	0	11,11,53	0.23	0
2	MC3	S	501	-	12,12,45	0.18	0	11,11,53	0.38	0
2	MC3	M	502	-	45,45,45	0.54	0	51,53,53	0.53	0
2	MC3	D	503	-	12,12,45	0.17	0	11,11,53	0.12	0
2	MC3	R	507	-	12,12,45	0.20	0	11,11,53	0.25	0
2	MC3	I	501	-	12,12,45	0.20	0	11,11,53	0.08	0
2	MC3	R	505	-	12,12,45	0.18	0	11,11,53	0.27	0
2	MC3	S	503	-	45,45,45	0.54	0	51,53,53	0.53	0
2	MC3	Y	505	-	12,12,45	0.22	0	11,11,53	0.24	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MC3	G	501	-	-	1/10/10/49	-
2	MC3	F	502	-	-	1/10/10/49	-
2	MC3	A	504	-	-	0/10/10/49	-
2	MC3	P	506	-	-	12/46/46/49	-
2	MC3	R	509	-	-	3/5/5/49	-
2	MC3	Q	503	-	-	12/37/37/49	-
2	MC3	A	508	-	-	1/10/10/49	-
2	MC3	O	502	-	-	1/10/10/49	-
2	MC3	V	502	-	-	1/10/10/49	-
2	MC3	C	502	-	-	1/10/10/49	-
2	MC3	H	502	-	-	5/10/10/49	-
2	MC3	X	504	-	-	3/10/10/49	-
2	MC3	B	503	-	-	28/48/48/49	-
2	MC3	L	502	-	-	0/10/10/49	-
2	MC3	C	506	-	-	1/8/8/49	-
2	MC3	D	505	-	-	1/10/10/49	-
2	MC3	C	505	-	-	1/10/10/49	-
2	MC3	L	507	-	-	10/17/17/49	-
2	MC3	T	506	-	-	0/10/10/49	-
2	MC3	Y	508	-	-	1/10/10/49	-
2	MC3	P	502	-	-	0/10/10/49	-
2	MC3	T	504	-	-	0/10/10/49	-
2	MC3	Y	506	-	-	0/10/10/49	-
2	MC3	L	505	-	-	0/10/10/49	-
2	MC3	B	502	-	-	5/10/10/49	-
2	MC3	G	506	-	-	9/33/33/49	-
2	MC3	V	504	-	-	0/10/10/49	-
2	MC3	C	504	-	-	0/10/10/49	-
2	MC3	K	505	-	-	0/10/10/49	-
2	MC3	M	507	-	-	4/26/26/49	-
2	MC3	D	502	-	-	0/10/10/49	-
2	MC3	L	509	-	-	0/10/10/49	-
2	MC3	N	502	-	-	5/10/10/49	-
2	MC3	L	501	-	-	3/5/5/49	-
2	MC3	M	501	-	-	0/7/7/49	-
2	MC3	V	501	-	-	3/10/10/49	-
2	MC3	Q	504	-	-	3/10/10/49	-
2	MC3	P	501	-	-	7/10/10/49	-
2	MC3	G	503	-	-	23/49/49/49	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MC3	D	506	-	-	12/46/46/49	-
2	MC3	Y	509	-	-	0/10/10/49	-
2	MC3	R	504	-	-	0/10/10/49	-
2	MC3	E	504	-	-	3/10/10/49	-
2	MC3	L	506	-	-	0/10/10/49	-
2	MC3	M	503	-	-	1/10/10/49	-
2	MC3	V	503	-	-	4/10/10/49	-
2	MC3	V	507	-	-	0/10/10/49	-
2	MC3	K	506	-	-	32/47/47/49	-
2	MC3	F	505	-	-	0/10/10/49	-
2	MC3	T	502	-	-	5/10/10/49	-
2	MC3	I	505	-	-	1/10/10/49	-
2	MC3	I	506	-	-	1/8/8/49	-
2	MC3	M	505	-	-	9/33/33/49	-
2	MC3	M	506	-	-	11/40/40/49	-
2	MC3	R	508	-	-	0/10/10/49	-
2	MC3	E	503	-	-	12/37/37/49	-
2	MC3	W	504	-	-	1/10/10/49	-
2	MC3	A	506	-	-	11/40/40/49	-
2	MC3	F	506	-	-	10/17/17/49	-
2	MC3	A	503	-	-	1/10/10/49	-
2	MC3	B	504	-	-	0/10/10/49	-
2	MC3	K	503	-	-	12/37/37/49	-
2	MC3	B	505	-	-	2/10/10/49	-
2	MC3	K	504	-	-	3/10/10/49	-
2	MC3	B	506	-	-	0/10/10/49	-
2	MC3	N	505	-	-	2/10/10/49	-
2	MC3	C	503	-	-	4/10/10/49	-
2	MC3	G	504	-	-	1/10/10/49	-
2	MC3	W	501	-	-	7/10/10/49	-
2	MC3	G	508	-	-	4/26/26/49	-
2	MC3	G	507	-	-	11/40/40/49	-
2	MC3	N	501	-	-	5/10/10/49	-
2	MC3	C	501	-	-	3/10/10/49	-
2	MC3	W	503	-	-	0/10/10/49	-
2	MC3	Y	503	-	-	1/10/10/49	-
2	MC3	H	504	-	-	0/10/10/49	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MC3	J	501	-	-	7/10/10/49	-
2	MC3	Y	501	-	-	3/5/5/49	-
2	MC3	J	504	-	-	1/10/10/49	-
2	MC3	X	506	-	-	32/47/47/49	-
2	MC3	K	501	-	-	0/10/10/49	-
2	MC3	F	503	-	-	0/9/9/49	-
2	MC3	X	503	-	-	12/37/37/49	-
2	MC3	S	502	-	-	0/7/7/49	-
2	MC3	F	504	-	-	0/10/10/49	-
2	MC3	O	503	-	-	4/10/10/49	-
2	MC3	N	506	-	-	0/10/10/49	-
2	MC3	G	505	-	-	0/10/10/49	-
2	MC3	E	506	-	-	32/47/47/49	-
2	MC3	A	502	-	-	23/49/49/49	-
2	MC3	L	503	-	-	1/10/10/49	-
2	MC3	R	501	-	-	0/10/10/49	-
2	MC3	I	504	-	-	0/10/10/49	-
2	MC3	S	507	-	-	11/40/40/49	-
2	MC3	Y	502	-	-	0/10/10/49	-
2	MC3	S	506	-	-	9/33/33/49	-
2	MC3	H	503	-	-	28/48/48/49	-
2	MC3	X	502	-	-	2/10/10/49	-
2	MC3	G	502	-	-	0/7/7/49	-
2	MC3	J	505	-	-	1/10/10/49	-
2	MC3	O	507	-	-	0/10/10/49	-
2	MC3	R	502	-	-	1/10/10/49	-
2	MC3	L	508	-	-	1/10/10/49	-
2	MC3	C	507	-	-	0/10/10/49	-
2	MC3	F	501	-	-	0/10/10/49	-
2	MC3	O	506	-	-	1/8/8/49	-
2	MC3	O	504	-	-	0/10/10/49	-
2	MC3	F	508	-	-	0/10/10/49	-
2	MC3	D	504	-	-	1/10/10/49	-
2	MC3	J	502	-	-	0/10/10/49	-
2	MC3	N	504	-	-	0/10/10/49	-
2	MC3	Y	507	-	-	10/17/17/49	-
2	MC3	A	501	-	-	0/7/7/49	-
2	MC3	S	508	-	-	4/26/26/49	-
2	MC3	J	506	-	-	12/46/46/49	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MC3	R	506	-	-	10/17/17/49	-
2	MC3	I	503	-	-	4/10/10/49	-
2	MC3	N	503	-	-	28/48/48/49	-
2	MC3	Q	505	-	-	0/10/10/49	-
2	MC3	W	505	-	-	1/10/10/49	-
2	MC3	W	506	-	-	12/46/46/49	-
2	MC3	Q	501	-	-	0/10/10/49	-
2	MC3	V	505	-	-	1/10/10/49	-
2	MC3	Y	504	-	-	0/9/9/49	-
2	MC3	O	501	-	-	3/10/10/49	-
2	MC3	B	501	-	-	5/10/10/49	-
2	MC3	H	501	-	-	5/10/10/49	-
2	MC3	M	504	-	-	0/10/10/49	-
2	MC3	X	505	-	-	0/10/10/49	-
2	MC3	V	506	-	-	1/8/8/49	-
2	MC3	E	502	-	-	2/10/10/49	-
2	MC3	X	501	-	-	0/10/10/49	-
2	MC3	S	505	-	-	0/10/10/49	-
2	MC3	S	504	-	-	1/10/10/49	-
2	MC3	Q	506	-	-	32/47/47/49	-
2	MC3	K	502	-	-	2/10/10/49	-
2	MC3	H	505	-	-	2/10/10/49	-
2	MC3	H	506	-	-	0/10/10/49	-
2	MC3	J	503	-	-	0/10/10/49	-
2	MC3	L	504	-	-	0/9/9/49	-
2	MC3	P	505	-	-	1/10/10/49	-
2	MC3	Q	502	-	-	2/10/10/49	-
2	MC3	R	503	-	-	0/9/9/49	-
2	MC3	T	501	-	-	5/10/10/49	-
2	MC3	T	505	-	-	2/10/10/49	-
2	MC3	F	509	-	-	3/5/5/49	-
2	MC3	E	505	-	-	0/10/10/49	-
2	MC3	E	501	-	-	0/10/10/49	-
2	MC3	A	507	-	-	4/26/26/49	-
2	MC3	I	502	-	-	1/10/10/49	-
2	MC3	T	503	-	-	28/48/48/49	-
2	MC3	W	502	-	-	0/10/10/49	-
2	MC3	M	508	-	-	1/10/10/49	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MC3	P	503	-	-	0/10/10/49	-
2	MC3	F	507	-	-	1/10/10/49	-
2	MC3	P	504	-	-	1/10/10/49	-
2	MC3	A	505	-	-	9/33/33/49	-
2	MC3	O	505	-	-	1/10/10/49	-
2	MC3	D	501	-	-	7/10/10/49	-
2	MC3	I	507	-	-	0/10/10/49	-
2	MC3	S	501	-	-	1/10/10/49	-
2	MC3	M	502	-	-	23/49/49/49	-
2	MC3	D	503	-	-	0/10/10/49	-
2	MC3	R	507	-	-	1/10/10/49	-
2	MC3	I	501	-	-	3/10/10/49	-
2	MC3	R	505	-	-	0/10/10/49	-
2	MC3	S	503	-	-	23/49/49/49	-
2	MC3	Y	505	-	-	0/10/10/49	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	503	MC3	P-O4P	2.83	1.65	1.54
2	K	503	MC3	P-O4P	2.83	1.65	1.54
2	Q	503	MC3	P-O4P	2.83	1.65	1.54
2	X	503	MC3	P-O4P	2.83	1.65	1.54
2	F	506	MC3	O2-C31	-2.28	1.34	1.42
2	R	506	MC3	O2-C31	-2.28	1.34	1.42
2	L	507	MC3	O2-C31	-2.25	1.34	1.42
2	Y	507	MC3	O2-C31	-2.25	1.34	1.42

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	503	MC3	O4P-P-O3P	-5.19	93.13	106.67
2	K	503	MC3	O4P-P-O3P	-5.19	93.13	106.67
2	Q	503	MC3	O4P-P-O3P	-5.19	93.13	106.67
2	X	503	MC3	O4P-P-O3P	-5.19	93.13	106.67
2	E	503	MC3	O2P-P-O1P	2.34	119.97	110.83
2	K	503	MC3	O2P-P-O1P	2.34	119.97	110.83
2	Q	503	MC3	O2P-P-O1P	2.34	119.97	110.83
2	X	503	MC3	C2-O2-C31	2.34	123.41	117.80
2	X	503	MC3	O2P-P-O1P	2.34	119.96	110.83
2	E	503	MC3	C2-O2-C31	2.34	123.40	117.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	Q	503	MC3	C2-O2-C31	2.34	123.40	117.80
2	K	503	MC3	C2-O2-C31	2.33	123.37	117.80
2	L	501	MC3	O2P-P-O1P	2.30	119.79	110.83
2	Y	501	MC3	O2P-P-O1P	2.30	119.79	110.83
2	F	509	MC3	O2P-P-O1P	2.29	119.77	110.83
2	R	509	MC3	O2P-P-O1P	2.29	119.77	110.83

There are no chirality outliers.

All (736) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	502	MC3	C4-O4P-P-O1P
2	A	502	MC3	C4-O4P-P-O2P
2	A	502	MC3	C4-O4P-P-O3P
2	A	505	MC3	O3P-C1-C2-C3
2	A	505	MC3	O3P-C1-C2-O2
2	A	506	MC3	C32-C31-O2-C2
2	A	506	MC3	C4-O4P-P-O2P
2	B	503	MC3	O4P-C4-C5-N
2	B	503	MC3	C5-C4-O4P-P
2	D	506	MC3	C1-O3P-P-O1P
2	D	506	MC3	C1-O3P-P-O4P
2	D	506	MC3	C4-O4P-P-O2P
2	D	506	MC3	C4-O4P-P-O3P
2	E	503	MC3	C1-O3P-P-O1P
2	E	503	MC3	C1-O3P-P-O2P
2	E	503	MC3	C1-O3P-P-O4P
2	E	506	MC3	O4P-C4-C5-N
2	E	506	MC3	C32-C31-O2-C2
2	E	506	MC3	C1-O3P-P-O1P
2	E	506	MC3	C1-O3P-P-O2P
2	E	506	MC3	C1-O3P-P-O4P
2	E	506	MC3	C4-O4P-P-O2P
2	F	506	MC3	C3-C2-O2-C31
2	F	506	MC3	C1-O3P-P-O1P
2	F	506	MC3	C4-O4P-P-O3P
2	F	509	MC3	O3P-C1-C2-O2
2	F	509	MC3	C1-O3P-P-O1P
2	G	503	MC3	C4-O4P-P-O1P
2	G	503	MC3	C4-O4P-P-O2P
2	G	503	MC3	C4-O4P-P-O3P
2	G	506	MC3	O3P-C1-C2-C3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	G	506	MC3	O3P-C1-C2-O2
2	G	507	MC3	C32-C31-O2-C2
2	G	507	MC3	C4-O4P-P-O2P
2	H	503	MC3	O4P-C4-C5-N
2	H	503	MC3	C5-C4-O4P-P
2	J	506	MC3	C1-O3P-P-O1P
2	J	506	MC3	C1-O3P-P-O4P
2	J	506	MC3	C4-O4P-P-O2P
2	J	506	MC3	C4-O4P-P-O3P
2	K	503	MC3	C1-O3P-P-O1P
2	K	503	MC3	C1-O3P-P-O2P
2	K	503	MC3	C1-O3P-P-O4P
2	K	506	MC3	O4P-C4-C5-N
2	K	506	MC3	C32-C31-O2-C2
2	K	506	MC3	C1-O3P-P-O1P
2	K	506	MC3	C1-O3P-P-O2P
2	K	506	MC3	C1-O3P-P-O4P
2	K	506	MC3	C4-O4P-P-O2P
2	L	501	MC3	O3P-C1-C2-O2
2	L	501	MC3	C1-O3P-P-O1P
2	L	507	MC3	C3-C2-O2-C31
2	L	507	MC3	C1-O3P-P-O1P
2	L	507	MC3	C4-O4P-P-O3P
2	M	502	MC3	C4-O4P-P-O1P
2	M	502	MC3	C4-O4P-P-O2P
2	M	502	MC3	C4-O4P-P-O3P
2	M	505	MC3	O3P-C1-C2-C3
2	M	505	MC3	O3P-C1-C2-O2
2	M	506	MC3	C32-C31-O2-C2
2	M	506	MC3	C4-O4P-P-O2P
2	N	503	MC3	O4P-C4-C5-N
2	N	503	MC3	C5-C4-O4P-P
2	P	506	MC3	C1-O3P-P-O1P
2	P	506	MC3	C1-O3P-P-O4P
2	P	506	MC3	C4-O4P-P-O2P
2	P	506	MC3	C4-O4P-P-O3P
2	Q	503	MC3	C1-O3P-P-O1P
2	Q	503	MC3	C1-O3P-P-O2P
2	Q	503	MC3	C1-O3P-P-O4P
2	Q	506	MC3	O4P-C4-C5-N
2	Q	506	MC3	C32-C31-O2-C2
2	Q	506	MC3	C1-O3P-P-O1P

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	Q	506	MC3	C1-O3P-P-O2P
2	Q	506	MC3	C1-O3P-P-O4P
2	Q	506	MC3	C4-O4P-P-O2P
2	R	506	MC3	C3-C2-O2-C31
2	R	506	MC3	C1-O3P-P-O1P
2	R	506	MC3	C4-O4P-P-O3P
2	R	509	MC3	O3P-C1-C2-O2
2	R	509	MC3	C1-O3P-P-O1P
2	S	503	MC3	C4-O4P-P-O1P
2	S	503	MC3	C4-O4P-P-O2P
2	S	503	MC3	C4-O4P-P-O3P
2	S	506	MC3	O3P-C1-C2-C3
2	S	506	MC3	O3P-C1-C2-O2
2	S	507	MC3	C32-C31-O2-C2
2	S	507	MC3	C4-O4P-P-O2P
2	T	503	MC3	O4P-C4-C5-N
2	T	503	MC3	C5-C4-O4P-P
2	W	506	MC3	C1-O3P-P-O1P
2	W	506	MC3	C1-O3P-P-O4P
2	W	506	MC3	C4-O4P-P-O2P
2	W	506	MC3	C4-O4P-P-O3P
2	X	503	MC3	C1-O3P-P-O1P
2	X	503	MC3	C1-O3P-P-O2P
2	X	503	MC3	C1-O3P-P-O4P
2	X	506	MC3	O4P-C4-C5-N
2	X	506	MC3	C32-C31-O2-C2
2	X	506	MC3	C1-O3P-P-O1P
2	X	506	MC3	C1-O3P-P-O2P
2	X	506	MC3	C1-O3P-P-O4P
2	X	506	MC3	C4-O4P-P-O2P
2	Y	501	MC3	O3P-C1-C2-O2
2	Y	501	MC3	C1-O3P-P-O1P
2	Y	507	MC3	C3-C2-O2-C31
2	Y	507	MC3	C1-O3P-P-O1P
2	Y	507	MC3	C4-O4P-P-O3P
2	B	503	MC3	O11-C11-O3-C3
2	H	503	MC3	O11-C11-O3-C3
2	N	503	MC3	O11-C11-O3-C3
2	T	503	MC3	O11-C11-O3-C3
2	A	506	MC3	O31-C31-O2-C2
2	E	506	MC3	O31-C31-O2-C2
2	G	507	MC3	O31-C31-O2-C2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	K	506	MC3	O31-C31-O2-C2
2	M	506	MC3	O31-C31-O2-C2
2	Q	506	MC3	O31-C31-O2-C2
2	S	507	MC3	O31-C31-O2-C2
2	X	506	MC3	O31-C31-O2-C2
2	B	503	MC3	C12-C11-O3-C3
2	H	503	MC3	C12-C11-O3-C3
2	N	503	MC3	C12-C11-O3-C3
2	T	503	MC3	C12-C11-O3-C3
2	F	506	MC3	C12-C11-O3-C3
2	L	507	MC3	C12-C11-O3-C3
2	R	506	MC3	C12-C11-O3-C3
2	Y	507	MC3	C12-C11-O3-C3
2	B	503	MC3	C16-C17-C18-C19
2	H	503	MC3	C16-C17-C18-C19
2	N	503	MC3	C16-C17-C18-C19
2	T	503	MC3	C16-C17-C18-C19
2	A	505	MC3	C32-C31-O2-C2
2	G	506	MC3	C32-C31-O2-C2
2	M	505	MC3	C32-C31-O2-C2
2	S	506	MC3	C32-C31-O2-C2
2	A	505	MC3	O31-C31-O2-C2
2	G	506	MC3	O31-C31-O2-C2
2	M	505	MC3	O31-C31-O2-C2
2	S	506	MC3	O31-C31-O2-C2
2	B	503	MC3	C36-C37-C38-C39
2	H	503	MC3	C36-C37-C38-C39
2	N	503	MC3	C36-C37-C38-C39
2	T	503	MC3	C36-C37-C38-C39
2	B	503	MC3	C40-C41-C42-C43
2	H	503	MC3	C40-C41-C42-C43
2	N	503	MC3	C40-C41-C42-C43
2	T	503	MC3	C40-C41-C42-C43
2	B	503	MC3	C18-C19-C20-C21
2	B	503	MC3	C38-C39-C40-C41
2	H	503	MC3	C18-C19-C20-C21
2	H	503	MC3	C38-C39-C40-C41
2	N	503	MC3	C18-C19-C20-C21
2	N	503	MC3	C38-C39-C40-C41
2	T	503	MC3	C18-C19-C20-C21
2	T	503	MC3	C38-C39-C40-C41
2	B	503	MC3	C4-C5-N-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	H	503	MC3	C4-C5-N-C7
2	N	503	MC3	C4-C5-N-C7
2	T	503	MC3	C4-C5-N-C7
2	B	503	MC3	C14-C15-C16-C17
2	H	503	MC3	C14-C15-C16-C17
2	N	503	MC3	C14-C15-C16-C17
2	T	503	MC3	C14-C15-C16-C17
2	F	506	MC3	O11-C11-O3-C3
2	L	507	MC3	O11-C11-O3-C3
2	R	506	MC3	O11-C11-O3-C3
2	Y	507	MC3	O11-C11-O3-C3
2	A	502	MC3	C32-C31-O2-C2
2	G	503	MC3	C32-C31-O2-C2
2	M	502	MC3	C32-C31-O2-C2
2	S	503	MC3	C32-C31-O2-C2
2	B	503	MC3	C4-C5-N-C8
2	H	503	MC3	C4-C5-N-C8
2	N	503	MC3	C4-C5-N-C8
2	T	503	MC3	C4-C5-N-C8
2	E	506	MC3	C31-C32-C33-C34
2	K	506	MC3	C31-C32-C33-C34
2	Q	506	MC3	C31-C32-C33-C34
2	X	506	MC3	C31-C32-C33-C34
2	E	506	MC3	C11-C12-C13-C14
2	K	506	MC3	C11-C12-C13-C14
2	Q	506	MC3	C11-C12-C13-C14
2	X	506	MC3	C11-C12-C13-C14
2	B	503	MC3	C34-C35-C36-C37
2	H	503	MC3	C34-C35-C36-C37
2	N	503	MC3	C34-C35-C36-C37
2	T	503	MC3	C34-C35-C36-C37
2	A	502	MC3	O31-C31-O2-C2
2	G	503	MC3	O31-C31-O2-C2
2	M	502	MC3	O31-C31-O2-C2
2	S	503	MC3	O31-C31-O2-C2
2	B	503	MC3	C32-C33-C34-C35
2	H	503	MC3	C32-C33-C34-C35
2	N	503	MC3	C32-C33-C34-C35
2	E	506	MC3	C38-C39-C40-C41
2	K	506	MC3	C38-C39-C40-C41
2	Q	506	MC3	C38-C39-C40-C41
2	T	503	MC3	C32-C33-C34-C35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	X	506	MC3	C38-C39-C40-C41
2	A	507	MC3	C12-C11-O3-C3
2	G	508	MC3	C12-C11-O3-C3
2	M	507	MC3	C12-C11-O3-C3
2	S	508	MC3	C12-C11-O3-C3
2	C	501	MC3	C34-C35-C36-C37
2	I	501	MC3	C34-C35-C36-C37
2	O	501	MC3	C34-C35-C36-C37
2	V	501	MC3	C34-C35-C36-C37
2	C	501	MC3	C32-C33-C34-C35
2	I	501	MC3	C32-C33-C34-C35
2	O	501	MC3	C32-C33-C34-C35
2	V	501	MC3	C32-C33-C34-C35
2	A	505	MC3	C32-C33-C34-C35
2	D	506	MC3	C32-C33-C34-C35
2	E	506	MC3	C37-C38-C39-C40
2	G	506	MC3	C32-C33-C34-C35
2	J	506	MC3	C32-C33-C34-C35
2	K	506	MC3	C37-C38-C39-C40
2	M	505	MC3	C32-C33-C34-C35
2	P	506	MC3	C32-C33-C34-C35
2	Q	506	MC3	C37-C38-C39-C40
2	S	506	MC3	C32-C33-C34-C35
2	W	506	MC3	C32-C33-C34-C35
2	X	506	MC3	C37-C38-C39-C40
2	E	506	MC3	C13-C14-C15-C16
2	K	506	MC3	C13-C14-C15-C16
2	Q	506	MC3	C13-C14-C15-C16
2	X	506	MC3	C13-C14-C15-C16
2	B	503	MC3	C4-C5-N-C6
2	H	503	MC3	C4-C5-N-C6
2	N	503	MC3	C4-C5-N-C6
2	T	503	MC3	C4-C5-N-C6
2	B	501	MC3	C40-C41-C42-C43
2	H	501	MC3	C40-C41-C42-C43
2	N	501	MC3	C40-C41-C42-C43
2	B	502	MC3	C38-C39-C40-C41
2	H	502	MC3	C38-C39-C40-C41
2	N	502	MC3	C38-C39-C40-C41
2	T	502	MC3	C38-C39-C40-C41
2	T	501	MC3	C40-C41-C42-C43
2	B	503	MC3	C20-C21-C22-C23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	H	503	MC3	C20-C21-C22-C23
2	N	503	MC3	C20-C21-C22-C23
2	T	503	MC3	C20-C21-C22-C23
2	B	503	MC3	C12-C13-C14-C15
2	H	503	MC3	C12-C13-C14-C15
2	N	503	MC3	C12-C13-C14-C15
2	T	503	MC3	C12-C13-C14-C15
2	C	503	MC3	C35-C36-C37-C38
2	I	503	MC3	C35-C36-C37-C38
2	O	503	MC3	C35-C36-C37-C38
2	V	503	MC3	C35-C36-C37-C38
2	D	501	MC3	C36-C37-C38-C39
2	E	506	MC3	C16-C17-C18-C19
2	J	501	MC3	C36-C37-C38-C39
2	K	506	MC3	C16-C17-C18-C19
2	P	501	MC3	C36-C37-C38-C39
2	Q	506	MC3	C16-C17-C18-C19
2	W	501	MC3	C36-C37-C38-C39
2	X	506	MC3	C16-C17-C18-C19
2	E	503	MC3	C15-C16-C17-C18
2	K	503	MC3	C15-C16-C17-C18
2	Q	503	MC3	C15-C16-C17-C18
2	X	503	MC3	C15-C16-C17-C18
2	G	506	MC3	C16-C17-C18-C19
2	A	505	MC3	C16-C17-C18-C19
2	B	503	MC3	C33-C34-C35-C36
2	D	501	MC3	C38-C39-C40-C41
2	H	503	MC3	C33-C34-C35-C36
2	J	501	MC3	C38-C39-C40-C41
2	M	505	MC3	C16-C17-C18-C19
2	N	503	MC3	C33-C34-C35-C36
2	P	501	MC3	C38-C39-C40-C41
2	S	506	MC3	C16-C17-C18-C19
2	T	503	MC3	C33-C34-C35-C36
2	W	501	MC3	C38-C39-C40-C41
2	E	503	MC3	C13-C14-C15-C16
2	K	503	MC3	C13-C14-C15-C16
2	Q	503	MC3	C13-C14-C15-C16
2	X	503	MC3	C13-C14-C15-C16
2	B	503	MC3	C32-C31-O2-C2
2	H	503	MC3	C32-C31-O2-C2
2	N	503	MC3	C32-C31-O2-C2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	T	503	MC3	C32-C31-O2-C2
2	A	502	MC3	C32-C33-C34-C35
2	G	503	MC3	C32-C33-C34-C35
2	M	502	MC3	C32-C33-C34-C35
2	S	503	MC3	C32-C33-C34-C35
2	A	502	MC3	C18-C19-C20-C21
2	G	503	MC3	C18-C19-C20-C21
2	M	502	MC3	C18-C19-C20-C21
2	S	503	MC3	C18-C19-C20-C21
2	A	507	MC3	O11-C11-O3-C3
2	M	507	MC3	O11-C11-O3-C3
2	S	508	MC3	O11-C11-O3-C3
2	G	508	MC3	O11-C11-O3-C3
2	B	503	MC3	C11-C12-C13-C14
2	H	503	MC3	C11-C12-C13-C14
2	N	503	MC3	C11-C12-C13-C14
2	T	503	MC3	C11-C12-C13-C14
2	C	501	MC3	C35-C36-C37-C38
2	E	503	MC3	C14-C15-C16-C17
2	I	501	MC3	C35-C36-C37-C38
2	K	503	MC3	C14-C15-C16-C17
2	O	501	MC3	C35-C36-C37-C38
2	Q	503	MC3	C14-C15-C16-C17
2	V	501	MC3	C35-C36-C37-C38
2	X	503	MC3	C14-C15-C16-C17
2	C	503	MC3	C37-C38-C39-C40
2	E	506	MC3	C39-C40-C41-C42
2	I	503	MC3	C37-C38-C39-C40
2	K	506	MC3	C39-C40-C41-C42
2	O	503	MC3	C37-C38-C39-C40
2	Q	506	MC3	C39-C40-C41-C42
2	V	503	MC3	C37-C38-C39-C40
2	X	506	MC3	C39-C40-C41-C42
2	B	503	MC3	C2-C1-O3P-P
2	H	503	MC3	C2-C1-O3P-P
2	N	503	MC3	C2-C1-O3P-P
2	T	503	MC3	C2-C1-O3P-P
2	B	502	MC3	C40-C41-C42-C43
2	H	502	MC3	C40-C41-C42-C43
2	N	502	MC3	C40-C41-C42-C43
2	T	502	MC3	C40-C41-C42-C43
2	B	503	MC3	O31-C31-O2-C2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	H	503	MC3	O31-C31-O2-C2
2	N	503	MC3	O31-C31-O2-C2
2	T	503	MC3	O31-C31-O2-C2
2	D	501	MC3	C39-C40-C41-C42
2	J	501	MC3	C39-C40-C41-C42
2	P	501	MC3	C39-C40-C41-C42
2	W	501	MC3	C39-C40-C41-C42
2	X	503	MC3	C31-C32-C33-C34
2	E	503	MC3	C31-C32-C33-C34
2	Q	503	MC3	C31-C32-C33-C34
2	D	501	MC3	C33-C34-C35-C36
2	P	501	MC3	C33-C34-C35-C36
2	J	501	MC3	C33-C34-C35-C36
2	W	501	MC3	C33-C34-C35-C36
2	K	503	MC3	C31-C32-C33-C34
2	J	501	MC3	C37-C38-C39-C40
2	W	501	MC3	C37-C38-C39-C40
2	D	501	MC3	C37-C38-C39-C40
2	P	501	MC3	C37-C38-C39-C40
2	E	502	MC3	C33-C34-C35-C36
2	K	502	MC3	C33-C34-C35-C36
2	Q	502	MC3	C33-C34-C35-C36
2	X	502	MC3	C33-C34-C35-C36
2	E	506	MC3	C4-C5-N-C6
2	K	506	MC3	C4-C5-N-C6
2	Q	506	MC3	C4-C5-N-C6
2	X	506	MC3	C4-C5-N-C6
2	F	506	MC3	O3P-C1-C2-O2
2	L	507	MC3	O3P-C1-C2-O2
2	R	506	MC3	O3P-C1-C2-O2
2	Y	507	MC3	O3P-C1-C2-O2
2	E	506	MC3	C34-C35-C36-C37
2	K	506	MC3	C34-C35-C36-C37
2	Q	506	MC3	C34-C35-C36-C37
2	X	506	MC3	C34-C35-C36-C37
2	X	506	MC3	C40-C41-C42-C43
2	D	501	MC3	C34-C35-C36-C37
2	J	501	MC3	C34-C35-C36-C37
2	P	501	MC3	C34-C35-C36-C37
2	W	501	MC3	C34-C35-C36-C37
2	B	502	MC3	C32-C33-C34-C35
2	E	506	MC3	C40-C41-C42-C43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	H	502	MC3	C32-C33-C34-C35
2	K	506	MC3	C40-C41-C42-C43
2	N	502	MC3	C32-C33-C34-C35
2	Q	506	MC3	C40-C41-C42-C43
2	T	502	MC3	C32-C33-C34-C35
2	E	504	MC3	C40-C41-C42-C43
2	K	504	MC3	C40-C41-C42-C43
2	Q	504	MC3	C40-C41-C42-C43
2	X	504	MC3	C40-C41-C42-C43
2	E	503	MC3	C12-C11-O3-C3
2	K	503	MC3	C12-C11-O3-C3
2	Q	503	MC3	C12-C11-O3-C3
2	X	503	MC3	C12-C11-O3-C3
2	C	503	MC3	C39-C40-C41-C42
2	I	503	MC3	C39-C40-C41-C42
2	O	503	MC3	C39-C40-C41-C42
2	V	503	MC3	C39-C40-C41-C42
2	A	506	MC3	C31-C32-C33-C34
2	B	503	MC3	C31-C32-C33-C34
2	G	507	MC3	C31-C32-C33-C34
2	H	503	MC3	C31-C32-C33-C34
2	M	506	MC3	C31-C32-C33-C34
2	N	503	MC3	C31-C32-C33-C34
2	S	507	MC3	C31-C32-C33-C34
2	T	503	MC3	C31-C32-C33-C34
2	D	506	MC3	O3P-C1-C2-C3
2	F	506	MC3	O3P-C1-C2-C3
2	J	506	MC3	O3P-C1-C2-C3
2	L	507	MC3	O3P-C1-C2-C3
2	P	506	MC3	O3P-C1-C2-C3
2	R	506	MC3	O3P-C1-C2-C3
2	W	506	MC3	O3P-C1-C2-C3
2	Y	507	MC3	O3P-C1-C2-C3
2	E	506	MC3	C4-C5-N-C8
2	K	506	MC3	C4-C5-N-C8
2	Q	506	MC3	C4-C5-N-C8
2	X	506	MC3	C4-C5-N-C8
2	B	503	MC3	C13-C14-C15-C16
2	H	503	MC3	C13-C14-C15-C16
2	N	503	MC3	C13-C14-C15-C16
2	T	503	MC3	C13-C14-C15-C16
2	A	502	MC3	C1-C2-C3-O3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	G	503	MC3	C1-C2-C3-O3
2	M	502	MC3	C1-C2-C3-O3
2	S	503	MC3	C1-C2-C3-O3
2	D	506	MC3	C38-C39-C40-C41
2	J	506	MC3	C38-C39-C40-C41
2	P	506	MC3	C38-C39-C40-C41
2	W	506	MC3	C38-C39-C40-C41
2	E	506	MC3	C35-C36-C37-C38
2	Q	506	MC3	C35-C36-C37-C38
2	K	506	MC3	C35-C36-C37-C38
2	X	506	MC3	C35-C36-C37-C38
2	A	506	MC3	C12-C11-O3-C3
2	G	507	MC3	C12-C11-O3-C3
2	M	506	MC3	C12-C11-O3-C3
2	S	507	MC3	C12-C11-O3-C3
2	C	503	MC3	C41-C42-C43-C44
2	I	503	MC3	C41-C42-C43-C44
2	O	503	MC3	C41-C42-C43-C44
2	V	503	MC3	C41-C42-C43-C44
2	E	506	MC3	C20-C21-C22-C23
2	K	506	MC3	C20-C21-C22-C23
2	Q	506	MC3	C20-C21-C22-C23
2	X	506	MC3	C20-C21-C22-C23
2	A	502	MC3	C35-C36-C37-C38
2	G	503	MC3	C35-C36-C37-C38
2	M	502	MC3	C35-C36-C37-C38
2	B	501	MC3	C36-C37-C38-C39
2	H	501	MC3	C36-C37-C38-C39
2	N	501	MC3	C36-C37-C38-C39
2	S	503	MC3	C35-C36-C37-C38
2	T	501	MC3	C36-C37-C38-C39
2	A	506	MC3	C32-C33-C34-C35
2	G	507	MC3	C32-C33-C34-C35
2	M	506	MC3	C32-C33-C34-C35
2	S	507	MC3	C32-C33-C34-C35
2	E	503	MC3	O11-C11-O3-C3
2	K	503	MC3	O11-C11-O3-C3
2	Q	503	MC3	O11-C11-O3-C3
2	X	503	MC3	O11-C11-O3-C3
2	F	509	MC3	C1-O3P-P-O4P
2	L	501	MC3	C1-O3P-P-O4P
2	R	509	MC3	C1-O3P-P-O4P

