Full wwPDB EM Validation Report ⓘ

Nov 29, 2022 – 12:31 AM JST

PDB ID	:	7W9K
EMDB ID	:	EMD-32368
Title	:	Cryo-EM structure of human Nav1.7-beta1-beta2 complex at 2.2 angstrom resolution
Authors	:	Yan, N.; Huang, G.; Liu, D.; Wei, P.; Shen, H.
Deposited on	:	2021-12-09
Resolution	:	2.20 Å(reported)

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

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

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

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

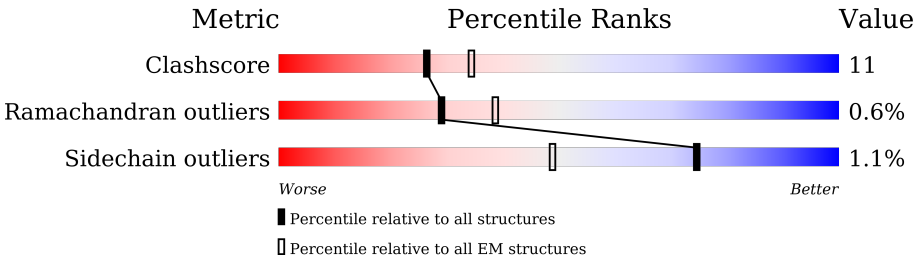
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	2031	13% 56% 14% 30%
2	B	218	67% 11% 21%
3	C	215	47% 50% 6% 45%
4	D	2	50% 100%
4	E	2	100%
4	F	2	100%

2 Entry composition (i)

There are 13 unique types of molecules in this entry. The entry contains 14933 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 Sodium channel protein type 9 subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1413	11412	7534	1796	1997	85	1	0

There are 43 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-42	MET	-	initiating methionine	UNP Q15858
A	-41	ALA	-	expression tag	UNP Q15858
A	-40	SER	-	expression tag	UNP Q15858
A	-39	TRP	-	expression tag	UNP Q15858
A	-38	SER	-	expression tag	UNP Q15858
A	-37	HIS	-	expression tag	UNP Q15858
A	-36	PRO	-	expression tag	UNP Q15858
A	-35	GLN	-	expression tag	UNP Q15858
A	-34	PHE	-	expression tag	UNP Q15858
A	-33	GLU	-	expression tag	UNP Q15858
A	-32	LYS	-	expression tag	UNP Q15858
A	-31	GLY	-	expression tag	UNP Q15858
A	-30	GLY	-	expression tag	UNP Q15858
A	-29	GLY	-	expression tag	UNP Q15858
A	-28	ALA	-	expression tag	UNP Q15858
A	-27	ARG	-	expression tag	UNP Q15858
A	-26	GLY	-	expression tag	UNP Q15858
A	-25	GLY	-	expression tag	UNP Q15858
A	-24	SER	-	expression tag	UNP Q15858
A	-23	GLY	-	expression tag	UNP Q15858
A	-22	GLY	-	expression tag	UNP Q15858
A	-21	GLY	-	expression tag	UNP Q15858
A	-20	SER	-	expression tag	UNP Q15858
A	-19	TRP	-	expression tag	UNP Q15858
A	-18	SER	-	expression tag	UNP Q15858
A	-17	HIS	-	expression tag	UNP Q15858
A	-16	PRO	-	expression tag	UNP Q15858
A	-15	GLN	-	expression tag	UNP Q15858

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-14	PHE	-	expression tag	UNP Q15858
A	-13	GLU	-	expression tag	UNP Q15858
A	-12	LYS	-	expression tag	UNP Q15858
A	-11	GLY	-	expression tag	UNP Q15858
A	-10	PHE	-	expression tag	UNP Q15858
A	-9	ASP	-	expression tag	UNP Q15858
A	-8	TYR	-	expression tag	UNP Q15858
A	-7	LYS	-	expression tag	UNP Q15858
A	-6	ASP	-	expression tag	UNP Q15858
A	-5	ASP	-	expression tag	UNP Q15858
A	-4	ASP	-	expression tag	UNP Q15858
A	-3	ASP	-	expression tag	UNP Q15858
A	-2	LYS	-	expression tag	UNP Q15858
A	-1	GLY	-	expression tag	UNP Q15858
A	0	THR	-	expression tag	UNP Q15858

- Molecule 2 is a protein called Sodium channel subunit beta-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	173	Total	C	N	O	S	0	0
			1416	902	232	272	10		

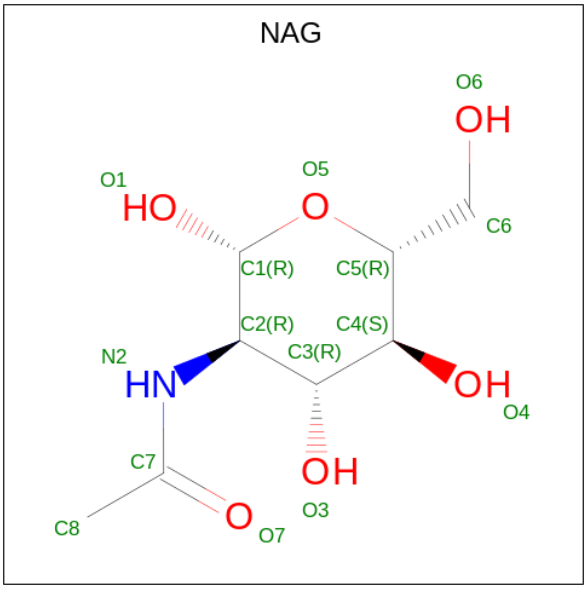
- Molecule 3 is a protein called Sodium channel subunit beta-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	119	Total	C	N	O	S	4	0
			980	615	172	183	10		

- Molecule 4 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

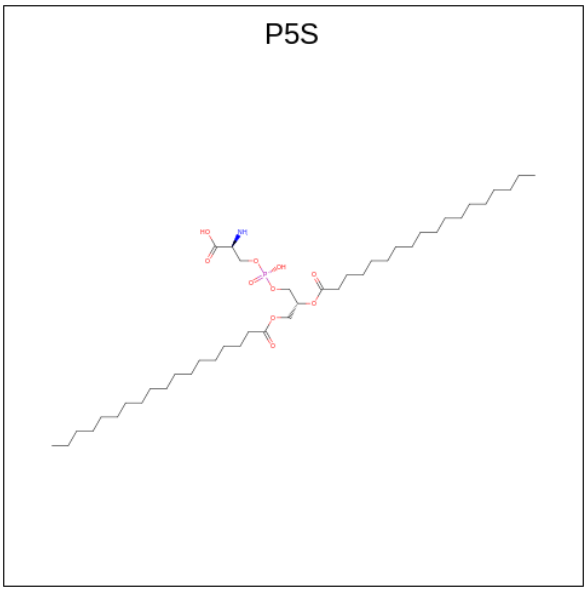
Mol	Chain	Residues	Atoms				AltConf	Trace
4	D	2	Total	C	N	O	0	0
			28	16	2	10		
4	E	2	Total	C	N	O	0	0
			28	16	2	10		
4	F	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).



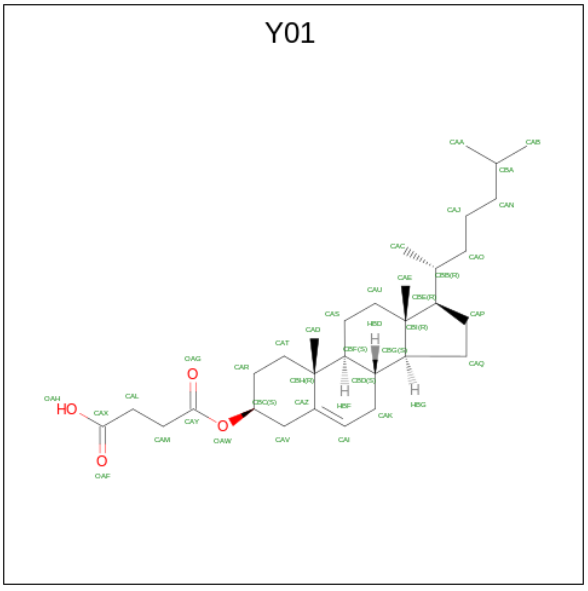
Mol	Chain	Residues	Atoms				AltConf
5	A	1	Total	C	N	O	0
			28	16	2	10	
5	A	1	Total	C	N	O	0
			28	16	2	10	
5	B	1	Total	C	N	O	0
			42	24	3	15	
5	B	1	Total	C	N	O	0
			42	24	3	15	
5	B	1	Total	C	N	O	0
			42	24	3	15	

- Molecule 6 is O-[(R)-{[(2R)-2,3-bis(octadecanoyloxy)propyl]oxy}(hydroxy)phosphoryl]-L-serine (three-letter code: P5S) (formula: $C_{42}H_{82}NO_{10}P$).



Mol	Chain	Residues	Atoms					AltConf
6	A	1	Total	C	N	O	P	0
			110	77	3	27	3	
6	A	1	Total	C	N	O	P	0
			110	77	3	27	3	
6	A	1	Total	C	N	O	P	0
			110	77	3	27	3	

- Molecule 7 is CHOLESTEROL HEMISUCCINATE (three-letter code: Y01) (formula: $C_{31}H_{50}O_4$).



Mol	Chain	Residues	Atoms			AltConf
7	A	1	Total	C	O	0
			210	186	24	

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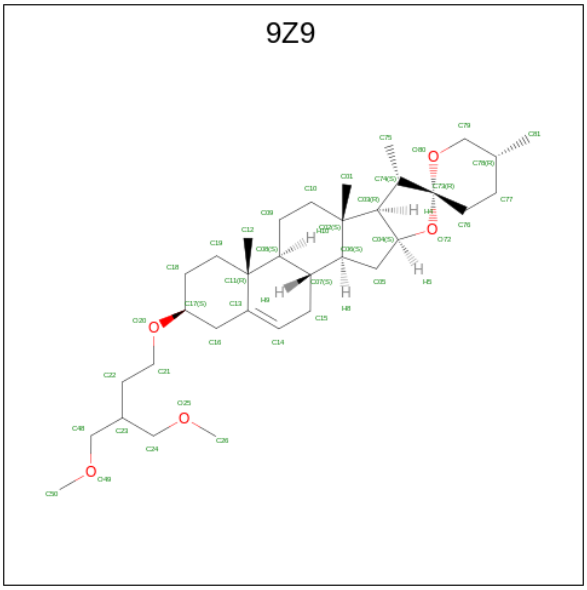
Mol	Chain	Residues	Atoms			AltConf
7	A	1	Total 210	C 186	O 24	0
7	A	1	Total 210	C 186	O 24	0
7	A	1	Total 210	C 186	O 24	0
7	A	1	Total 210	C 186	O 24	0
7	A	1	Total 210	C 186	O 24	0

- Molecule 8 is (3beta,14beta,17beta,25R)-3-[4-methoxy-3-(methoxymethyl)butoxy]spirost-5-en (three-letter code: 9Z9) (formula: $C_{34}H_{56}O_5$).

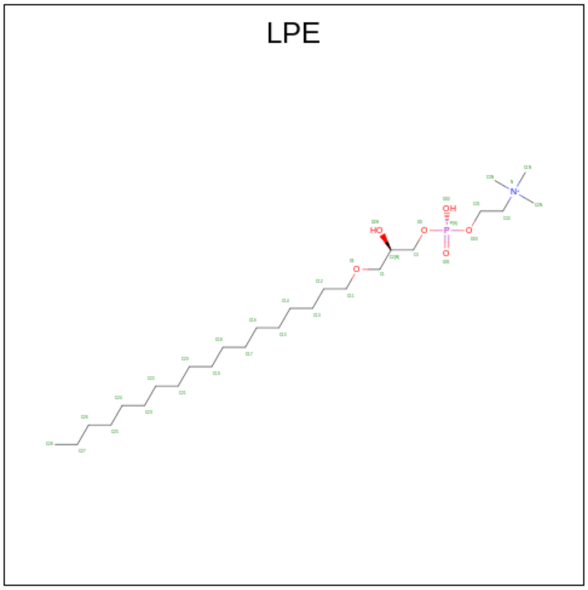


Mol	Chain	Residues	Atoms			AltConf
8	A	1	Total 39	C 34	O 5	0

- Molecule 9 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		AltConf
9	A	1	Total 1	Na 1	0

- Molecule 10 is 1-O-OCTADECYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: LPE) (formula: $C_{26}H_{57}NO_6P$).