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	Y	501	MC3	C1-O3P-P-O4P
2	A	506	MC3	O11-C11-O3-C3
2	G	507	MC3	O11-C11-O3-C3
2	M	506	MC3	O11-C11-O3-C3
2	E	506	MC3	C15-C16-C17-C18
2	K	506	MC3	C15-C16-C17-C18
2	Q	506	MC3	C15-C16-C17-C18
2	S	507	MC3	O11-C11-O3-C3
2	X	506	MC3	C15-C16-C17-C18
2	A	502	MC3	O3P-C1-C2-O2
2	D	506	MC3	O3P-C1-C2-O2
2	G	503	MC3	O3P-C1-C2-O2
2	J	506	MC3	O3P-C1-C2-O2
2	M	502	MC3	O3P-C1-C2-O2
2	P	506	MC3	O3P-C1-C2-O2
2	S	503	MC3	O3P-C1-C2-O2
2	W	506	MC3	O3P-C1-C2-O2
2	T	501	MC3	C34-C35-C36-C37
2	B	501	MC3	C34-C35-C36-C37
2	H	501	MC3	C34-C35-C36-C37
2	N	501	MC3	C34-C35-C36-C37
2	E	506	MC3	C5-C4-O4P-P
2	K	506	MC3	C5-C4-O4P-P
2	Q	506	MC3	C5-C4-O4P-P
2	X	506	MC3	C5-C4-O4P-P
2	A	502	MC3	O2-C2-C3-O3
2	A	506	MC3	O2-C2-C3-O3
2	G	503	MC3	O2-C2-C3-O3
2	G	507	MC3	O2-C2-C3-O3
2	M	502	MC3	O2-C2-C3-O3
2	M	506	MC3	O2-C2-C3-O3
2	S	503	MC3	O2-C2-C3-O3
2	S	507	MC3	O2-C2-C3-O3
2	B	501	MC3	C35-C36-C37-C38
2	C	506	MC3	C40-C41-C42-C43
2	H	501	MC3	C35-C36-C37-C38
2	I	506	MC3	C40-C41-C42-C43
2	N	501	MC3	C35-C36-C37-C38
2	O	506	MC3	C40-C41-C42-C43
2	T	501	MC3	C35-C36-C37-C38
2	V	506	MC3	C40-C41-C42-C43
2	B	505	MC3	C36-C37-C38-C39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	H	505	MC3	C36-C37-C38-C39
2	N	505	MC3	C36-C37-C38-C39
2	T	505	MC3	C36-C37-C38-C39
2	A	506	MC3	O4P-C4-C5-N
2	A	507	MC3	O4P-C4-C5-N
2	D	506	MC3	O4P-C4-C5-N
2	G	507	MC3	O4P-C4-C5-N
2	G	508	MC3	O4P-C4-C5-N
2	J	506	MC3	O4P-C4-C5-N
2	M	506	MC3	O4P-C4-C5-N
2	M	507	MC3	O4P-C4-C5-N
2	P	506	MC3	O4P-C4-C5-N
2	S	507	MC3	O4P-C4-C5-N
2	S	508	MC3	O4P-C4-C5-N
2	W	506	MC3	O4P-C4-C5-N
2	A	502	MC3	C33-C34-C35-C36
2	G	503	MC3	C33-C34-C35-C36
2	M	502	MC3	C33-C34-C35-C36
2	S	503	MC3	C33-C34-C35-C36
2	T	501	MC3	C41-C42-C43-C44
2	B	501	MC3	C41-C42-C43-C44
2	H	501	MC3	C41-C42-C43-C44
2	N	501	MC3	C41-C42-C43-C44
2	E	506	MC3	O3P-C1-C2-O2
2	K	506	MC3	O3P-C1-C2-O2
2	Q	506	MC3	O3P-C1-C2-O2
2	X	506	MC3	O3P-C1-C2-O2
2	D	506	MC3	C37-C38-C39-C40
2	J	506	MC3	C37-C38-C39-C40
2	P	506	MC3	C37-C38-C39-C40
2	W	506	MC3	C37-C38-C39-C40
2	A	505	MC3	O2-C2-C3-O3
2	G	506	MC3	O2-C2-C3-O3
2	M	505	MC3	O2-C2-C3-O3
2	S	506	MC3	O2-C2-C3-O3
2	S	506	MC3	C34-C35-C36-C37
2	A	505	MC3	C34-C35-C36-C37
2	G	506	MC3	C34-C35-C36-C37
2	M	505	MC3	C34-C35-C36-C37
2	A	506	MC3	C1-O3P-P-O4P
2	A	506	MC3	C4-O4P-P-O3P
2	B	503	MC3	C4-O4P-P-O1P

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	B	503	MC3	C4-O4P-P-O2P
2	B	503	MC3	C4-O4P-P-O3P
2	D	506	MC3	C1-O3P-P-O2P
2	E	506	MC3	C4-C5-N-C7
2	E	506	MC3	C4-O4P-P-O1P
2	E	506	MC3	C4-O4P-P-O3P
2	F	506	MC3	C4-O4P-P-O1P
2	G	507	MC3	C1-O3P-P-O4P
2	G	507	MC3	C4-O4P-P-O3P
2	H	503	MC3	C4-O4P-P-O1P
2	H	503	MC3	C4-O4P-P-O2P
2	H	503	MC3	C4-O4P-P-O3P
2	J	506	MC3	C1-O3P-P-O2P
2	K	506	MC3	C4-C5-N-C7
2	K	506	MC3	C4-O4P-P-O1P
2	K	506	MC3	C4-O4P-P-O3P
2	L	507	MC3	C4-O4P-P-O1P
2	M	506	MC3	C1-O3P-P-O4P
2	M	506	MC3	C4-O4P-P-O3P
2	N	503	MC3	C4-O4P-P-O1P
2	N	503	MC3	C4-O4P-P-O2P
2	N	503	MC3	C4-O4P-P-O3P
2	P	506	MC3	C1-O3P-P-O2P
2	Q	506	MC3	C4-C5-N-C7
2	Q	506	MC3	C4-O4P-P-O1P
2	Q	506	MC3	C4-O4P-P-O3P
2	R	506	MC3	C4-O4P-P-O1P
2	S	507	MC3	C1-O3P-P-O4P
2	S	507	MC3	C4-O4P-P-O3P
2	T	503	MC3	C4-O4P-P-O1P
2	T	503	MC3	C4-O4P-P-O2P
2	T	503	MC3	C4-O4P-P-O3P
2	W	506	MC3	C1-O3P-P-O2P
2	X	506	MC3	C4-C5-N-C7
2	X	506	MC3	C4-O4P-P-O1P
2	X	506	MC3	C4-O4P-P-O3P
2	Y	507	MC3	C4-O4P-P-O1P
2	K	506	MC3	C32-C33-C34-C35
2	X	506	MC3	C32-C33-C34-C35
2	E	506	MC3	C32-C33-C34-C35
2	Q	506	MC3	C32-C33-C34-C35
2	D	501	MC3	C35-C36-C37-C38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	E	506	MC3	C17-C18-C19-C20
2	J	501	MC3	C35-C36-C37-C38
2	K	506	MC3	C17-C18-C19-C20
2	P	501	MC3	C35-C36-C37-C38
2	Q	506	MC3	C17-C18-C19-C20
2	W	501	MC3	C35-C36-C37-C38
2	X	506	MC3	C17-C18-C19-C20
2	H	502	MC3	C41-C42-C43-C44
2	A	502	MC3	C4-C5-N-C8
2	G	503	MC3	C4-C5-N-C8
2	M	502	MC3	C4-C5-N-C8
2	S	503	MC3	C4-C5-N-C8
2	B	502	MC3	C41-C42-C43-C44
2	N	502	MC3	C41-C42-C43-C44
2	T	502	MC3	C41-C42-C43-C44
2	E	506	MC3	O3P-C1-C2-C3
2	K	506	MC3	O3P-C1-C2-C3
2	Q	506	MC3	O3P-C1-C2-C3
2	X	506	MC3	O3P-C1-C2-C3
2	E	502	MC3	C32-C33-C34-C35
2	K	502	MC3	C32-C33-C34-C35
2	Q	502	MC3	C32-C33-C34-C35
2	X	502	MC3	C32-C33-C34-C35
2	E	503	MC3	O3-C11-C12-C13
2	K	503	MC3	O3-C11-C12-C13
2	Q	503	MC3	O3-C11-C12-C13
2	X	503	MC3	O3-C11-C12-C13
2	F	506	MC3	C5-C4-O4P-P
2	L	507	MC3	C5-C4-O4P-P
2	R	506	MC3	C5-C4-O4P-P
2	Y	507	MC3	C5-C4-O4P-P
2	E	506	MC3	O3-C11-C12-C13
2	K	506	MC3	O3-C11-C12-C13
2	Q	506	MC3	O3-C11-C12-C13
2	X	506	MC3	O3-C11-C12-C13
2	C	502	MC3	C34-C35-C36-C37
2	I	502	MC3	C34-C35-C36-C37
2	O	502	MC3	C34-C35-C36-C37
2	V	502	MC3	C34-C35-C36-C37
2	G	503	MC3	C19-C20-C21-C22
2	A	502	MC3	C19-C20-C21-C22
2	M	502	MC3	C19-C20-C21-C22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	S	503	MC3	C19-C20-C21-C22
2	A	502	MC3	O3P-C1-C2-C3
2	G	503	MC3	O3P-C1-C2-C3
2	M	502	MC3	O3P-C1-C2-C3
2	S	503	MC3	O3P-C1-C2-C3
2	G	501	MC3	C35-C36-C37-C38
2	M	508	MC3	C35-C36-C37-C38
2	S	501	MC3	C35-C36-C37-C38
2	E	503	MC3	C2-C1-O3P-P
2	K	503	MC3	C2-C1-O3P-P
2	Q	503	MC3	C2-C1-O3P-P
2	X	503	MC3	C2-C1-O3P-P
2	A	508	MC3	C35-C36-C37-C38
2	T	502	MC3	C39-C40-C41-C42
2	B	502	MC3	C39-C40-C41-C42
2	H	502	MC3	C39-C40-C41-C42
2	N	502	MC3	C39-C40-C41-C42
2	E	503	MC3	C1-C2-O2-C31
2	K	503	MC3	C1-C2-O2-C31
2	Q	503	MC3	C1-C2-O2-C31
2	X	503	MC3	C1-C2-O2-C31
2	Y	508	MC3	C37-C38-C39-C40
2	F	507	MC3	C37-C38-C39-C40
2	L	508	MC3	C37-C38-C39-C40
2	R	507	MC3	C37-C38-C39-C40
2	K	504	MC3	C37-C38-C39-C40
2	E	504	MC3	C37-C38-C39-C40
2	K	506	MC3	C12-C13-C14-C15
2	Q	504	MC3	C37-C38-C39-C40
2	X	504	MC3	C37-C38-C39-C40
2	X	506	MC3	C12-C13-C14-C15
2	F	506	MC3	C1-C2-O2-C31
2	L	507	MC3	C1-C2-O2-C31
2	R	506	MC3	C1-C2-O2-C31
2	Y	507	MC3	C1-C2-O2-C31
2	E	506	MC3	C12-C13-C14-C15
2	Q	506	MC3	C12-C13-C14-C15
2	E	504	MC3	C35-C36-C37-C38
2	K	504	MC3	C35-C36-C37-C38
2	Q	504	MC3	C35-C36-C37-C38
2	X	504	MC3	C35-C36-C37-C38
2	D	506	MC3	C2-C1-O3P-P

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	J	506	MC3	C2-C1-O3P-P
2	P	506	MC3	C2-C1-O3P-P
2	W	506	MC3	C2-C1-O3P-P
2	A	507	MC3	C13-C14-C15-C16
2	G	508	MC3	C13-C14-C15-C16
2	M	507	MC3	C13-C14-C15-C16
2	S	508	MC3	C13-C14-C15-C16
2	B	503	MC3	O2-C31-C32-C33
2	H	503	MC3	O2-C31-C32-C33
2	N	503	MC3	O2-C31-C32-C33
2	T	503	MC3	O2-C31-C32-C33
2	A	505	MC3	C1-C2-C3-O3
2	G	506	MC3	C1-C2-C3-O3
2	M	505	MC3	C1-C2-C3-O3
2	S	506	MC3	C1-C2-C3-O3
2	B	505	MC3	C37-C38-C39-C40
2	H	505	MC3	C37-C38-C39-C40
2	N	505	MC3	C37-C38-C39-C40
2	T	505	MC3	C37-C38-C39-C40
2	W	504	MC3	C36-C37-C38-C39
2	D	504	MC3	C36-C37-C38-C39
2	J	504	MC3	C36-C37-C38-C39
2	P	504	MC3	C36-C37-C38-C39
2	A	502	MC3	C41-C42-C43-C44
2	G	503	MC3	C41-C42-C43-C44
2	M	502	MC3	C41-C42-C43-C44
2	S	503	MC3	C41-C42-C43-C44
2	A	502	MC3	O2-C31-C32-C33
2	G	503	MC3	O2-C31-C32-C33
2	M	502	MC3	O2-C31-C32-C33
2	S	503	MC3	O2-C31-C32-C33
2	A	502	MC3	O3-C11-C12-C13
2	G	503	MC3	O3-C11-C12-C13
2	M	502	MC3	O3-C11-C12-C13
2	S	503	MC3	O3-C11-C12-C13
2	D	505	MC3	C38-C39-C40-C41
2	J	505	MC3	C38-C39-C40-C41
2	P	505	MC3	C38-C39-C40-C41
2	W	505	MC3	C38-C39-C40-C41
2	S	503	MC3	C15-C16-C17-C18
2	A	502	MC3	C15-C16-C17-C18
2	M	502	MC3	C15-C16-C17-C18

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	G	503	MC3	C15-C16-C17-C18
2	E	506	MC3	C19-C20-C21-C22
2	K	506	MC3	C19-C20-C21-C22
2	Q	506	MC3	C19-C20-C21-C22
2	X	506	MC3	C19-C20-C21-C22
2	A	502	MC3	C4-C5-N-C6
2	A	502	MC3	C4-C5-N-C7
2	G	503	MC3	C4-C5-N-C6
2	G	503	MC3	C4-C5-N-C7
2	M	502	MC3	C4-C5-N-C6
2	M	502	MC3	C4-C5-N-C7
2	S	503	MC3	C4-C5-N-C6
2	S	503	MC3	C4-C5-N-C7
2	I	505	MC3	C33-C34-C35-C36
2	C	505	MC3	C33-C34-C35-C36
2	O	505	MC3	C33-C34-C35-C36
2	V	505	MC3	C33-C34-C35-C36
2	A	502	MC3	O11-C11-C12-C13
2	G	503	MC3	O11-C11-C12-C13
2	M	502	MC3	O11-C11-C12-C13
2	S	503	MC3	O11-C11-C12-C13
2	A	503	MC3	C40-C41-C42-C43
2	G	504	MC3	C40-C41-C42-C43
2	M	503	MC3	C40-C41-C42-C43
2	G	503	MC3	O31-C31-C32-C33
2	F	502	MC3	C39-C40-C41-C42
2	R	502	MC3	C39-C40-C41-C42
2	S	504	MC3	C40-C41-C42-C43
2	A	502	MC3	O31-C31-C32-C33
2	M	502	MC3	O31-C31-C32-C33
2	S	503	MC3	O31-C31-C32-C33
2	L	503	MC3	C39-C40-C41-C42
2	Y	503	MC3	C39-C40-C41-C42

There are no ring outliers.

54 monomers are involved in 73 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	501	MC3	1	0
2	R	509	MC3	1	0
2	A	508	MC3	1	0
2	B	503	MC3	4	0

Continued on next page...

Continued from previous page...

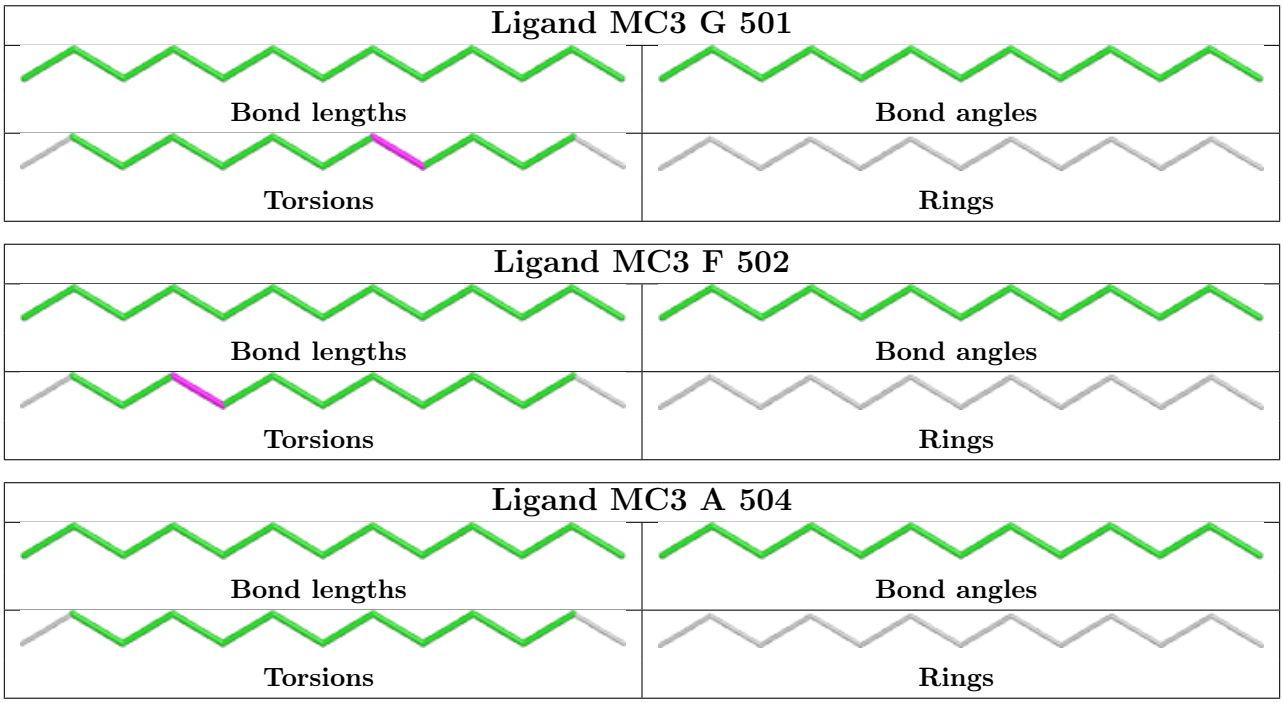
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	506	MC3	1	0
2	Y	508	MC3	1	0
2	Y	506	MC3	1	0
2	G	506	MC3	3	0
2	V	504	MC3	1	0
2	C	504	MC3	1	0
2	K	505	MC3	1	0
2	L	501	MC3	1	0
2	G	503	MC3	3	0
2	L	506	MC3	1	0
2	M	503	MC3	2	0
2	K	506	MC3	3	0
2	F	505	MC3	1	0
2	I	506	MC3	1	0
2	M	505	MC3	3	0
2	A	503	MC3	2	0
2	G	504	MC3	2	0
2	W	501	MC3	1	0
2	J	501	MC3	1	0
2	Y	501	MC3	1	0
2	X	506	MC3	3	0
2	E	506	MC3	2	0
2	A	502	MC3	2	0
2	I	504	MC3	1	0
2	S	506	MC3	3	0
2	H	503	MC3	3	0
2	L	508	MC3	1	0
2	O	506	MC3	1	0
2	O	504	MC3	1	0
2	J	502	MC3	1	0
2	J	506	MC3	1	0
2	N	503	MC3	5	0
2	W	506	MC3	2	0
2	X	505	MC3	1	0
2	V	506	MC3	1	0
2	E	502	MC3	1	0
2	S	504	MC3	2	0
2	Q	506	MC3	1	0
2	Q	502	MC3	1	0
2	F	509	MC3	1	0
2	T	503	MC3	3	0
2	W	502	MC3	1	0

Continued on next page...

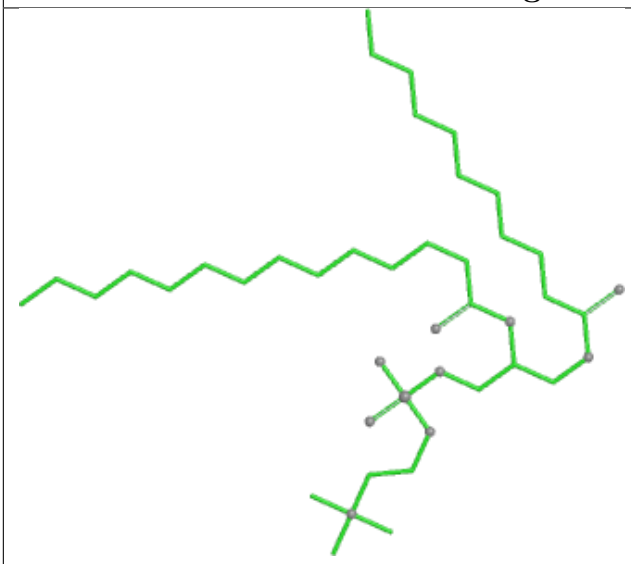
Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	M	508	MC3	1	0
2	F	507	MC3	1	0
2	A	505	MC3	3	0
2	S	501	MC3	1	0
2	M	502	MC3	2	0
2	R	507	MC3	1	0
2	R	505	MC3	1	0
2	S	503	MC3	3	0

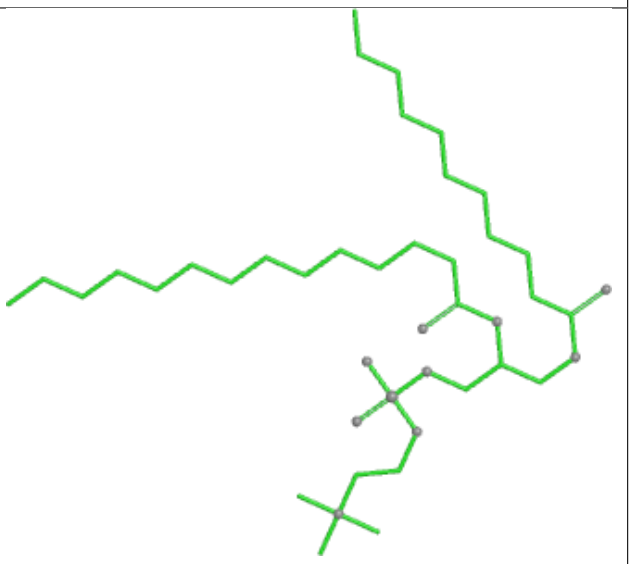
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



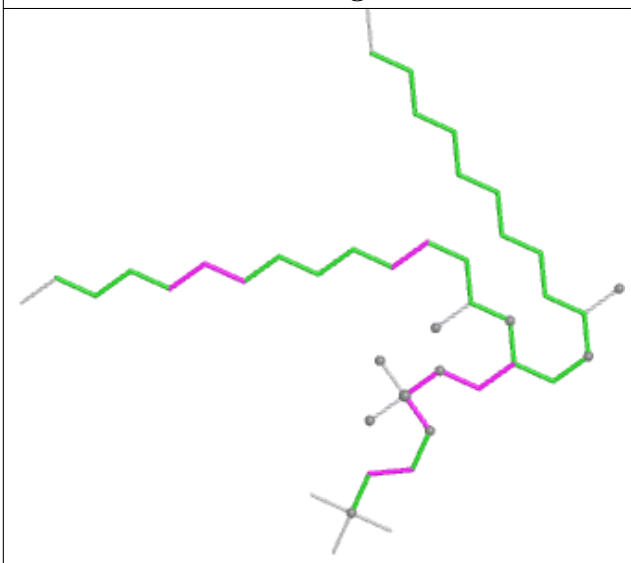
Ligand MC3 P 506



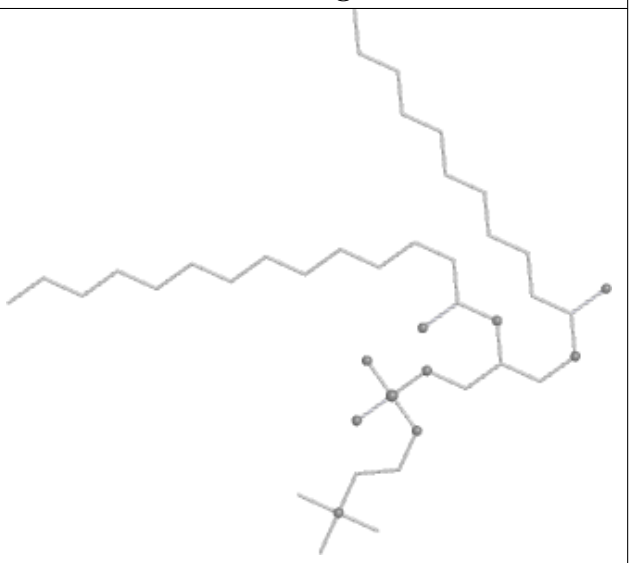
Bond lengths



Bond angles

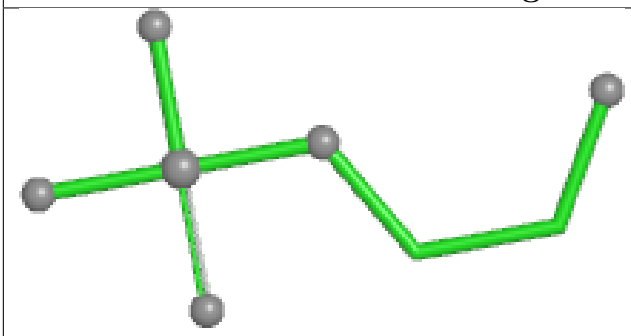


Torsions

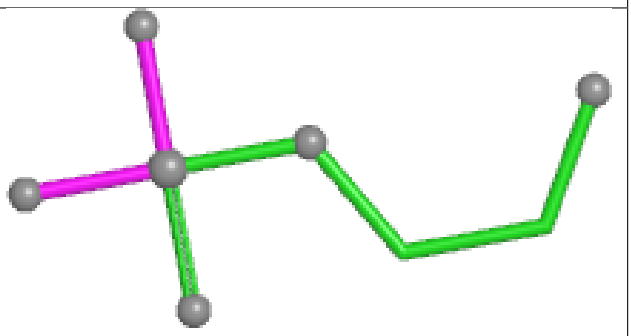


Rings

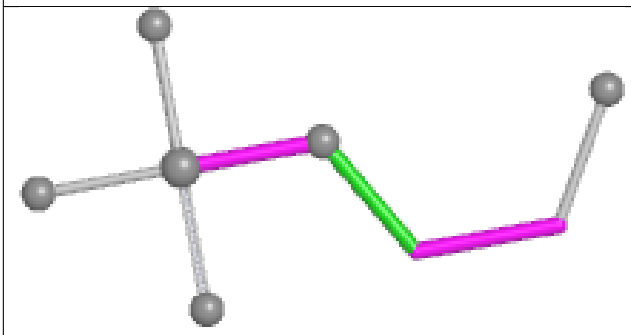
Ligand MC3 R 509



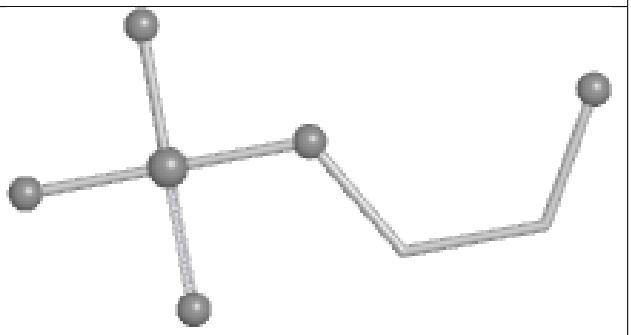
Bond lengths



Bond angles

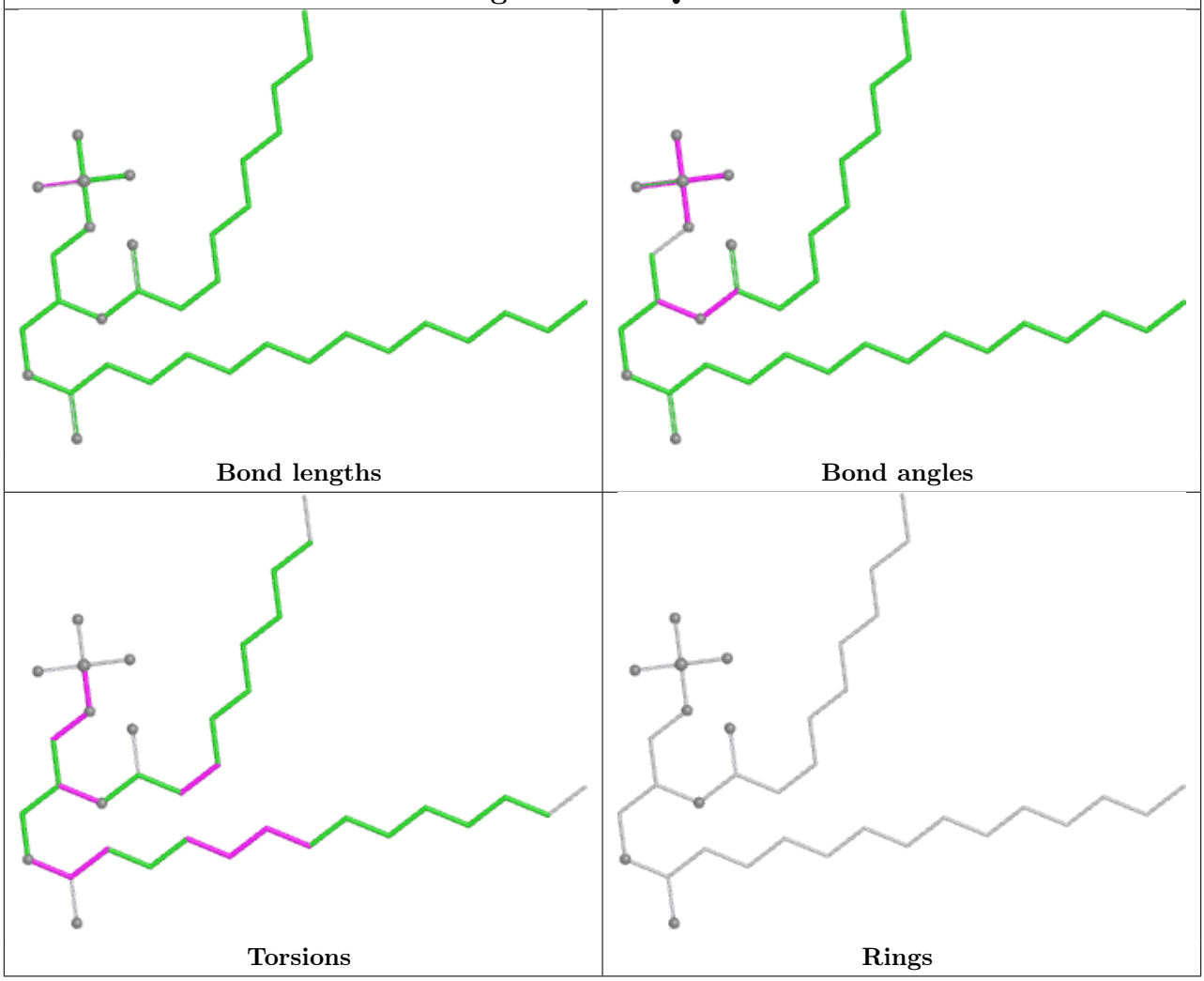


Torsions

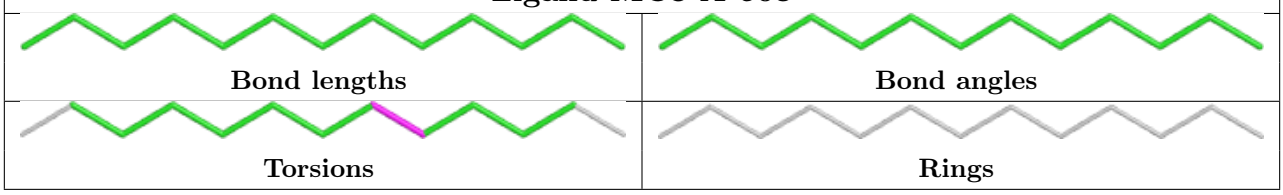


Rings

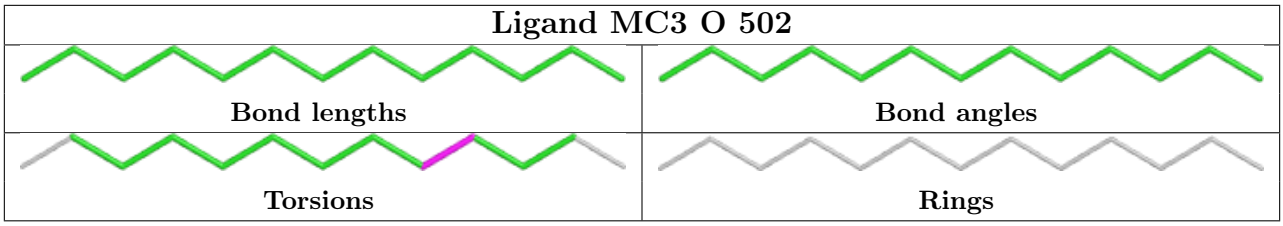
Ligand MC3 Q 503



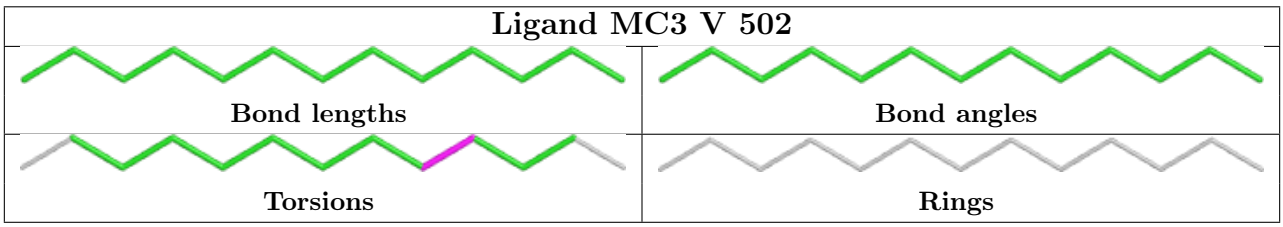
Ligand MC3 A 508



Ligand MC3 O 502



Ligand MC3 V 502

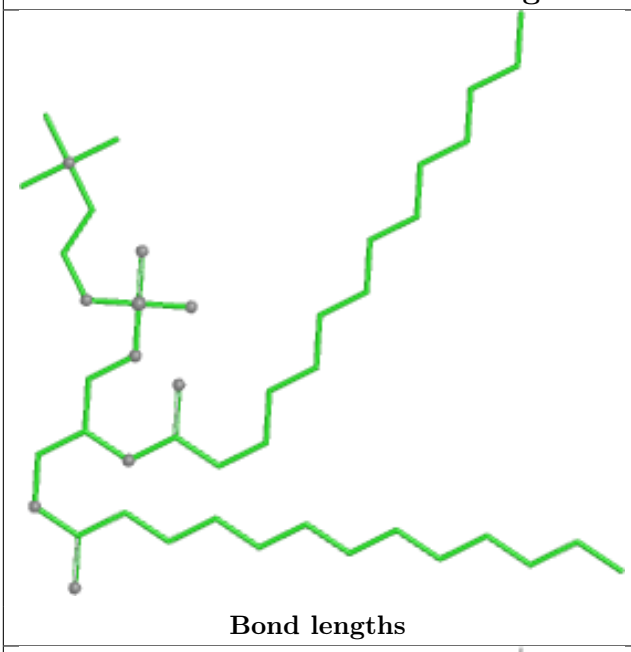


Ligand MC3 C 502	
 Bond lengths	 Bond angles
 Torsions	 Rings

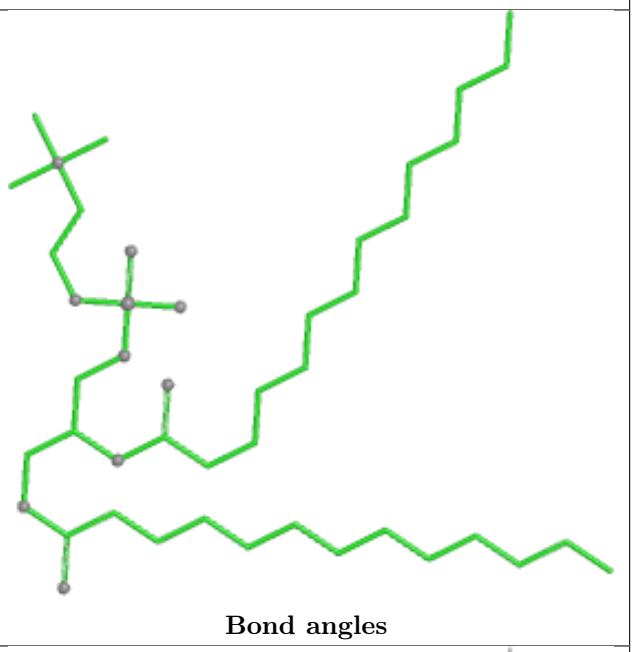
Ligand MC3 H 502	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand MC3 X 504	
 Bond lengths	 Bond angles
 Torsions	 Rings