Mol	Chain	Residues	Atoms	AltConf
10	A	1	Total C N O P 329 217 14 84 14	0
10	A	1	Total C N O P 329 217 14 84 14	0
10	A	1	Total C N O P 329 217 14 84 14	0
10	A	1	Total C N O P 329 217 14 84 14	0
10	A	1	Total C N O P 329 217 14 84 14	0
10	A	1	Total C N O P 329 217 14 84 14	0
10	A	1	Total C N O P 329 217 14 84 14	0
10	A	1	Total C N O P 329 217 14 84 14	0
10	A	1	Total C N O P 329 217 14 84 14	0
10	A	1	Total C N O P 329 217 14 84 14	0
10	A	1	Total C N O P 329 217 14 84 14	0
10	A	1	Total C N O P 329 217 14 84 14	0
10	A	1	Total C N O P 329 217 14 84 14	0
10	A	1	Total C N O P 329 217 14 84 14	0

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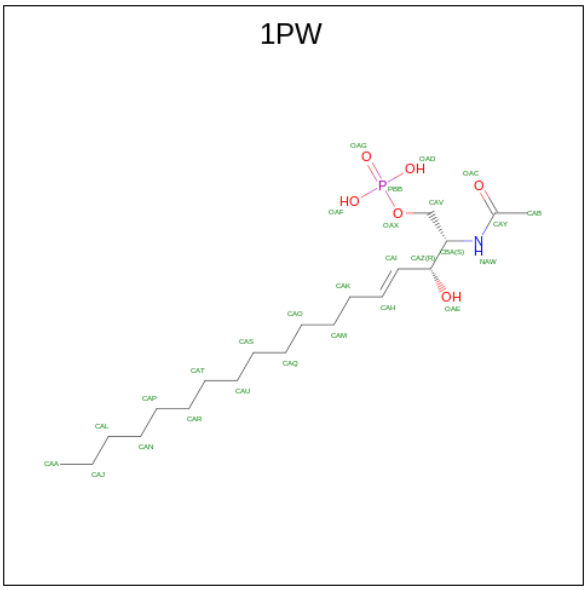
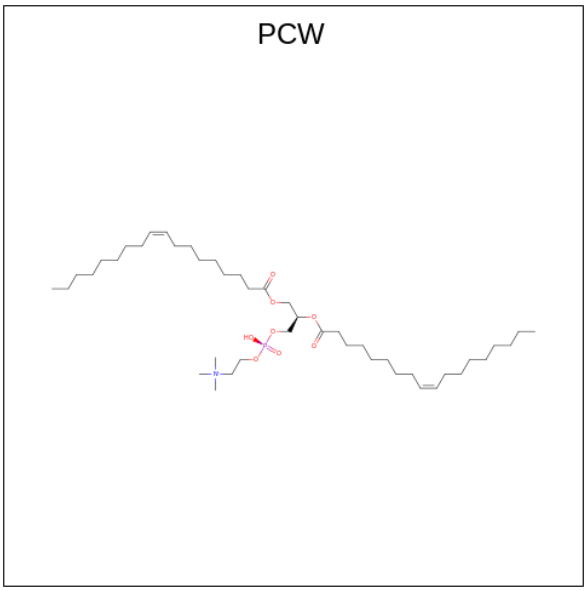
Mol	Chain	Residues	Atoms					AltConf
10	B	1	Total	C	N	O	P	0
			17	9	1	6	1	

- Molecule 11 is (2S,3R,4E)-2-(acetylamino)-3-hydroxyoctadec-4-en-1-yl dihydrogen phosphate (three-letter code: 1PW) (formula: $C_{20}H_{40}NO_6P$).



Mol	Chain	Residues	Atoms				AltConf
11	A	1	Total	C	O	P	0
			24	18	5	1	

- Molecule 12 is 1,2-DIOLEOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PCW) (formula: $C_{44}H_{85}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
12	A	1	Total	C	N	O	P	0
			232	182	5	40	5	
12	A	1	Total	C	N	O	P	0
			232	182	5	40	5	
12	A	1	Total	C	N	O	P	0
			232	182	5	40	5	
12	A	1	Total	C	N	O	P	0
			232	182	5	40	5	
12	A	1	Total	C	N	O	P	0
			232	182	5	40	5	

- Molecule 13 is water.

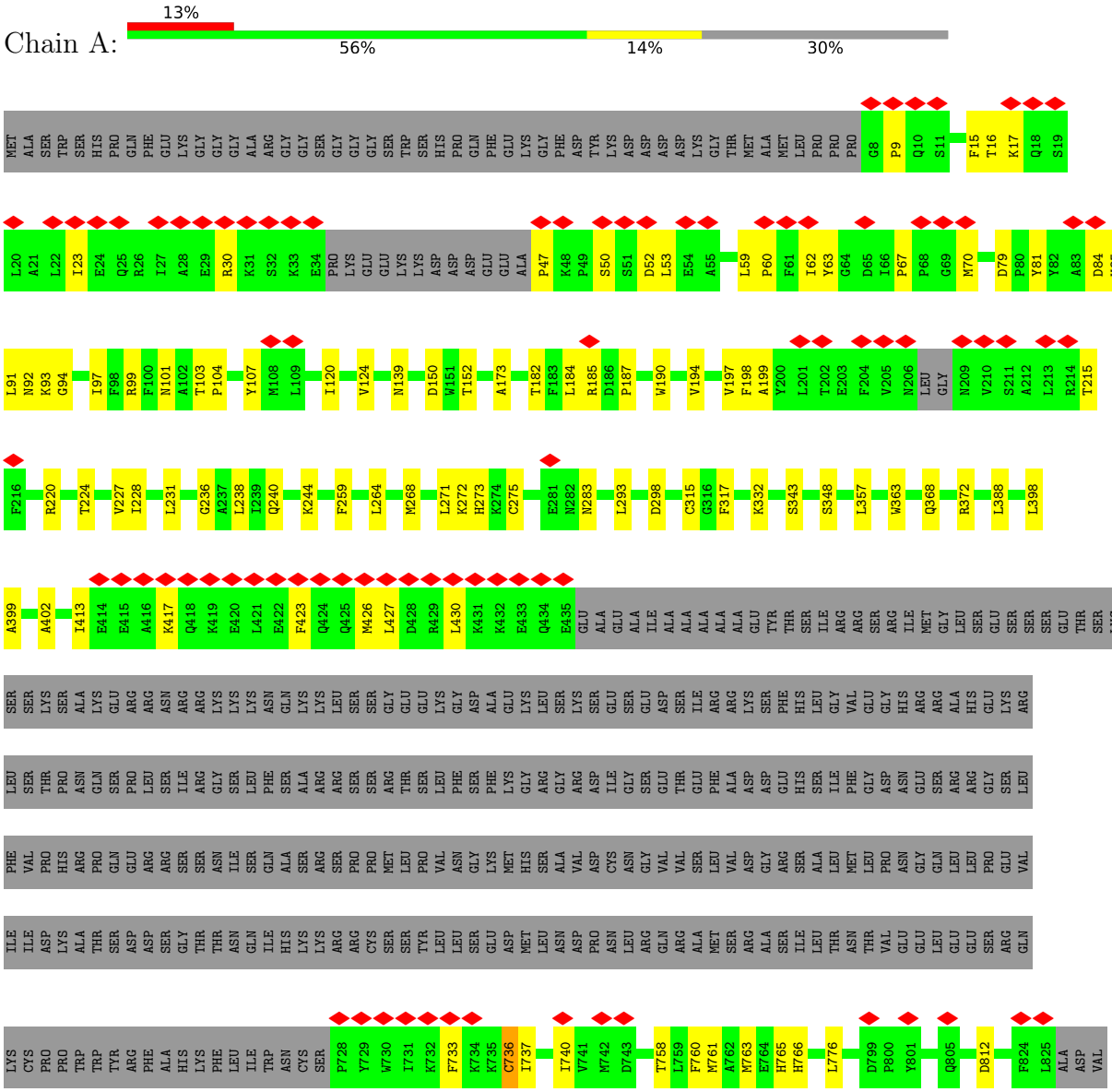
Mol	Chain	Residues	Atoms		AltConf
13	A	9	Total	O	0
			9	9	

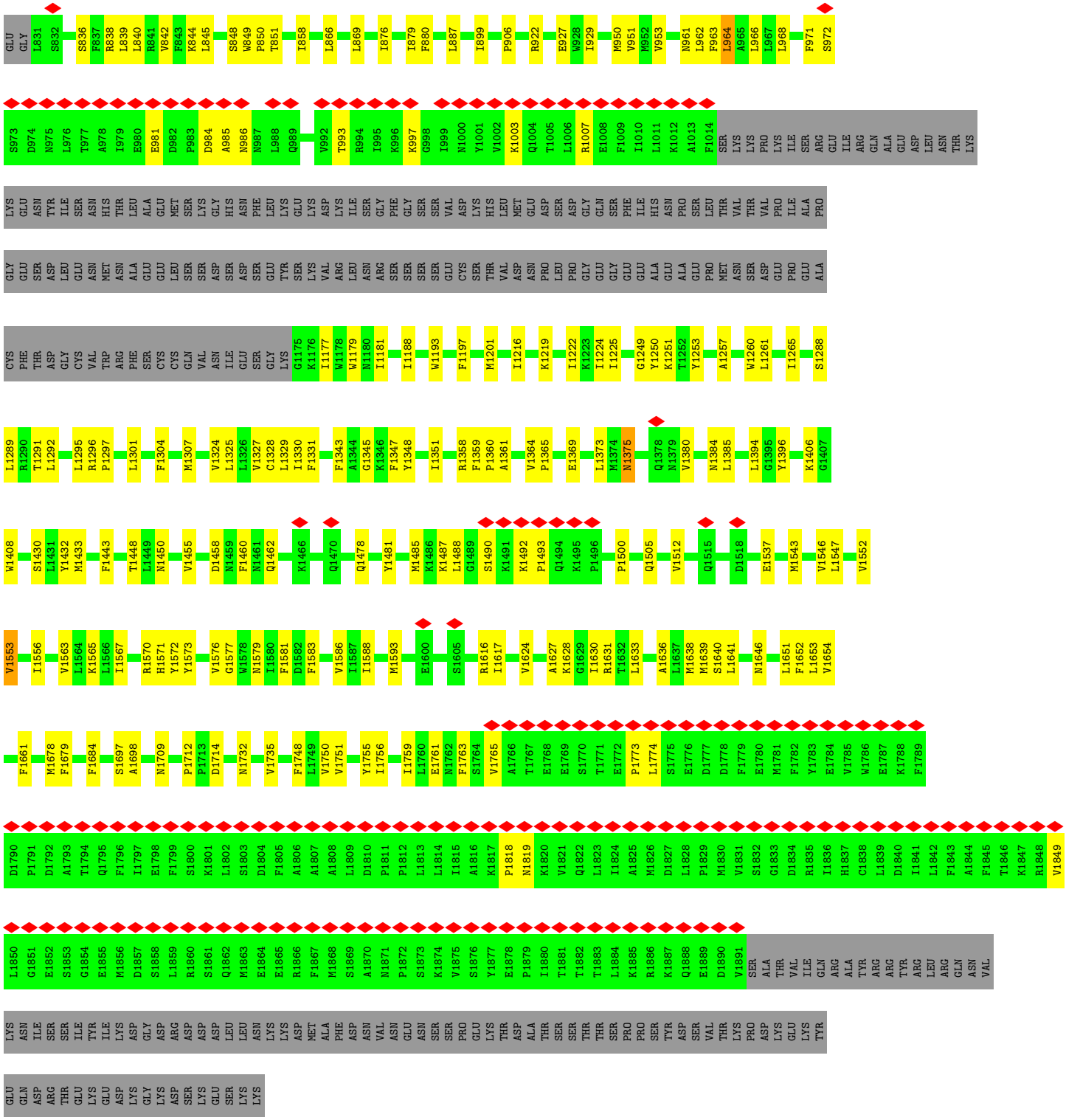
3 Residue-property plots (i)

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: Sodium channel protein type 9 subunit alpha

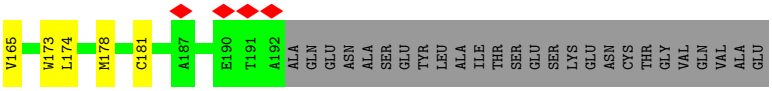
Chain A:





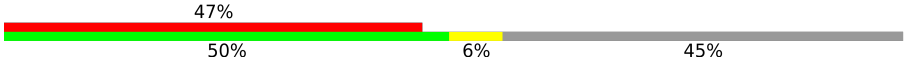
• Molecule 2: Sodium channel subunit beta-1

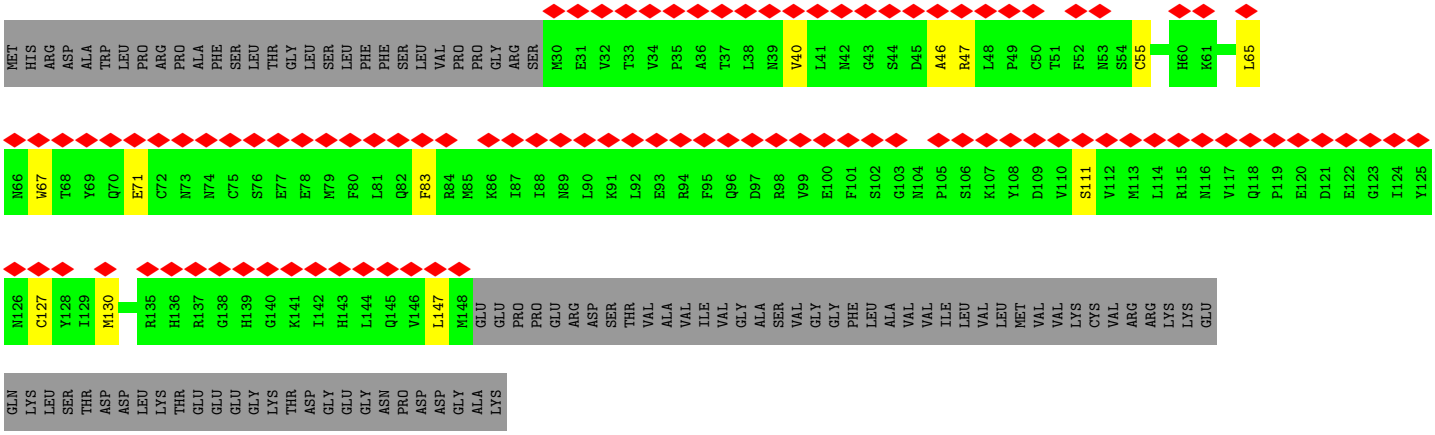
Chain B:



• Molecule 3: Sodium channel subunit beta-2

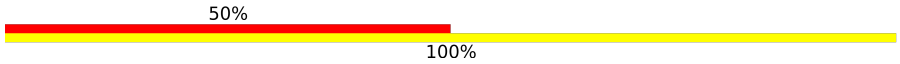
Chain C:





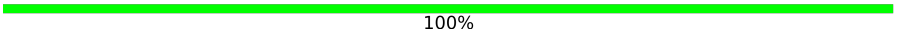
• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:



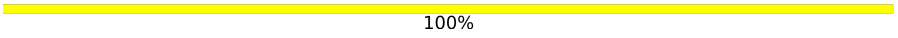
• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:



• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	785228	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.145	Depositor
Minimum map value	-0.060	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.022	Depositor
Map size (Å)	421.59363, 421.59363, 421.59363	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0979, 1.0979, 1.0979	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: P5S, NA, Y01, 1PW, 9Z9, PCW, NAG, LPE

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	0.85	0/11686	0.89	0/15823
2	B	1.03	0/1442	0.95	0/1949
3	C	0.35	0/1011	0.58	0/1367
All	All	0.85	0/14139	0.88	0/19139

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	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1712	PRO	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11412	0	11617	250	0
2	B	1416	0	1380	26	0
3	C	980	0	935	4	0
4	D	28	0	25	2	0
4	E	28	0	25	0	0
4	F	28	0	25	0	0
5	A	28	0	26	1	0
5	B	42	0	39	7	0
6	A	110	0	130	9	0
7	A	210	0	294	71	0
8	A	39	0	0	14	0
9	A	1	0	0	0	0
10	A	329	0	445	34	0
10	B	17	0	19	0	0
11	A	24	0	33	2	0
12	A	232	0	323	29	0
13	A	9	0	0	0	0
All	All	14933	0	15316	337	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 11.

All (337) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:ILE:HD11	1:A:99:ARG:NH1	1.60	1.16
2:B:112:THR:HG21	5:B:303:NAG:C8	1.84	1.06
1:A:1250:TYR:HB3	7:A:2004:Y01:HAU1	1.36	1.03
1:A:950:MET:HE3	7:A:2007:Y01:HAU2	1.40	1.02
1:A:1324:VAL:HG21	1:A:1455:VAL:HG21	1.47	0.96
1:A:1759:ILE:HG21	8:A:2006:9Z9:C09	1.99	0.93
2:B:112:THR:HG21	5:B:303:NAG:H81	1.49	0.93
1:A:964:LEU:HD11	8:A:2006:9Z9:C04	2.00	0.92
1:A:398:LEU:HD13	8:A:2006:9Z9:C75	2.02	0.89
1:A:182:THR:HG22	1:A:185:ARG:HD3	1.57	0.87
2:B:112:THR:HG21	5:B:303:NAG:H82	1.57	0.86
1:A:268:MET:HG2	1:A:1537:GLU:HG2	1.56	0.86
1:A:964:LEU:HD11	8:A:2006:9Z9:C05	2.08	0.84
12:A:2015:PCW:H372	7:A:2032:Y01:CAQ	2.10	0.81
12:A:2015:PCW:H372	7:A:2032:Y01:HAQ2	1.63	0.81
1:A:950:MET:CE	7:A:2007:Y01:HAU2	2.11	0.80
1:A:1224:ILE:HD11	2:B:155:ALA:HB1	1.62	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:51:ALA:HB2	2:B:127:LEU:HD13	1.64	0.78
1:A:858:ILE:HG21	1:A:1450:ASN:HD22	1.48	0.76
1:A:1759:ILE:HG13	8:A:2006:9Z9:C10	2.16	0.76
1:A:963:PHE:CE2	8:A:2006:9Z9:C81	2.69	0.75
2:B:85:ARG:O	2:B:115:HIS:HE1	1.71	0.74
2:B:125:ARG:HG2	2:B:127:LEU:CD2	2.18	0.74
12:A:2015:PCW:C37	7:A:2032:Y01:CAQ	2.66	0.73
1:A:849:TRP:HB2	7:A:2005:Y01:HAD3	1.71	0.73
12:A:2015:PCW:H81	7:A:2032:Y01:OAF	1.89	0.73
1:A:1460:PHE:CD2	1:A:1756:ILE:HG13	2.24	0.72
10:A:2033:LPE:H3N1	2:B:181:CYS:SG	2.30	0.72
1:A:60:PRO:HB2	1:A:62:ILE:HG12	1.70	0.71
2:B:112:THR:CG2	5:B:303:NAG:H82	2.20	0.71
1:A:101:ASN:ND2	1:A:103:THR:HB	2.06	0.70
1:A:1301:LEU:HD21	10:A:2016:LPE:H152	1.74	0.70
1:A:47:PRO:HB2	1:A:81:TYR:CE2	2.27	0.69
2:B:125:ARG:HG2	2:B:127:LEU:HD21	1.75	0.69
1:A:91:LEU:HD23	1:A:97:ILE:HA	1.74	0.69
1:A:426:MET:O	1:A:430:LEU:HG	1.91	0.69
1:A:1224:ILE:CD1	2:B:155:ALA:HB1	2.23	0.69
1:A:1250:TYR:CB	7:A:2004:Y01:HAU1	2.19	0.68
1:A:1328:CYS:HB3	12:A:2015:PCW:H281	1.75	0.68
1:A:1640:SER:HB3	1:A:1761:GLU:HG3	1.74	0.68
1:A:67:PRO:HB2	1:A:70:MET:HG3	1.75	0.67
1:A:1432:TYR:CD2	7:A:2009:Y01:HBF	2.29	0.67
1:A:59:LEU:HD22	1:A:91:LEU:HD13	1.76	0.67
2:B:57:TRP:HB2	2:B:71:LEU:HG	1.76	0.67
1:A:1627:ALA:HA	10:A:2026:LPE:H1N2	1.76	0.66
1:A:398:LEU:CD1	8:A:2006:9Z9:C75	2.73	0.66
1:A:30:ARG:NH2	1:A:84:ASP:OD2	2.29	0.65
1:A:89:ILE:HD11	1:A:99:ARG:HH11	1.59	0.65
1:A:1328:CYS:SG	1:A:1448:THR:HG23	2.37	0.65
1:A:1577:GLY:H	12:A:2020:PCW:H51	1.62	0.65
6:A:2019:P5S:H22	12:A:2020:PCW:H131	1.79	0.65
1:A:1330:ILE:HG13	7:A:2005:Y01:HAB2	1.77	0.65
1:A:963:PHE:CZ	8:A:2006:9Z9:C81	2.80	0.65
1:A:964:LEU:CD1	8:A:2006:9Z9:C05	2.74	0.64
1:A:413:ILE:HB	1:A:417:LYS:HE3	1.80	0.64
1:A:1478:GLN:HG2	10:A:2021:LPE:H311	1.79	0.64
12:A:2015:PCW:C8	7:A:2032:Y01:HAM2	2.28	0.63
1:A:1478:GLN:HE22	1:A:1646:ASN:HD21	1.47	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:271:LEU:HD12	1:A:343:SER:HA	1.81	0.62
1:A:1432:TYR:CE2	7:A:2009:Y01:HBF	2.34	0.62
1:A:1571:HIS:HB3	6:A:2031:P5S:N	2.15	0.62
1:A:139:ASN:HD21	1:A:220:ARG:HD3	1.64	0.62
12:A:2015:PCW:H371	7:A:2032:Y01:HAP1	1.81	0.61
1:A:139:ASN:ND2	1:A:220:ARG:HD3	2.16	0.61
7:A:2003:Y01:HAE2	7:A:2003:Y01:HAC1	1.83	0.60
1:A:1653:LEU:HD13	10:A:2025:LPE:H162	1.82	0.60
1:A:887:LEU:HD11	7:A:2007:Y01:HAT1	1.84	0.60
7:A:2004:Y01:HAC1	7:A:2004:Y01:HAE2	1.84	0.60
1:A:120:ILE:HD13	1:A:173:ALA:HB1	1.84	0.60
7:A:2005:Y01:HAE2	7:A:2005:Y01:HAC1	1.84	0.60
1:A:1295:LEU:HD21	10:A:2017:LPE:H192	1.83	0.60
1:A:9:PRO:HB3	1:A:63:TYR:O	2.00	0.60
1:A:950:MET:HE1	7:A:2007:Y01:CAS	2.32	0.60
7:A:2009:Y01:HAC1	7:A:2009:Y01:HAE2	1.84	0.60
7:A:2007:Y01:HAE2	7:A:2007:Y01:HAC1	1.84	0.59
1:A:50:SER:HB2	1:A:53:LEU:HB2	1.83	0.59
1:A:1661:PHE:CD2	10:A:2016:LPE:H3N3	2.36	0.59
1:A:1478:GLN:HE22	1:A:1646:ASN:ND2	2.00	0.59
1:A:1478:GLN:HG2	10:A:2021:LPE:C31	2.33	0.58
1:A:1331:PHE:CZ	1:A:1443:PHE:HB3	2.38	0.58
1:A:761:MET:SD	1:A:838:ARG:HD2	2.43	0.58
1:A:187:PRO:HA	1:A:190[B]:TRP:HD1	1.67	0.58
1:A:858:ILE:CG2	1:A:1450:ASN:HD22	2.15	0.58
10:A:2012:LPE:H21	12:A:2015:PCW:H131	1.84	0.58
10:A:2014:LPE:H112	7:A:2032:Y01:HAO1	1.84	0.58
1:A:963:PHE:CE2	8:A:2006:9Z9:C77	2.86	0.58
1:A:1325:LEU:HD13	11:A:2013:1PW:H16	1.85	0.58
1:A:47:PRO:HB2	1:A:81:TYR:CD2	2.39	0.57
2:B:112:THR:CB	5:B:303:NAG:H82	2.35	0.57
1:A:880:PHE:HE1	7:A:2007:Y01:HAC2	1.70	0.57
1:A:1249:GLY:HA2	6:A:2002:P5S:H48A	1.86	0.57
1:A:1636:ALA:HB2	1:A:1765:VAL:HG11	1.86	0.57
1:A:1641:LEU:HB3	10:A:2021:LPE:H11	1.85	0.56
1:A:293:LEU:HD22	1:A:298:ASP:HB3	1.86	0.56
1:A:1288:SER:O	1:A:1291:THR:HG22	2.05	0.56
1:A:1347:PHE:HB3	1:A:1385:LEU:HD13	1.87	0.56
1:A:1373:LEU:HG	1:A:1380:VAL:HG21	1.87	0.56
1:A:89:ILE:CD1	1:A:99:ARG:NH1	2.51	0.56
12:A:2015:PCW:H82	7:A:2032:Y01:HAM2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1329:LEU:HD23	12:A:2015:PCW:H271	1.87	0.56
1:A:1364:VAL:HG21	1:A:1373:LEU:HD22	1.88	0.56
6:A:2019:P5S:C35	6:A:2019:P5S:C46	2.83	0.56
1:A:1571:HIS:HB3	6:A:2031:P5S:HN	1.71	0.56
1:A:1458:ASP:O	1:A:1462:GLN:HG2	2.06	0.56
1:A:1460:PHE:CE2	1:A:1756:ILE:HG13	2.41	0.56
1:A:1570:ARG:HG3	6:A:2031:P5S:H1	1.88	0.56
1:A:89:ILE:HG12	1:A:99:ARG:HG3	1.86	0.55
1:A:1512:VAL:CG1	1:A:1565:LYS:HG2	2.36	0.55
1:A:357:LEU:HD23	1:A:363:TRP:HB2	1.88	0.55
1:A:1219:LYS:HE3	1:A:1222:ILE:HD11	1.89	0.55
1:A:851:THR:HG23	1:A:1327:VAL:HG21	1.89	0.55
1:A:1324:VAL:CG2	1:A:1455:VAL:HG21	2.30	0.55
1:A:1224:ILE:HD12	1:A:1225:ILE:N	2.21	0.54
2:B:33:GLY:O	5:B:302:NAG:H82	2.07	0.54
1:A:194:VAL:HA	1:A:197:VAL:HG22	1.89	0.54
1:A:224:THR:HA	1:A:227:VAL:HG22	1.90	0.54
1:A:1485:MET:HB3	1:A:1639:MET:HE3	1.88	0.54
1:A:91:LEU:CD2	1:A:97:ILE:HA	2.37	0.54
1:A:1460:PHE:HD2	1:A:1756:ILE:HG13	1.71	0.54
1:A:1552:VAL:HG22	1:A:1593:MET:SD	2.47	0.54
1:A:1553:VAL:HA	1:A:1556:ILE:HG13	1.88	0.54
1:A:1628:LYS:HG3	1:A:1631:ARG:HH12	1.73	0.54
1:A:92:ASN:HB2	1:A:124:VAL:HG22	1.89	0.53
1:A:836:SER:O	1:A:839:LEU:HB2	2.09	0.53
1:A:1485:MET:HB3	1:A:1639:MET:CE	2.39	0.53
1:A:1638:MET:HB2	6:A:2019:P5S:H44A	1.90	0.53
1:A:1748:PHE:HB2	11:A:2013:1PW:H30	1.90	0.53
1:A:812:ASP:HB2	1:A:844:LYS:NZ	2.23	0.53
1:A:1588:ILE:HD13	12:A:2020:PCW:H221	1.90	0.53
1:A:849:TRP:CZ3	7:A:2005:Y01:HAE3	2.43	0.53
1:A:966:LEU:HB3	1:A:1450:ASN:HD21	1.74	0.53
2:B:35:THR:HG22	2:B:109:THR:O	2.08	0.53
1:A:1396:TYR:OH	7:A:2032:Y01:HAA2	2.09	0.52
1:A:1500:PRO:HB2	1:A:1505:GLN:HB3	1.91	0.52
1:A:1627:ALA:HA	10:A:2026:LPE:C1N	2.39	0.52
12:A:2015:PCW:H371	7:A:2032:Y01:CAP	2.39	0.52
3:C:67:TRP:CZ2	3:C:127:CYS:HB3	2.45	0.52
1:A:182:THR:CG2	1:A:185:ARG:HD3	2.35	0.52
1:A:1331:PHE:HZ	1:A:1443:PHE:HB3	1.75	0.52
1:A:1661:PHE:CZ	10:A:2016:LPE:H3N1	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:47:ARG:NH2	3:C:111[B]:SER:OG	2.43	0.52
1:A:1406:LYS:HD2	1:A:1698:ALA:HA	1.92	0.52
1:A:1348:TYR:CE1	1:A:1384:ASN:HB2	2.45	0.51
12:A:2015:PCW:H61	7:A:2032:Y01:CAX	2.39	0.51
1:A:848:SER:HB3	1:A:986:ASN:HD21	1.74	0.51
1:A:1188:ILE:HG13	10:A:2033:LPE:H3N3	1.91	0.51
1:A:1257:ALA:HB1	10:A:2017:LPE:H31	1.92	0.51
12:A:2015:PCW:H371	7:A:2032:Y01:CAQ	2.39	0.51
1:A:1351:ILE:HG22	1:A:1358:ARG:HA	1.93	0.51
1:A:899:ILE:HD12	1:A:906:PRO:HG3	1.93	0.50
7:A:2007:Y01:HAE2	7:A:2007:Y01:CAC	2.41	0.50
4:D:1:NAG:C3	4:D:2:NAG:O7	2.59	0.50
1:A:950:MET:CE	7:A:2007:Y01:CAU	2.87	0.50
10:A:2033:LPE:H21	2:B:173:TRP:CZ3	2.47	0.50
12:A:2015:PCW:C37	7:A:2032:Y01:CAP	2.90	0.50
1:A:1481:TYR:CE1	10:A:2021:LPE:H1N3	2.46	0.50
1:A:981:GLU:OE2	7:A:2005:Y01:OAF	2.30	0.50
1:A:1406:LYS:HD2	1:A:1697:SER:O	2.12	0.50
1:A:848:SER:CB	1:A:986:ASN:HD21	2.25	0.50
7:A:2003:Y01:HAE2	7:A:2003:Y01:CAC	2.41	0.50
7:A:2005:Y01:HAE2	7:A:2005:Y01:CAC	2.41	0.50
2:B:125:ARG:CG	2:B:127:LEU:CD2	2.89	0.50
1:A:59:LEU:HD22	1:A:91:LEU:CD1	2.41	0.50
1:A:1478:GLN:NE2	1:A:1646:ASN:HD21	2.10	0.50
1:A:1512:VAL:HG13	1:A:1565:LYS:HG2	1.95	0.49
1:A:971:PHE:HD1	1:A:972:SER:HB2	1.78	0.49
1:A:858:ILE:HG21	1:A:1450:ASN:ND2	2.24	0.49
1:A:1177:ILE:O	1:A:1181:ILE:HG12	2.13	0.49
1:A:228:ILE:HB	1:A:231:LEU:HD22	1.93	0.49
1:A:92:ASN:C	1:A:94:GLY:H	2.15	0.49