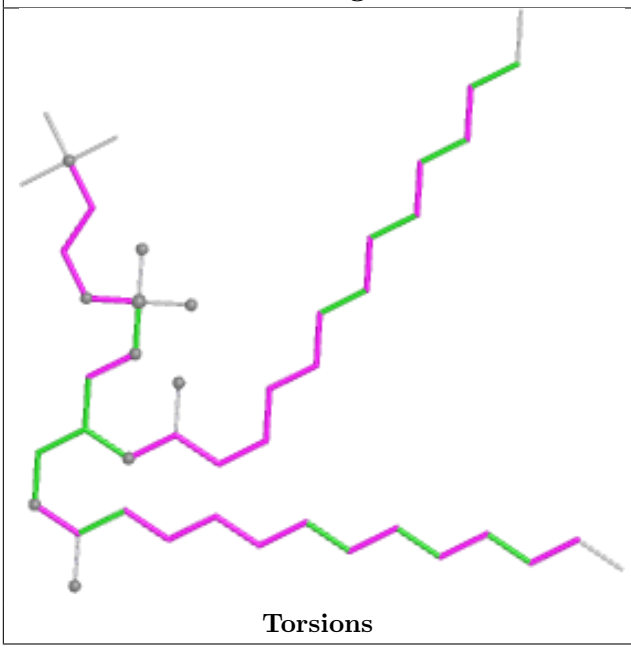
Ligand MC3 B 503



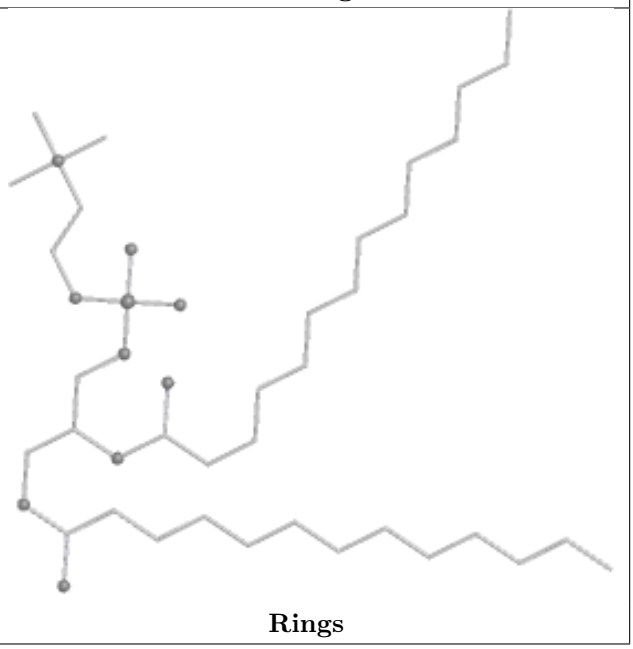
Bond lengths



Bond angles



Torsions



Rings

Ligand MC3 L 502



Bond lengths



Bond angles

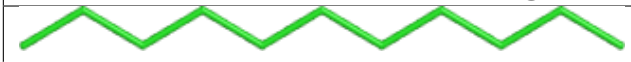


Torsions

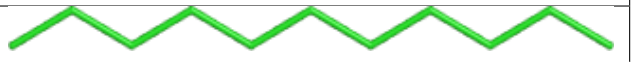


Rings

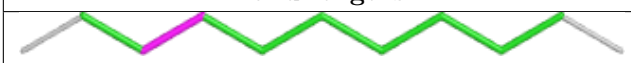
Ligand MC3 C 506



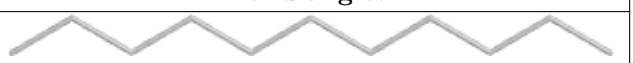
Bond lengths



Bond angles

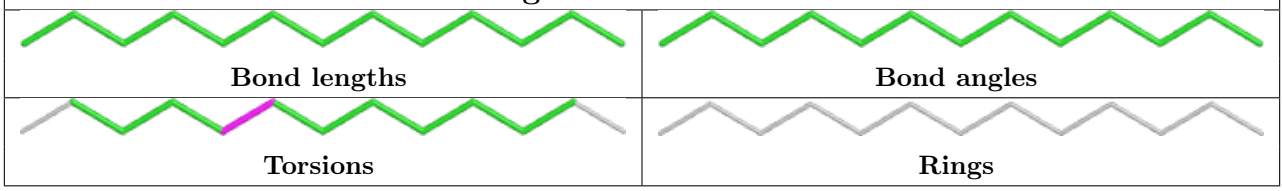


Torsions

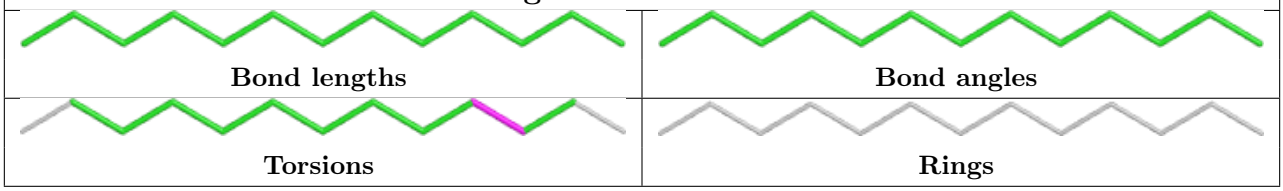


Rings

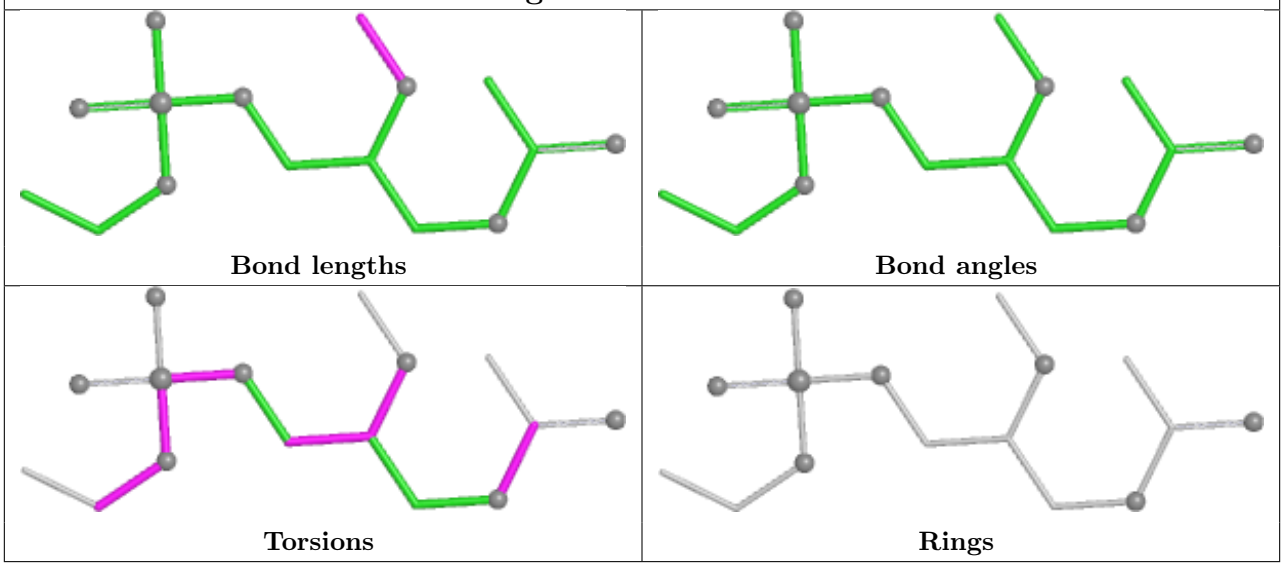
Ligand MC3 D 505



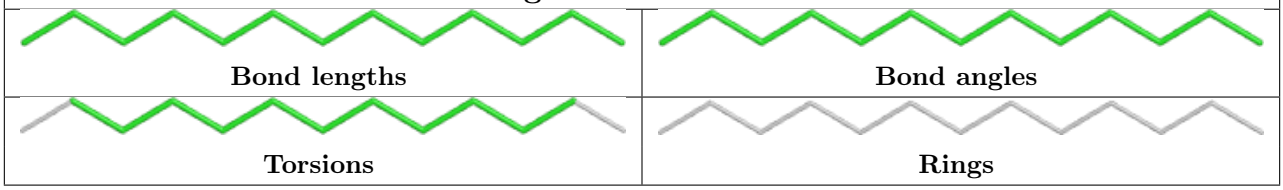
Ligand MC3 C 505



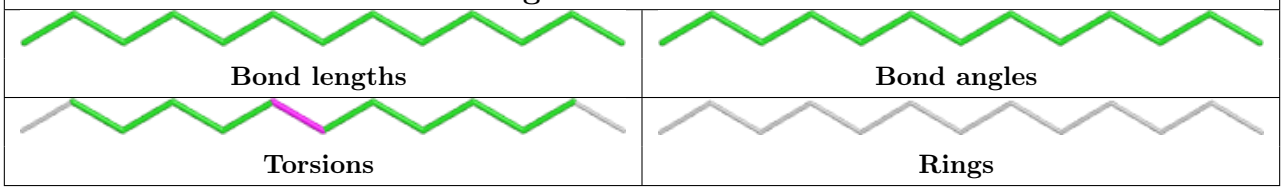
Ligand MC3 L 507



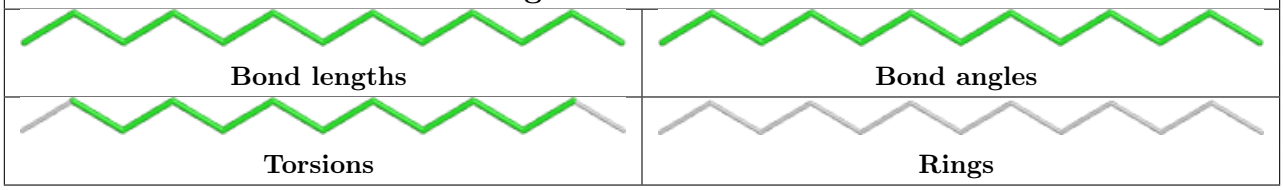
Ligand MC3 T 506



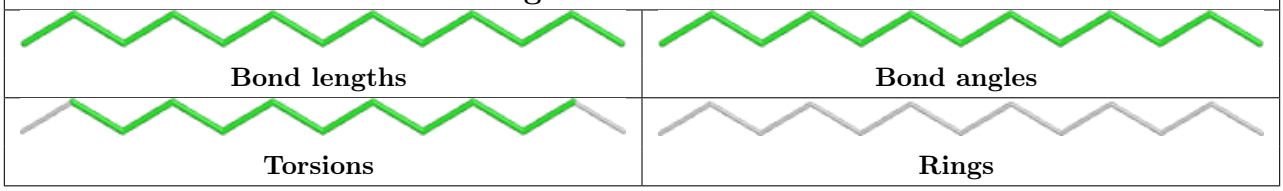
Ligand MC3 Y 508



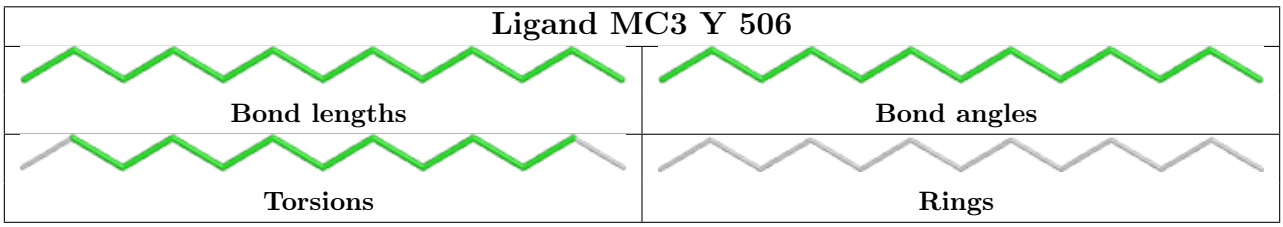
Ligand MC3 P 502



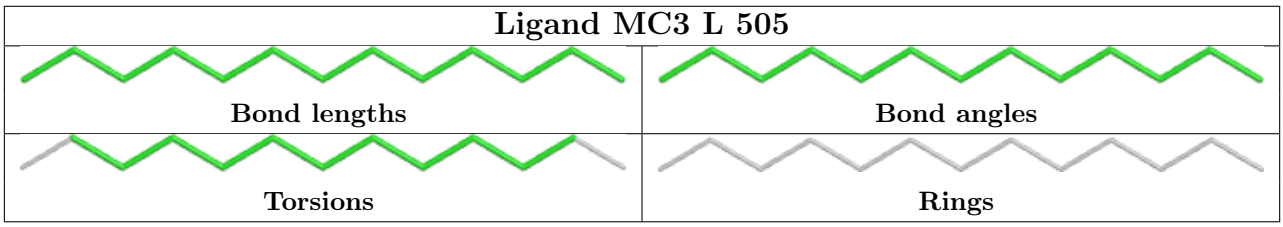
Ligand MC3 T 504



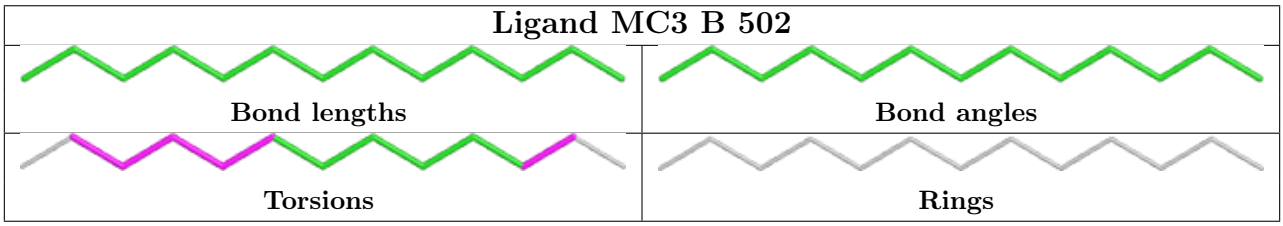
Ligand MC3 Y 506



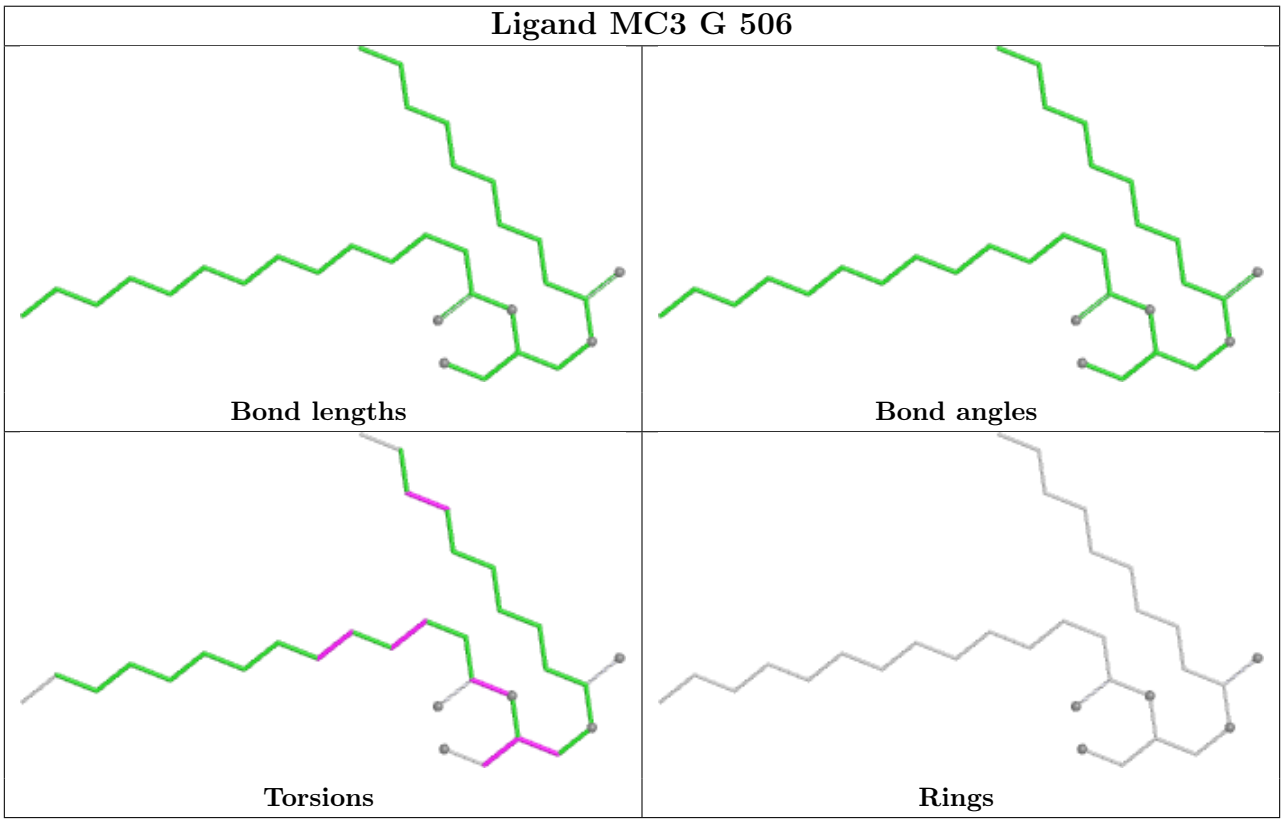
Ligand MC3 L 505



Ligand MC3 B 502



Ligand MC3 G 506



Ligand MC3 V 504


Bond lengths


Bond angles


Torsions


Rings

Ligand MC3 C 504


Bond lengths


Bond angles


Torsions


Rings

Ligand MC3 K 505

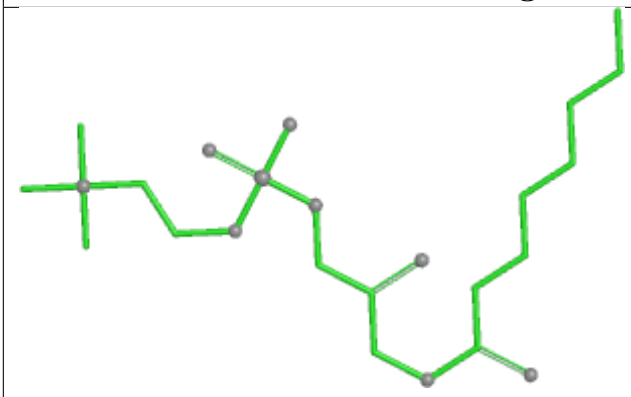

Bond lengths

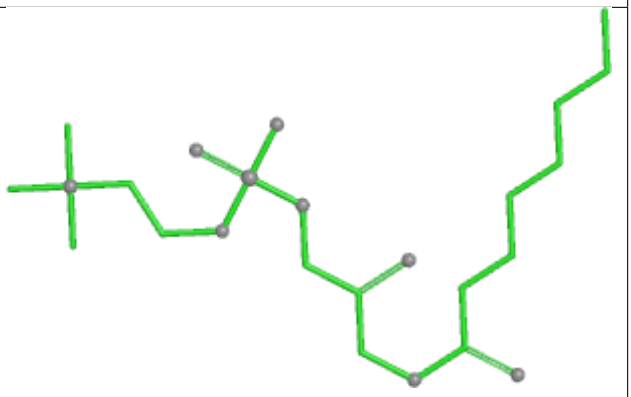

Bond angles

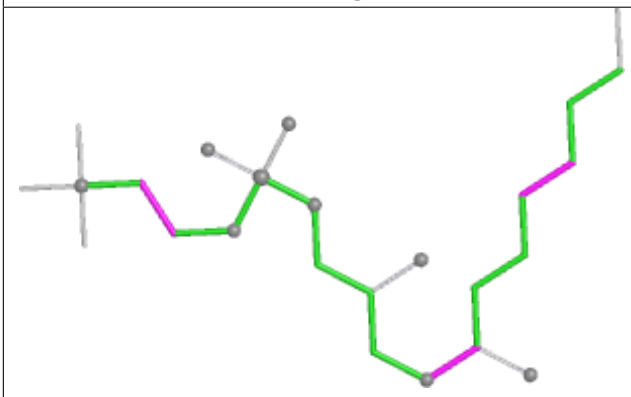

Torsions

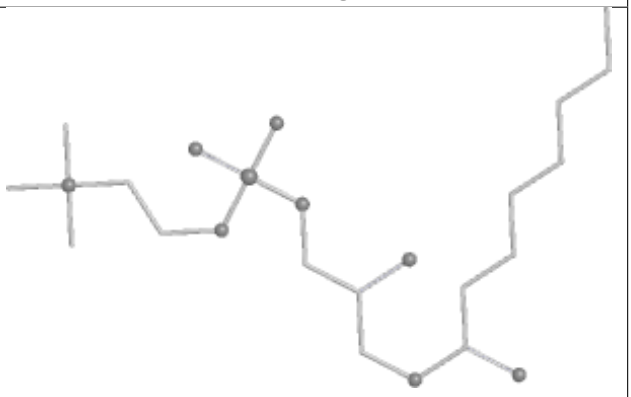

Rings

Ligand MC3 M 507

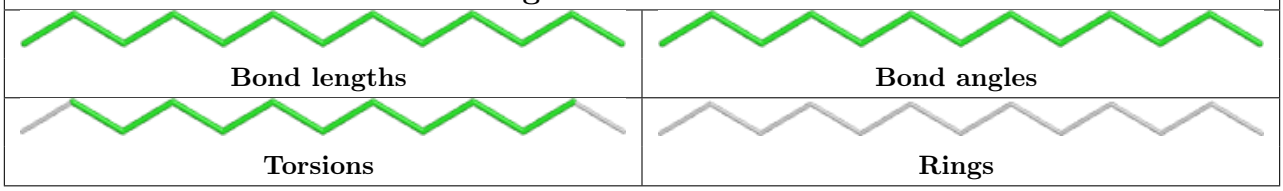

Bond lengths


Bond angles

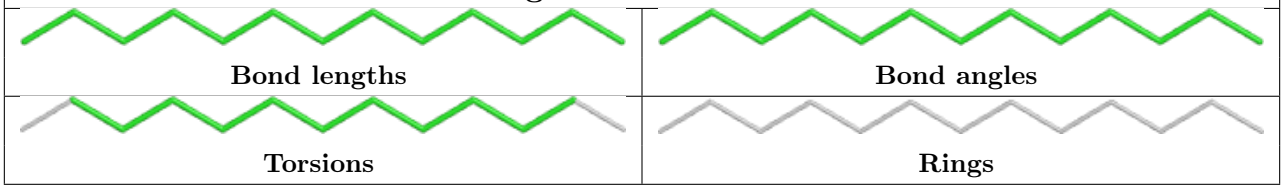

Torsions


Rings

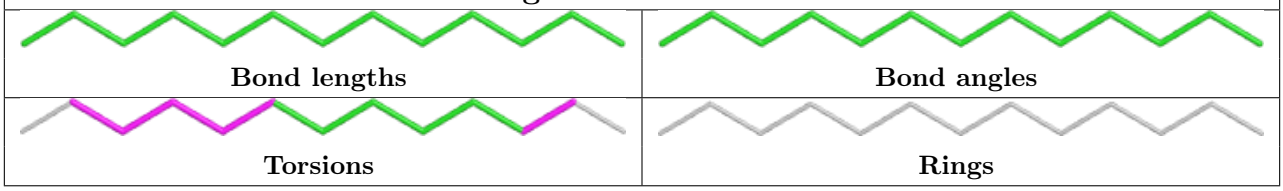
Ligand MC3 D 502



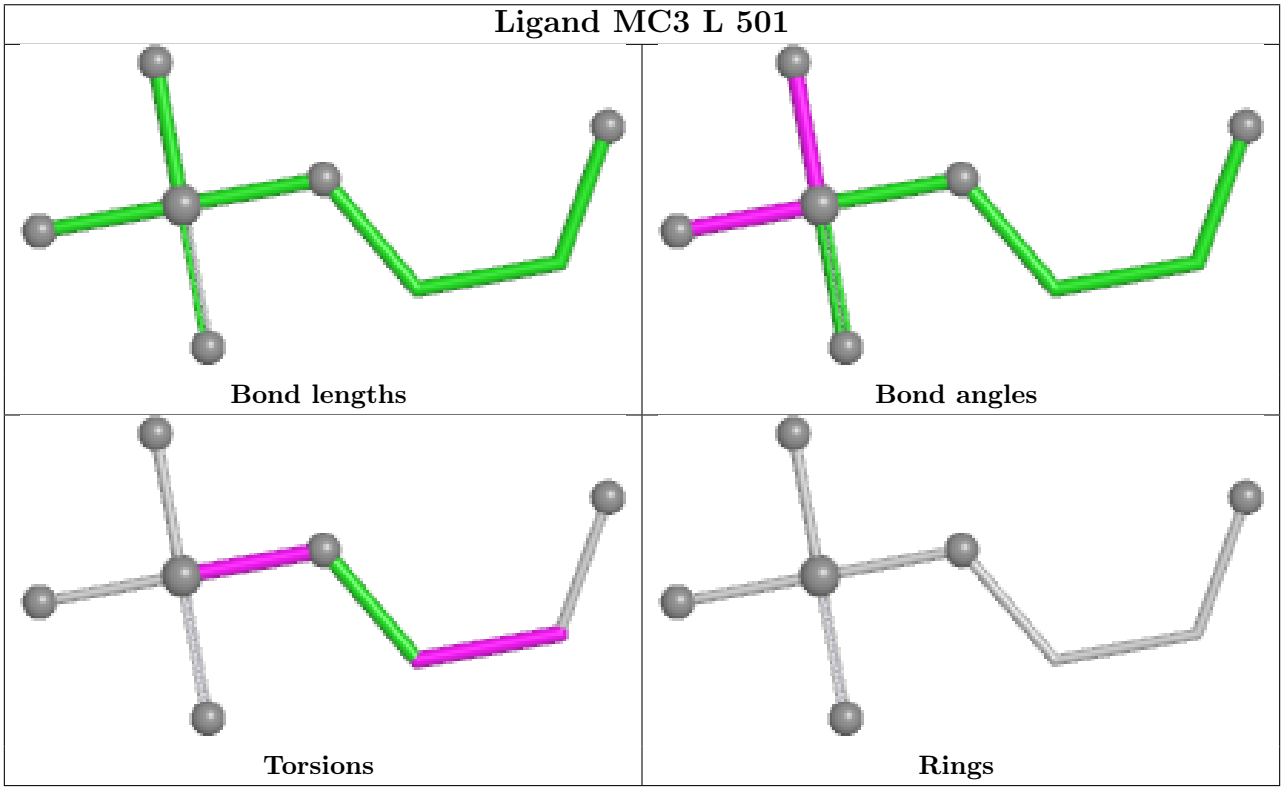
Ligand MC3 L 509



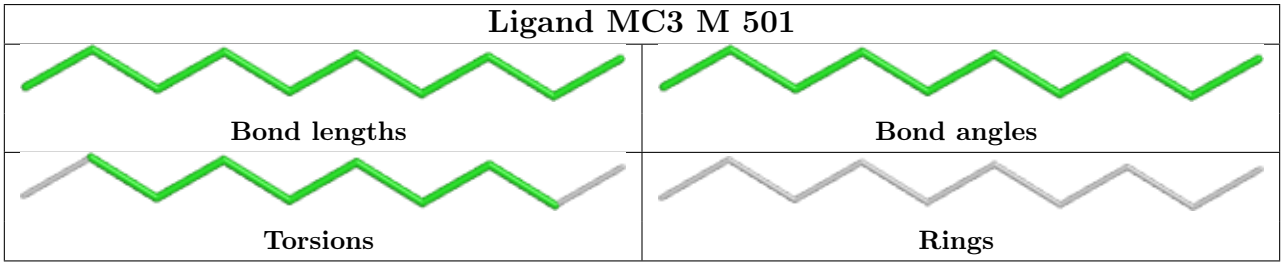
Ligand MC3 N 502



Ligand MC3 L 501



Ligand MC3 M 501

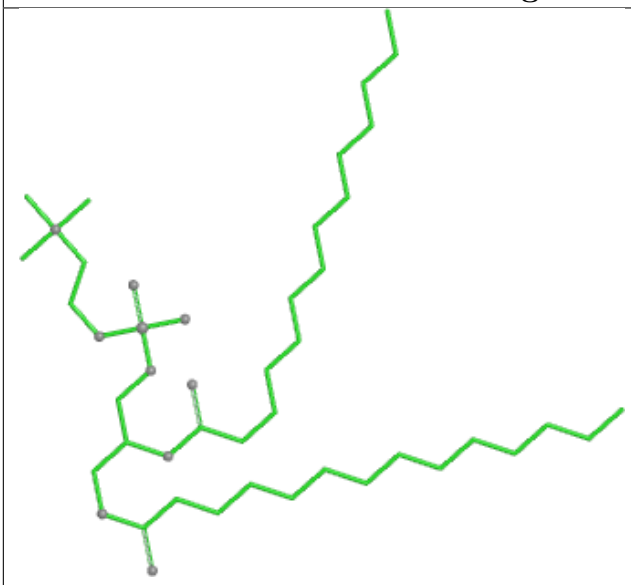


Ligand MC3 V 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

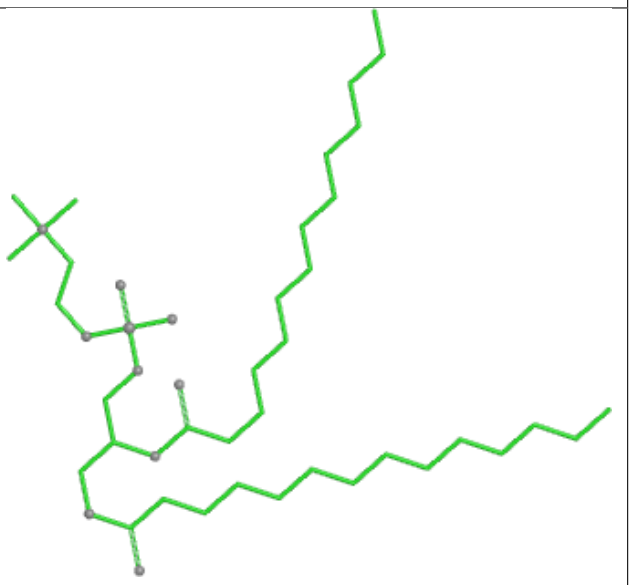
Ligand MC3 Q 504	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand MC3 P 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

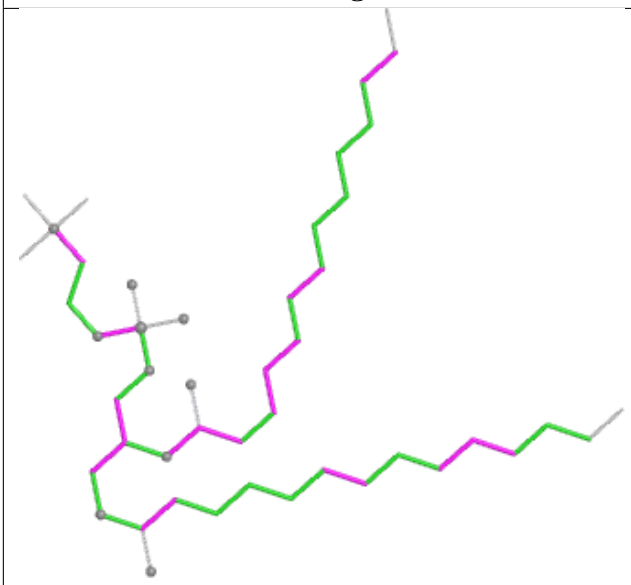
Ligand MC3 G 503



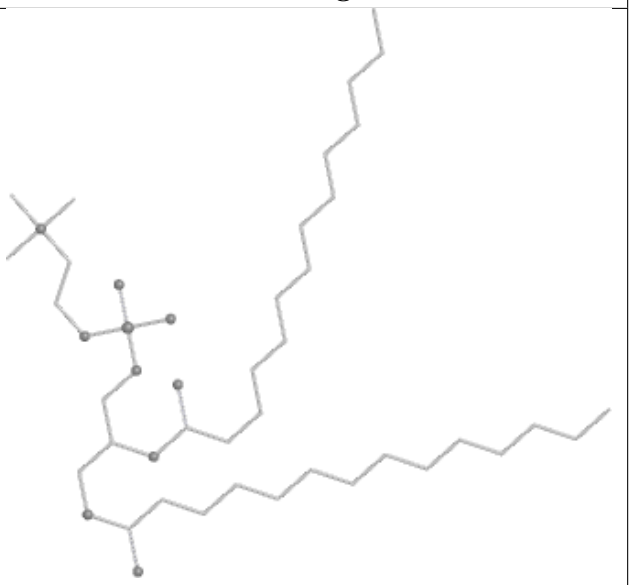
Bond lengths



Bond angles

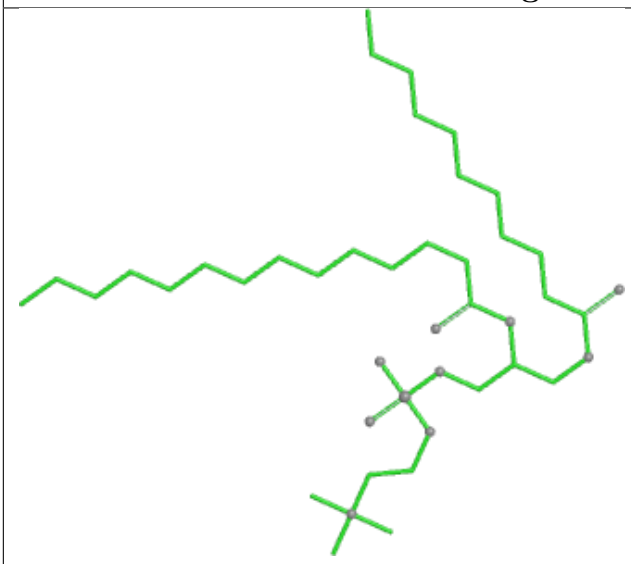


Torsions

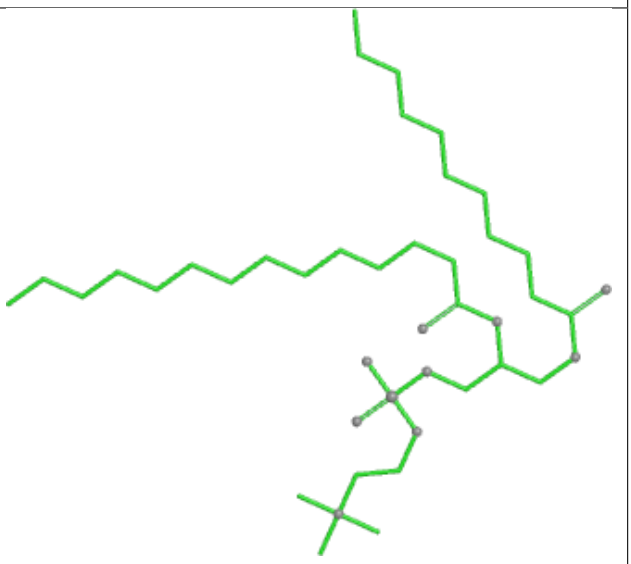


Rings

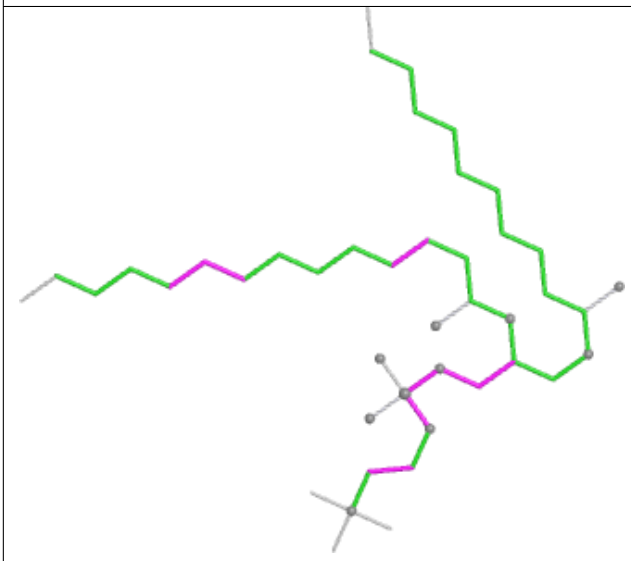
Ligand MC3 D 506



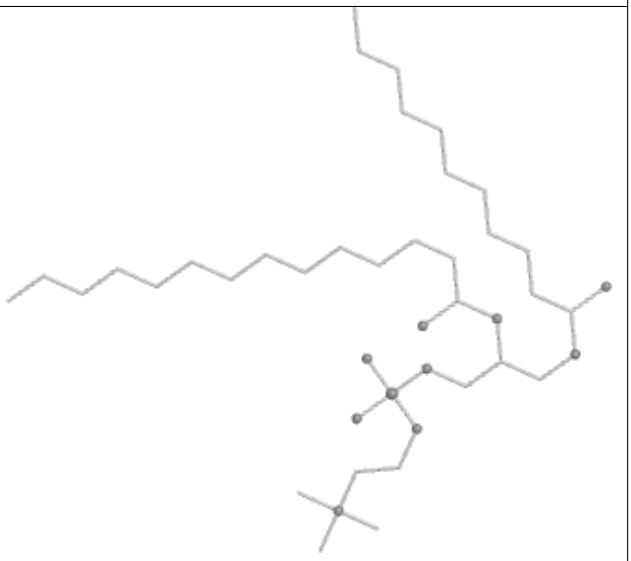
Bond lengths



Bond angles



Torsions



Rings

Ligand MC3 Y 509



Bond lengths



Bond angles



Torsions



Rings

Ligand MC3 R 504



Bond lengths



Bond angles



Torsions



Rings

Ligand MC3 E 504	
 Bond lengths	 Bond angles
 Torsions	 Rings

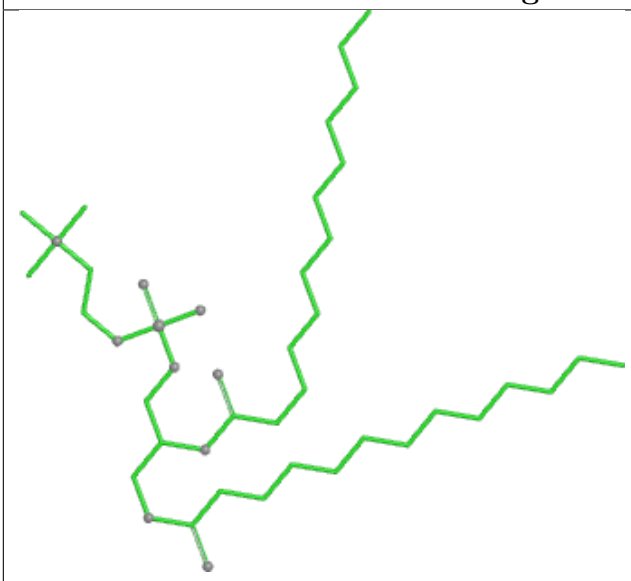
Ligand MC3 L 506	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand MC3 M 503	
 Bond lengths	 Bond angles
 Torsions	 Rings

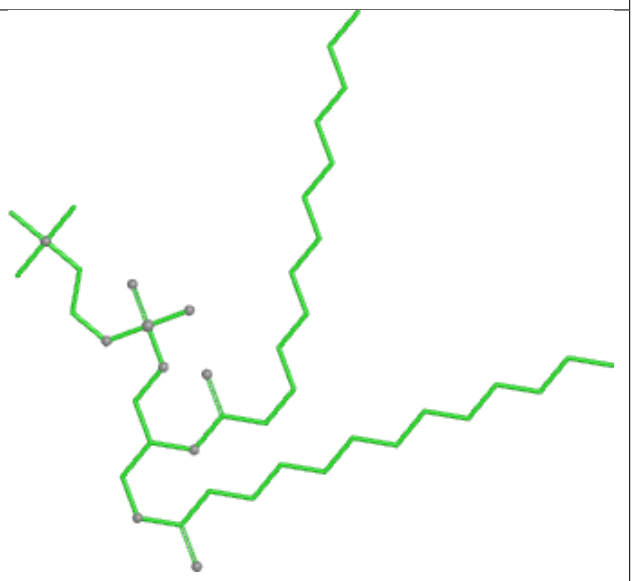
Ligand MC3 V 503	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand MC3 V 507	
 Bond lengths	 Bond angles
 Torsions	 Rings

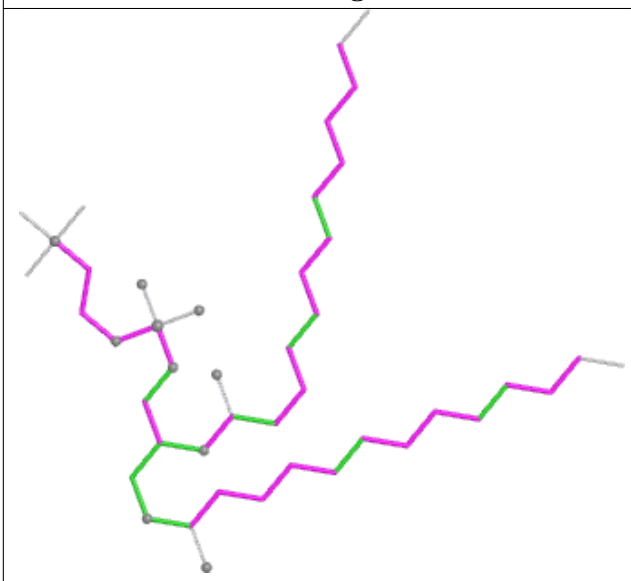
Ligand MC3 K 506



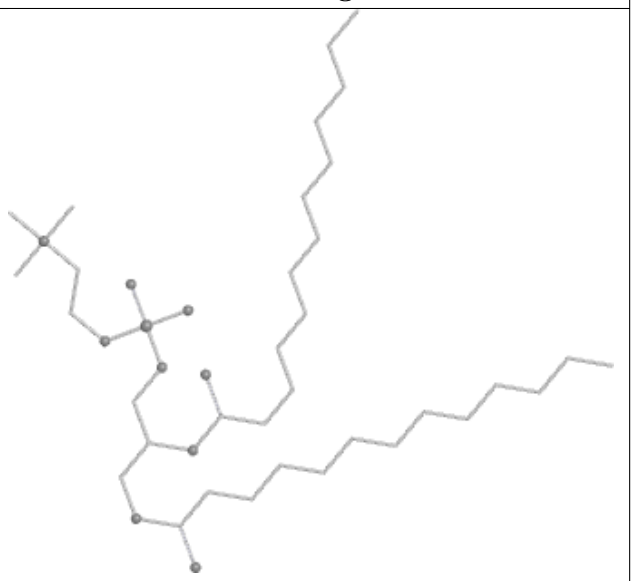
Bond lengths



Bond angles



Torsions



Rings

Ligand MC3 F 505



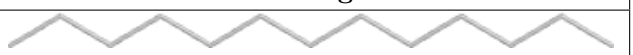
Bond lengths



Bond angles



Torsions



Rings

Ligand MC3 T 502



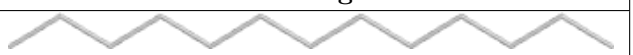
Bond lengths



Bond angles

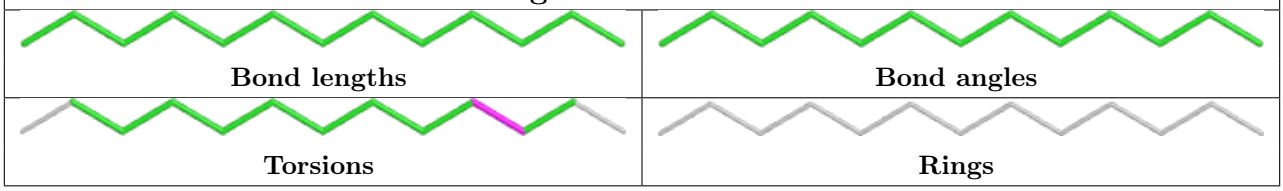


Torsions

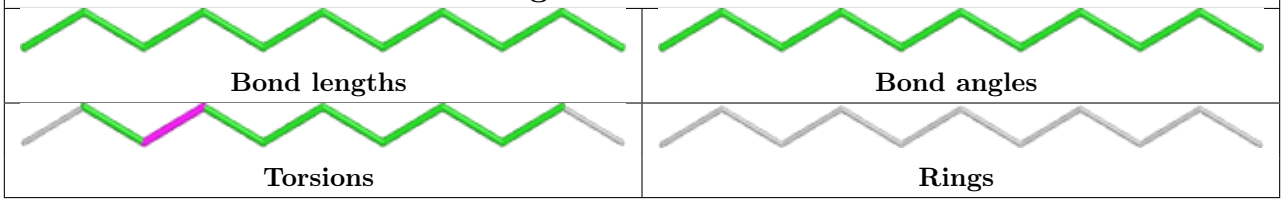


Rings

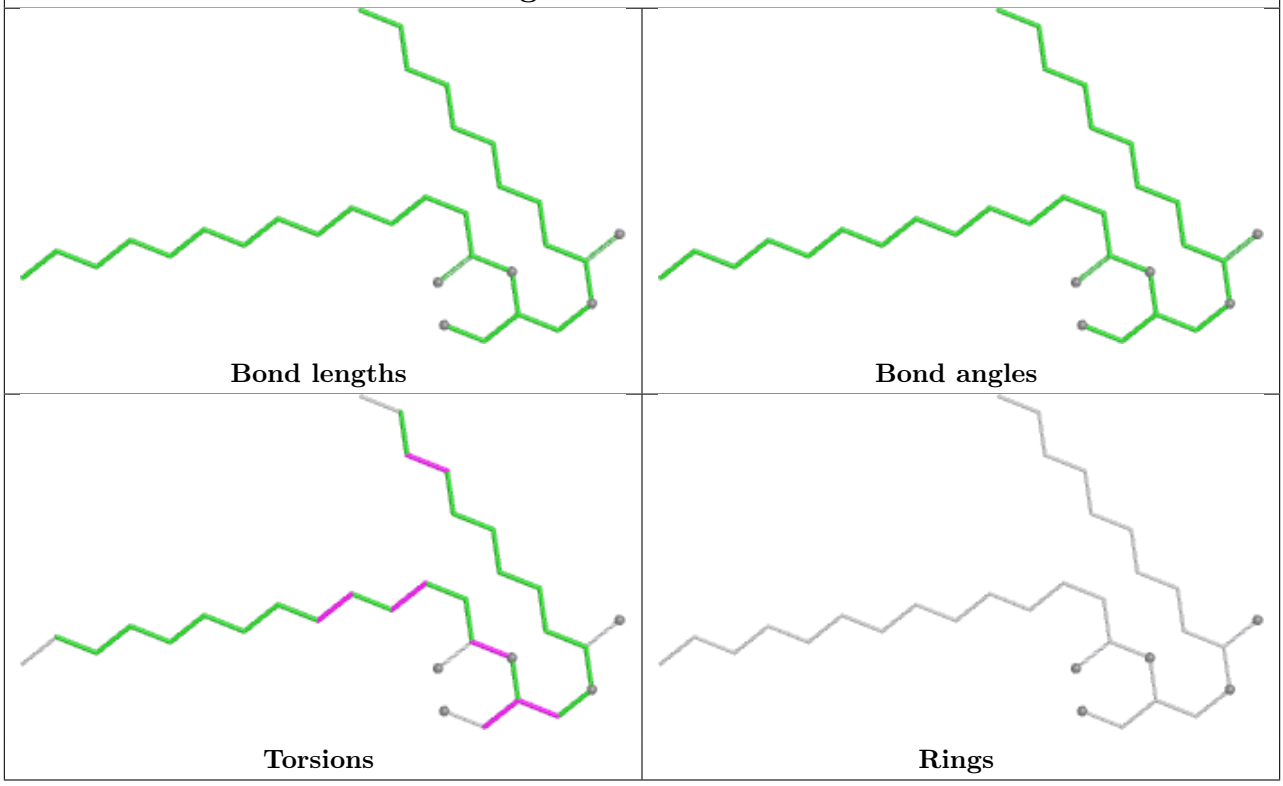
Ligand MC3 I 505



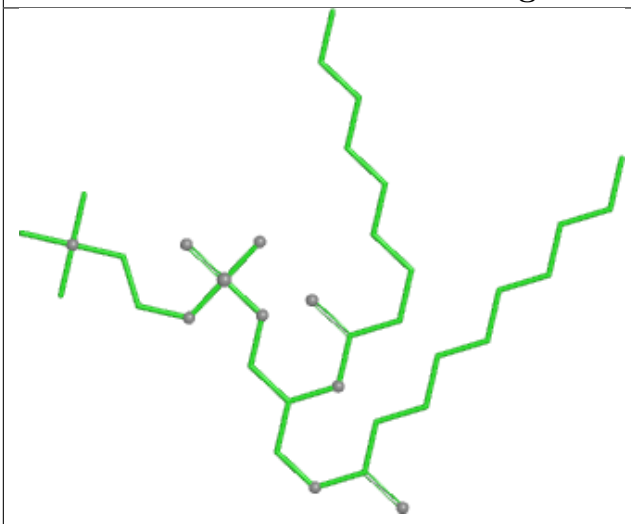
Ligand MC3 I 506



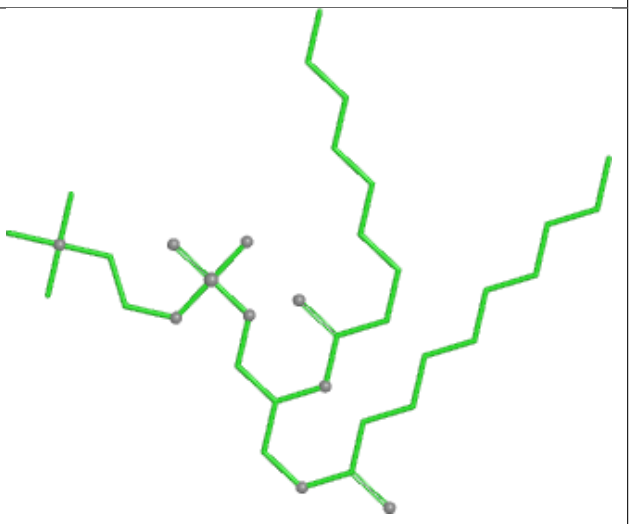
Ligand MC3 M 505



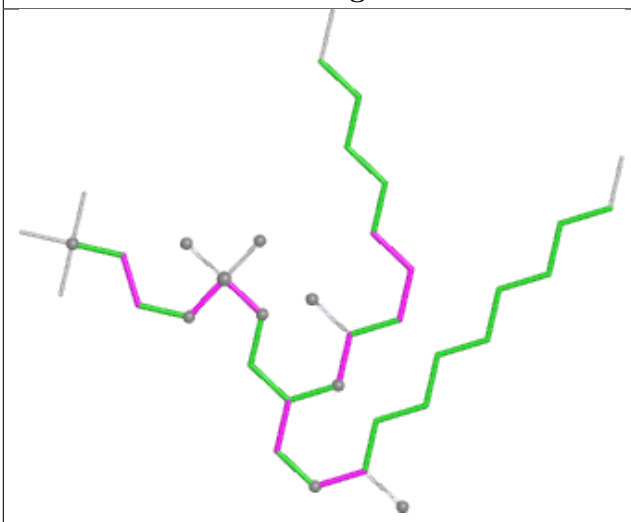
Ligand MC3 M 506



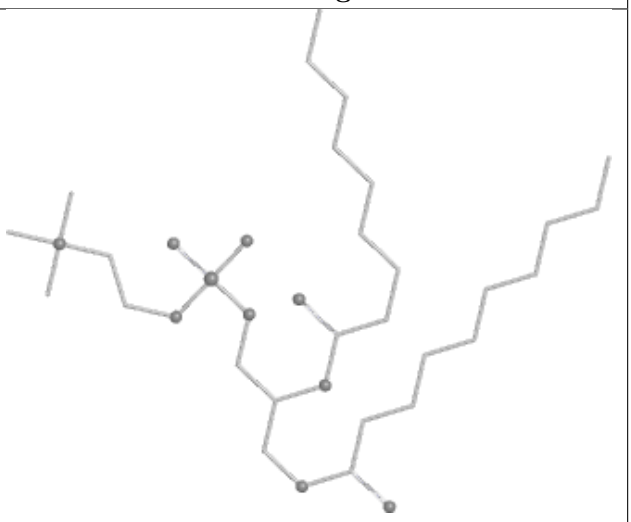
Bond lengths



Bond angles



Torsions



Rings

Ligand MC3 R 508



Bond lengths



Bond angles

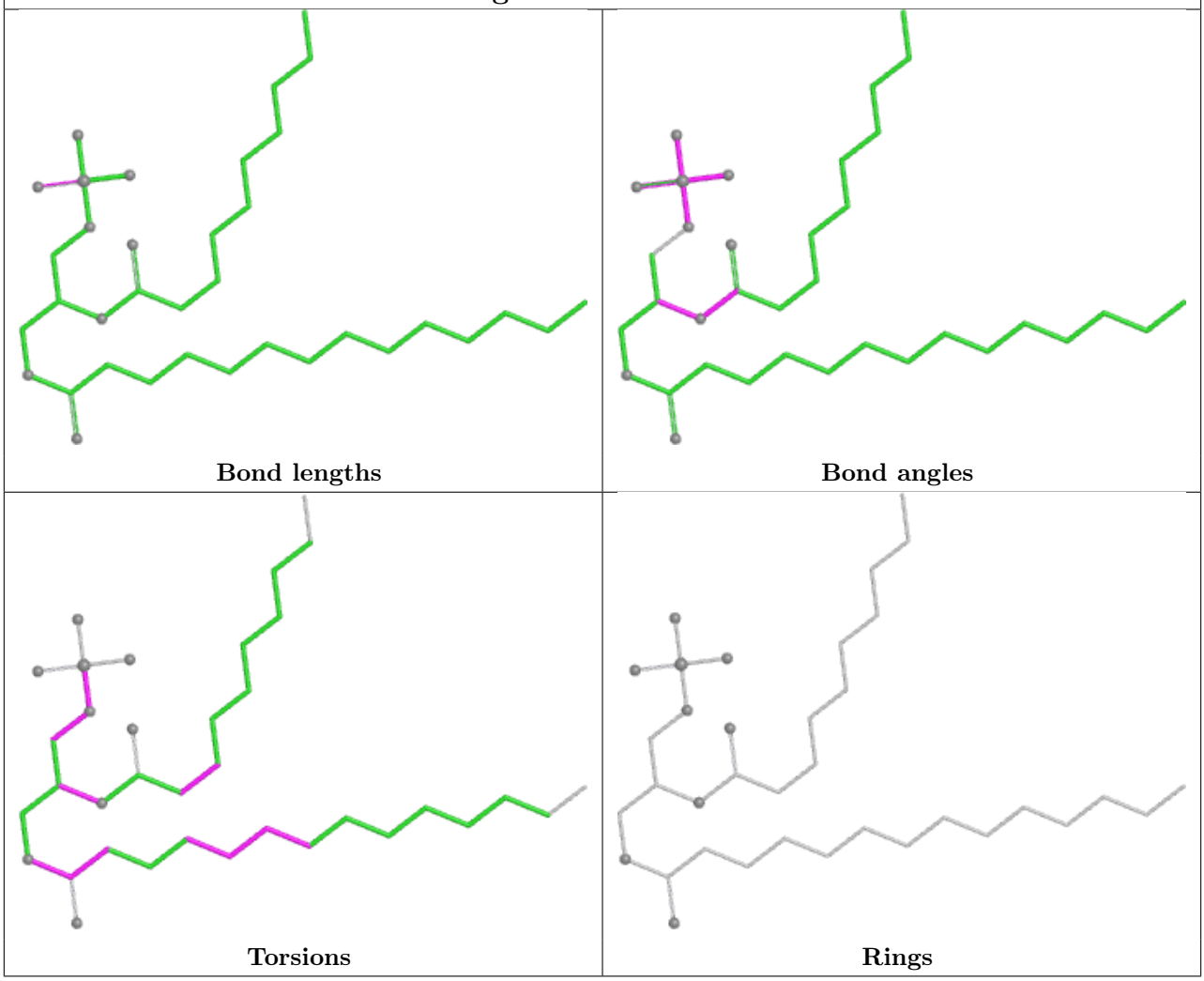


Torsions

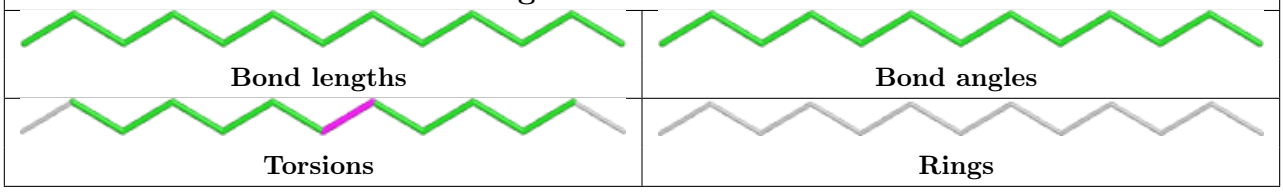


Rings

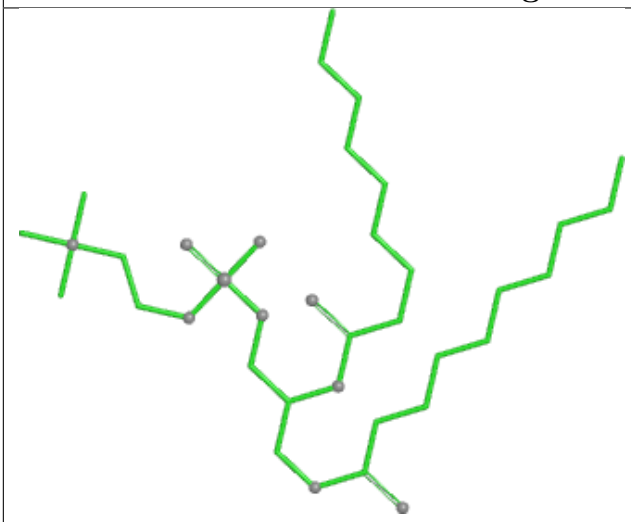
Ligand MC3 E 503



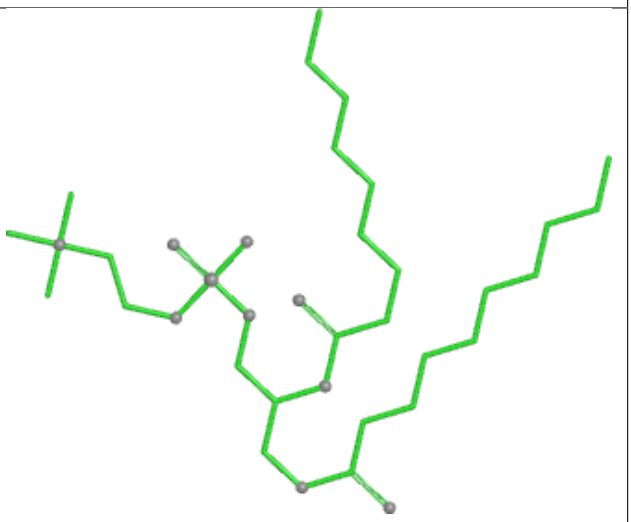
Ligand MC3 W 504



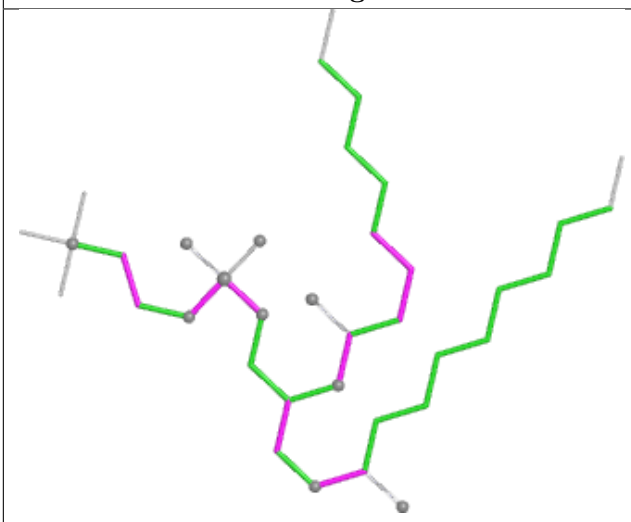
Ligand MC3 A 506



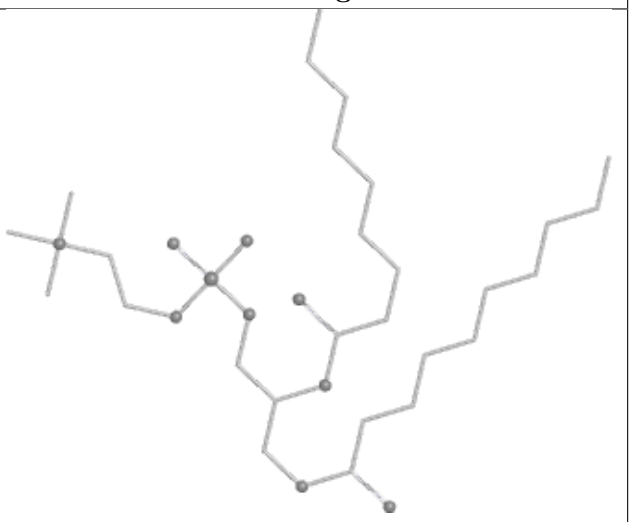
Bond lengths



Bond angles

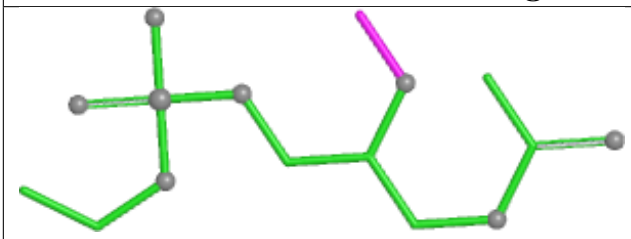


Torsions

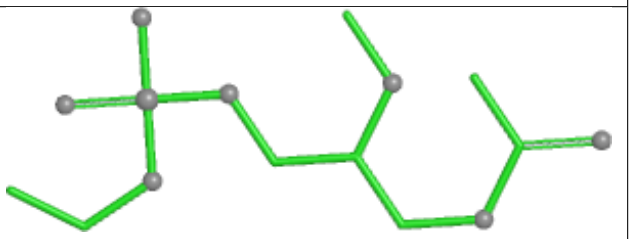


Rings

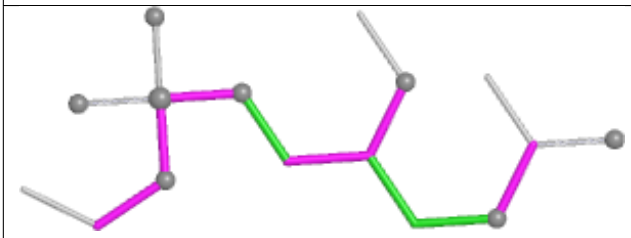
Ligand MC3 F 506



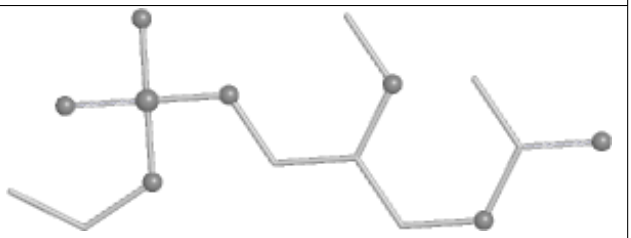
Bond lengths



Bond angles



Torsions



Rings

Ligand MC3 A 503



Bond lengths



Bond angles

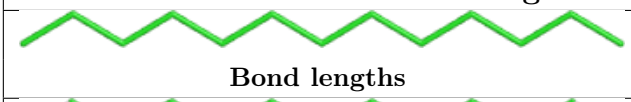


Torsions



Rings

Ligand MC3 B 504



Bond lengths



Bond angles

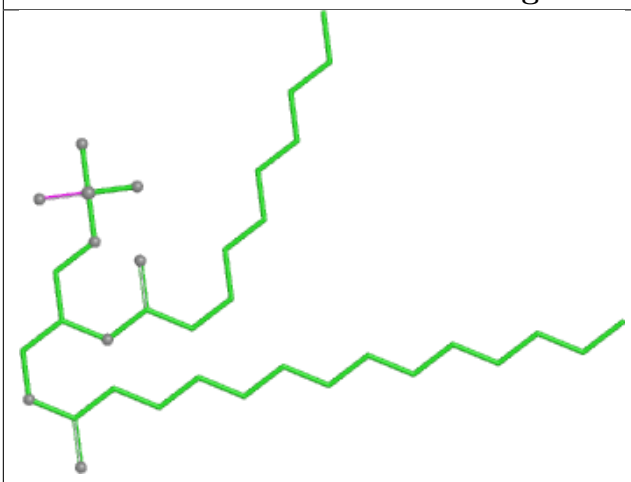


Torsions

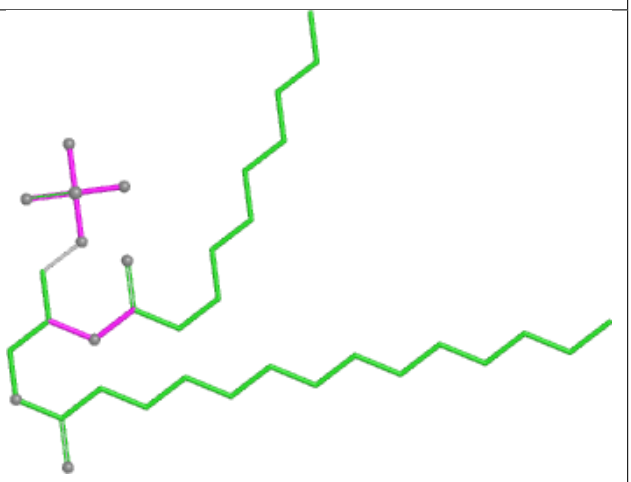


Rings

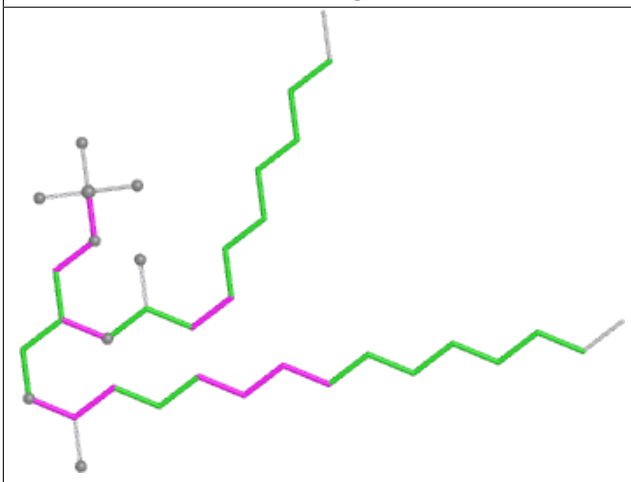
Ligand MC3 K 503



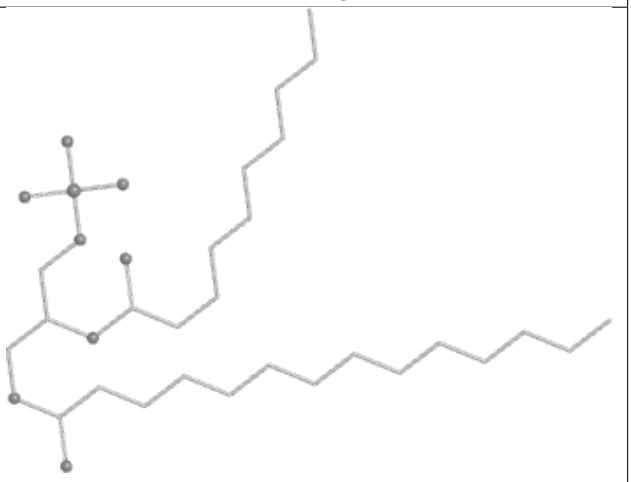
Bond lengths



Bond angles



Torsions



Rings

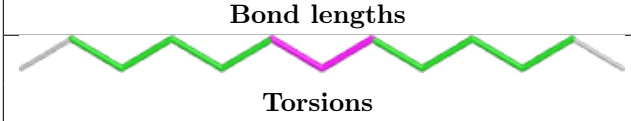
Ligand MC3 B 505



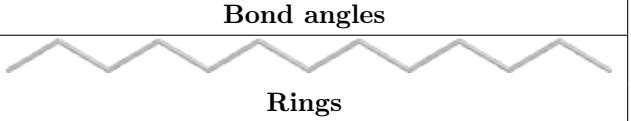
Bond lengths



Bond angles



Torsions



Rings

Ligand MC3 K 504	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand MC3 B 506	
 Bond lengths	 Bond angles
 Torsions	 Rings

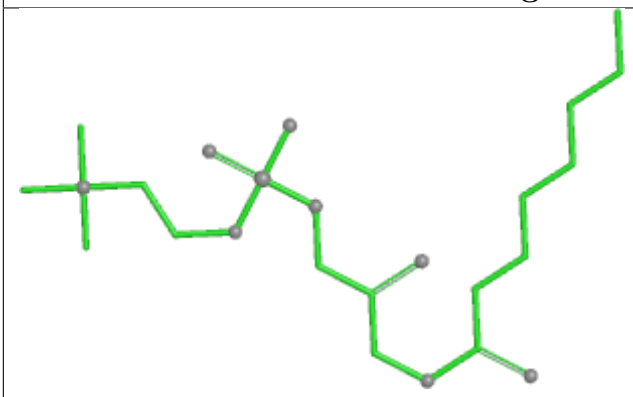
Ligand MC3 N 505	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand MC3 C 503	
 Bond lengths	 Bond angles
 Torsions	 Rings

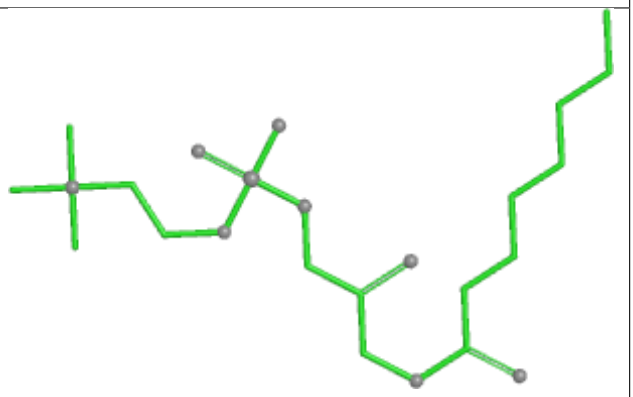
Ligand MC3 G 504	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand MC3 W 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