1:A:150:ASP:C	1:A:152:THR:H	2.16	0.49
1:A:1325:LEU:O	1:A:1329:LEU:HG	2.13	0.49
1:A:1301:LEU:HA	1:A:1307:MET:HE3	1.95	0.49
10:A:2014:LPE:H3N2	7:A:2032:Y01:HAV1	1.93	0.49
1:A:849:TRP:CZ2	1:A:1327:VAL:HG23	2.48	0.49
1:A:1343:PHE:HB3	1:A:1347:PHE:CE1	2.48	0.49
1:A:268:MET:CG	1:A:1537:GLU:HG2	2.33	0.48
1:A:950:MET:HE1	7:A:2007:Y01:HAS2	1.94	0.48
1:A:968:LEU:HD21	8:A:2006:9Z9:C14	2.43	0.48
1:A:1654:VAL:HG22	10:A:2016:LPE:H141	1.94	0.48
1:A:275:CYS:SG	1:A:315:CYS:HB3	2.52	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:368:GLN:HG2	1:A:1679:PHE:CZ	2.48	0.48
1:A:876:ILE:O	1:A:879:ILE:HG13	2.13	0.48
1:A:60:PRO:CB	1:A:62:ILE:HG12	2.42	0.48
7:A:2005:Y01:HAV2	7:A:2005:Y01:OAG	2.14	0.48
1:A:273:HIS:CE1	1:A:317:PHE:HE2	2.32	0.48
7:A:2009:Y01:OAG	7:A:2009:Y01:HAV2	2.14	0.48
12:A:2015:PCW:H61	7:A:2032:Y01:OAF	2.14	0.48
2:B:34:MET:O	2:B:111:VAL:HG23	2.14	0.48
1:A:845:LEU:HD11	7:A:2005:Y01:HAA1	1.94	0.48
7:A:2007:Y01:HAU2	7:A:2007:Y01:HAC1	1.96	0.48
1:A:120:ILE:CD1	1:A:173:ALA:HB1	2.43	0.48
7:A:2005:Y01:HAC1	7:A:2005:Y01:HAU2	1.96	0.47
7:A:2009:Y01:HAC1	7:A:2009:Y01:HAU2	1.96	0.47
1:A:1375:ASN:HD22	1:A:1375:ASN:HA	1.52	0.47
1:A:240:GLN:O	1:A:244:LYS:HD2	2.14	0.47
1:A:851:THR:HG23	1:A:1327:VAL:CG2	2.45	0.47
7:A:2004:Y01:HAC1	7:A:2004:Y01:HAU2	1.96	0.47
1:A:1485:MET:SD	1:A:1639:MET:HE1	2.55	0.47
1:A:984:ASP:O	1:A:985:ALA:C	2.53	0.47
7:A:2003:Y01:HAC1	7:A:2003:Y01:HAU2	1.96	0.47
1:A:273:HIS:CE1	1:A:332:LYS:HB2	2.50	0.46
1:A:89:ILE:HD11	1:A:99:ARG:HH12	1.66	0.46
1:A:961:ASN:HD22	1:A:961:ASN:N	2.13	0.46
1:A:950:MET:HE3	7:A:2007:Y01:CAU	2.28	0.46
1:A:1358:ARG:HG2	1:A:1359:PHE:O	2.16	0.46
4:D:1:NAG:H3	4:D:2:NAG:O7	2.14	0.46
1:A:737:ILE:HD13	1:A:740:ILE:HD12	1.97	0.46
1:A:1732:ASN:HD22	1:A:1735:VAL:HG23	1.80	0.46
7:A:2004:Y01:HAE2	7:A:2004:Y01:CAC	2.41	0.46
7:A:2009:Y01:HAE2	7:A:2009:Y01:CAC	2.41	0.46
12:A:2029:PCW:H341	12:A:2029:PCW:H371	1.56	0.46
1:A:92:ASN:HB2	1:A:124:VAL:CG2	2.46	0.46
1:A:423:PHE:O	1:A:427:LEU:HG	2.15	0.46
10:A:2023:LPE:H3N2	10:A:2024:LPE:H31	1.97	0.46
1:A:758:THR:HG21	7:A:2005:Y01:HBA	1.98	0.46
1:A:1003:LYS:HE2	1:A:1007:ARG:HH21	1.80	0.46
12:A:2015:PCW:C37	7:A:2032:Y01:HAQ1	2.43	0.46
1:A:849:TRP:HB2	7:A:2005:Y01:CAD	2.43	0.45
1:A:1651:LEU:HD13	1:A:1750:VAL:HG21	1.98	0.45
12:A:2020:PCW:H31	12:A:2029:PCW:H31	1.98	0.45
1:A:101:ASN:HD21	1:A:103:THR:HB	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:2032:Y01:HBB	7:A:2032:Y01:HAE2	1.60	0.45
2:B:71:LEU:HB3	2:B:80:LEU:HD12	1.97	0.45
1:A:1365:PRO:HD2	1:A:1369:GLU:HG3	1.99	0.45
1:A:858:ILE:CG2	1:A:1450:ASN:ND2	2.80	0.45
1:A:1653:LEU:HD22	10:A:2025:LPE:H182	1.99	0.45
10:A:2028:LPE:H3N2	10:A:2028:LPE:H312	1.72	0.45
1:A:348:SER:HB2	12:A:2018:PCW:H332	1.99	0.45
1:A:1301:LEU:HD21	10:A:2016:LPE:C15	2.44	0.45
2:B:125:ARG:CG	2:B:127:LEU:HD22	2.47	0.45
1:A:1430:SER:HB3	1:A:1433:MET:HG2	1.98	0.44
1:A:842:VAL:HG13	7:A:2005:Y01:HAA2	1.99	0.44
1:A:866:LEU:HD12	1:A:966:LEU:HD23	1.99	0.44
1:A:104:PRO:HB2	1:A:107:TYR:HA	1.98	0.44
1:A:736:CYS:O	1:A:740:ILE:HG13	2.17	0.44
1:A:1197:PHE:O	1:A:1201:MET:HG2	2.17	0.44
2:B:162:MET:HA	2:B:165:VAL:HG22	1.99	0.44
1:A:760:PHE:CE2	1:A:776:LEU:HA	2.52	0.44
1:A:849:TRP:CE3	7:A:2005:Y01:HAE3	2.53	0.44
1:A:187:PRO:HA	1:A:190[B]:TRP:CD1	2.51	0.44
1:A:272:LYS:HB2	1:A:332:LYS:HG3	2.00	0.44
1:A:1361:ALA:O	1:A:1365:PRO:HB3	2.17	0.44
7:A:2007:Y01:HAS2	7:A:2007:Y01:HAE1	1.81	0.44
1:A:1219:LYS:HB3	1:A:1222:ILE:HG13	1.99	0.44
1:A:1261:LEU:O	1:A:1265:ILE:HG13	2.18	0.44
1:A:1543:MET:HA	1:A:1546:VAL:HG22	2.00	0.44
1:A:1624:VAL:HG13	1:A:1630:ILE:HD12	2.00	0.44
10:A:2021:LPE:H311	10:A:2021:LPE:H2N3	1.61	0.44
1:A:850:PRO:HD3	7:A:2005:Y01:HAV1	1.99	0.44
7:A:2005:Y01:HAN2	7:A:2005:Y01:HAC3	2.00	0.44
1:A:1250:TYR:OH	10:A:2027:LPE:H172	2.18	0.44
1:A:1251:LYS:C	1:A:1253:TYR:H	2.22	0.44
1:A:1260:TRP:CE3	7:A:2003:Y01:CAE	3.01	0.43
1:A:1774:LEU:HD21	1:A:1849:VAL:HG11	2.00	0.43
2:B:112:THR:H	2:B:115:HIS:CD2	2.36	0.43
1:A:1583:PHE:HA	1:A:1586:VAL:HG22	2.00	0.43
1:A:1394:LEU:HG	12:A:2015:PCW:H121	2.00	0.43
2:B:44:LYS:HG2	2:B:102:GLN:OE1	2.18	0.43
1:A:89:ILE:CG1	1:A:99:ARG:HG3	2.48	0.43
1:A:981:GLU:CG	7:A:2005:Y01:OAF	2.65	0.43
1:A:1652:PHE:HE1	10:A:2023:LPE:H141	1.84	0.43
1:A:733:PHE:O	1:A:737:ILE:HG12	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:880:PHE:CG	1:A:951:VAL:HG22	2.54	0.43
12:A:2020:PCW:H73	12:A:2020:PCW:H41	1.57	0.43
1:A:259:PHE:HZ	1:A:388:LEU:HD12	1.84	0.42
1:A:1296:ARG:HG2	1:A:1297:PRO:HD3	2.01	0.42
7:A:2032:Y01:HAS2	7:A:2032:Y01:HAE1	1.81	0.42
1:A:372:ARG:HA	1:A:1678:MET:SD	2.59	0.42
2:B:112:THR:HB	5:B:303:NAG:H82	2.01	0.42
1:A:1641:LEU:HD23	10:A:2021:LPE:H12	2.01	0.42
12:A:2015:PCW:H81	7:A:2032:Y01:HAM2	2.01	0.42
1:A:91:LEU:HD21	1:A:97:ILE:HG12	2.01	0.42
1:A:1563:VAL:O	1:A:1567:ILE:HG13	2.19	0.42
1:A:1571:HIS:C	1:A:1573:TYR:N	2.73	0.42
1:A:1577:GLY:N	12:A:2020:PCW:H51	2.32	0.42
1:A:1304:PHE:HB2	1:A:1307:MET:HE2	2.01	0.42
1:A:50:SER:N	1:A:79:ASP:OD2	2.48	0.42
1:A:198:PHE:HD1	1:A:198:PHE:HA	1.77	0.42
1:A:985:ALA:O	1:A:986:ASN:C	2.57	0.42
1:A:1488:LEU:O	1:A:1490:SER:N	2.52	0.42
7:A:2009:Y01:HAS2	7:A:2009:Y01:HAE1	1.81	0.42
1:A:236:GLY:O	1:A:240:GLN:HG2	2.19	0.42
1:A:922:ARG:HG2	1:A:927:GLU:HB2	2.02	0.42
6:A:2002:P5S:H56A	6:A:2002:P5S:H53	1.86	0.42
7:A:2009:Y01:HAN2	7:A:2009:Y01:HAC3	2.00	0.42
1:A:16:THR:O	1:A:17:LYS:C	2.57	0.42
1:A:1751:VAL:O	1:A:1755:TYR:HD1	2.01	0.42
3:C:65:LEU:HB3	3:C:83:PHE:HB3	2.02	0.42
1:A:766:HIS:CD2	1:A:1345:GLY:HA3	2.54	0.42
1:A:215:THR:HB	7:A:2007:Y01:HAK2	2.02	0.41
1:A:283:ASN:HB2	5:A:2001:NAG:H2	2.02	0.41
1:A:981:GLU:HG3	7:A:2005:Y01:OAF	2.19	0.41
1:A:1289:LEU:O	1:A:1292:LEU:HB2	2.20	0.41
1:A:264:LEU:O	1:A:268:MET:HB2	2.20	0.41
1:A:332:LYS:HB3	1:A:332:LYS:HE3	1.92	0.41
1:A:1570:ARG:HB3	1:A:1571:HIS:H	1.56	0.41
2:B:174:LEU:O	2:B:178:MET:HG3	2.20	0.41
3:C:40:VAL:HG11	3:C:46:ALA:HB2	2.03	0.41
1:A:23:ILE:HG23	1:A:84:ASP:O	2.20	0.41
1:A:763:MET:O	1:A:765:HIS:HD2	2.03	0.41
1:A:968:LEU:HD21	8:A:2006:9Z9:C15	2.49	0.41
1:A:1759:ILE:HG23	1:A:1763:PHE:CE1	2.55	0.41
1:A:1216:ILE:HA	1:A:1219:LYS:HE2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:A:2029:PCW:H63	12:A:2029:PCW:H42	1.59	0.41
1:A:238:LEU:HD23	1:A:961:ASN:OD1	2.20	0.41
1:A:963:PHE:CD2	8:A:2006:9Z9:C81	3.03	0.41
1:A:993:THR:HG22	1:A:997:LYS:HE3	2.02	0.41
7:A:2005:Y01:HAS2	7:A:2005:Y01:HAE1	1.81	0.41
1:A:1684:PHE:HD2	10:A:2024:LPE:H141	1.85	0.41
10:A:2017:LPE:H311	10:A:2017:LPE:H2N2	1.87	0.41
10:A:2022:LPE:H112	10:A:2022:LPE:H142	1.98	0.41
7:A:2032:Y01:HAP1	7:A:2032:Y01:HAO2	1.36	0.41
1:A:402:ALA:HB1	8:A:2006:9Z9:C15	2.51	0.41
1:A:869:LEU:HD22	1:A:962:LEU:HD13	2.03	0.41
1:A:1481:TYR:CD1	10:A:2021:LPE:H1N3	2.56	0.41
7:A:2004:Y01:HAS2	7:A:2004:Y01:HAE1	1.81	0.41
1:A:184:LEU:HD23	1:A:184:LEU:HA	1.59	0.41
1:A:1325:LEU:HD11	12:A:2015:PCW:C47	2.51	0.41
1:A:1432:TYR:CE2	7:A:2009:Y01:HAT1	2.57	0.41
1:A:1576:VAL:HB	1:A:1579:ASN:HB2	2.03	0.41
1:A:1487:LYS:O	1:A:1488:LEU:C	2.58	0.40
1:A:1709:ASN:ND2	1:A:1714:ASP:HB3	2.36	0.40
10:A:2027:LPE:H312	10:A:2027:LPE:H2N2	1.81	0.40
1:A:1617:ILE:HB	12:A:2020:PCW:H261	2.03	0.40
10:A:2023:LPE:H311	10:A:2023:LPE:H2N3	1.78	0.40
1:A:85:LYS:HE2	1:A:85:LYS:HB2	1.87	0.40
1:A:399:ALA:HB2	1:A:1759:ILE:HD12	2.04	0.40
2:B:37:LYS:HE3	2:B:93:ASN:HB3	2.03	0.40
1:A:845:LEU:CD1	7:A:2005:Y01:HAA1	2.51	0.40
1:A:1251:LYS:C	1:A:1253:TYR:N	2.74	0.40
1:A:1488:LEU:C	1:A:1490:SER:H	2.25	0.40
1:A:1492:LYS:HD3	1:A:1493:PRO:HD2	2.03	0.40
1:A:1512:VAL:HG11	1:A:1565:LYS:HG2	2.03	0.40
1:A:1581:PHE:CD1	6:A:2019:P5S:H24A	2.56	0.40
1:A:388:LEU:HD23	1:A:388:LEU:HA	1.86	0.40
1:A:1179:TRP:HZ3	10:A:2027:LPE:O31	2.04	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	1402/2031 (69%)	1318 (94%)	75 (5%)	9 (1%)	25 26
2	B	171/218 (78%)	167 (98%)	3 (2%)	1 (1%)	25 26
3	C	120/215 (56%)	117 (98%)	3 (2%)	0	100 100
All	All	1693/2464 (69%)	1602 (95%)	81 (5%)	10 (1%)	29 26