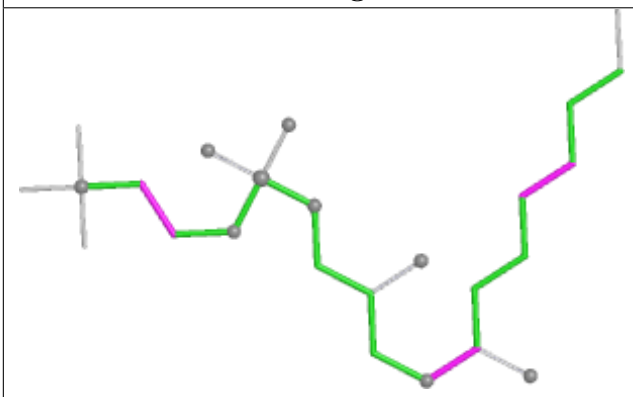
Ligand MC3 G 508



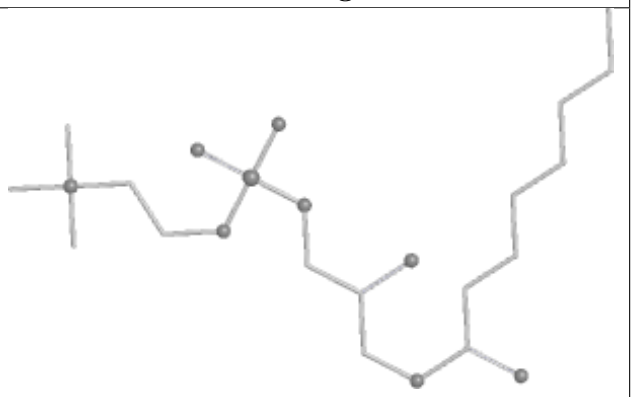
Bond lengths



Bond angles

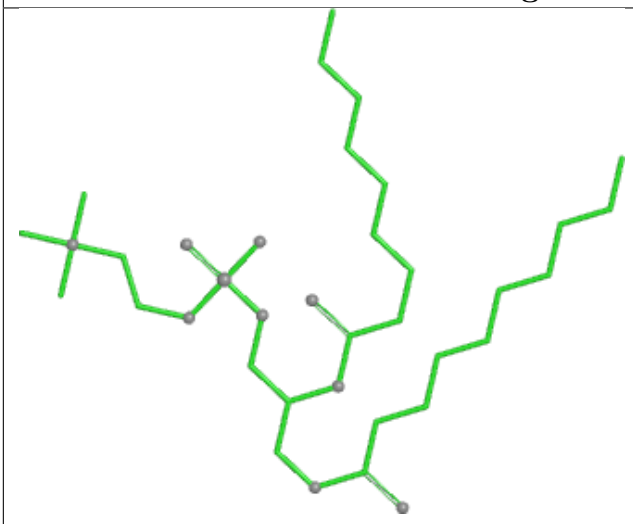


Torsions

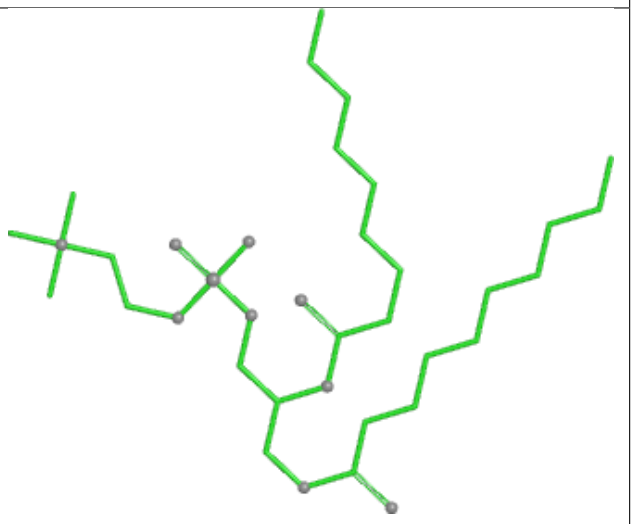


Rings

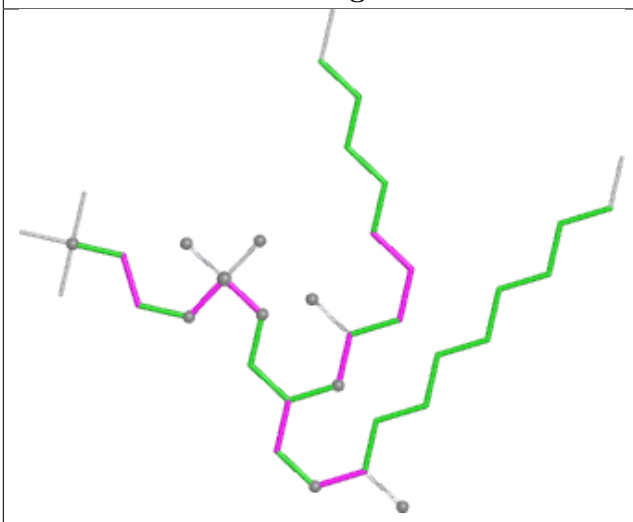
Ligand MC3 G 507



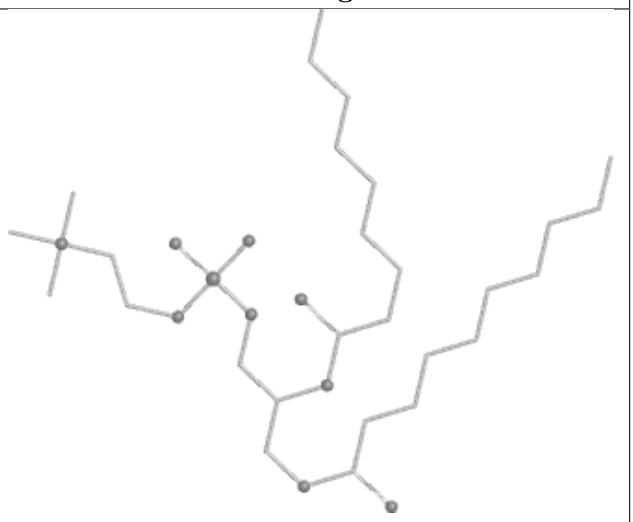
Bond lengths



Bond angles



Torsions



Rings

Ligand MC3 N 501



Bond lengths



Bond angles



Torsions



Rings

Ligand MC3 C 501



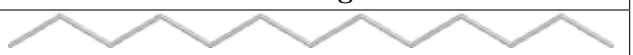
Bond lengths



Bond angles

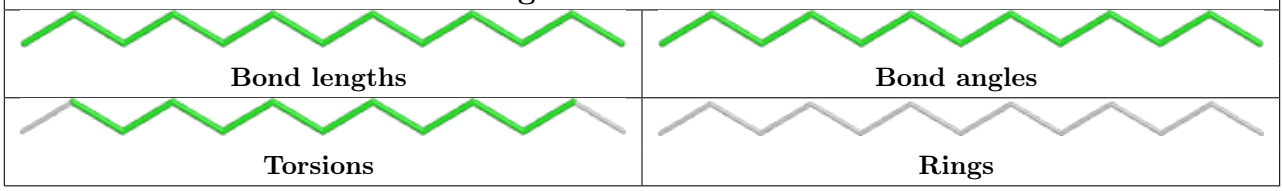


Torsions

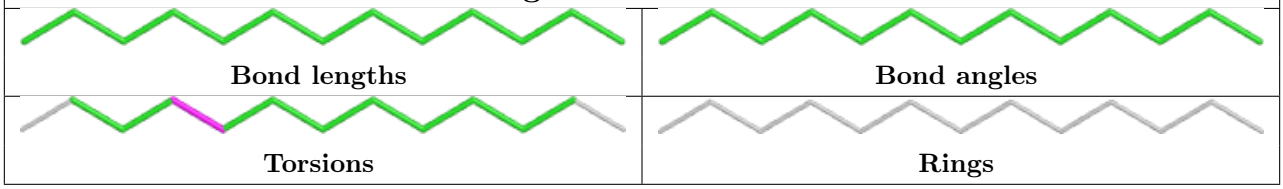


Rings

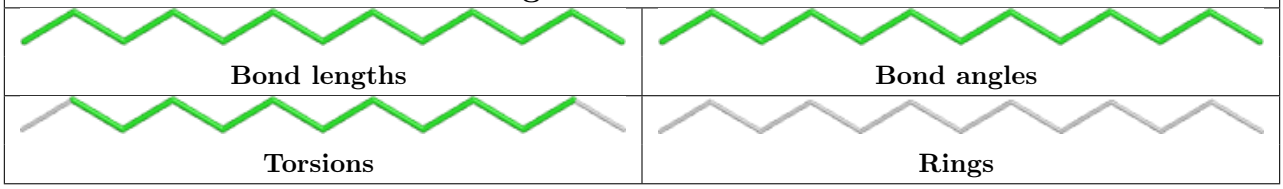
Ligand MC3 W 503



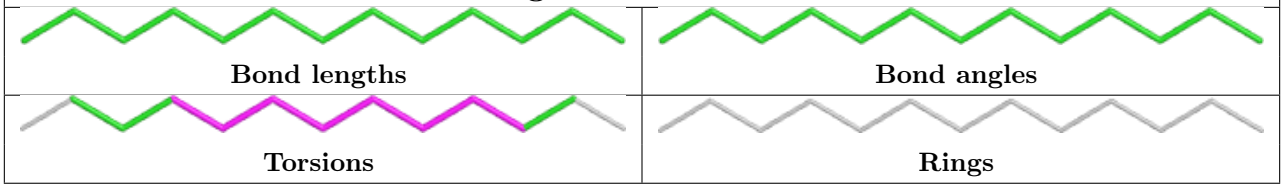
Ligand MC3 Y 503



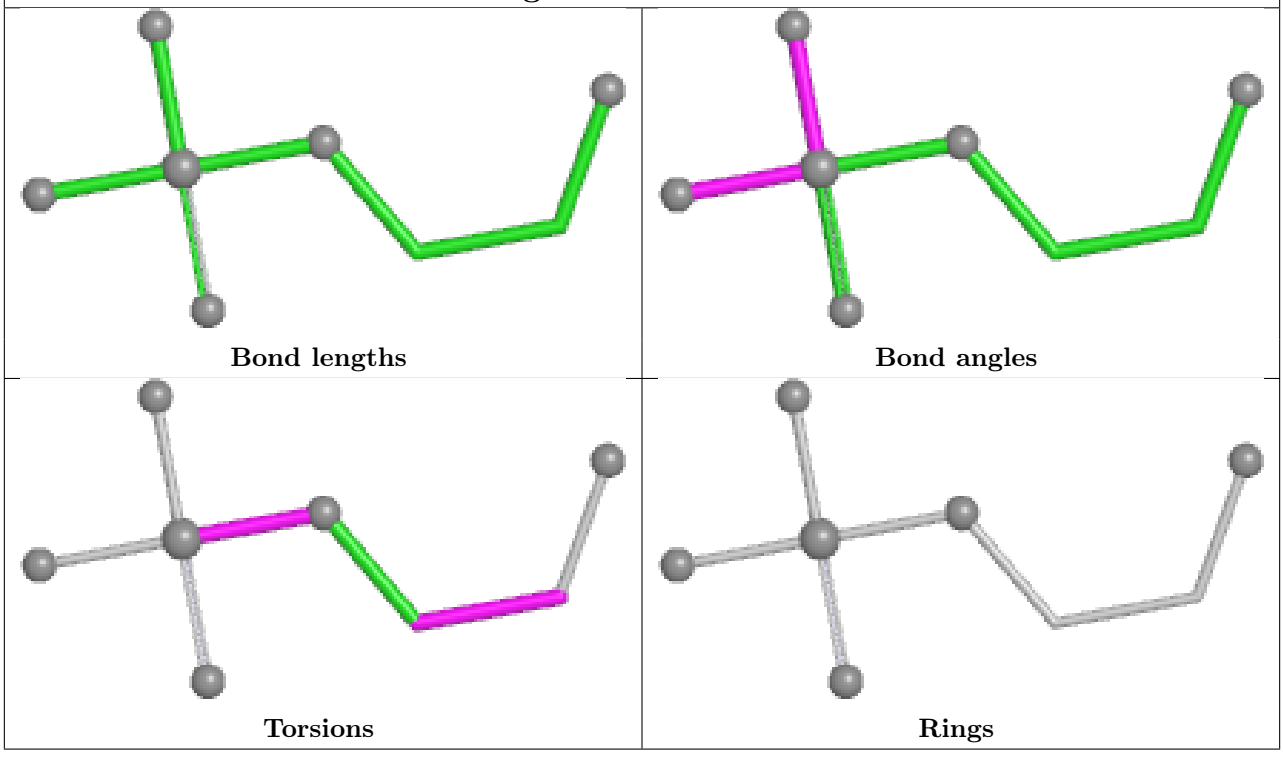
Ligand MC3 H 504



Ligand MC3 J 501



Ligand MC3 Y 501



Ligand MC3 J 504



Bond lengths



Bond angles

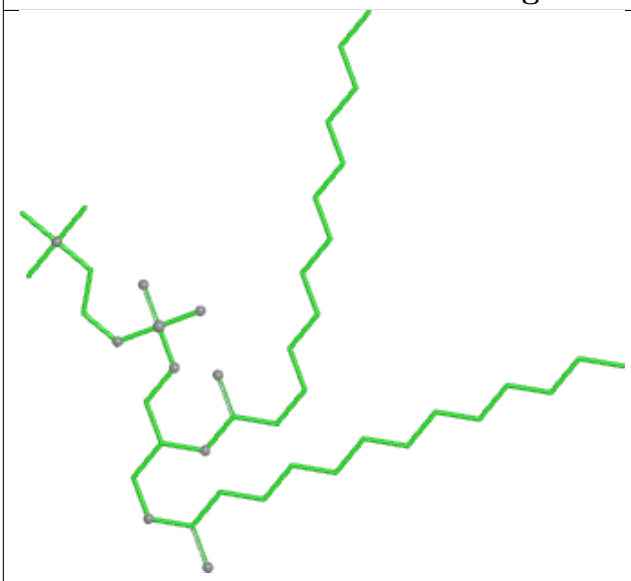


Torsions

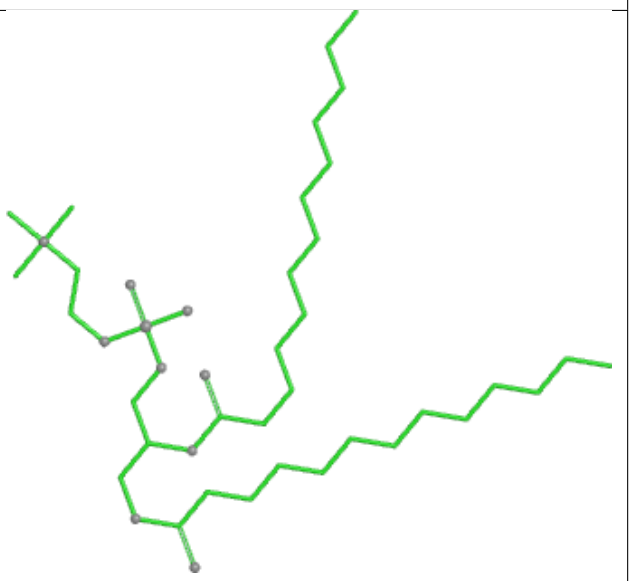


Rings

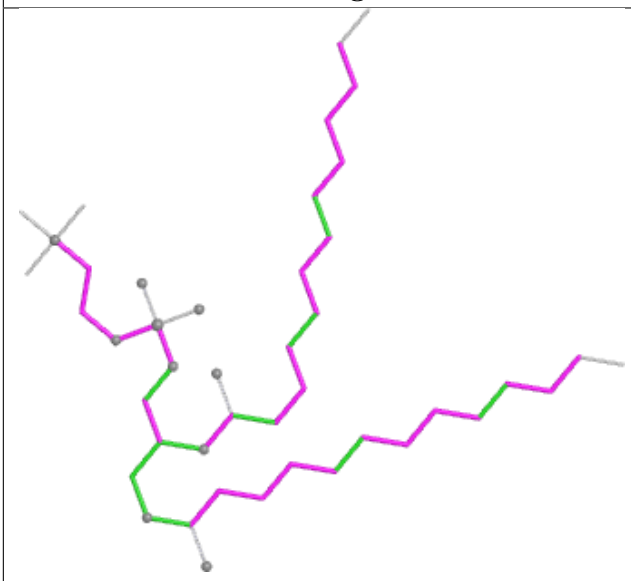
Ligand MC3 X 506



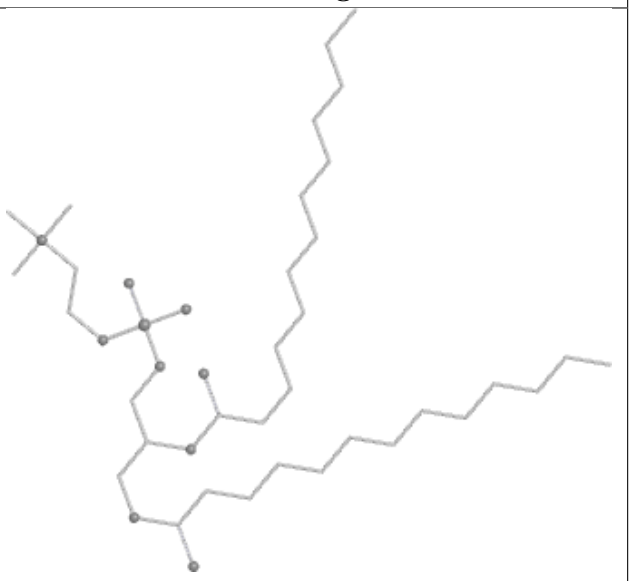
Bond lengths



Bond angles



Torsions



Rings

Ligand MC3 K 501



Bond lengths



Bond angles



Torsions



Rings

Ligand MC3 F 503



Bond lengths



Bond angles

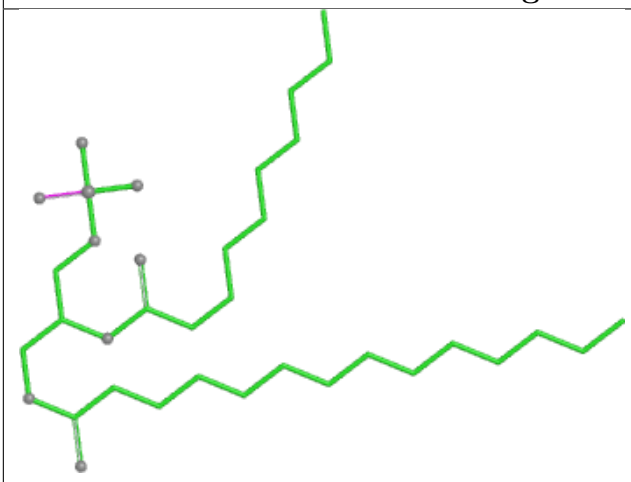


Torsions

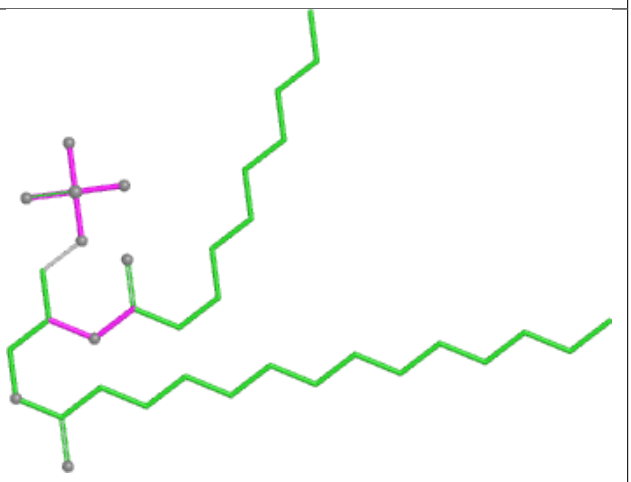


Rings

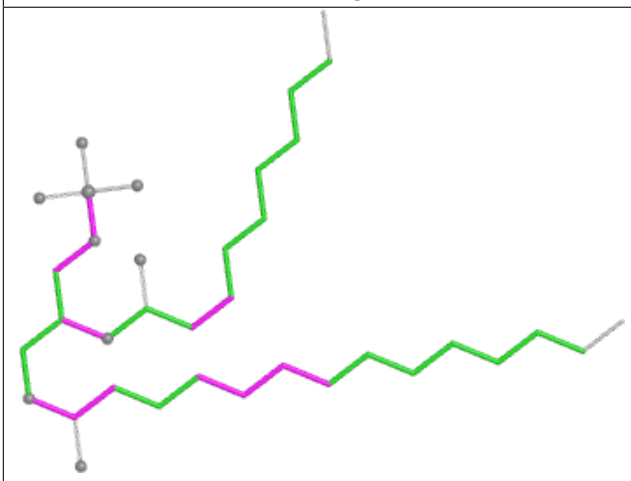
Ligand MC3 X 503



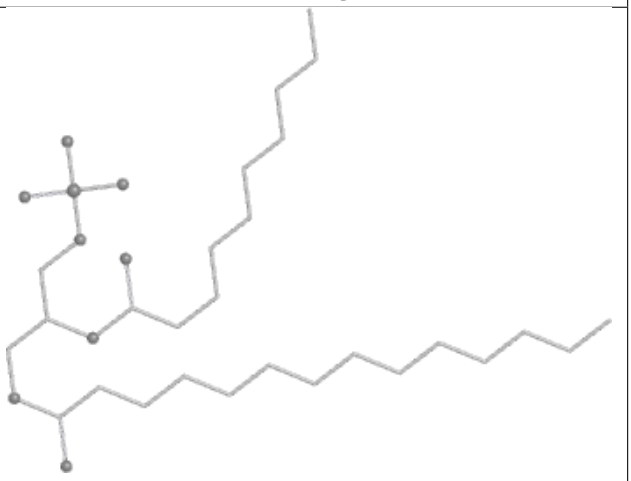
Bond lengths



Bond angles



Torsions



Rings

Ligand MC3 S 502



Bond lengths



Bond angles



Torsions



Rings

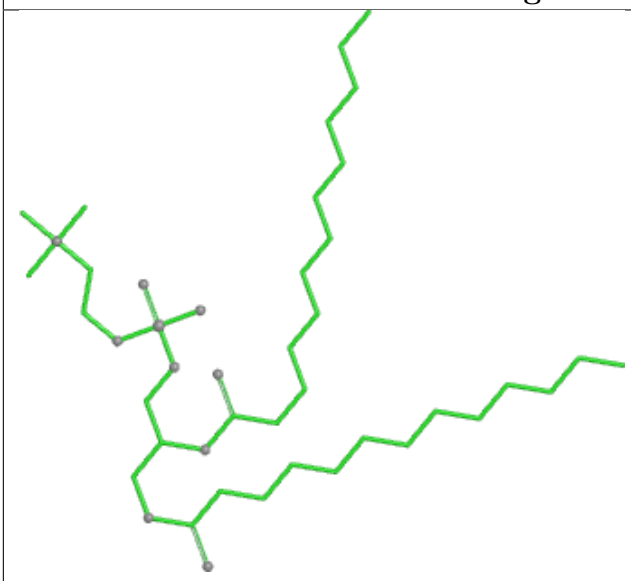
Ligand MC3 F 504	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand MC3 O 503	
 Bond lengths	 Bond angles
 Torsions	 Rings

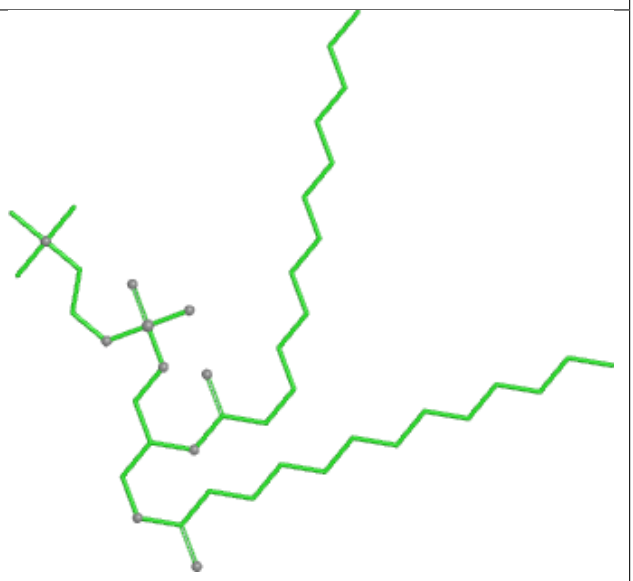
Ligand MC3 N 506	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand MC3 G 505	
 Bond lengths	 Bond angles
 Torsions	 Rings

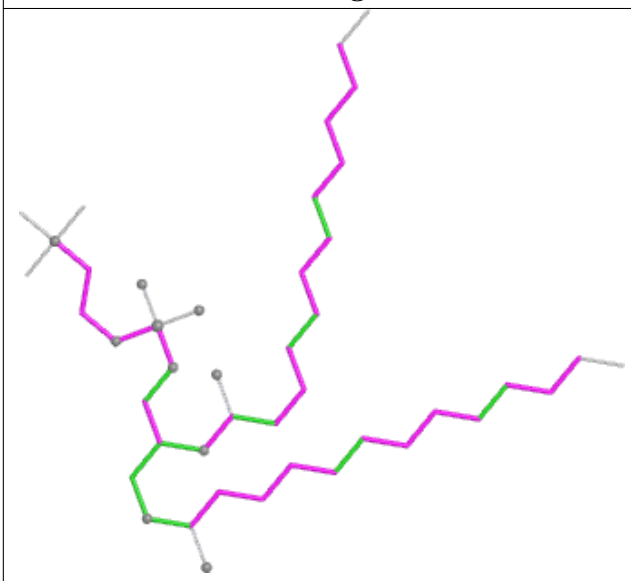
Ligand MC3 E 506



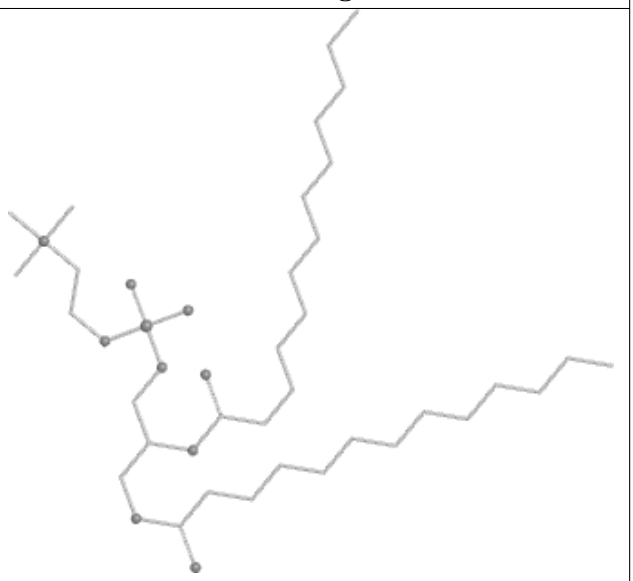
Bond lengths



Bond angles

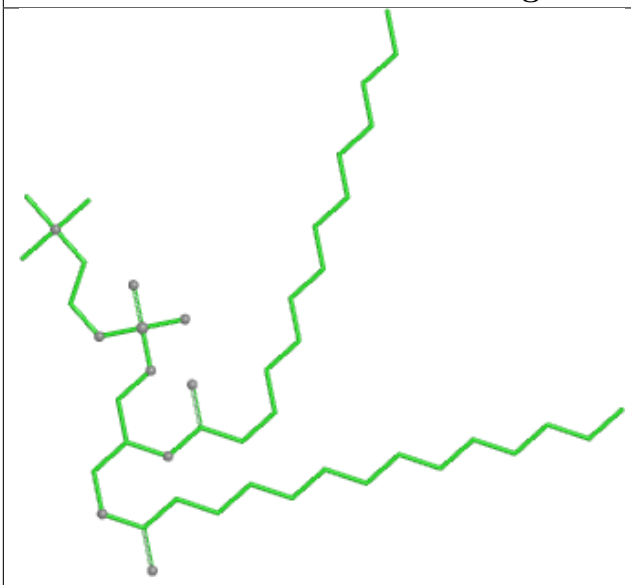


Torsions

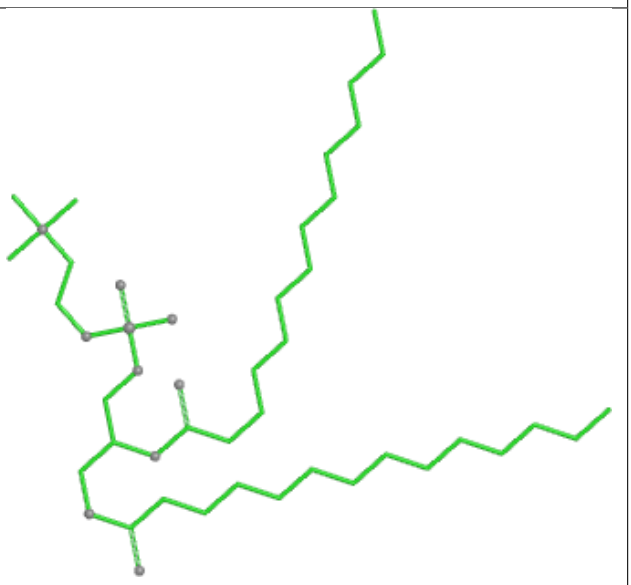


Rings

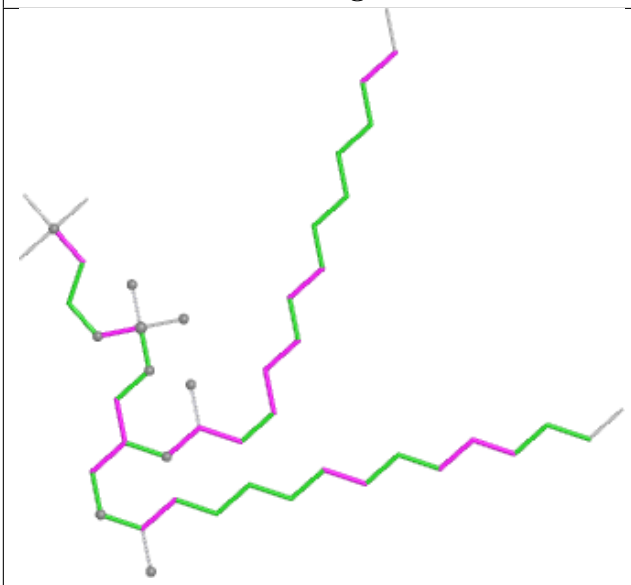
Ligand MC3 A 502



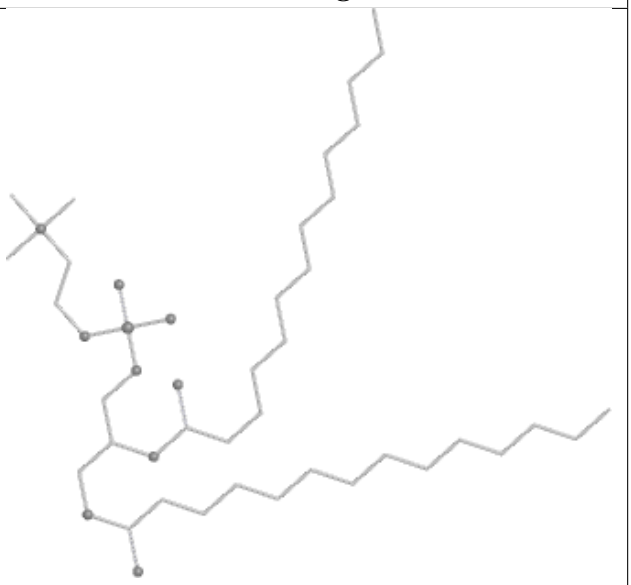
Bond lengths



Bond angles



Torsions



Rings

Ligand MC3 L 503



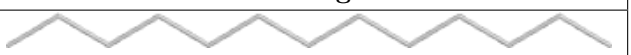
Bond lengths



Bond angles



Torsions



Rings

Ligand MC3 R 501



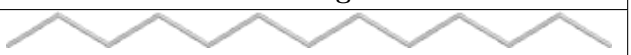
Bond lengths



Bond angles



Torsions



Rings

Ligand MC3 I 504

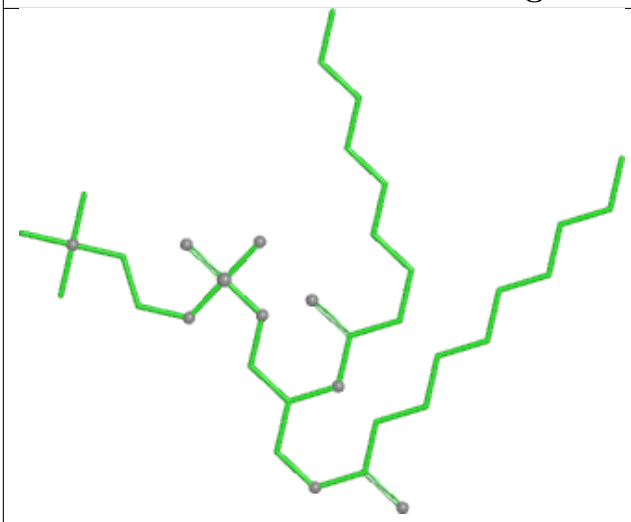

Bond lengths

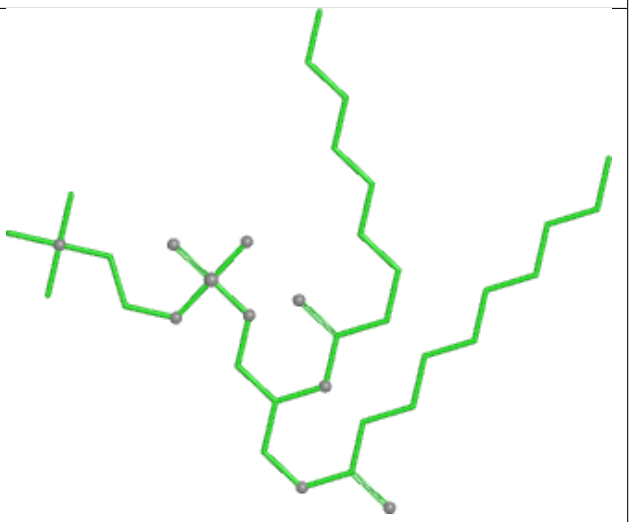

Bond angles

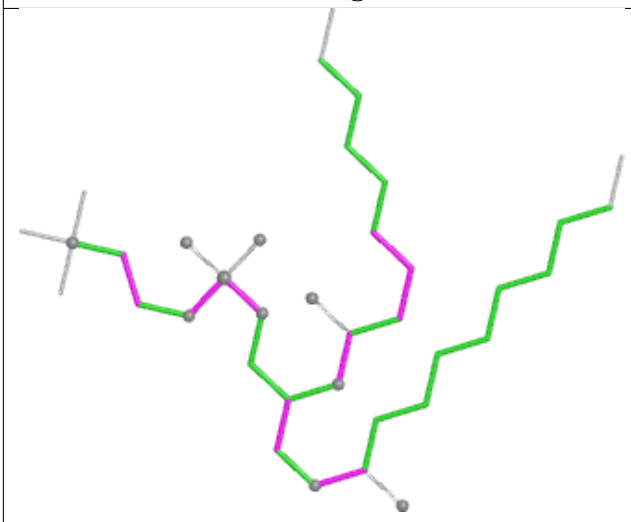

Torsions

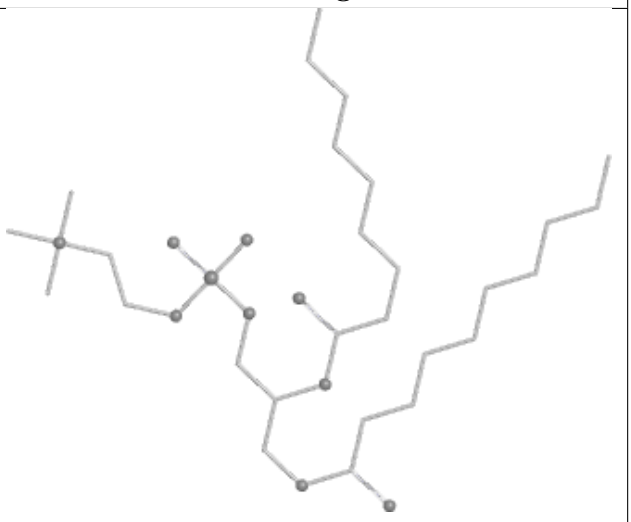

Rings

Ligand MC3 S 507


Bond lengths


Bond angles


Torsions


Rings

Ligand MC3 Y 502

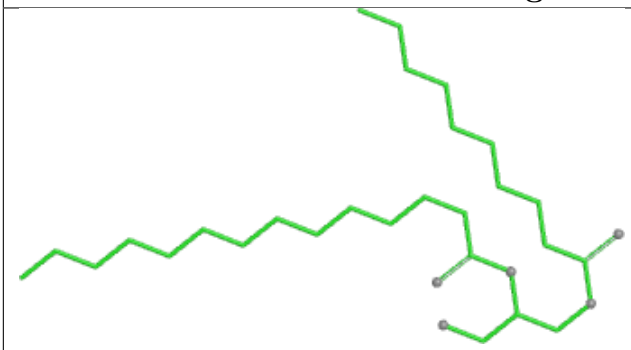

Bond lengths


Bond angles

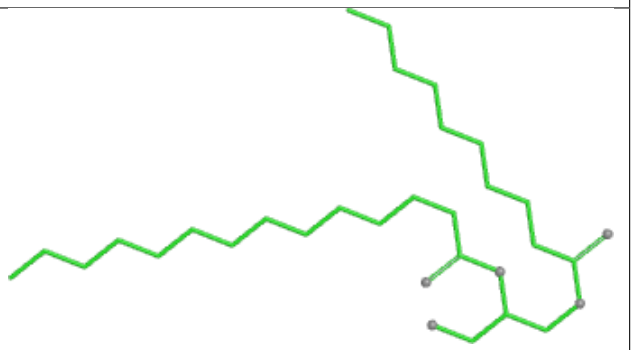

Torsions


Rings

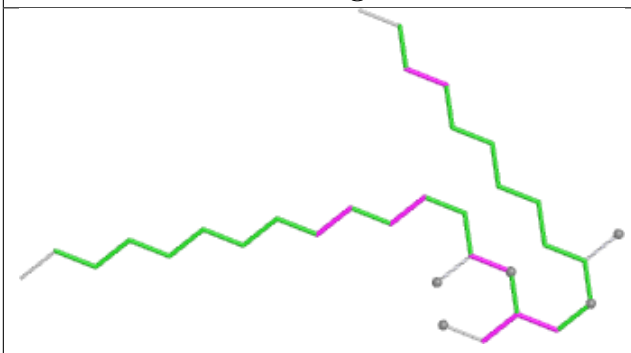
Ligand MC3 S 506



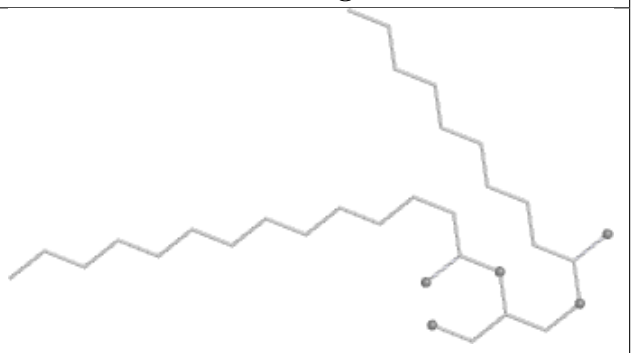
Bond lengths



Bond angles

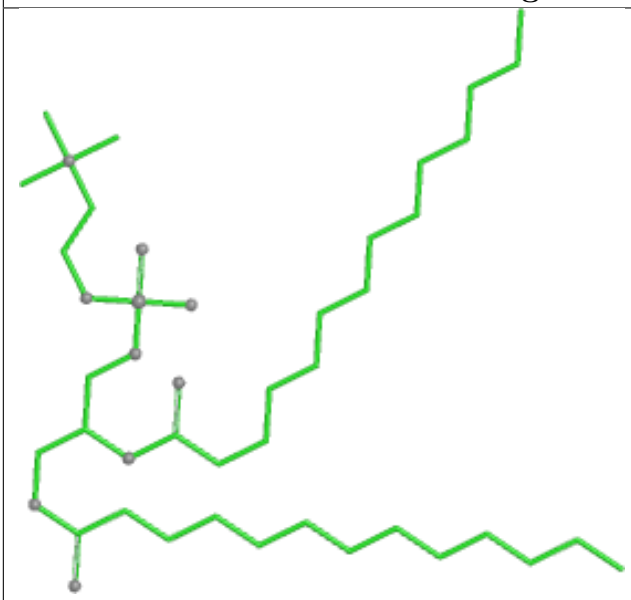


Torsions

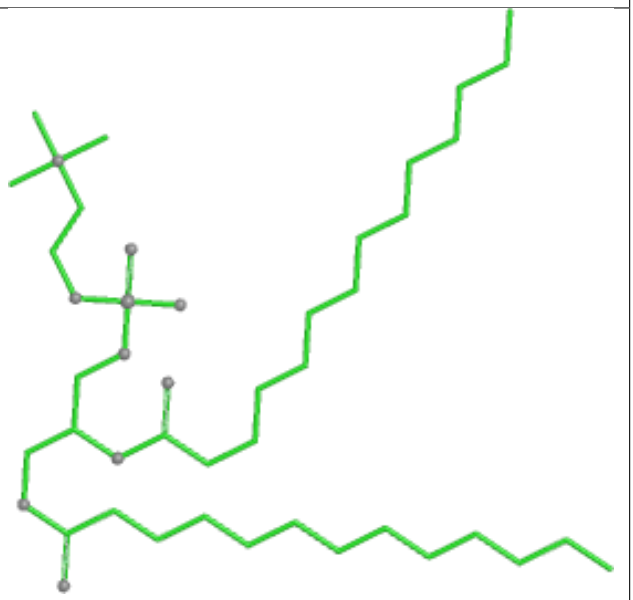


Rings

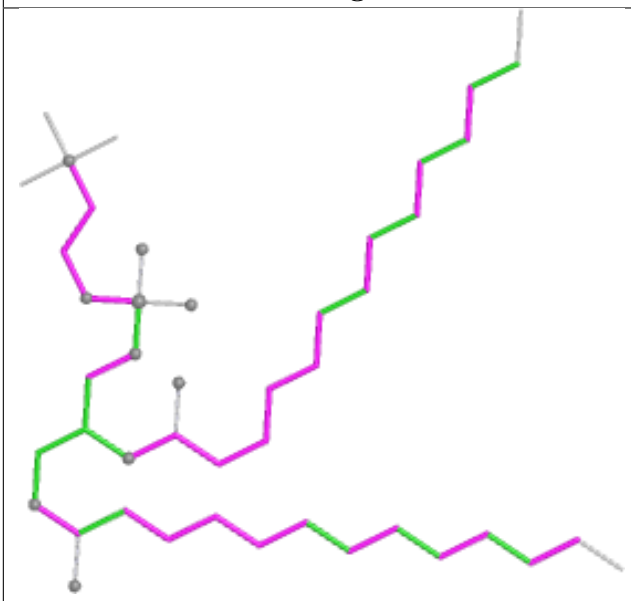
Ligand MC3 H 503



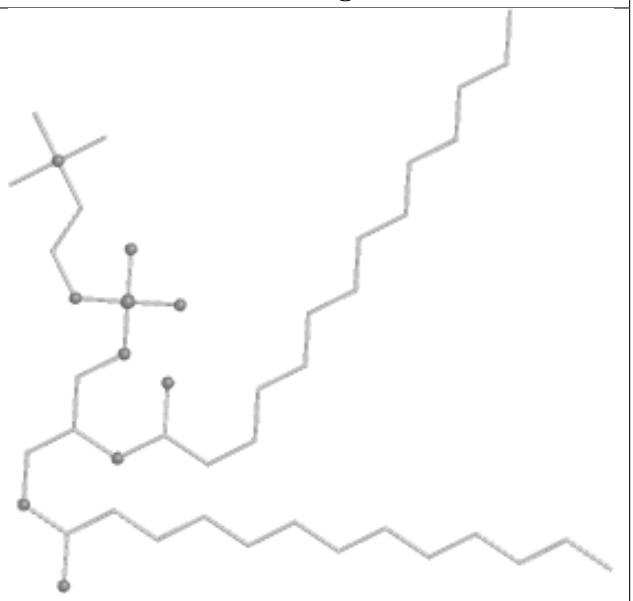
Bond lengths



Bond angles



Torsions



Rings

Ligand MC3 X 502



Bond lengths



Bond angles



Torsions



Rings

Ligand MC3 G 502	
Bond lengths	Bond angles
Torsions	Rings

Ligand MC3 J 505	
Bond lengths	Bond angles
Torsions	Rings

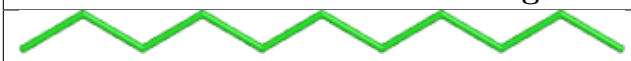
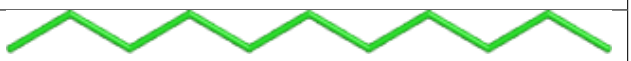
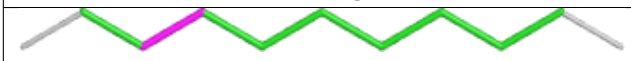
Ligand MC3 O 507	
Bond lengths	Bond angles
Torsions	Rings