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1773	PRO
2	B	150	ALA
1	A	15	PHE
1	A	93	LYS
1	A	953	VAL
1	A	1572	TYR
1	A	52	ASP
1	A	199	ALA
1	A	1360	PRO
1	A	1818	PRO

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	1265/1809 (70%)	1253 (99%)	12 (1%)	78 88
2	B	157/190 (83%)	156 (99%)	1 (1%)	86 93

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	C	114/193 (59%)	110 (96%)	4 (4%)	36 46
All	All	1536/2192 (70%)	1519 (99%)	17 (1%)	74 85

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	736	CYS
1	A	840	LEU
1	A	929	ILE
1	A	964	LEU
1	A	1193	TRP
1	A	1375	ASN
1	A	1408	TRP
1	A	1547	LEU
1	A	1553	VAL
1	A	1616	ARG
1	A	1633	LEU
1	A	1819	ASN
2	B	93	ASN
3	C	55	CYS
3	C	71	GLU
3	C	130	MET
3	C	147	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	101	ASN
1	A	139	ASN
1	A	278	ASN
1	A	336	ASN
1	A	410	GLN
1	A	766	HIS
1	A	774	ASN
1	A	886	GLN
1	A	909	HIS
1	A	961	ASN
1	A	986	ASN
1	A	1276	ASN
1	A	1323	ASN
1	A	1341	ASN

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Mol	Chain	Res	Type
1	A	1378	GLN
1	A	1384	ASN
1	A	1450	ASN
1	A	1461	ASN
1	A	1462	GLN
1	A	1478	GLN
1	A	1494	GLN
1	A	1665	ASN
1	A	1709	ASN
1	A	1721	HIS
1	A	1732	ASN
2	B	115	HIS
2	B	143	HIS
3	C	53	ASN
3	C	82	GLN
3	C	118	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

6 monosaccharides 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	$\#\|Z\| > 2$
4	NAG	D	1	1,4	14,14,15	0.35	0	17,19,21	0.55	0
4	NAG	D	2	4	14,14,15	0.28	0	17,19,21	0.76	0
4	NAG	E	1	1,4	14,14,15	0.19	0	17,19,21	0.45	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	NAG	E	2	4	14,14,15	0.45	0	17,19,21	0.66	0
4	NAG	F	1	2,4	14,14,15	0.57	0	17,19,21	1.19	2 (11%)
4	NAG	F	2	4	14,14,15	0.65	0	17,19,21	1.20	1 (5%)

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
4	NAG	D	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	D	2	4	-	2/6/23/26	0/1/1/1
4	NAG	E	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	E	2	4	-	2/6/23/26	0/1/1/1
4	NAG	F	1	2,4	-	2/6/23/26	0/1/1/1
4	NAG	F	2	4	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	F	1	NAG	C1-O5-C5	2.75	115.92	112.19
4	F	1	NAG	C3-C4-C5	-2.64	105.52	110.24
4	F	2	NAG	C4-C3-C2	-2.40	107.50	111.02

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	2	NAG	C8-C7-N2-C2
4	D	2	NAG	O7-C7-N2-C2
4	E	1	NAG	O5-C5-C6-O6
4	F	2	NAG	C4-C5-C6-O6
4	F	2	NAG	O5-C5-C6-O6
4	E	1	NAG	C4-C5-C6-O6
4	E	2	NAG	C4-C5-C6-O6
4	F	1	NAG	C4-C5-C6-O6
4	E	2	NAG	O5-C5-C6-O6
4	F	1	NAG	O5-C5-C6-O6

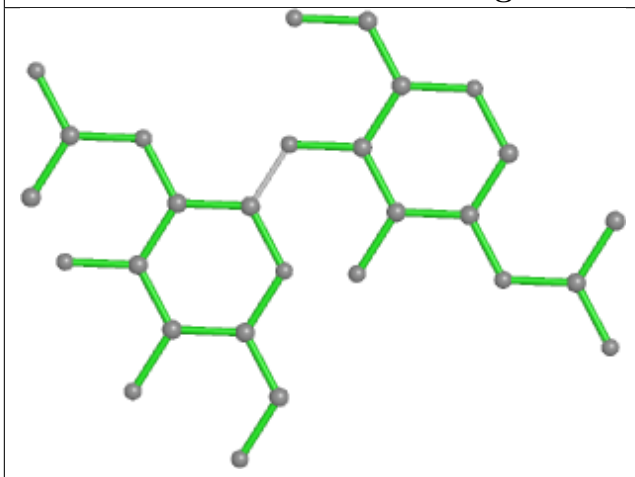
There are no ring outliers.

2 monomers are involved in 2 short contacts:

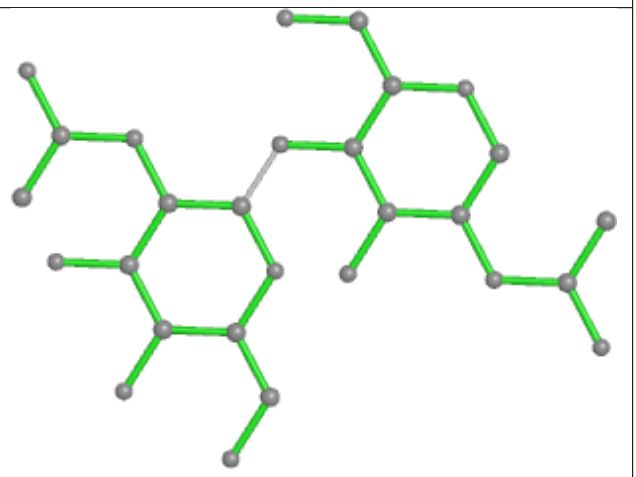
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	2	NAG	2	0
4	D	1	NAG	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