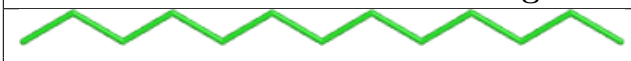
Ligand MC3 R 502	
Bond lengths	Bond angles
Torsions	Rings

Ligand MC3 L 508	
Bond lengths	Bond angles
Torsions	Rings

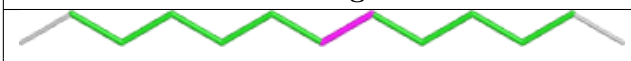
Ligand MC3 C 507	
Bond lengths	Bond angles
Torsions	Rings

Ligand MC3 F 501	
Bond lengths	Bond angles
Torsions	Rings

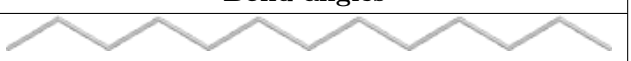
Ligand MC3 O 506	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand MC3 O 504	
 Bond lengths	 Bond angles
 Torsions	 Rings

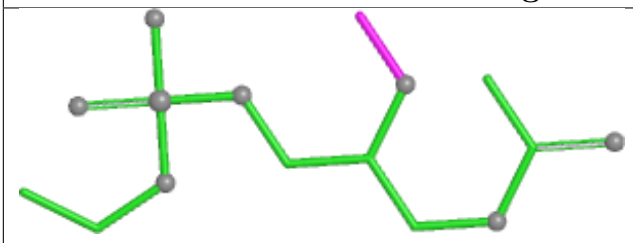
Ligand MC3 F 508	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand MC3 D 504	
 Bond lengths	 Bond angles
 Torsions	 Rings

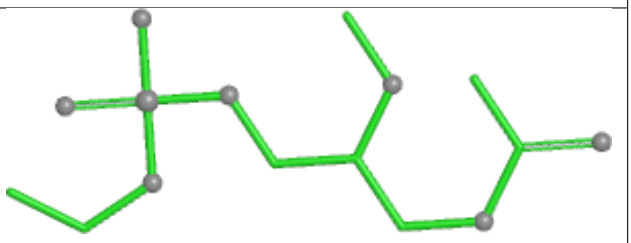
Ligand MC3 J 502	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand MC3 N 504	
 Bond lengths	 Bond angles
 Torsions	 Rings

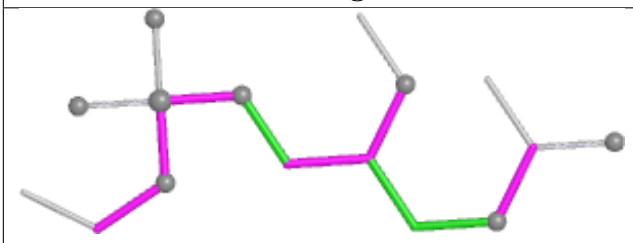
Ligand MC3 Y 507



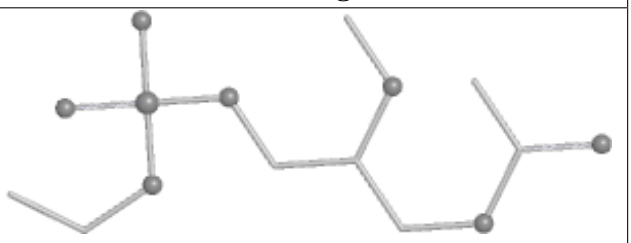
Bond lengths



Bond angles



Torsions



Rings

Ligand MC3 A 501



Bond lengths



Bond angles

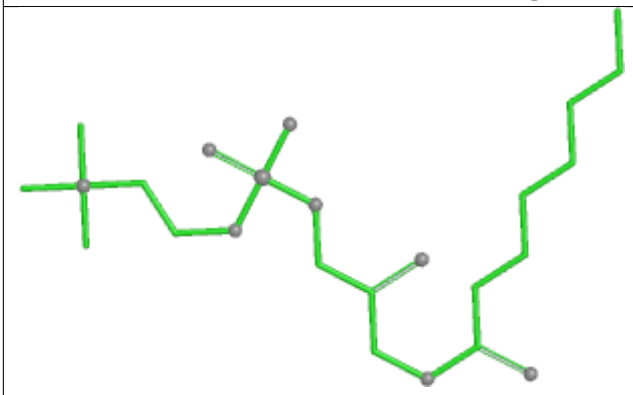


Torsions

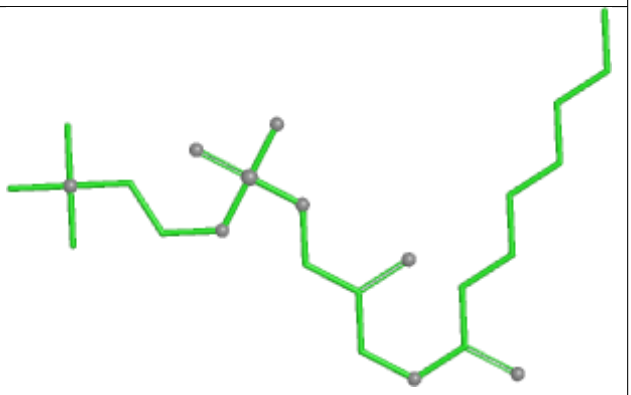


Rings

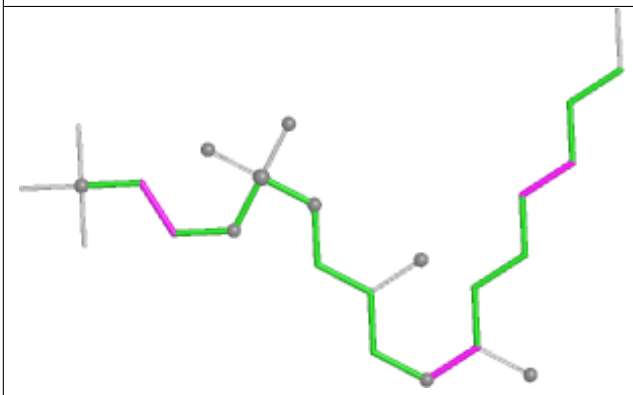
Ligand MC3 S 508



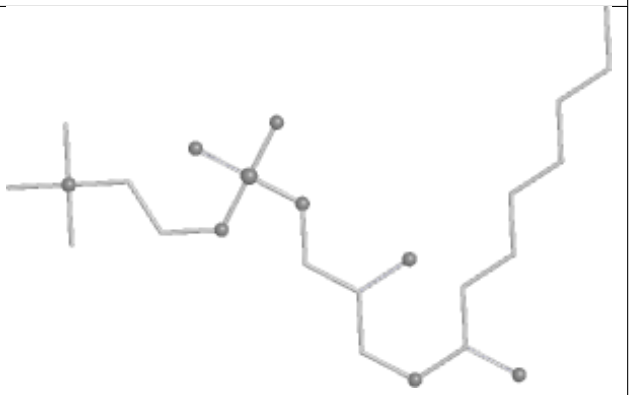
Bond lengths



Bond angles

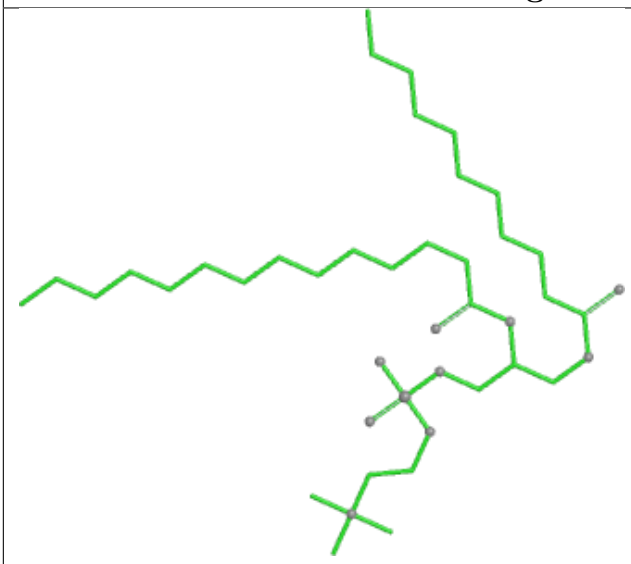


Torsions

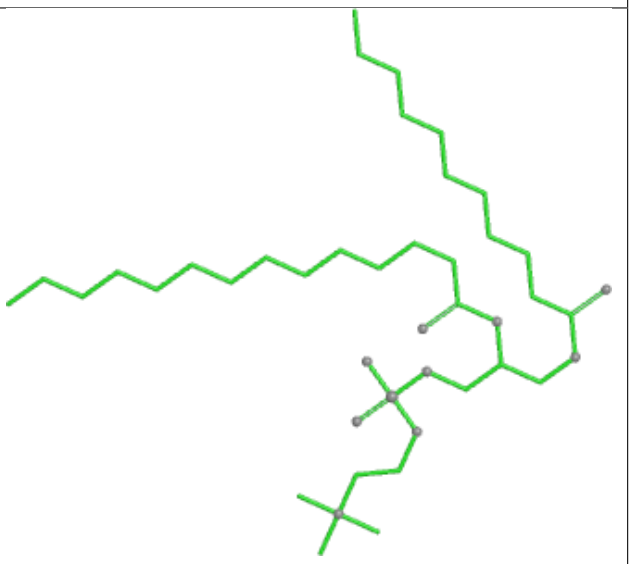


Rings

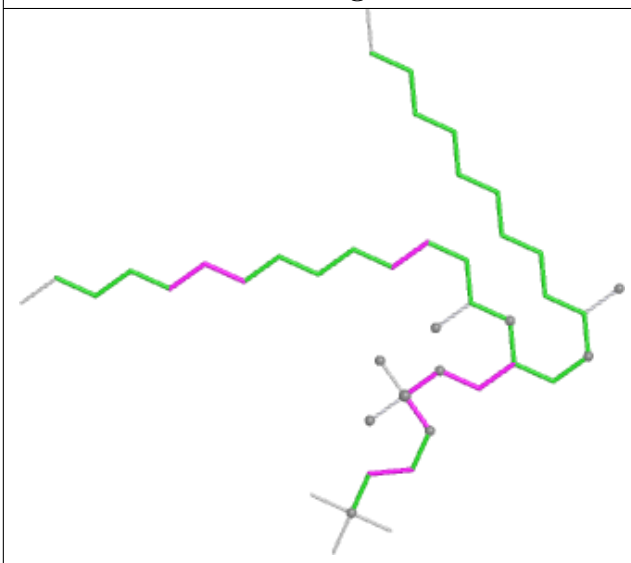
Ligand MC3 J 506



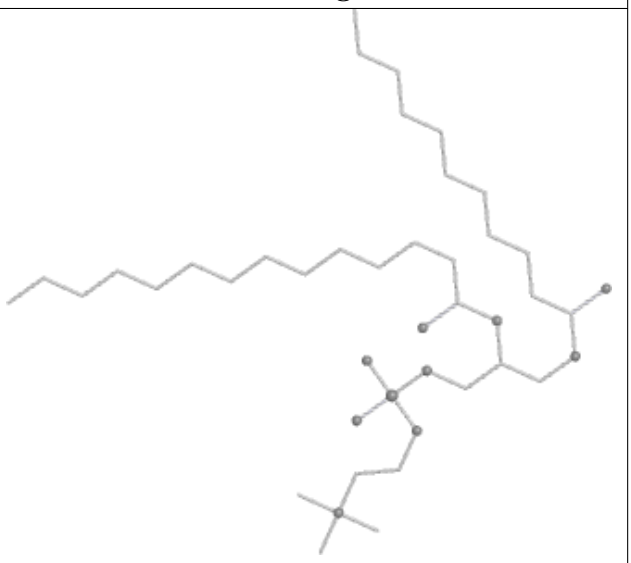
Bond lengths



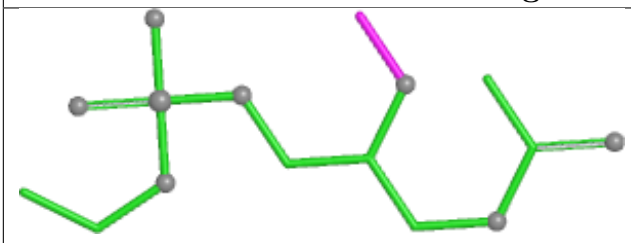
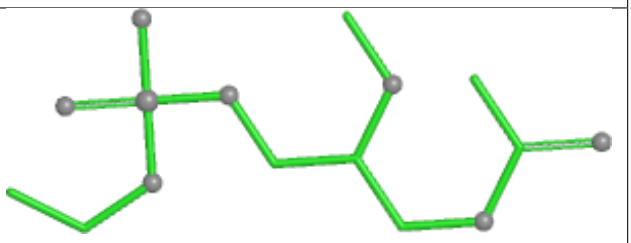
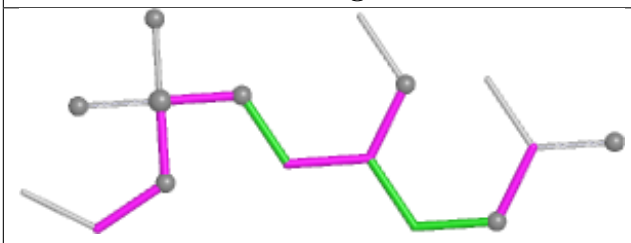
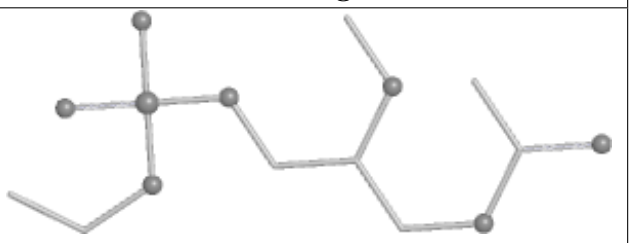
Bond angles



Torsions

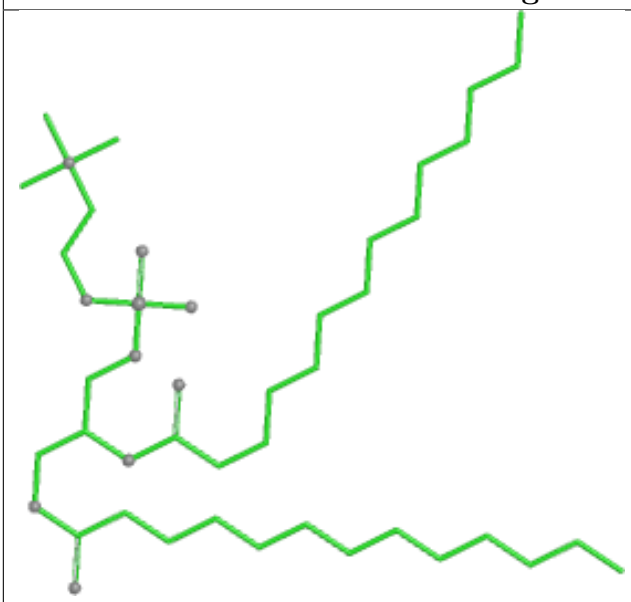


Rings

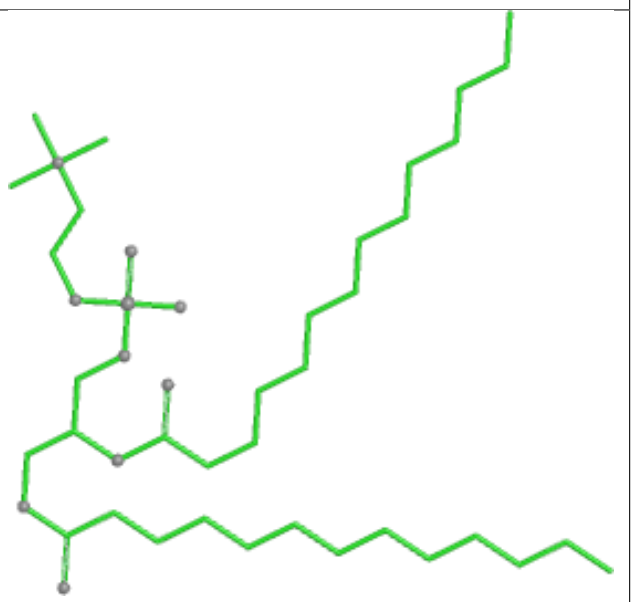
Ligand MC3 R 506	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand MC3 I 503	
 Bond lengths	 Bond angles
 Torsions	 Rings

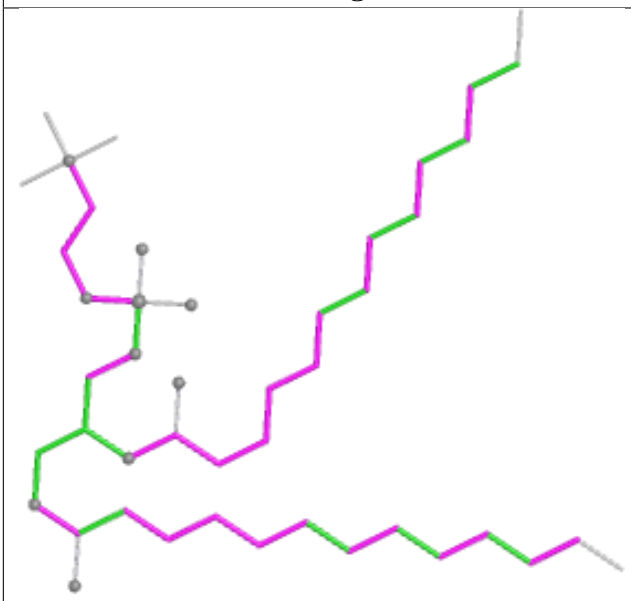
Ligand MC3 N 503



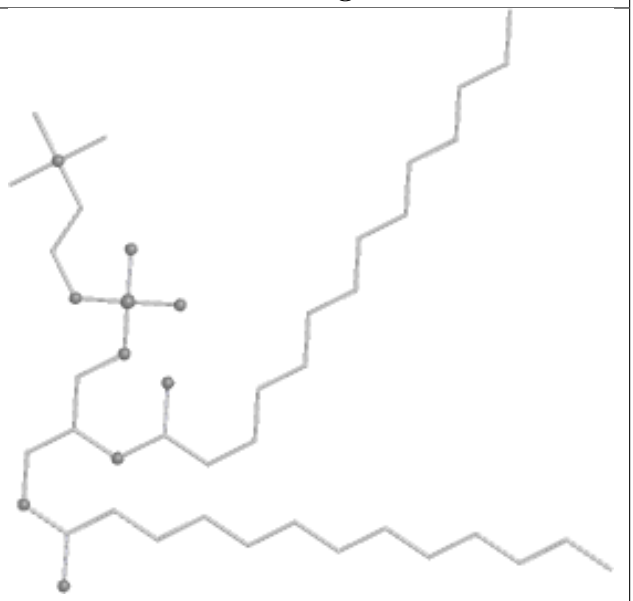
Bond lengths



Bond angles



Torsions



Rings

Ligand MC3 Q 505



Bond lengths



Bond angles



Torsions



Rings

Ligand MC3 W 505



Bond lengths



Bond angles

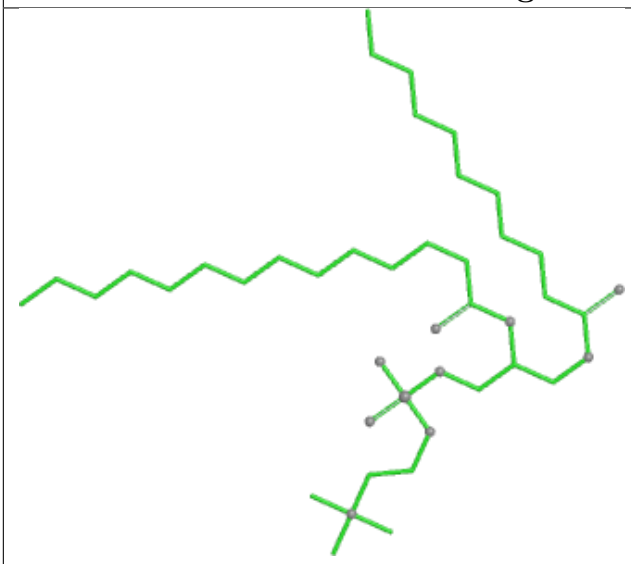


Torsions

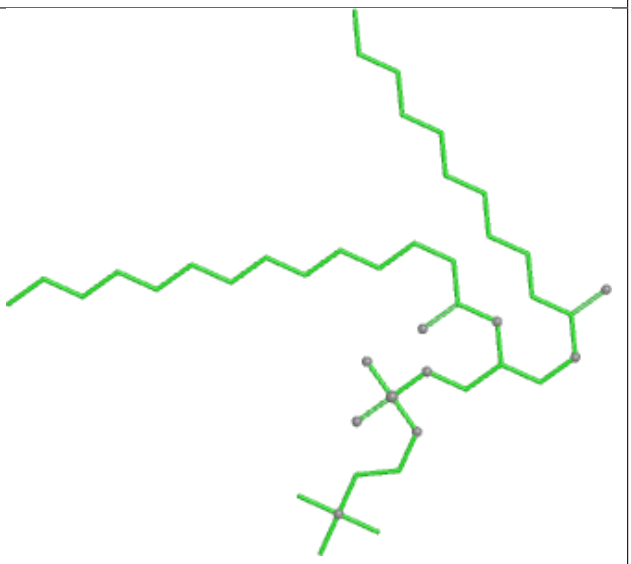


Rings

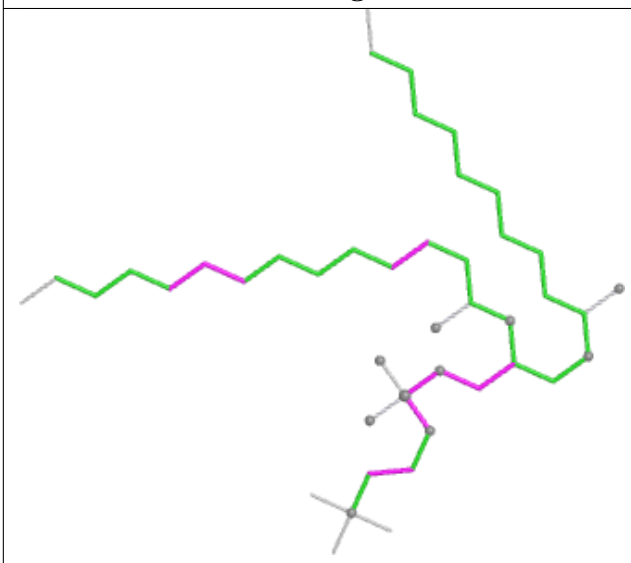
Ligand MC3 W 506



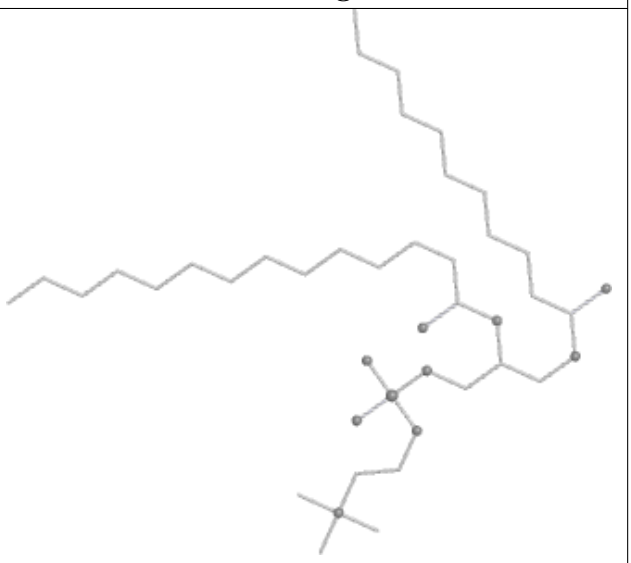
Bond lengths



Bond angles



Torsions



Rings

Ligand MC3 Q 501



Bond lengths



Bond angles



Torsions



Rings

Ligand MC3 V 505



Bond lengths



Bond angles

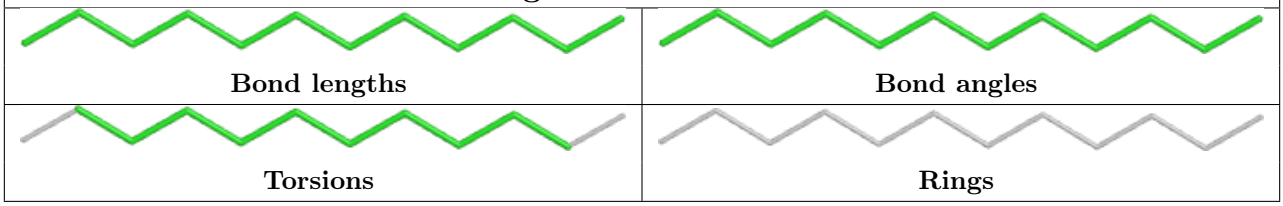


Torsions

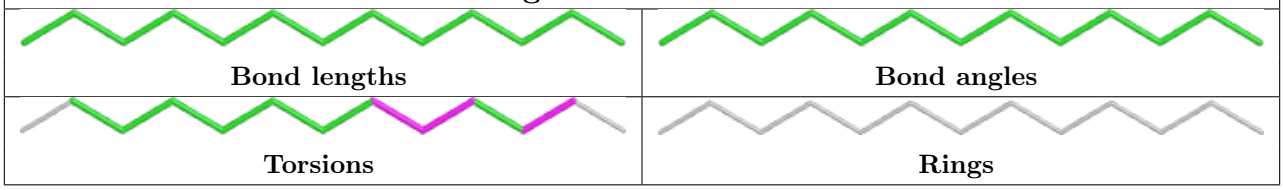


Rings

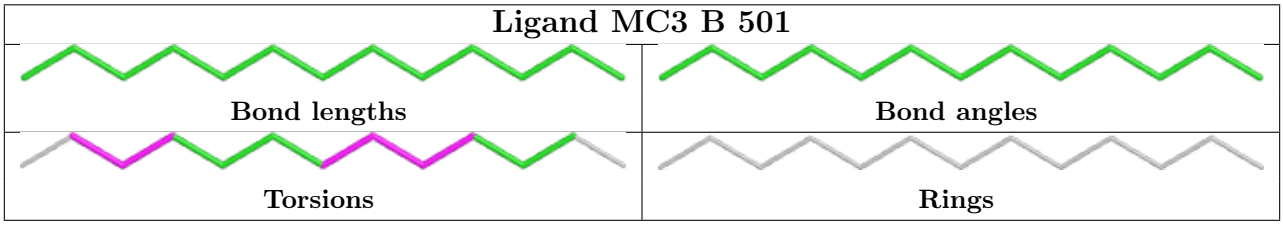
Ligand MC3 Y 504



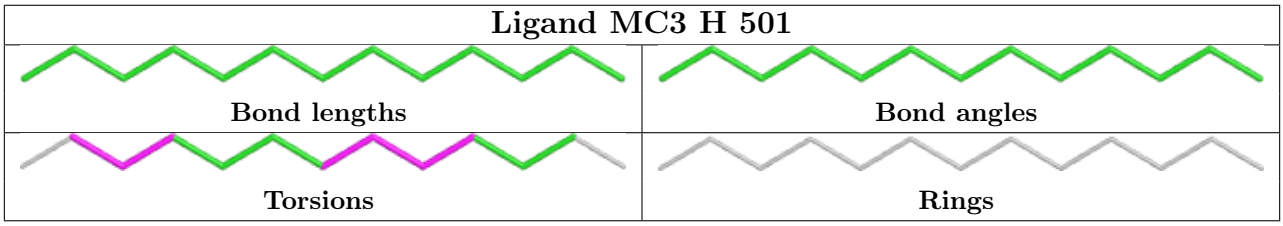
Ligand MC3 O 501



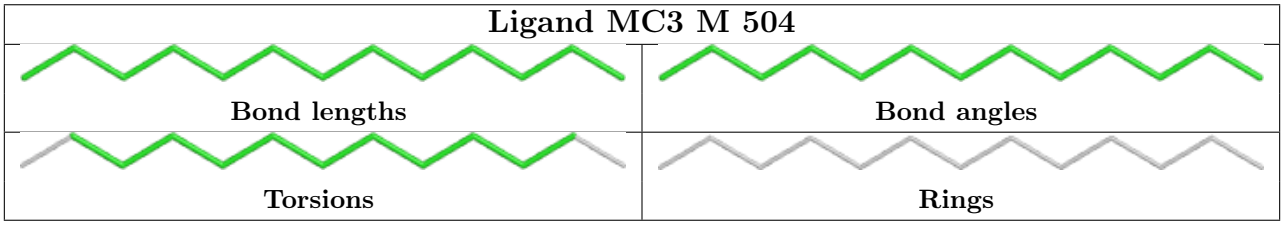
Ligand MC3 B 501



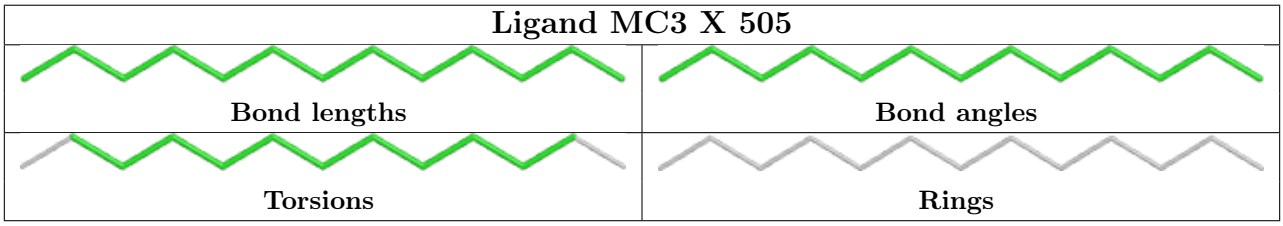
Ligand MC3 H 501



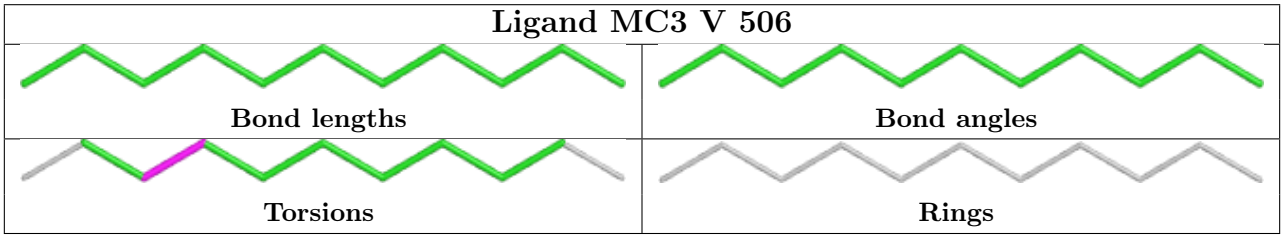
Ligand MC3 M 504



Ligand MC3 X 505



Ligand MC3 V 506



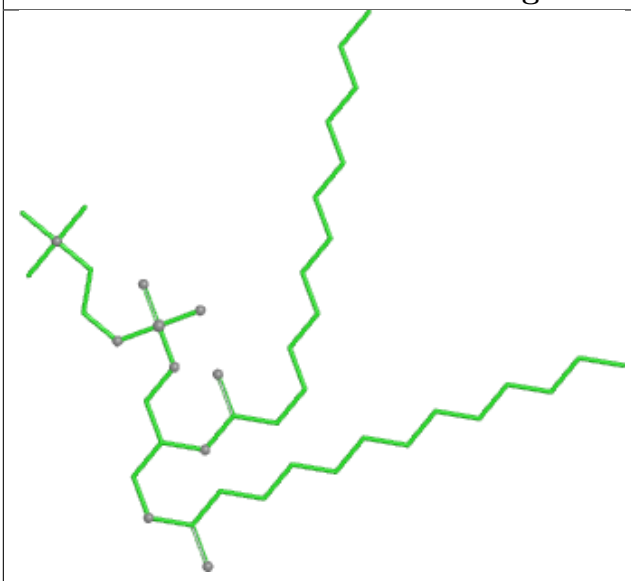
Ligand MC3 E 502	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand MC3 X 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

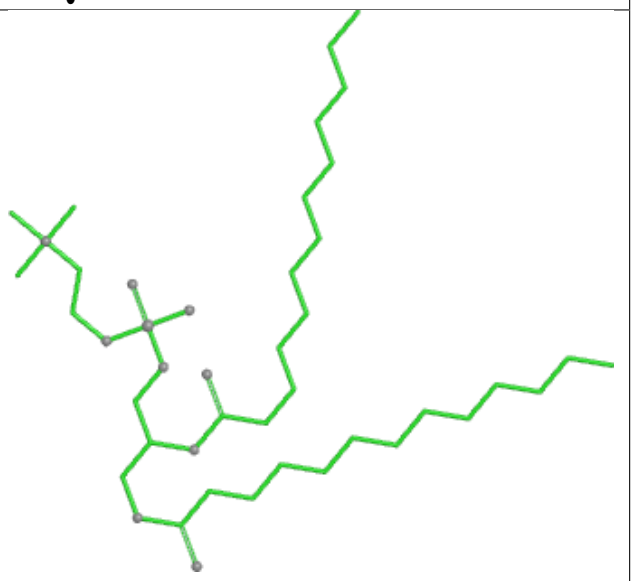
Ligand MC3 S 505	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand MC3 S 504	
 Bond lengths	 Bond angles
 Torsions	 Rings