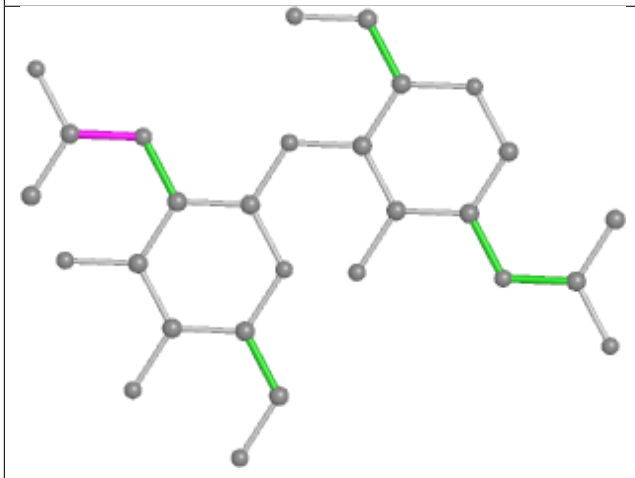
Oligosaccharide Chain D



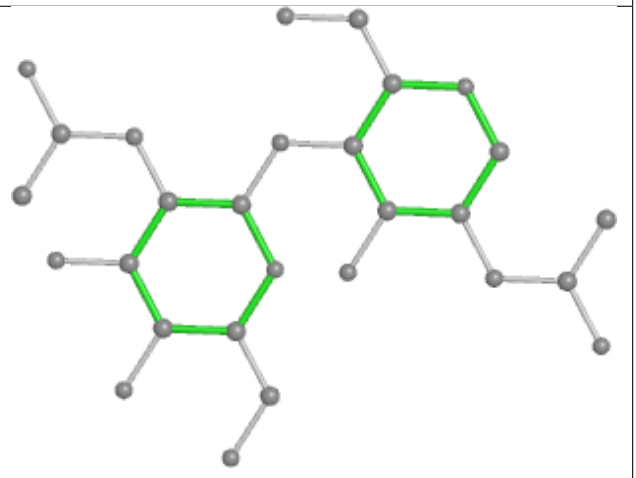
Bond lengths



Bond angles

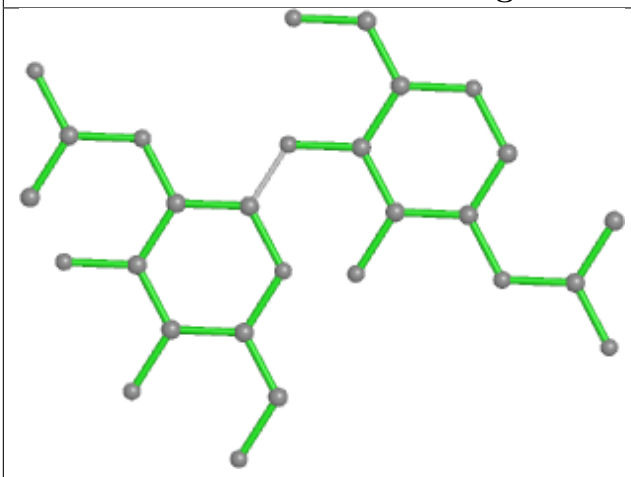


Torsions

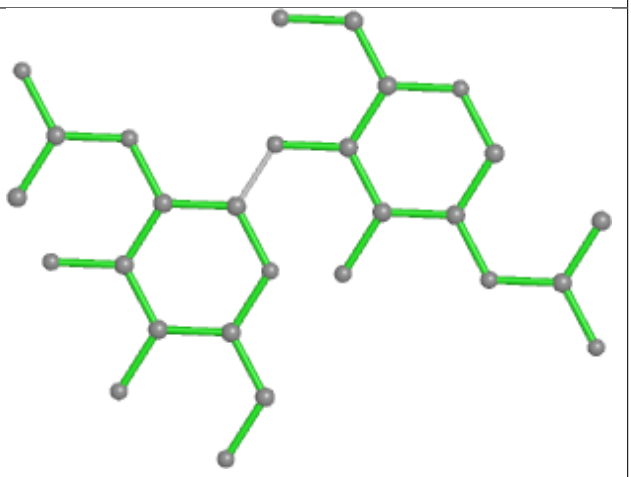


Rings

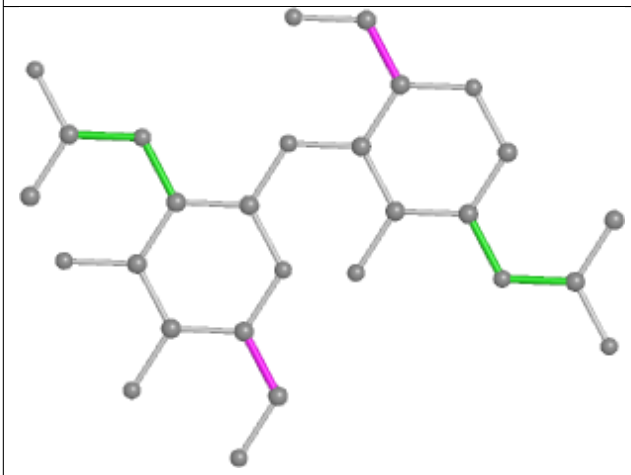
Oligosaccharide Chain E



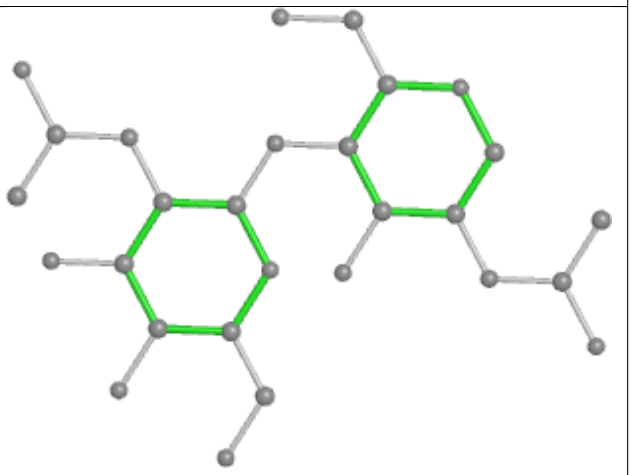
Bond lengths



Bond angles

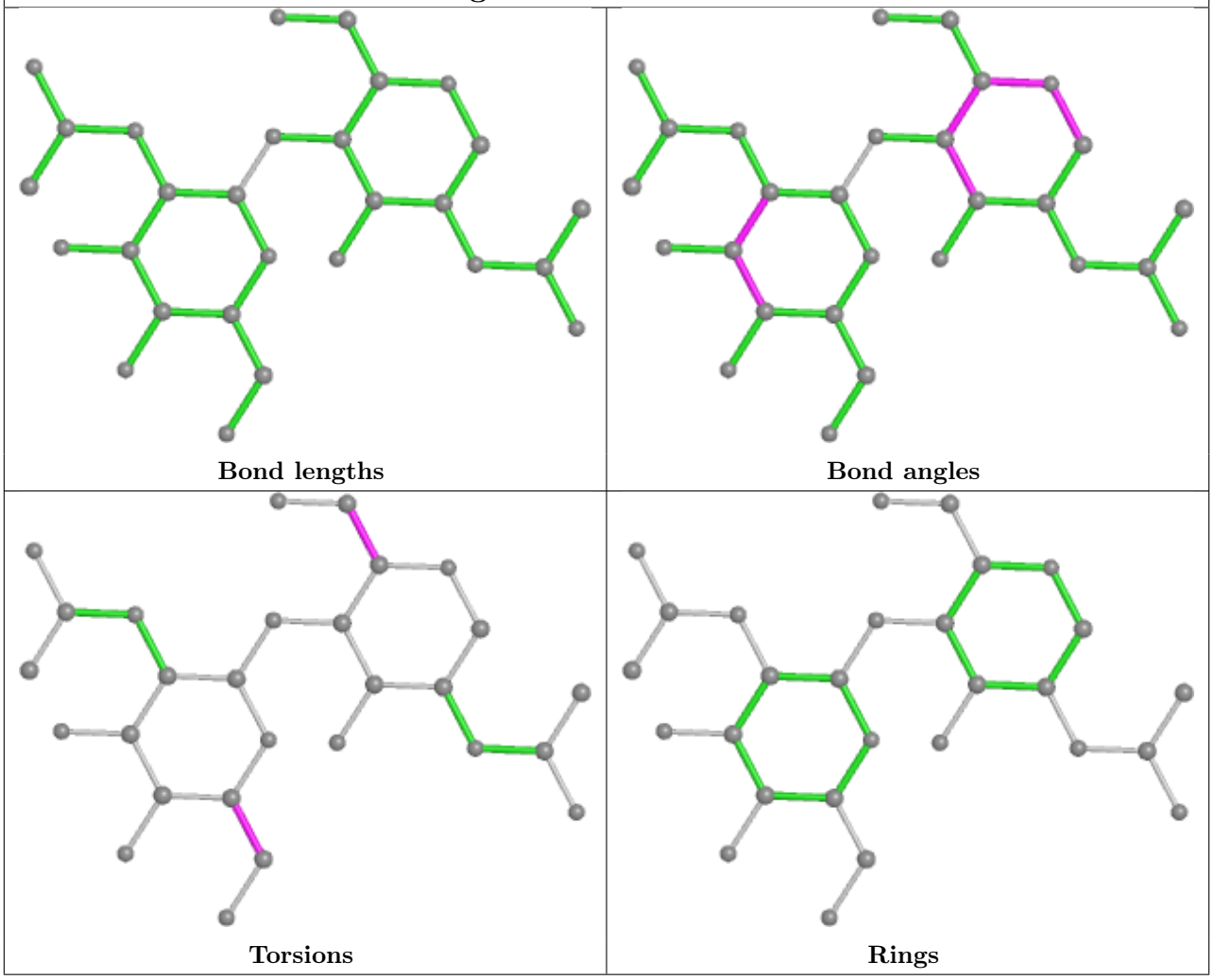


Torsions



Rings

Oligosaccharide Chain F



5.6 Ligand geometry (i)

Of 37 ligands modelled in this entry, 1 is monoatomic - leaving 36 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
7	Y01	A	2032	-	38,38,38	1.62	7 (18%)	57,57,57	1.63	9 (15%)
5	NAG	A	2008	1	14,14,15	0.38	0	17,19,21	0.90	1 (5%)
5	NAG	B	301	2	14,14,15	0.64	0	17,19,21	0.98	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
10	LPE	A	2017	-	27,27,33	0.54	0	31,33,39	0.61	0
10	LPE	A	2016	-	21,21,33	0.68	0	25,27,39	1.03	2 (8%)
5	NAG	A	2001	1	14,14,15	0.35	0	17,19,21	0.44	0
7	Y01	A	2007	-	38,38,38	0.66	1 (2%)	57,57,57	1.78	10 (17%)
6	P5S	A	2031	-	32,33,53	1.17	4 (12%)	36,40,60	1.04	3 (8%)
10	LPE	A	2025	-	24,24,33	0.53	0	28,30,39	0.53	0
5	NAG	B	302	2	14,14,15	0.18	0	17,19,21	0.41	0
6	P5S	A	2002	-	33,34,53	0.76	1 (3%)	36,40,60	1.81	5 (13%)
10	LPE	A	2021	-	24,24,33	0.60	0	28,30,39	0.89	1 (3%)
10	LPE	A	2024	-	24,24,33	0.53	0	28,30,39	0.63	0
10	LPE	A	2033	-	16,16,33	0.67	0	20,22,39	0.67	0
10	LPE	A	2023	-	24,24,33	0.54	0	28,30,39	0.68	1 (3%)
10	LPE	A	2014	-	19,19,33	0.62	0	23,25,39	0.51	0
12	PCW	A	2020	-	43,43,53	1.01	2 (4%)	49,51,61	1.12	5 (10%)
10	LPE	A	2022	-	24,24,33	0.85	0	28,30,39	0.92	1 (3%)
10	LPE	A	2011	-	24,24,33	0.51	0	28,30,39	0.60	0
7	Y01	A	2005	-	38,38,38	1.15	4 (10%)	57,57,57	1.74	12 (21%)
7	Y01	A	2003	-	38,38,38	0.66	1 (2%)	57,57,57	1.79	11 (19%)
12	PCW	A	2029	-	43,43,53	1.03	2 (4%)	49,51,61	0.94	2 (4%)
12	PCW	A	2018	-	46,46,53	0.99	3 (6%)	52,54,61	1.18	4 (7%)
12	PCW	A	2030	-	43,43,53	1.03	2 (4%)	49,51,61	1.00	2 (4%)
8	9Z9	A	2006	-	44,44,44	0.70	1 (2%)	66,68,68	1.45	12 (18%)
10	LPE	A	2026	-	24,24,33	0.51	0	28,30,39	0.62	0
10	LPE	A	2028	-	16,16,33	0.69	0	20,22,39	0.67	0
11	1PW	A	2013	-	23,23,27	0.44	0	24,26,32	0.61	0
10	LPE	B	304	-	16,16,33	0.67	0	20,22,39	0.60	0
10	LPE	A	2027	-	24,24,33	0.54	0	28,30,39	0.50	0
12	PCW	A	2015	-	52,52,53	0.93	2 (3%)	58,60,61	0.97	2 (3%)
5	NAG	B	303	2	14,14,15	0.25	0	17,19,21	0.42	0
6	P5S	A	2019	-	40,40,53	1.13	3 (7%)	43,45,60	1.37	3 (6%)
7	Y01	A	2004	-	38,38,38	0.65	1 (2%)	57,57,57	1.79	11 (19%)
10	LPE	A	2012	-	24,24,33	0.33	0	25,27,39	0.60	0
7	Y01	A	2009	-	38,38,38	1.15	4 (10%)	57,57,57	1.74	11 (19%)

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
7	Y01	A	2032	-	-	7/19/77/77	0/4/4/4
5	NAG	A	2008	1	-	2/6/23/26	0/1/1/1
5	NAG	B	301	2	-	0/6/23/26	0/1/1/1
10	LPE	A	2017	-	-	10/28/28/34	-
10	LPE	A	2016	-	-	15/22/22/34	-
5	NAG	A	2001	1	-	2/6/23/26	0/1/1/1
7	Y01	A	2007	-	-	0/19/77/77	0/4/4/4
6	P5S	A	2031	-	-	16/39/39/59	-
10	LPE	A	2025	-	-	8/25/25/34	-
5	NAG	B	302	2	-	0/6/23/26	0/1/1/1
6	P5S	A	2002	-	-	28/39/39/59	-
10	LPE	A	2021	-	-	7/25/25/34	-
10	LPE	A	2024	-	-	3/25/25/34	-
10	LPE	A	2033	-	-	8/17/17/34	-
10	LPE	A	2023	-	-	3/25/25/34	-
10	LPE	A	2014	-	-	10/20/20/34	-
12	PCW	A	2020	-	-	12/47/47/57	-
10	LPE	A	2022	-	-	12/25/25/34	-
10	LPE	A	2011	-	-	10/25/25/34	-
7	Y01	A	2005	-	-	4/19/77/77	0/4/4/4
7	Y01	A	2003	-	-	0/19/77/77	0/4/4/4
12	PCW	A	2029	-	-	16/47/47/57	-
12	PCW	A	2018	-	-	13/50/50/57	-
12	PCW	A	2030	-	-	11/47/47/57	-
8	9Z9	A	2006	-	-	0/12/100/100	0/6/6/6
10	LPE	A	2026	-	-	6/25/25/34	-
10	LPE	A	2028	-	-	7/17/17/34	-
11	1PW	A	2013	-	-	4/22/22/29	-
10	LPE	B	304	-	-	9/17/17/34	-
10	LPE	A	2027	-	-	10/25/25/34	-
12	PCW	A	2015	-	-	16/56/56/57	-
5	NAG	B	303	2	-	0/6/23/26	0/1/1/1
6	P5S	A	2019	-	-	8/44/44/59	-
7	Y01	A	2004	-	-	0/19/77/77	0/4/4/4
10	LPE	A	2012	-	-	8/25/25/34	-
7	Y01	A	2009	-	-	4/19/77/77	0/4/4/4

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	A	2029	PCW	O3-C11	4.40	1.46	1.33
6	A	2019	P5S	O37-C38	4.40	1.46	1.34
7	A	2032	Y01	CBB-CBE	-4.36	1.46	1.54
12	A	2030	PCW	O3-C11	4.26	1.45	1.33
12	A	2030	PCW	O2-C31	4.20	1.46	1.34
12	A	2015	PCW	O2-C31	4.19	1.46	1.34
7	A	2032	Y01	CAR-CBC	-4.17	1.39	1.51
12	A	2015	PCW	O3-C11	4.13	1.45	1.33
12	A	2020	PCW	O2-C31	3.92	1.45	1.34
6	A	2019	P5S	O19-C17	3.92	1.44	1.33
12	A	2018	PCW	O3-C11	3.89	1.44	1.33
12	A	2029	PCW	O2-C31	3.88	1.45	1.34
12	A	2020	PCW	O3-C11	3.88	1.44	1.33
7	A	2032	Y01	OAW-CAY	3.70	1.44	1.34
12	A	2018	PCW	O2-C31	3.66	1.44	1.34
7	A	2009	Y01	OAW-CAY	3.63	1.44	1.34
7	A	2005	Y01	OAW-CAY	3.62	1.44	1.34
6	A	2002	P5S	O37-C38	3.40	1.43	1.34
6	A	2019	P5S	C28-C27	-3.34	1.32	1.51
7	A	2032	Y01	CAV-CBC	2.90	1.59	1.52
6	A	2031	P5S	O19-C17	2.74	1.41	1.33
6	A	2031	P5S	O37-C2	-2.52	1.40	1.46
7	A	2032	Y01	CAM-CAY	2.39	1.57	1.50
7	A	2005	Y01	CAM-CAY	2.37	1.57	1.50
7	A	2009	Y01	CAM-CAY	2.36	1.57	1.50
6	A	2031	P5S	O19-C1	-2.28	1.39	1.45
6	A	2031	P5S	O37-C38	2.27	1.40	1.34
7	A	2009	Y01	CAL-CAX	2.25	1.55	1.50
7	A	2005	Y01	CAL-CAX	2.23	1.55	1.50
7	A	2003	Y01	CBH-CBF	-2.22	1.52	1.56
7	A	2032	Y01	CBH-CBF	-2.20	1.52	1.56
8	A	2006	9Z9	C11-C08	-2.19	1.52	1.56
7	A	2005	Y01	CBH-CBF	-2.18	1.52	1.56
7	A	2032	Y01	CAL-CAX	2.17	1.55	1.50
7	A	2007	Y01	CBH-CBF	-2.16	1.52	1.56
12	A	2018	PCW	C6-N	-2.14	1.43	1.50
7	A	2009	Y01	CBH-CBF	-2.13	1.52	1.56
7	A	2004	Y01	CBH-CBF	-2.13	1.52	1.56