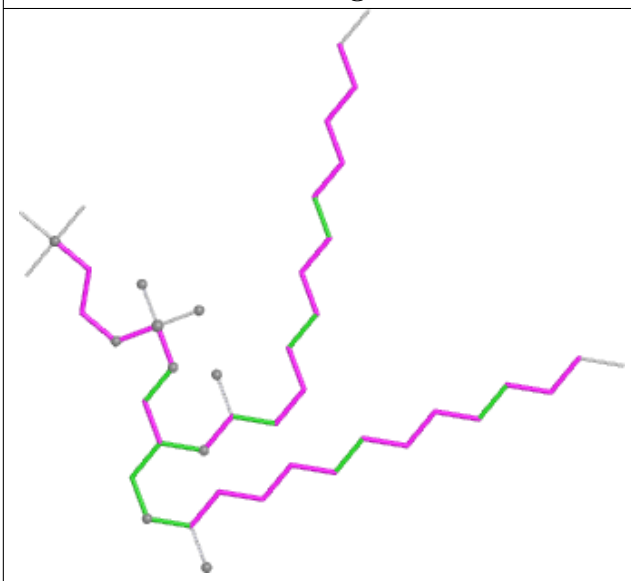
Ligand MC3 Q 506



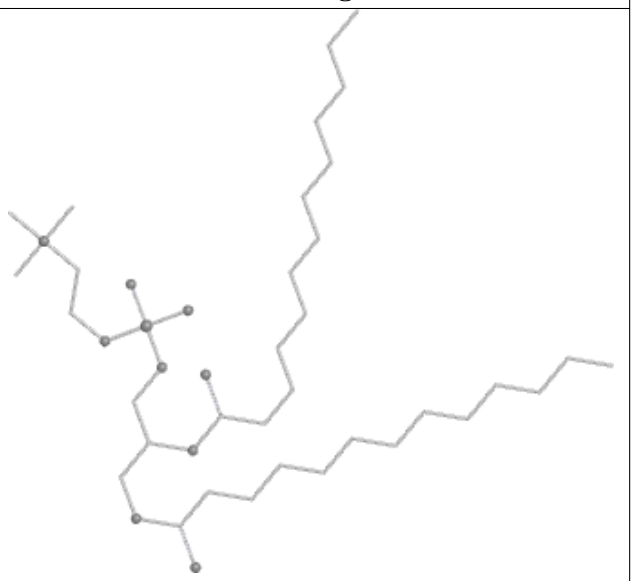
Bond lengths



Bond angles



Torsions



Rings

Ligand MC3 K 502



Bond lengths



Bond angles

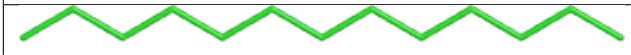


Torsions



Rings

Ligand MC3 H 505



Bond lengths



Bond angles

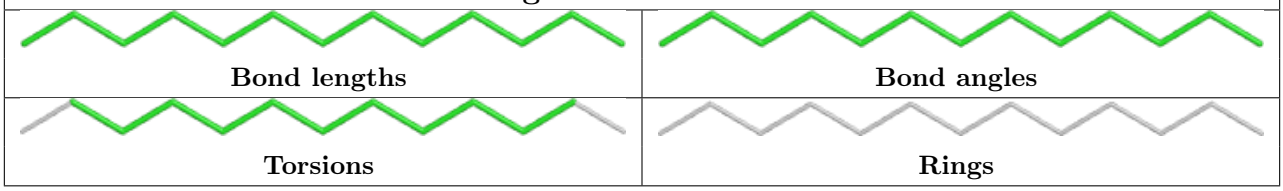


Torsions

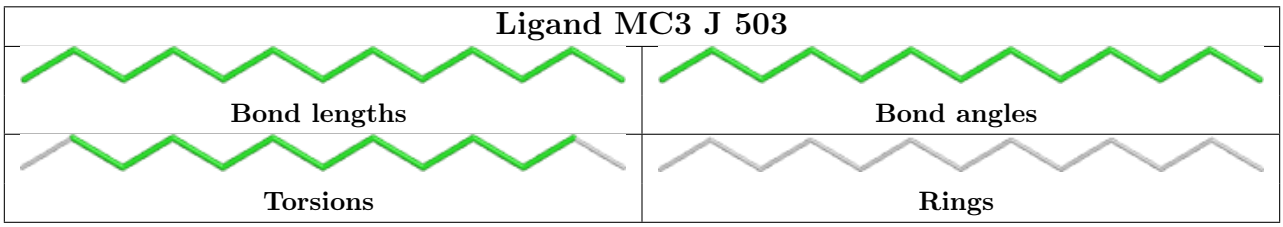


Rings

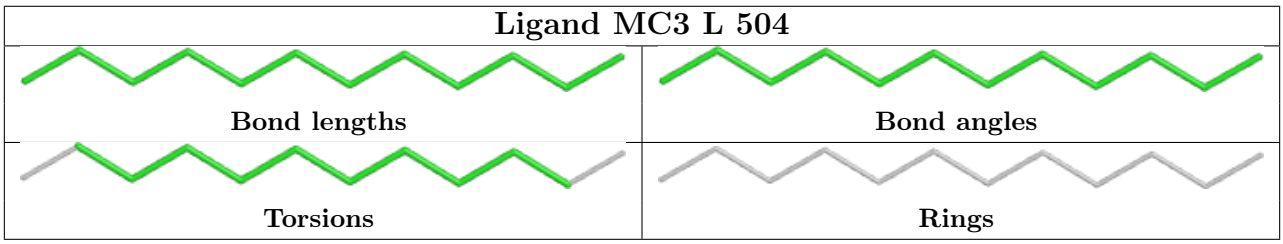
Ligand MC3 H 506



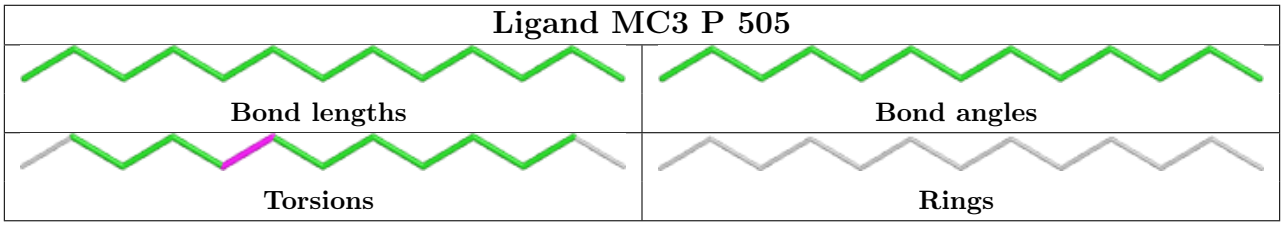
Ligand MC3 J 503



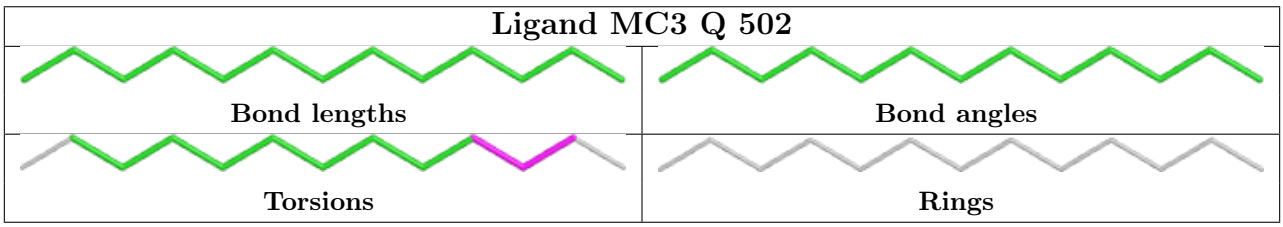
Ligand MC3 L 504



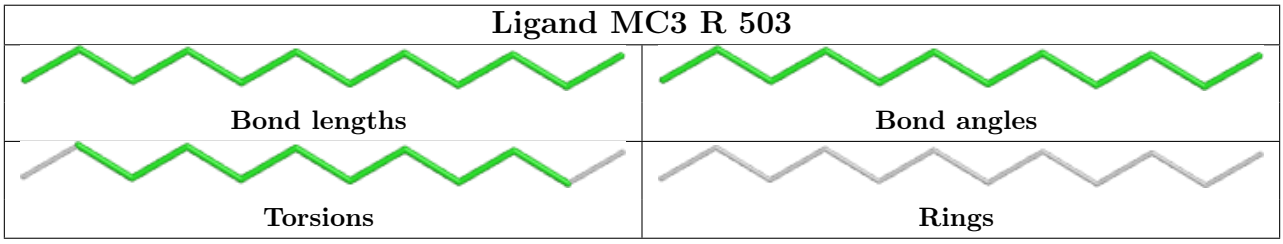
Ligand MC3 P 505



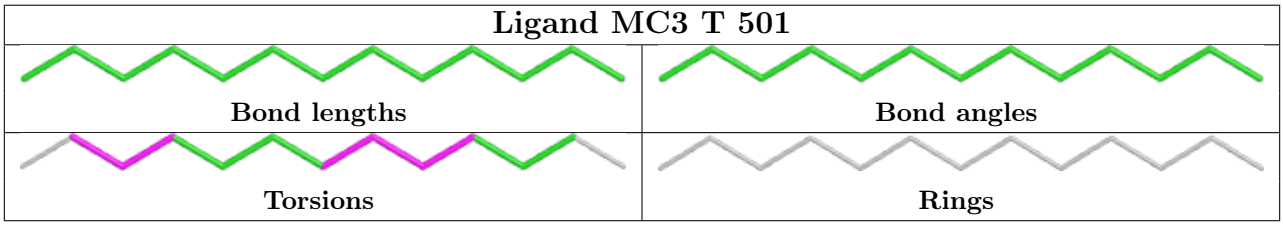
Ligand MC3 Q 502



Ligand MC3 R 503



Ligand MC3 T 501



Ligand MC3 T 505



Bond lengths



Bond angles

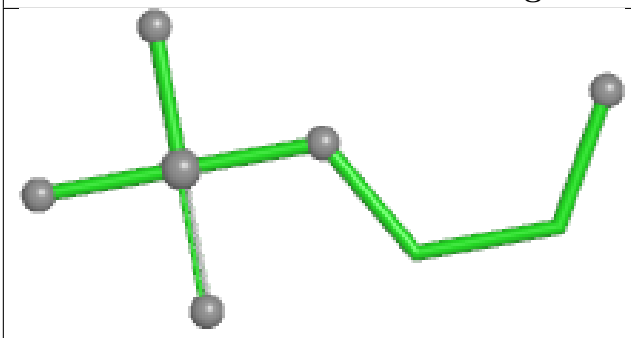


Torsions

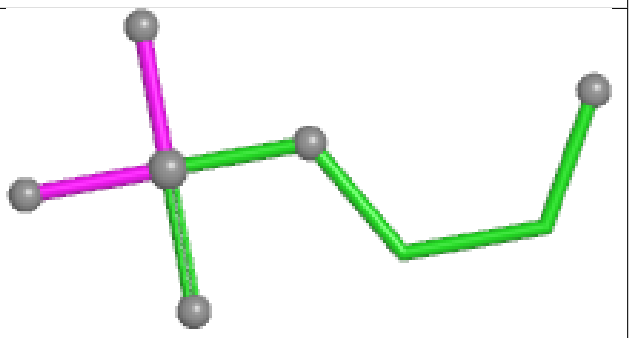


Rings

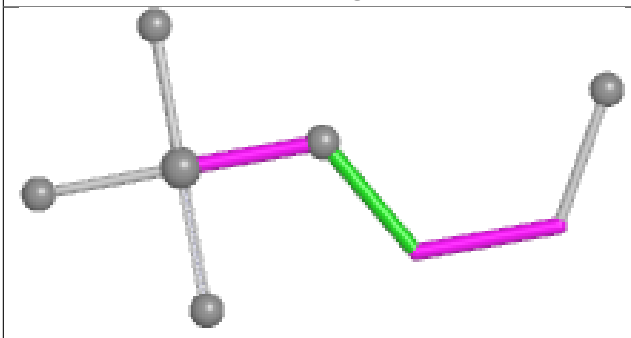
Ligand MC3 F 509



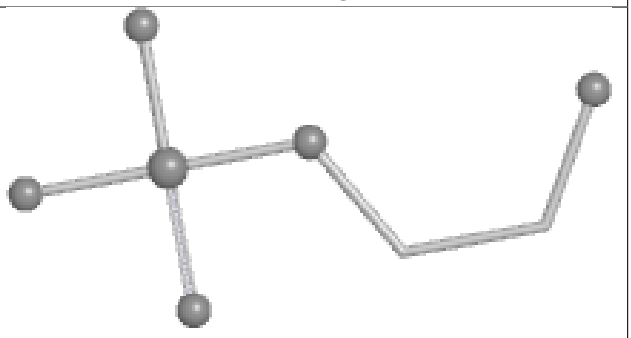
Bond lengths



Bond angles



Torsions



Rings

Ligand MC3 E 505



Bond lengths



Bond angles



Torsions



Rings

Ligand MC3 E 501



Bond lengths



Bond angles

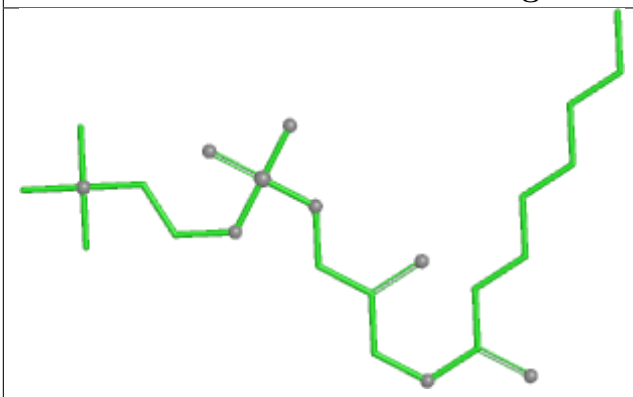


Torsions

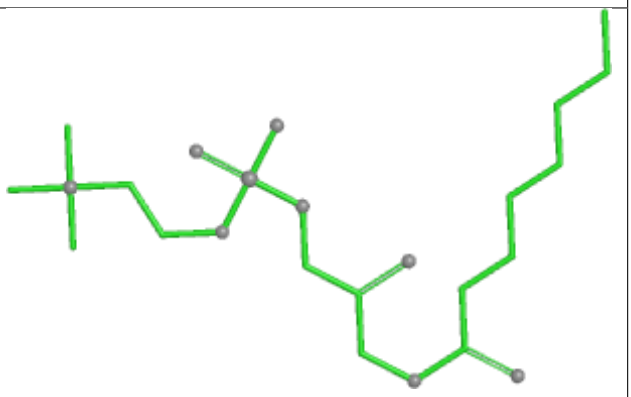


Rings

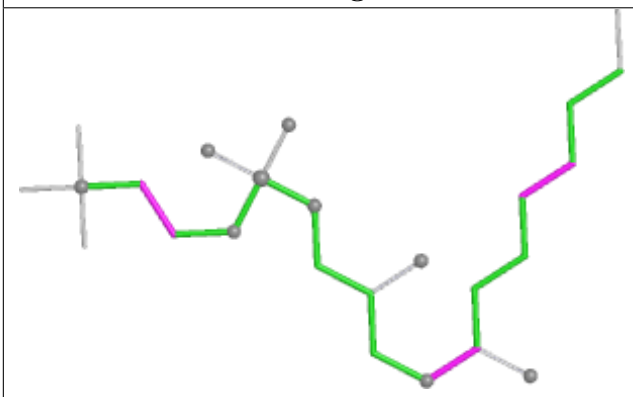
Ligand MC3 A 507



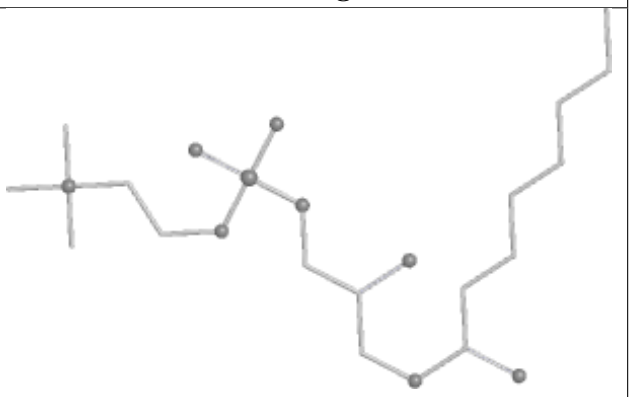
Bond lengths



Bond angles



Torsions



Rings

Ligand MC3 I 502



Bond lengths



Bond angles

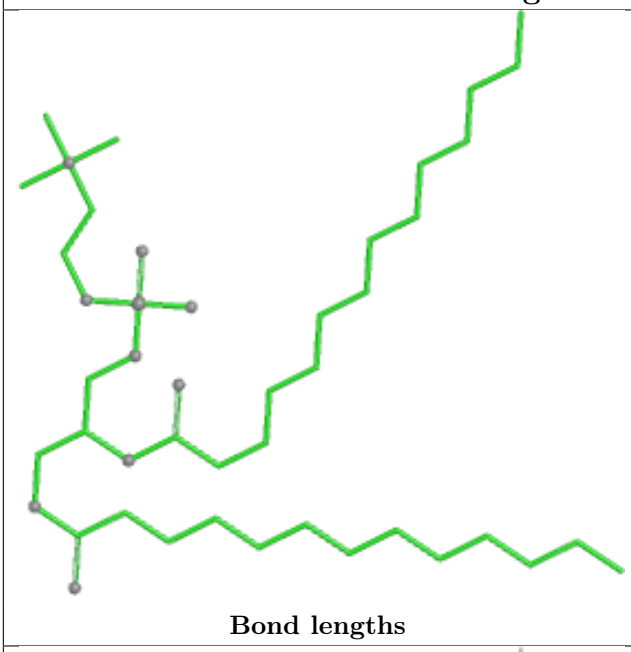


Torsions

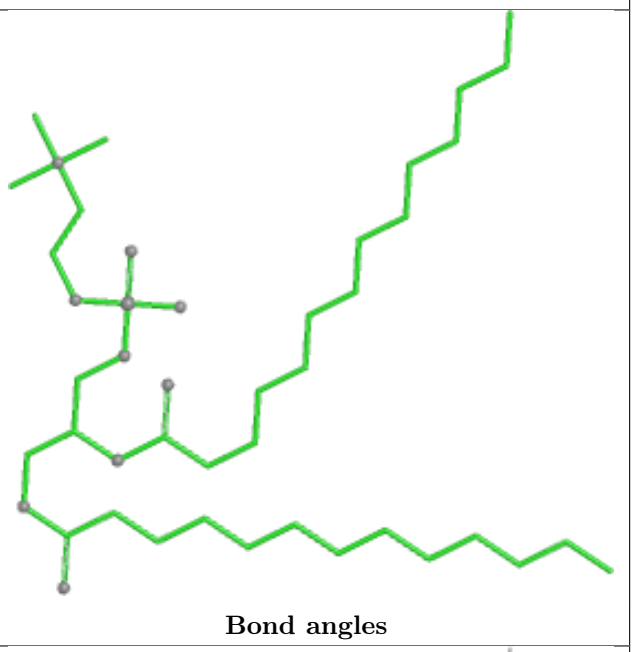


Rings

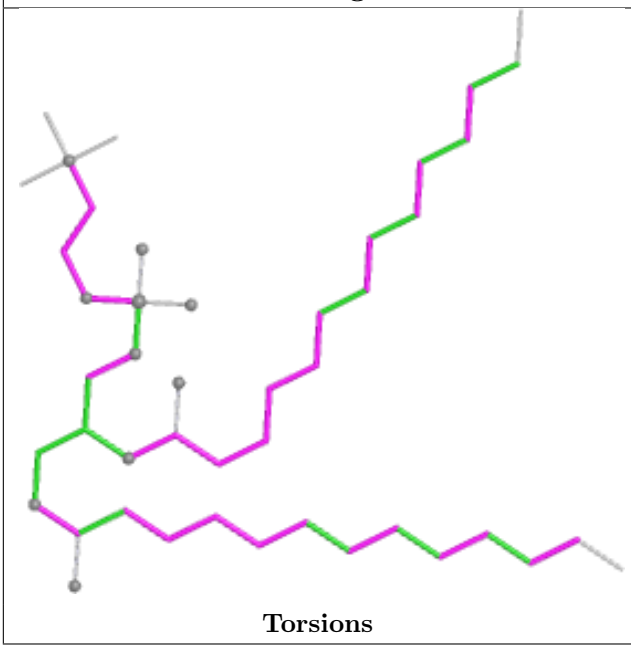
Ligand MC3 T 503



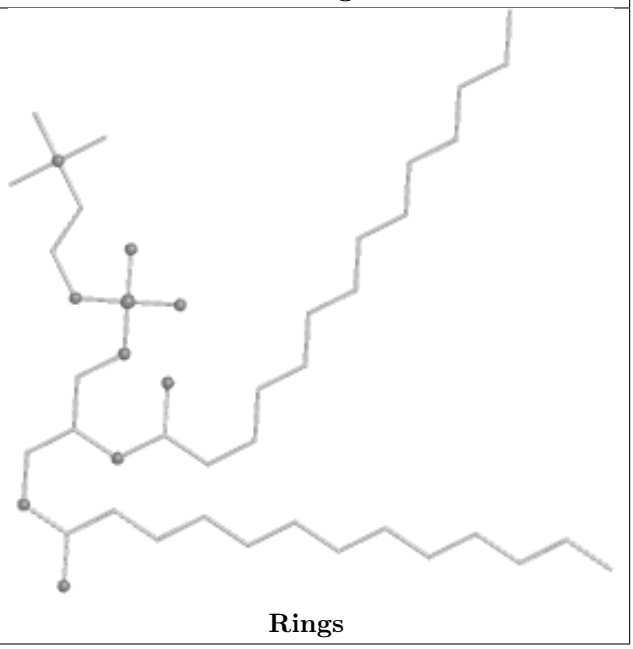
Bond lengths



Bond angles



Torsions



Rings

Ligand MC3 W 502



Bond lengths



Bond angles



Torsions



Rings

Ligand MC3 M 508



Bond lengths



Bond angles

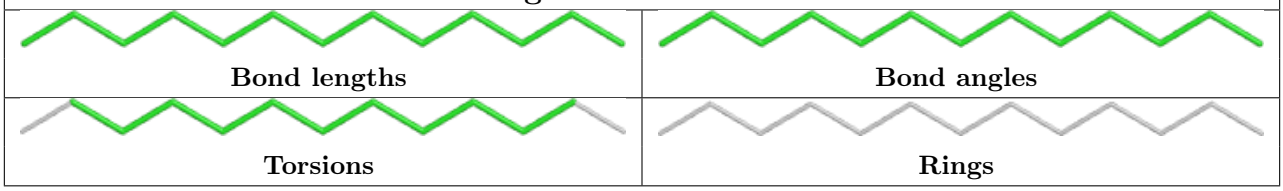


Torsions

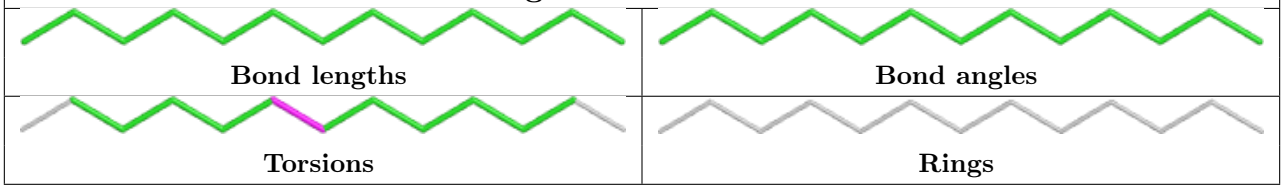


Rings

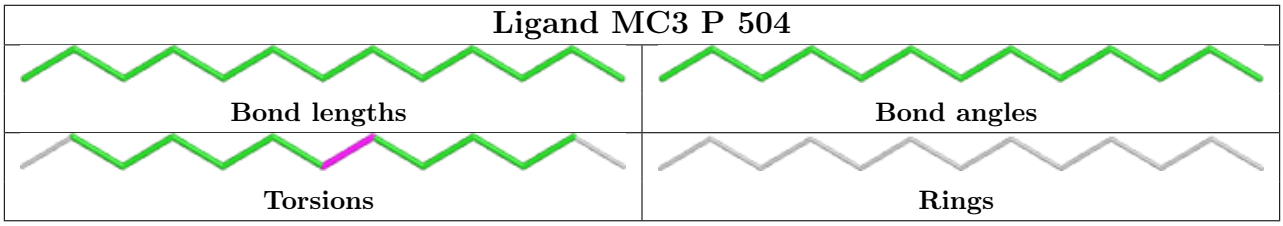
Ligand MC3 P 503



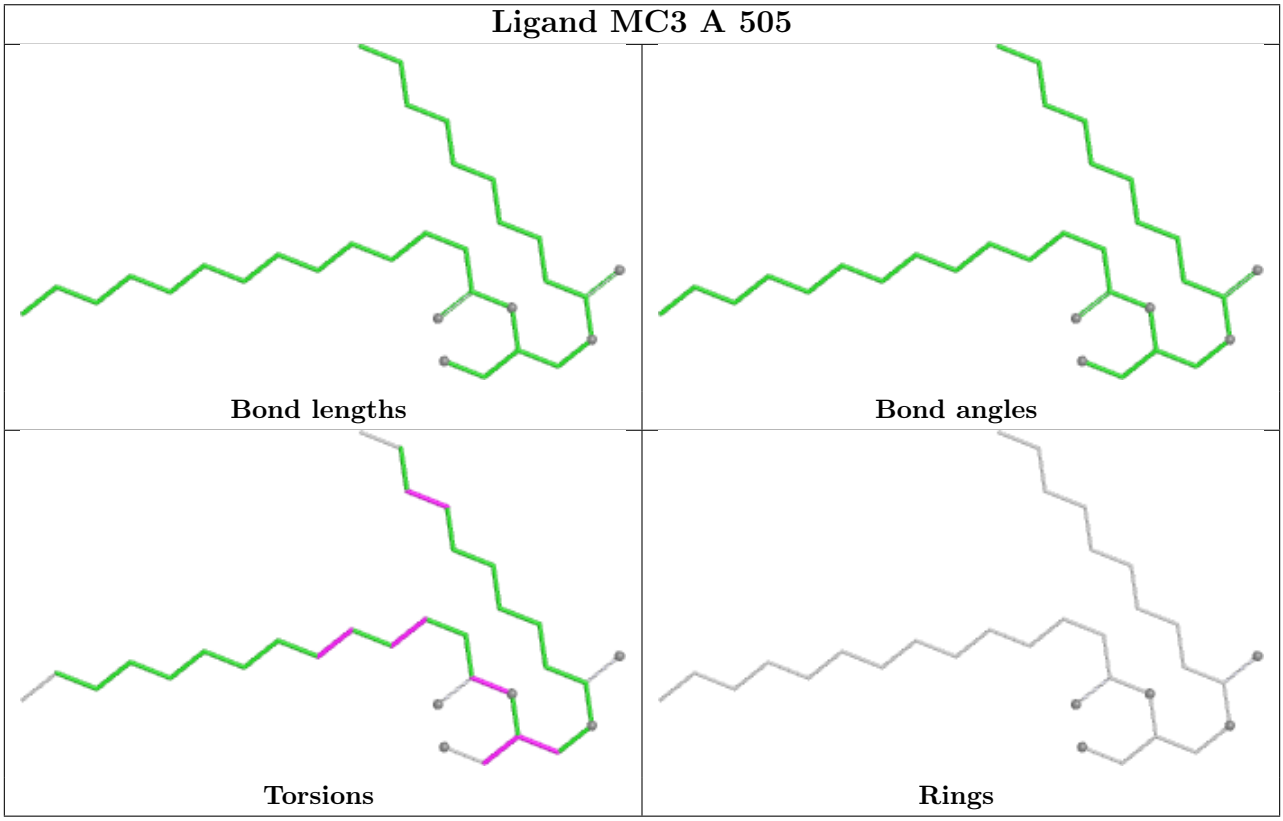
Ligand MC3 F 507



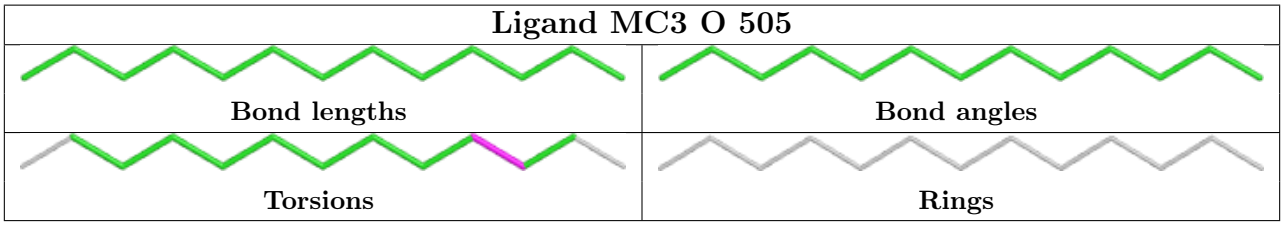
Ligand MC3 P 504



Ligand MC3 A 505



Ligand MC3 O 505

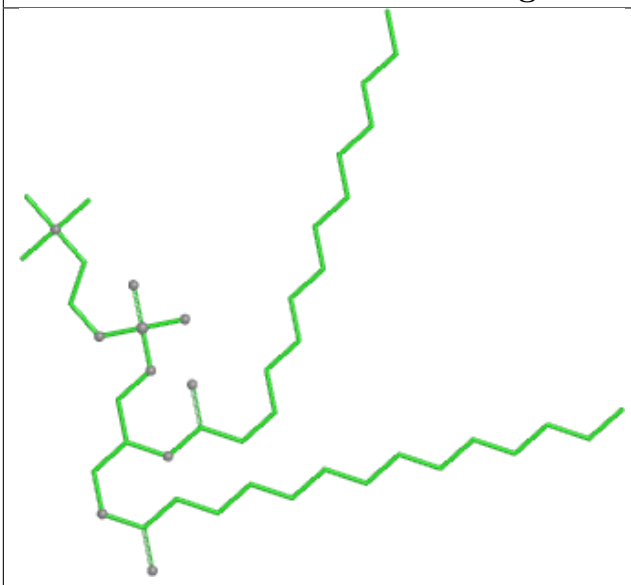


Ligand MC3 D 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

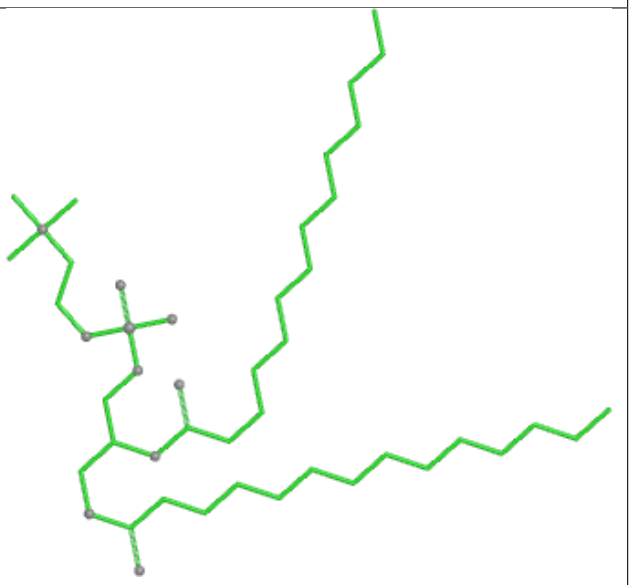
Ligand MC3 I 507	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand MC3 S 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

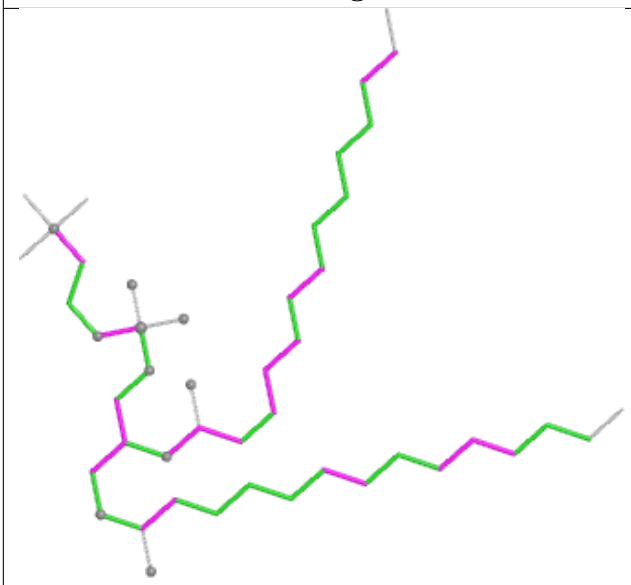
Ligand MC3 M 502



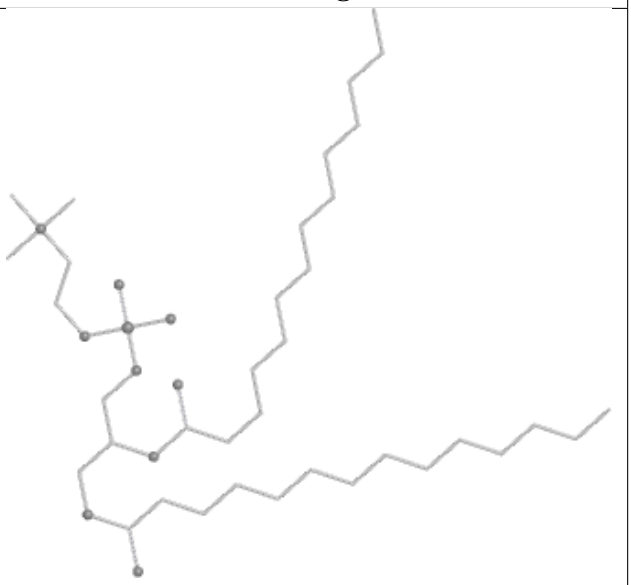
Bond lengths



Bond angles



Torsions



Rings

Ligand MC3 D 503



Bond lengths



Bond angles



Torsions



Rings

Ligand MC3 R 507



Bond lengths



Bond angles



Torsions



Rings

Ligand MC3 I 501



Bond lengths



Bond angles



Torsions



Rings

Ligand MC3 R 505



Bond lengths



Bond angles

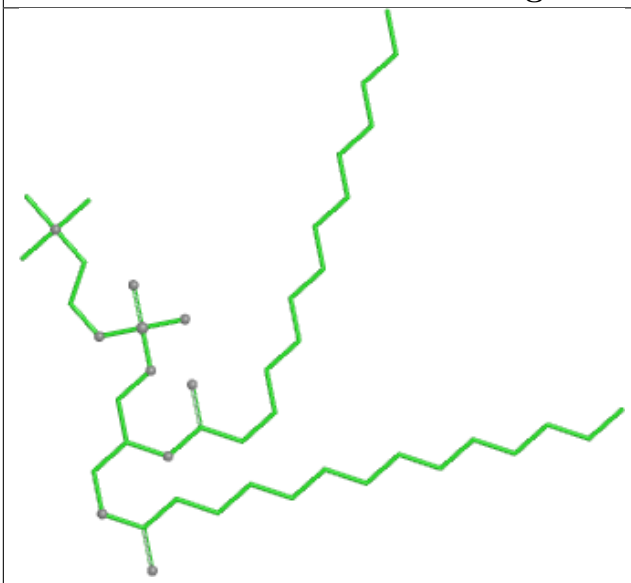


Torsions

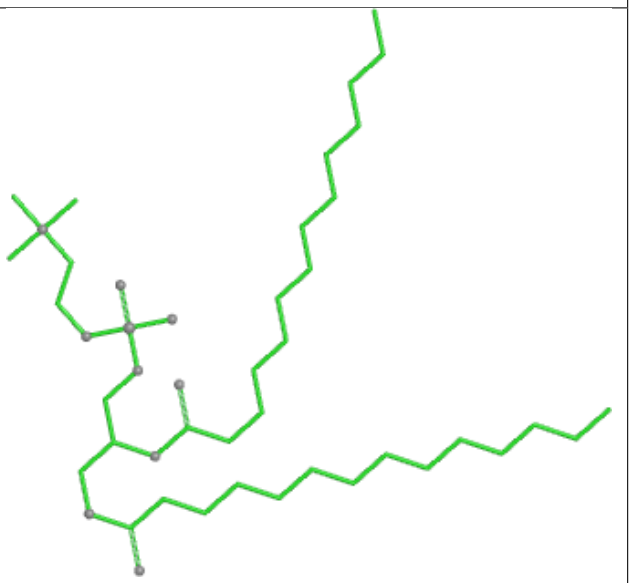


Rings

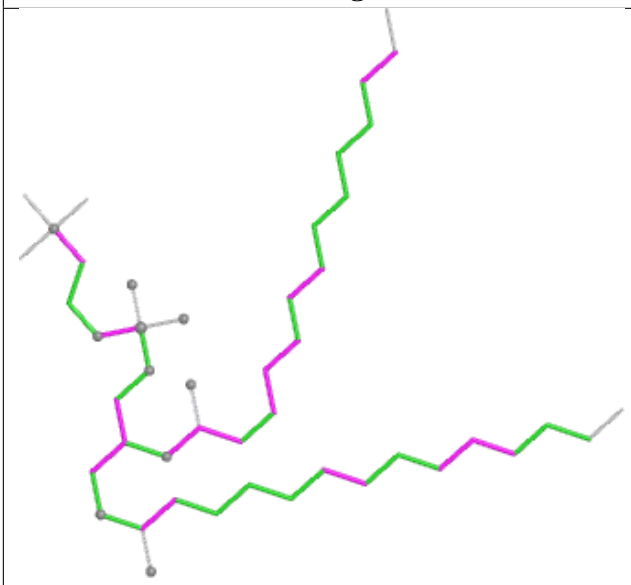
Ligand MC3 S 503



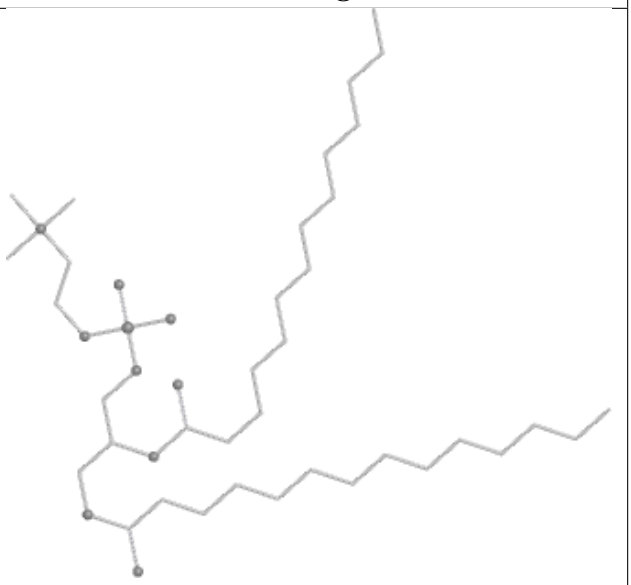
Bond lengths



Bond angles



Torsions



Rings

Ligand MC3 Y 505	
 Bond lengths	 Bond angles
 Torsions	 Rings

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.

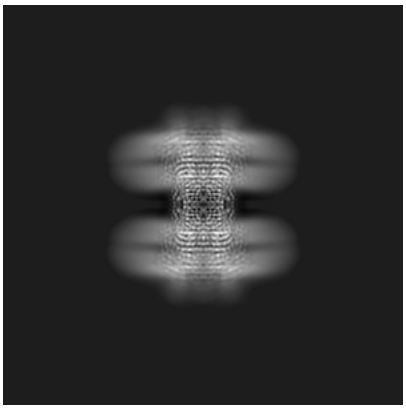
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-78870. These allow visual inspection of the internal detail of the map and identification of artifacts.

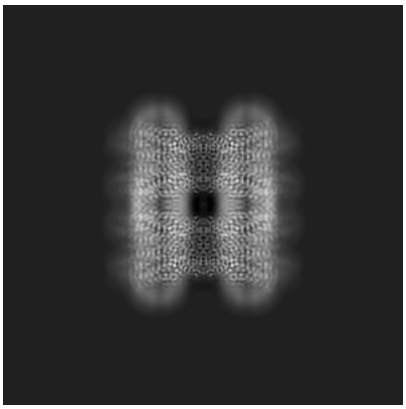
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

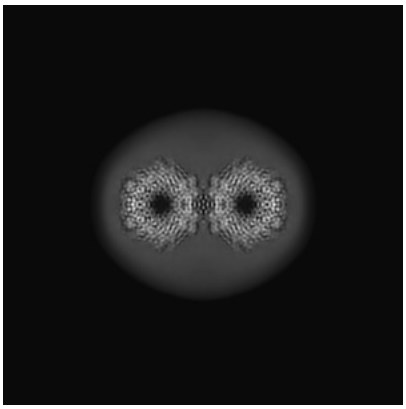
6.1.1 Primary map



X

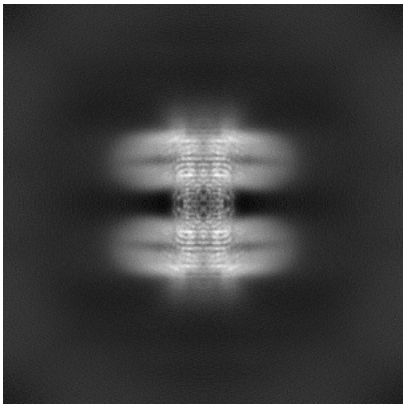


Y

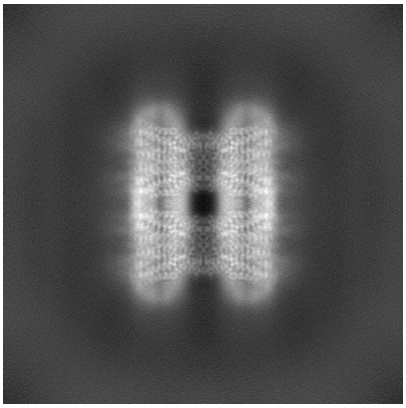


Z

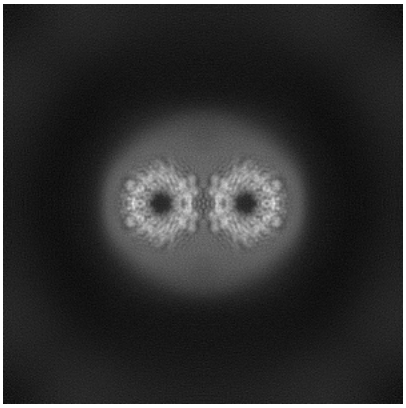
6.1.2 Raw map



X



Y



Z

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

6.2 Central slices (i)

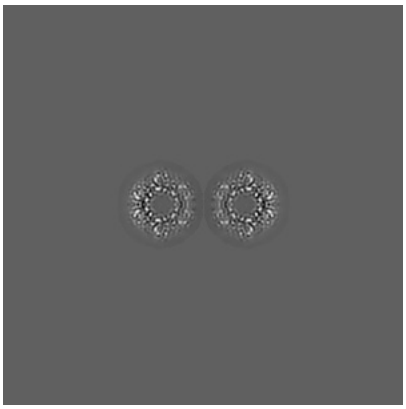
6.2.1 Primary map



X Index: 216

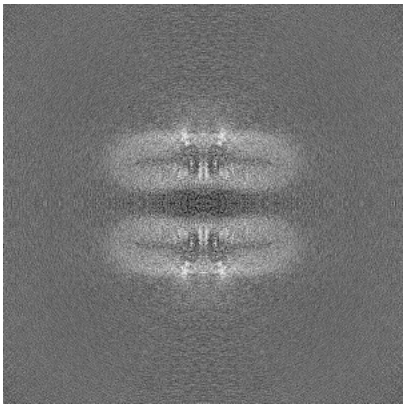


Y Index: 216

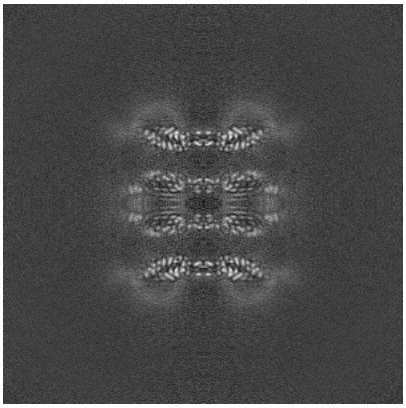


Z Index: 216

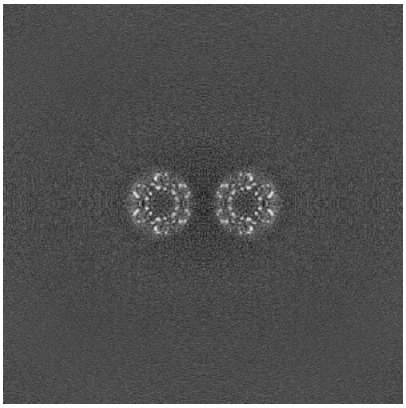
6.2.2 Raw map



X Index: 216



Y Index: 216

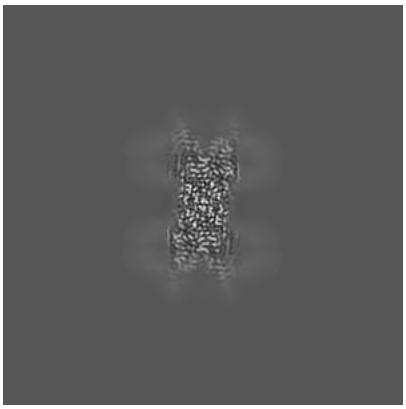


Z Index: 216

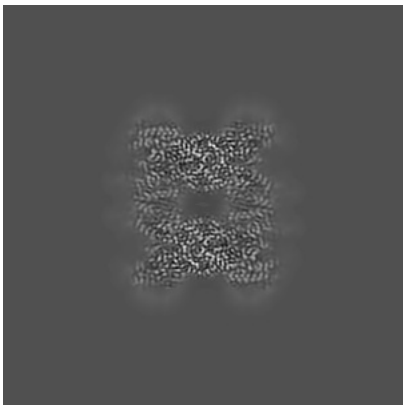
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

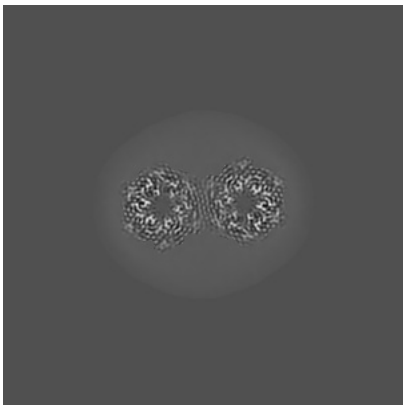
6.3.1 Primary map



X Index: 280

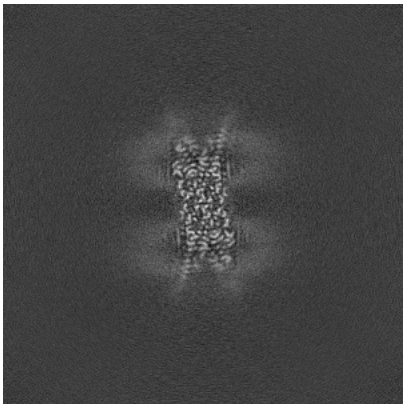


Y Index: 233

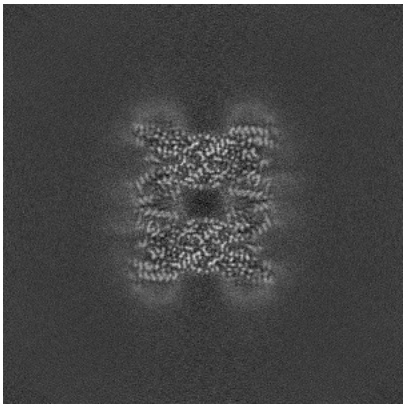


Z Index: 246

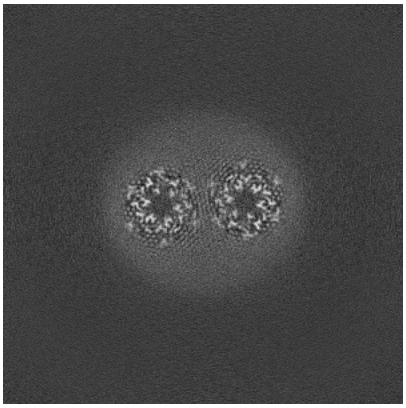
6.3.2 Raw map



X Index: 151



Y Index: 199

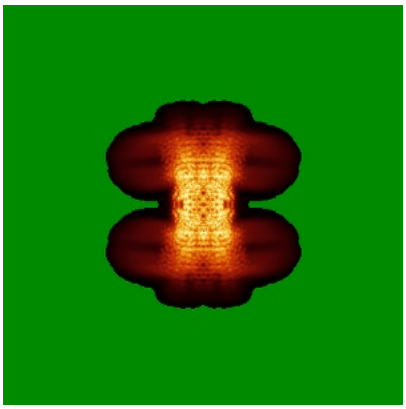


Z Index: 246

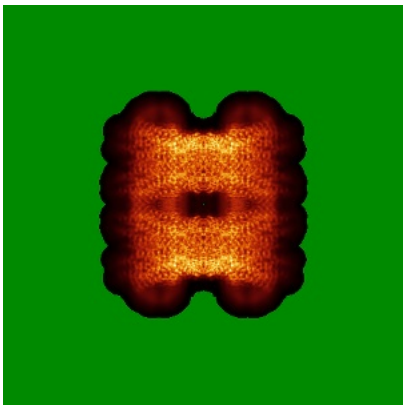
The images above show the largest variance slices of the map in three orthogonal directions.

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

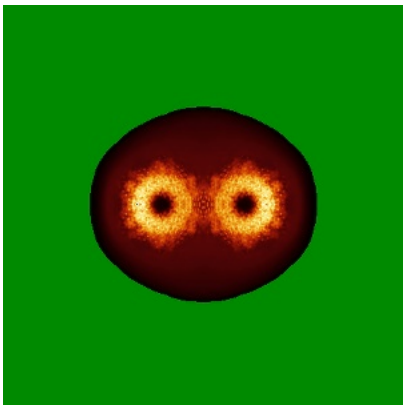
6.4.1 Primary map



X

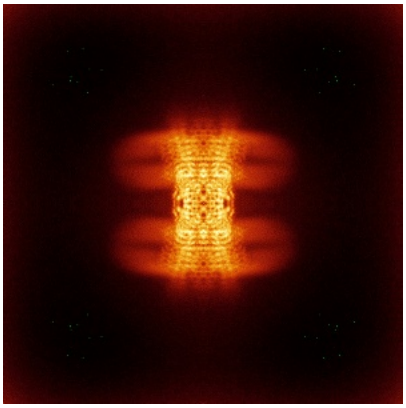


Y

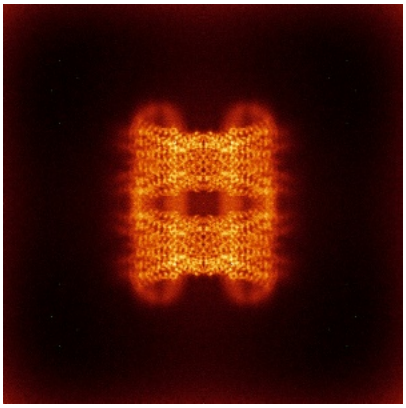


Z

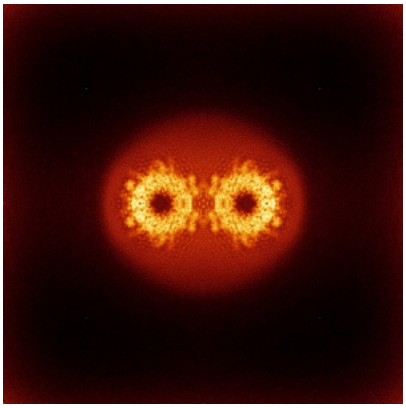
6.4.2 Raw map



X



Y

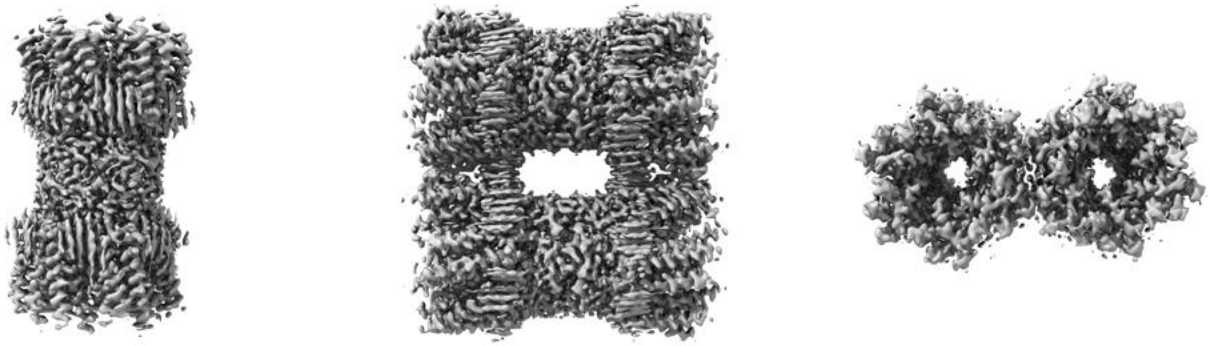


Z

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)

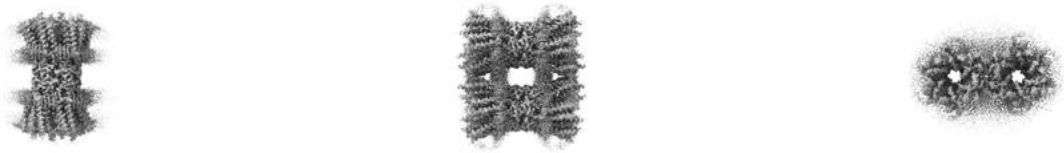
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.65. 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.

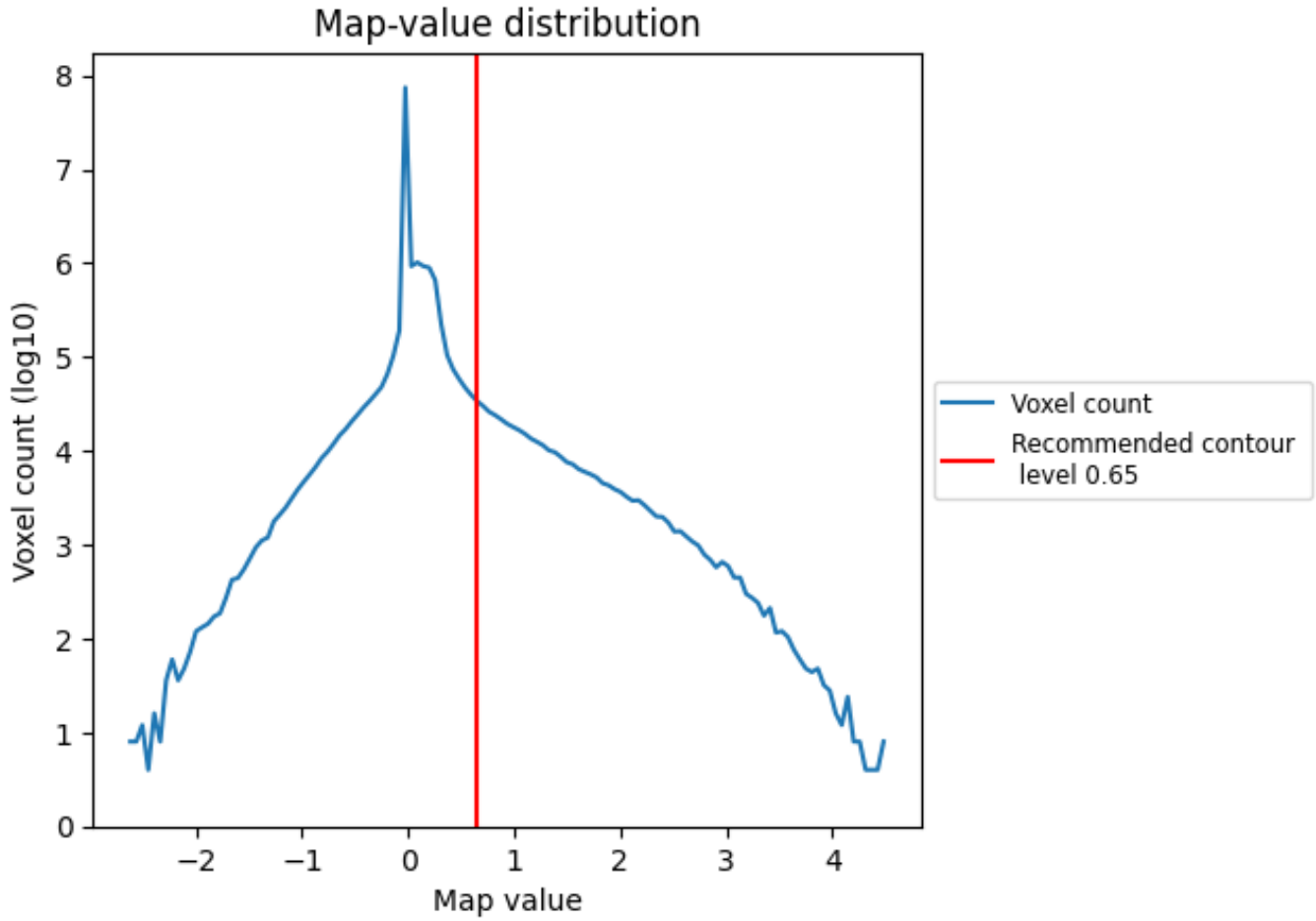
6.6 Mask visualisation (i)

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

7 Map analysis

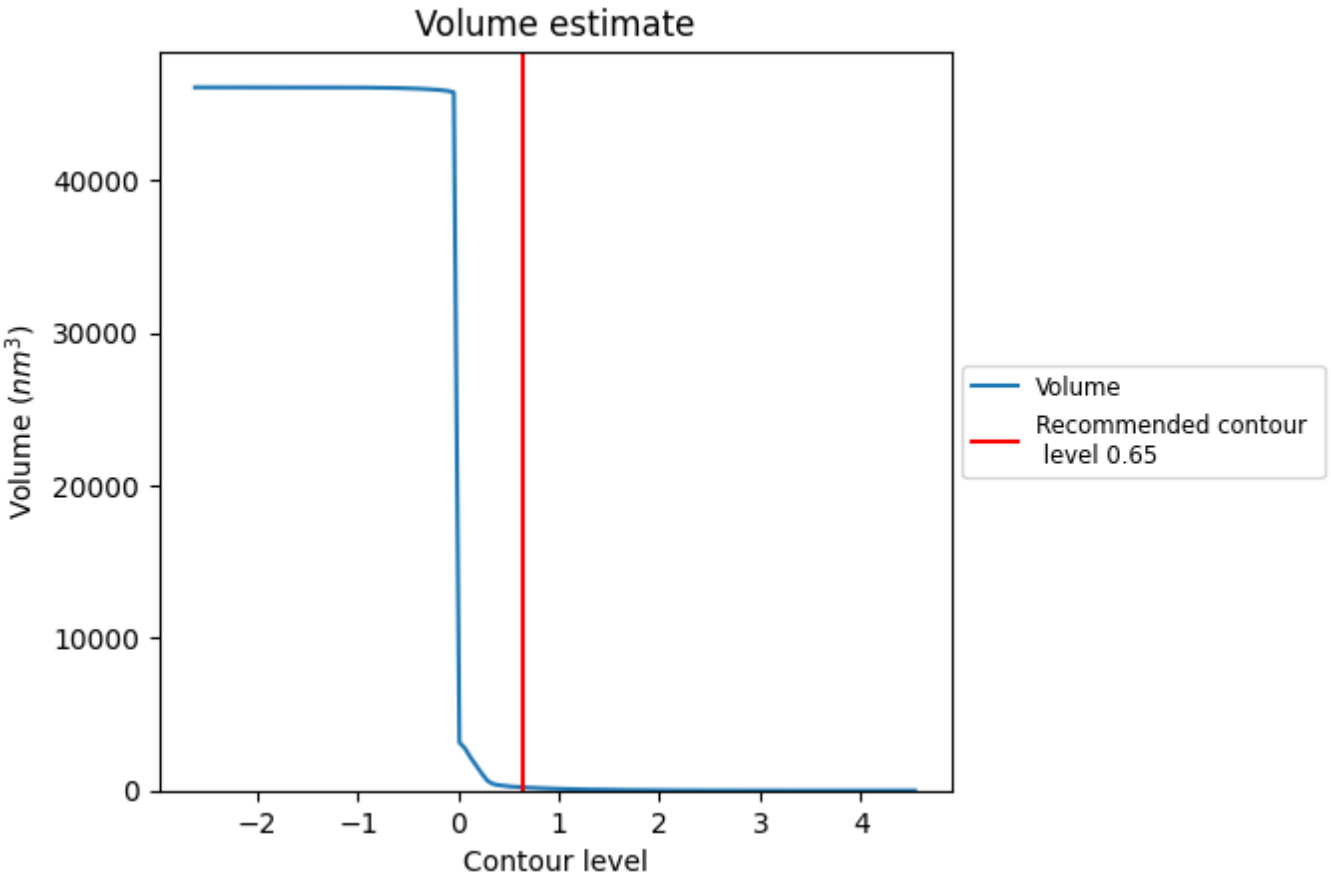
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

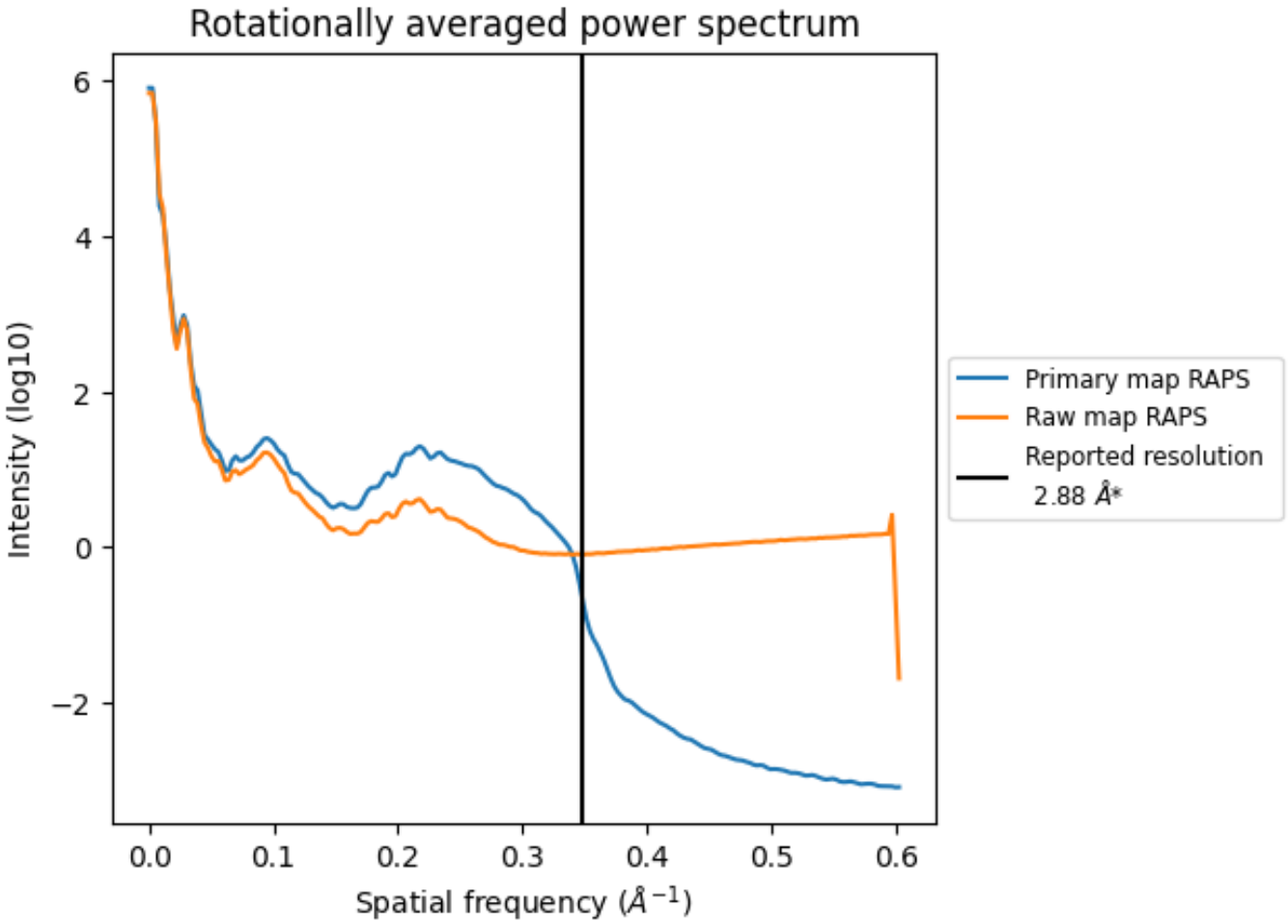
7.2 Volume estimate



The volume at the recommended contour level is 206 nm^3; this corresponds to an approximate mass of 186 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)

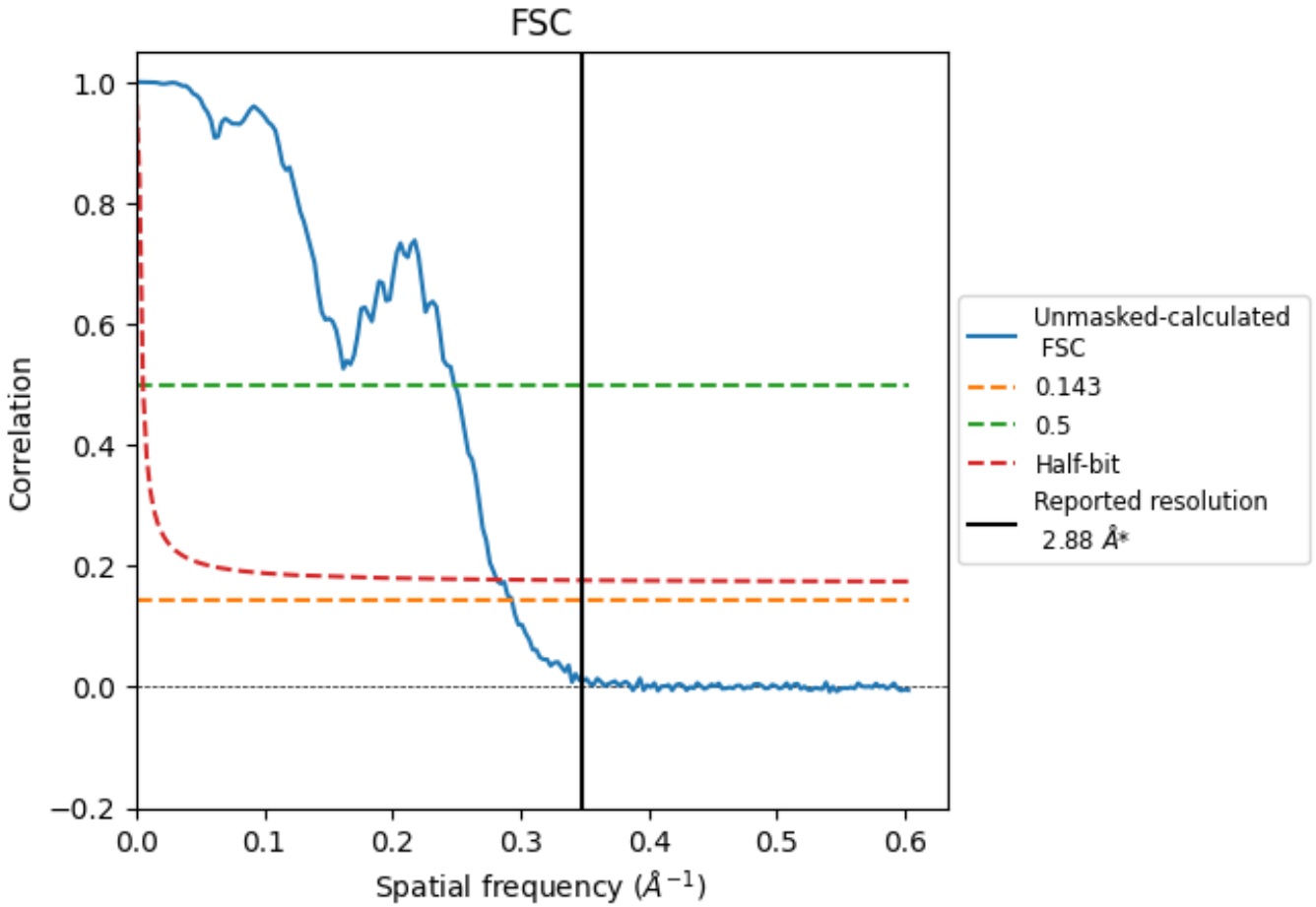


*Reported resolution corresponds to spatial frequency of 0.347 Å^{-1}

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 0.347 Å^{-1}

8.2 Resolution estimates (i)

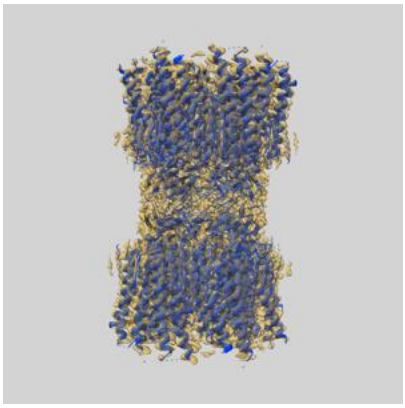
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.88	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.41	4.02	3.55

*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 3.41 differs from the reported value 2.88 by more than 10 %

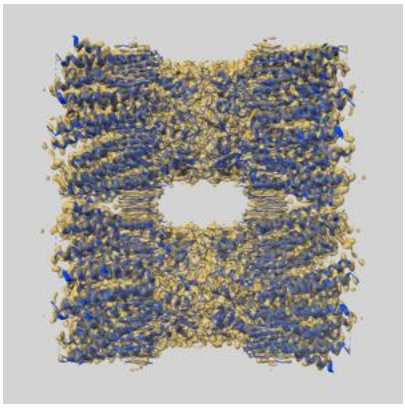
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-78870 and PDB model 38KG. Per-residue inclusion information can be found in section 3 on page 16.

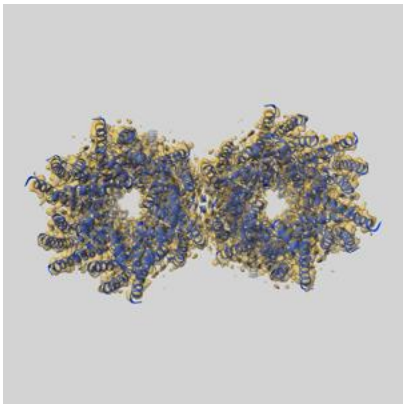
9.1 Map-model overlay



X



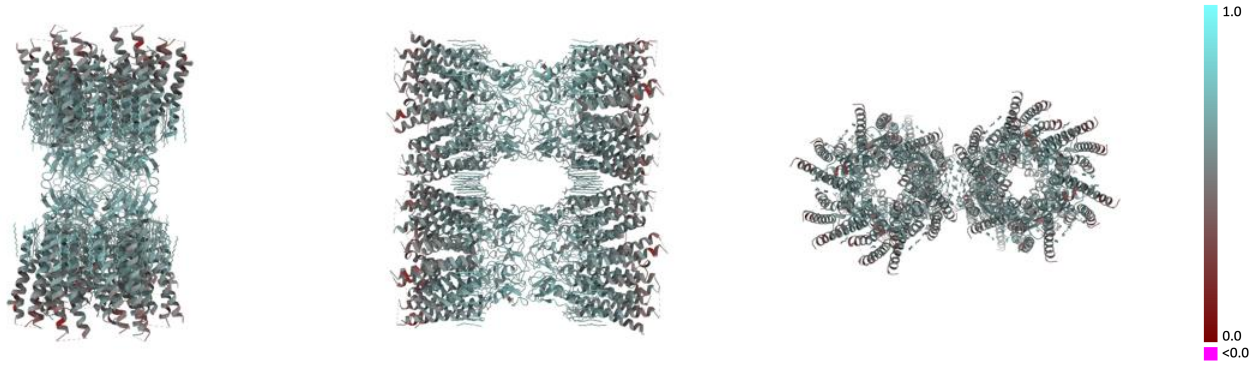
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.65 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

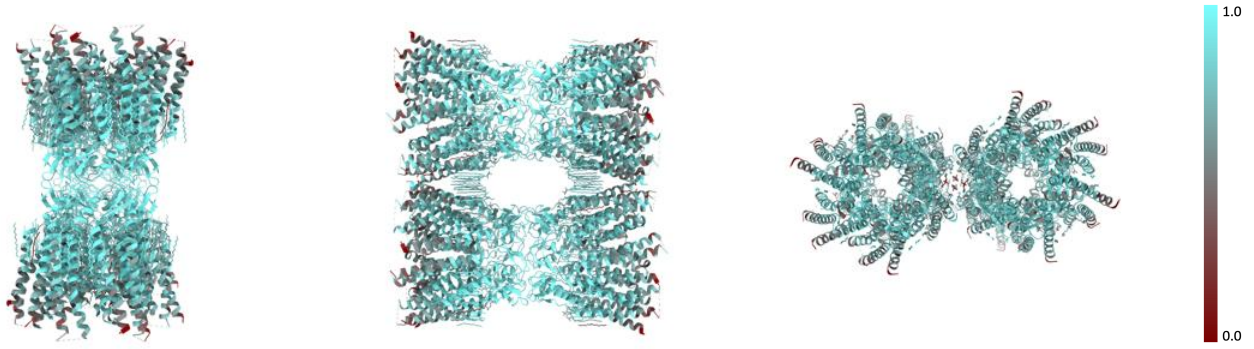
9.2 Q-score mapped to coordinate model



X Y Z

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

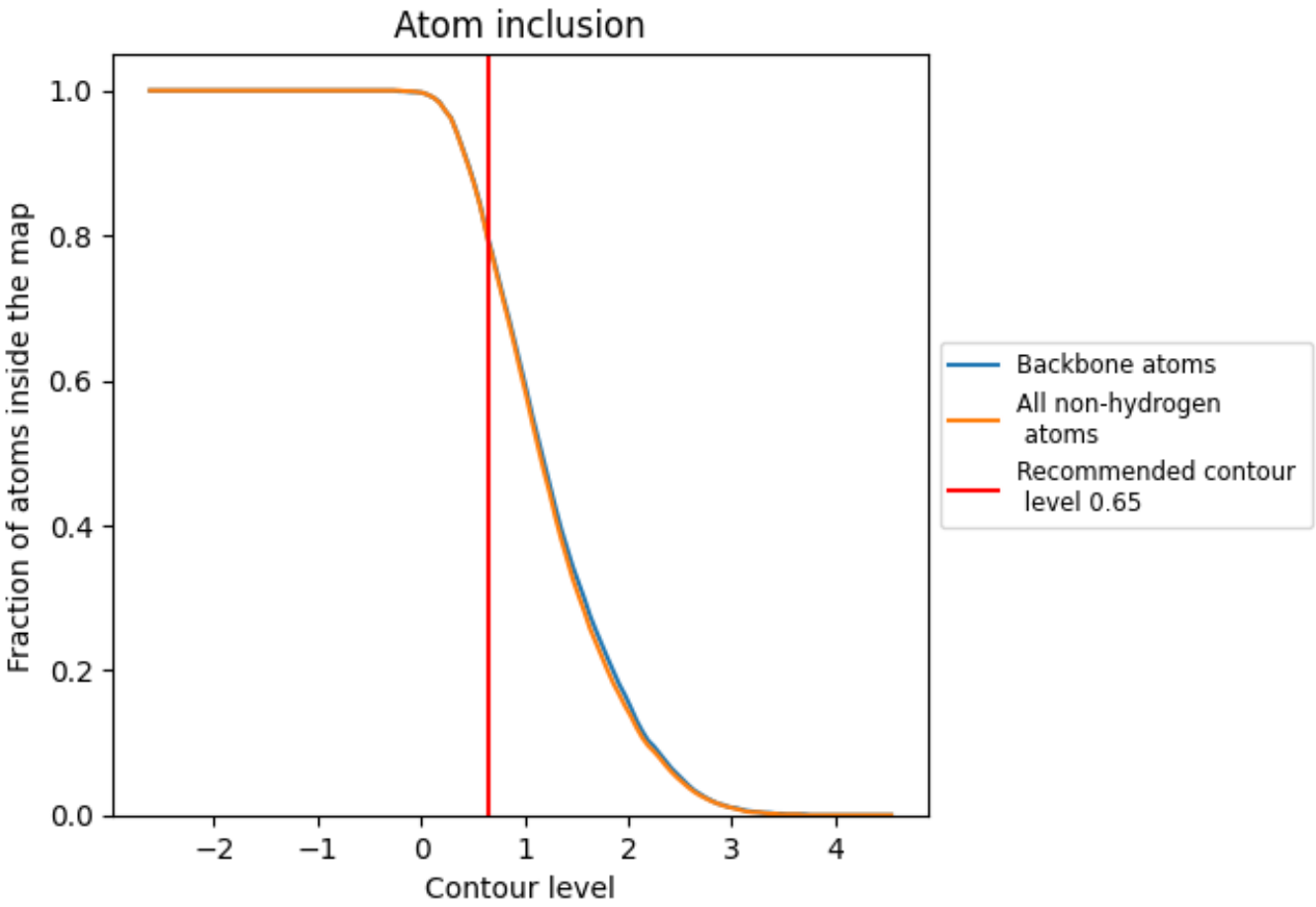
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.65).

9.4 Atom inclusion (i)



At the recommended contour level, 79% of all backbone atoms, 79% 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 (0.65) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7910	0.5570
A	0.7950	0.5520
B	0.7830	0.5510
C	0.8070	0.5620
D	0.7990	0.5650
E	0.7900	0.5540
F	0.8030	0.5600
G	0.7950	0.5500
H	0.7830	0.5500
I	0.8070	0.5640
J	0.7990	0.5650
K	0.7900	0.5520
L	0.8030	0.5620
M	0.7950	0.5510
N	0.7830	0.5510
O	0.8070	0.5610
P	0.7990	0.5650
Q	0.7900	0.5550
R	0.8030	0.5610
S	0.7950	0.5500
T	0.7830	0.5500
V	0.8070	0.5620
W	0.7990	0.5660
X	0.7900	0.5530
Y	0.8030	0.5610