All (108) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	2002	P5S	OG-CB-CA	7.10	114.25	108.06
7	A	2009	Y01	CBI-CBE-CBB	-5.94	110.19	119.49
7	A	2005	Y01	CBI-CBE-CBB	-5.92	110.21	119.49
7	A	2004	Y01	CBI-CBE-CBB	-5.91	110.23	119.49
7	A	2007	Y01	CBI-CBE-CBB	-5.91	110.23	119.49
7	A	2003	Y01	CBI-CBE-CBB	-5.90	110.24	119.49
6	A	2019	P5S	O37-C38-C39	5.47	123.29	111.50
12	A	2018	PCW	O2-C31-C32	4.83	121.92	111.50
7	A	2004	Y01	CBI-CBG-CBD	-4.81	107.25	114.38
7	A	2007	Y01	CBI-CBG-CBD	-4.81	107.26	114.38
7	A	2003	Y01	CBI-CBG-CBD	-4.77	107.32	114.38
7	A	2032	Y01	CBI-CBG-CBD	-4.73	107.37	114.38
7	A	2005	Y01	CBI-CBG-CBD	-4.73	107.38	114.38
7	A	2009	Y01	CBI-CBG-CBD	-4.72	107.39	114.38
8	A	2006	9Z9	C02-C06-C07	-4.38	107.89	114.38
7	A	2032	Y01	CBI-CBE-CBB	-4.15	112.98	119.49
6	A	2002	P5S	OXT-C-O	-4.06	114.87	124.09
7	A	2004	Y01	OAW-CAY-CAM	3.98	120.08	111.50
7	A	2003	Y01	OAW-CAY-CAM	3.97	120.06	111.50
7	A	2007	Y01	OAW-CAY-CAM	3.95	120.02	111.50
12	A	2030	PCW	O2-C31-C32	3.94	119.99	111.50
10	A	2022	LPE	C3N-N-C2N	3.92	119.06	108.97
12	A	2015	PCW	O2-C31-C32	3.87	119.83	111.50
7	A	2009	Y01	OAW-CAY-CAM	3.75	119.58	111.50
7	A	2005	Y01	OAW-CAY-CAM	3.74	119.56	111.50
6	A	2002	P5S	O37-C38-C39	3.69	119.46	111.50
7	A	2032	Y01	OAW-CAY-CAM	3.58	119.23	111.50
8	A	2006	9Z9	C21-C22-C23	-3.51	109.44	113.88
6	A	2031	P5S	O37-C38-C39	3.43	118.90	111.50
7	A	2009	Y01	CAS-CAU-CBI	-3.32	107.08	112.78
7	A	2032	Y01	CAS-CAU-CBI	-3.31	107.10	112.78
7	A	2003	Y01	CAS-CAU-CBI	-3.31	107.10	112.78
7	A	2005	Y01	CAS-CAU-CBI	-3.31	107.11	112.78
7	A	2004	Y01	CAS-CAU-CBI	-3.31	107.11	112.78
7	A	2007	Y01	CAS-CAU-CBI	-3.29	107.14	112.78
8	A	2006	9Z9	C09-C10-C02	-3.28	107.16	112.78
12	A	2029	PCW	O2-C31-C32	3.24	118.49	111.50
8	A	2006	9Z9	C02-C03-C74	-3.24	109.53	120.56
12	A	2018	PCW	O3-C11-C12	3.06	121.51	111.91
7	A	2003	Y01	CAD-CBH-CBF	-2.93	108.19	111.68
6	A	2002	P5S	OXT-C-CA	2.93	123.36	113.38
7	A	2009	Y01	CAD-CBH-CBF	-2.93	108.19	111.68
7	A	2004	Y01	CAD-CBH-CBF	-2.90	108.22	111.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A	2005	Y01	CAD-CBH-CBF	-2.90	108.22	111.68
12	A	2020	PCW	C3-C2-C1	-2.89	104.95	111.79
7	A	2007	Y01	CAD-CBH-CBF	-2.88	108.25	111.68
7	A	2032	Y01	CAD-CBH-CBF	-2.87	108.26	111.68
10	A	2016	LPE	C3-C2-C1	-2.86	104.37	112.79
8	A	2006	9Z9	C12-C11-C08	-2.86	108.28	111.68
12	A	2020	PCW	O2-C31-C32	2.81	117.55	111.50
8	A	2006	9Z9	C76-C73-C74	-2.78	109.98	115.69
7	A	2007	Y01	CBG-CBI-CBE	2.72	103.30	100.07
7	A	2032	Y01	CBG-CBI-CBE	2.71	103.28	100.07
7	A	2005	Y01	CBG-CBI-CBE	2.71	103.28	100.07
7	A	2003	Y01	CBG-CBI-CBE	2.71	103.28	100.07
7	A	2009	Y01	CBG-CBI-CBE	2.71	103.28	100.07
7	A	2004	Y01	CBG-CBI-CBE	2.69	103.26	100.07
12	A	2030	PCW	O3-C11-C12	2.69	120.36	111.91
5	A	2008	NAG	C1-O5-C5	2.64	115.77	112.19
7	A	2007	Y01	CAS-CBF-CBH	-2.58	109.69	113.08
10	A	2016	LPE	C31-C32-N	-2.55	107.27	115.78
7	A	2004	Y01	CAS-CBF-CBH	-2.54	109.73	113.08
7	A	2032	Y01	CAS-CBF-CBH	-2.53	109.74	113.08
8	A	2006	9Z9	C75-C74-C73	-2.52	110.32	114.92
12	A	2020	PCW	O3-C11-C12	2.50	119.75	111.91
7	A	2009	Y01	CAS-CBF-CBH	-2.50	109.79	113.08
7	A	2003	Y01	CAS-CBF-CBH	-2.49	109.80	113.08
7	A	2005	Y01	CAS-CBF-CBH	-2.48	109.81	113.08
7	A	2003	Y01	CBD-CAK-CAI	-2.47	109.18	112.73
7	A	2009	Y01	CBD-CAK-CAI	-2.47	109.19	112.73
8	A	2006	9Z9	C09-C08-C11	-2.46	109.84	113.08
12	A	2015	PCW	O3-C11-C12	2.45	119.60	111.91
7	A	2005	Y01	CBD-CAK-CAI	-2.44	109.22	112.73
7	A	2032	Y01	CBD-CAK-CAI	-2.43	109.24	112.73
6	A	2031	P5S	O19-C17-C20	2.43	119.54	111.91
7	A	2007	Y01	CBD-CAK-CAI	-2.43	109.24	112.73
7	A	2004	Y01	CBD-CAK-CAI	-2.42	109.25	112.73
8	A	2006	9Z9	C07-C15-C14	-2.40	109.28	112.73
6	A	2019	P5S	C41-C40-C39	-2.38	104.64	113.19
7	A	2003	Y01	CBF-CBH-CAZ	2.34	113.33	109.65
7	A	2005	Y01	CBF-CBH-CAZ	2.32	113.29	109.65
7	A	2032	Y01	CBF-CBH-CAZ	2.32	113.28	109.65
12	A	2029	PCW	O3-C11-C12	2.31	119.17	111.91
7	A	2007	Y01	CBF-CBH-CAZ	2.31	113.28	109.65
7	A	2009	Y01	CBF-CBH-CAZ	2.31	113.27	109.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	2002	P5S	C2-O37-C38	-2.29	112.16	117.79
8	A	2006	9Z9	C08-C11-C13	2.28	113.23	109.65
7	A	2007	Y01	CAC-CBB-CBE	-2.27	109.44	112.92
7	A	2004	Y01	CBF-CBH-CAZ	2.27	113.21	109.65
7	A	2004	Y01	CAC-CBB-CBE	-2.24	109.50	112.92
7	A	2005	Y01	CAC-CBB-CBE	-2.22	109.52	112.92
7	A	2003	Y01	CAC-CBB-CBE	-2.22	109.53	112.92
7	A	2009	Y01	CAC-CBB-CBE	-2.21	109.54	112.92
12	A	2020	PCW	C34-C33-C32	-2.17	105.39	113.19
10	A	2023	LPE	C31-C32-N	-2.17	108.53	115.78
10	A	2021	LPE	C31-C32-N	-2.13	108.67	115.78
12	A	2018	PCW	O2-C31-O31	-2.11	118.61	123.70
6	A	2031	P5S	OXT-C-CA	2.11	120.56	113.38
6	A	2019	P5S	O15-P12-O13	2.11	122.65	112.24
12	A	2020	PCW	O3-C3-C2	2.07	114.45	108.43
12	A	2018	PCW	O3-C11-O11	-2.05	118.41	123.59
7	A	2004	Y01	CAQ-CBG-CBD	-2.05	115.70	119.08
7	A	2003	Y01	CAQ-CBG-CBD	-2.04	115.73	119.08
7	A	2005	Y01	CAQ-CBG-CBD	-2.03	115.73	119.08
8	A	2006	9Z9	O80-C79-C78	-2.03	109.26	112.18
8	A	2006	9Z9	C17-C16-C13	-2.02	108.37	111.52
7	A	2009	Y01	CAQ-CBG-CBD	-2.02	115.76	119.08
7	A	2005	Y01	CBC-CAV-CAZ	-2.00	108.41	111.52

There are no chirality outliers.

All (269) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	2002	P5S	C-CA-CB-OG
6	A	2002	P5S	N-CA-CB-OG
6	A	2002	P5S	CB-OG-P12-O13
6	A	2002	P5S	C3-O16-P12-OG
6	A	2002	P5S	C3-O16-P12-O13
6	A	2002	P5S	C3-O16-P12-O15
6	A	2019	P5S	CB-OG-P12-O15
6	A	2019	P5S	C3-O16-P12-OG
6	A	2019	P5S	C3-O16-P12-O13
6	A	2019	P5S	C3-O16-P12-O15
6	A	2031	P5S	C3-O16-P12-O13
10	A	2011	LPE	C3-O3-P-O31
10	A	2012	LPE	C3-O3-P-O31
10	A	2014	LPE	C3-O3-P-O32

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Mol	Chain	Res	Type	Atoms
10	A	2014	LPE	C31-O33-P-O31
10	A	2016	LPE	O1-C1-C2-C3
10	A	2016	LPE	C3-O3-P-O32
10	A	2016	LPE	C31-O33-P-O3
10	A	2016	LPE	C31-O33-P-O31
10	A	2016	LPE	C32-C31-O33-P
10	A	2016	LPE	O33-C31-C32-N
10	A	2017	LPE	C3-O3-P-O32
10	A	2021	LPE	C31-O33-P-O31
10	A	2021	LPE	O33-C31-C32-N
10	A	2022	LPE	C31-O33-P-O31
10	A	2023	LPE	C31-O33-P-O31
10	A	2025	LPE	C31-O33-P-O32
10	A	2026	LPE	C31-O33-P-O31
10	A	2027	LPE	O1-C1-C2-C3
10	A	2027	LPE	C3-O3-P-O32
10	A	2027	LPE	C31-O33-P-O3
10	A	2027	LPE	C31-O33-P-O31
10	A	2027	LPE	C31-O33-P-O32
10	A	2033	LPE	C3-O3-P-O32
10	A	2033	LPE	C31-O33-P-O31
10	A	2033	LPE	C31-O33-P-O32
10	B	304	LPE	C3-O3-P-O31
10	B	304	LPE	C3-O3-P-O32
10	B	304	LPE	C3-O3-P-O33
11	A	2013	1PW	CAH-CAI-CAZ-OAE
11	A	2013	1PW	CAH-CAI-CAZ-CBA
12	A	2018	PCW	O4P-C4-C5-N
12	A	2020	PCW	C32-C31-O2-C2
12	A	2029	PCW	O4P-C4-C5-N
12	A	2029	PCW	C1-O3P-P-O2P
12	A	2030	PCW	C4-O4P-P-O1P
6	A	2031	P5S	O18-C17-O19-C1
6	A	2031	P5S	C20-C17-O19-C1
7	A	2032	Y01	CAC-CBB-CBE-CAP
7	A	2032	Y01	CAC-CBB-CBE-CBI
12	A	2020	PCW	O31-C31-O2-C2
7	A	2032	Y01	CAJ-CAO-CBB-CAC
7	A	2032	Y01	CAO-CBB-CBE-CBI
12	A	2029	PCW	O11-C11-O3-C3
12	A	2029	PCW	C12-C11-O3-C3
5	A	2001	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
7	A	2032	Y01	CAO-CBB-CBE-CAP
5	A	2008	NAG	C8-C7-N2-C2
5	A	2008	NAG	O7-C7-N2-C2
10	A	2027	LPE	O1-C1-C2-O2H
5	A	2001	NAG	C4-C5-C6-O6
7	A	2005	Y01	CAR-CBC-OAW-CAY
10	A	2025	LPE	C31-C32-N-C2N
10	A	2025	LPE	C31-C32-N-C3N
12	A	2018	PCW	C4-C5-N-C8
12	A	2020	PCW	C4-C5-N-C7
12	A	2030	PCW	C12-C11-O3-C3
7	A	2009	Y01	CAR-CBC-OAW-CAY
7	A	2032	Y01	CAJ-CAO-CBB-CBE
10	A	2016	LPE	O1-C1-C2-O2H
10	A	2028	LPE	C31-C32-N-C3N
12	A	2018	PCW	C4-C5-N-C7
6	A	2002	P5S	C38-C39-C40-C41
12	A	2030	PCW	O11-C11-O3-C3
10	A	2016	LPE	O1-C11-C12-C13
10	A	2022	LPE	O1-C1-C2-O2H
6	A	2002	P5S	CB-OG-P12-O16
10	A	2012	LPE	C31-O33-P-O3
10	A	2016	LPE	C3-O3-P-O33
10	A	2017	LPE	C3-O3-P-O33
10	A	2024	LPE	C3-O3-P-O33
10	A	2025	LPE	C31-O33-P-O3
10	A	2027	LPE	C3-O3-P-O33
10	A	2028	LPE	C31-O33-P-O3
10	A	2033	LPE	C3-O3-P-O33
10	A	2033	LPE	C31-O33-P-O3
10	B	304	LPE	C31-O33-P-O3
12	A	2015	PCW	C4-O4P-P-O3P
12	A	2018	PCW	C4-O4P-P-O3P
12	A	2020	PCW	C4-O4P-P-O3P
12	A	2030	PCW	C1-O3P-P-O4P
12	A	2030	PCW	C4-O4P-P-O3P
7	A	2005	Y01	CAV-CBC-OAW-CAY
7	A	2009	Y01	CAV-CBC-OAW-CAY
10	A	2011	LPE	O1-C11-C12-C13
10	A	2016	LPE	C31-C32-N-C1N
10	A	2016	LPE	C31-C32-N-C2N
10	A	2016	LPE	C31-C32-N-C3N

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Mol	Chain	Res	Type	Atoms
12	A	2020	PCW	C4-C5-N-C6
10	A	2022	LPE	O1-C1-C2-C3
6	A	2002	P5S	C46-C48-C49-C50
6	A	2019	P5S	C25-C26-C27-C28
6	A	2031	P5S	C17-C20-C21-C22
6	A	2031	P5S	C42-C43-C44-C45
10	A	2012	LPE	O1-C11-C12-C13
10	A	2025	LPE	C31-C32-N-C1N
10	A	2022	LPE	C12-C13-C14-C15
6	A	2002	P5S	C51-C52-C53-C54
6	A	2019	P5S	C27-C28-C29-C30
6	A	2002	P5S	C41-C42-C43-C44
12	A	2029	PCW	C33-C34-C35-C36
6	A	2002	P5S	C52-C53-C54-C55
10	A	2022	LPE	C14-C15-C16-C17
12	A	2018	PCW	C4-C5-N-C6
12	A	2020	PCW	C4-C5-N-C8
12	A	2015	PCW	C24-C25-C26-C27
12	A	2015	PCW	C32-C33-C34-C35
12	A	2015	PCW	C32-C31-O2-C2
6	A	2031	P5S	C21-C22-C23-C24
6	A	2002	P5S	C48-C49-C50-C51
12	A	2029	PCW	C31-C32-C33-C34
10	A	2026	LPE	C13-C14-C15-C16
10	A	2012	LPE	C13-C14-C15-C16
10	A	2028	LPE	C31-C32-N-C1N
10	A	2028	LPE	C31-C32-N-C2N
6	A	2031	P5S	C38-C39-C40-C41
12	A	2015	PCW	O31-C31-O2-C2
6	A	2002	P5S	C39-C38-O37-C2
6	A	2031	P5S	C3-O16-P12-OG
10	A	2012	LPE	C3-O3-P-O33
12	A	2018	PCW	C35-C36-C37-C38
6	A	2031	P5S	C40-C41-C42-C43
6	A	2031	P5S	C43-C44-C45-C46
10	A	2011	LPE	C2-C1-O1-C11
7	A	2032	Y01	CAN-CAJ-CAO-CBB
12	A	2015	PCW	C41-C42-C43-C44
12	A	2018	PCW	C34-C35-C36-C37
6	A	2002	P5S	O47-C38-O37-C2
6	A	2002	P5S	C1-C2-C3-O16
10	B	304	LPE	C2-C3-O3-P

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Mol	Chain	Res	Type	Atoms
10	A	2028	LPE	C2-C1-O1-C11
10	A	2017	LPE	O1-C1-C2-C3
10	A	2017	LPE	O1-C1-C2-O2H
10	A	2014	LPE	C3-O3-P-O33
10	A	2022	LPE	C16-C17-C18-C19
10	A	2022	LPE	C11-C12-C13-C14
6	A	2002	P5S	C2-C3-O16-P12
6	A	2031	P5S	C2-C3-O16-P12
12	A	2020	PCW	C2-C1-O3P-P
11	A	2013	1PW	CAK-CAM-CAO-CAQ
7	A	2009	Y01	CAO-CAJ-CAN-CBA
10	A	2021	LPE	C2-C1-O1-C11
7	A	2005	Y01	CAO-CAJ-CAN-CBA
6	A	2031	P5S	C39-C38-O37-C2
6	A	2002	P5S	O37-C2-C3-O16
10	A	2022	LPE	C12-C11-O1-C1
6	A	2002	P5S	C40-C41-C42-C43
6	A	2031	P5S	CA-CB-OG-P12
6	A	2031	P5S	O47-C38-O37-C2
12	A	2029	PCW	O31-C31-O2-C2
10	B	304	LPE	C2-C1-O1-C11
10	A	2014	LPE	C12-C11-O1-C1
10	A	2014	LPE	C31-O33-P-O3
10	A	2022	LPE	C31-O33-P-O3
10	A	2023	LPE	C31-O33-P-O3
10	A	2026	LPE	C31-O33-P-O3
12	A	2029	PCW	C1-O3P-P-O4P
10	A	2011	LPE	C2-C3-O3-P
10	A	2014	LPE	C2-C3-O3-P
6	A	2002	P5S	CB-OG-P12-O15
6	A	2031	P5S	C3-O16-P12-O15
10	A	2012	LPE	C3-O3-P-O32
10	A	2012	LPE	C31-O33-P-O31
10	A	2014	LPE	C3-O3-P-O31
10	A	2022	LPE	C3-O3-P-O32
10	A	2024	LPE	C3-O3-P-O31
10	A	2025	LPE	C31-O33-P-O31
10	A	2027	LPE	C3-O3-P-O31
10	A	2028	LPE	C31-O33-P-O31
10	B	304	LPE	C31-O33-P-O31
12	A	2015	PCW	C4-C5-N-C6
12	A	2015	PCW	C4-C5-N-C7

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Mol	Chain	Res	Type	Atoms
12	A	2015	PCW	C4-O4P-P-O2P
12	A	2018	PCW	C4-O4P-P-O2P
12	A	2020	PCW	C4-O4P-P-O2P
12	A	2029	PCW	C4-O4P-P-O2P
12	A	2030	PCW	C1-O3P-P-O2P
12	A	2030	PCW	C4-O4P-P-O2P
10	A	2012	LPE	C32-C31-O33-P
10	A	2033	LPE	C32-C31-O33-P
10	B	304	LPE	C32-C31-O33-P
10	A	2016	LPE	C12-C11-O1-C1
10	A	2021	LPE	C12-C11-O1-C1
10	A	2011	LPE	C11-C12-C13-C14
10	A	2033	LPE	C2-C1-O1-C11
10	A	2026	LPE	C2-C1-O1-C11
10	A	2016	LPE	C13-C14-C15-C16
12	A	2029	PCW	C34-C35-C36-C37
12	A	2030	PCW	C4-C5-N-C6
10	A	2011	LPE	O33-C31-C32-N
10	A	2014	LPE	O33-C31-C32-N
10	A	2017	LPE	O33-C31-C32-N
10	A	2022	LPE	O33-C31-C32-N
10	A	2023	LPE	O33-C31-C32-N
10	A	2024	LPE	O33-C31-C32-N
10	A	2025	LPE	O33-C31-C32-N
10	A	2026	LPE	O33-C31-C32-N
10	A	2027	LPE	O33-C31-C32-N
10	A	2033	LPE	O33-C31-C32-N
10	B	304	LPE	O33-C31-C32-N
12	A	2030	PCW	O4P-C4-C5-N
6	A	2002	P5S	C50-C51-C52-C53
10	A	2017	LPE	C12-C11-O1-C1
12	A	2015	PCW	C4-C5-N-C8
12	A	2029	PCW	C32-C31-O2-C2
6	A	2019	P5S	CB-OG-P12-O16
10	A	2011	LPE	C3-O3-P-O33
10	A	2017	LPE	C31-O33-P-O3
10	A	2021	LPE	C31-O33-P-O3
10	A	2026	LPE	C3-O3-P-O33
10	A	2028	LPE	C3-O3-P-O33
12	A	2018	PCW	C1-O3P-P-O4P
12	A	2020	PCW	C1-O3P-P-O4P
12	A	2029	PCW	C4-O4P-P-O3P

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Mol	Chain	Res	Type	Atoms
12	A	2018	PCW	C17-C18-C19-C20
12	A	2018	PCW	C37-C38-C39-C40
12	A	2015	PCW	C23-C24-C25-C26
12	A	2029	PCW	C11-C12-C13-C14
10	A	2027	LPE	C2-C1-O1-C11
12	A	2030	PCW	C4-C5-N-C8
10	A	2016	LPE	C11-C12-C13-C14
11	A	2013	1PW	CAN-CAP-CAR-CAT
6	A	2002	P5S	C43-C44-C45-C46
12	A	2030	PCW	C4-C5-N-C7
12	A	2015	PCW	C44-C45-C46-C47
6	A	2002	P5S	C39-C40-C41-C42
12	A	2029	PCW	C21-C22-C23-C24
6	A	2031	P5S	C41-C42-C43-C44
6	A	2002	P5S	O19-C1-C2-O37
10	A	2017	LPE	C2-C3-O3-P
6	A	2002	P5S	C53-C54-C55-C56
12	A	2015	PCW	C17-C18-C19-C20
12	A	2015	PCW	C13-C14-C15-C16
12	A	2015	PCW	C39-C40-C41-C42
12	A	2020	PCW	O3-C11-C12-C13
12	A	2018	PCW	C39-C40-C41-C42
10	A	2011	LPE	C31-C32-N-C2N
10	A	2011	LPE	C16-C17-C18-C19
10	A	2014	LPE	C1-C2-C3-O3
10	A	2022	LPE	C13-C14-C15-C16
12	A	2015	PCW	C19-C20-C21-C22
6	A	2019	P5S	CB-OG-P12-O13
10	A	2017	LPE	C31-O33-P-O31
10	A	2021	LPE	C3-O3-P-O31
12	A	2018	PCW	C1-O3P-P-O2P
12	A	2020	PCW	C1-O3P-P-O2P
12	A	2029	PCW	C4-C5-N-C6
10	A	2011	LPE	C32-C31-O33-P
10	A	2017	LPE	C32-C31-O33-P
10	A	2021	LPE	C32-C31-O33-P
10	A	2025	LPE	C32-C31-O33-P
12	A	2020	PCW	C5-C4-O4P-P
6	A	2002	P5S	C49-C50-C51-C52
10	A	2014	LPE	C31-C32-N-C2N
12	A	2029	PCW	O3-C11-C12-C13
6	A	2002	P5S	O37-C38-C39-C40

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Mol	Chain	Res	Type	Atoms
7	A	2005	Y01	CAN-CAJ-CAO-CBB
7	A	2009	Y01	CAN-CAJ-CAO-CBB
6	A	2002	P5S	O47-C38-C39-C40

There are no ring outliers.

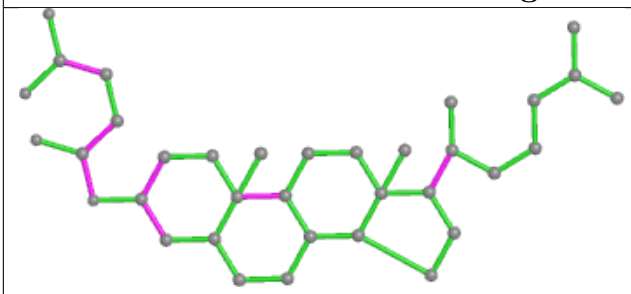
31 monomers are involved in 149 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	2032	Y01	20	0
10	A	2017	LPE	3	0
10	A	2016	LPE	5	0
5	A	2001	NAG	1	0
7	A	2007	Y01	13	0
6	A	2031	P5S	3	0
10	A	2025	LPE	2	0
5	B	302	NAG	1	0
6	A	2002	P5S	2	0
10	A	2021	LPE	7	0
10	A	2024	LPE	2	0
10	A	2033	LPE	3	0
10	A	2023	LPE	3	0
10	A	2014	LPE	2	0
12	A	2020	PCW	7	0
10	A	2022	LPE	1	0
7	A	2005	Y01	19	0
7	A	2003	Y01	4	0
12	A	2029	PCW	3	0
12	A	2018	PCW	1	0
8	A	2006	9Z9	14	0
10	A	2026	LPE	2	0
10	A	2028	LPE	1	0
11	A	2013	1PW	2	0
10	A	2027	LPE	3	0
12	A	2015	PCW	19	0
5	B	303	NAG	6	0
6	A	2019	P5S	4	0
7	A	2004	Y01	6	0
10	A	2012	LPE	1	0
7	A	2009	Y01	9	0

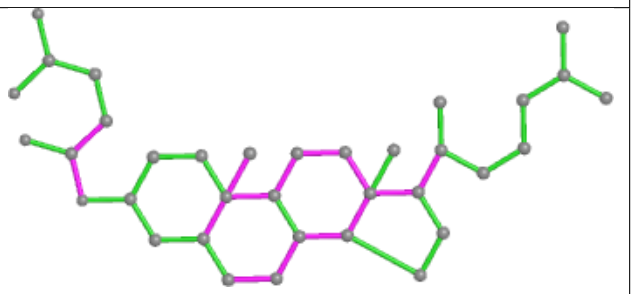
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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.

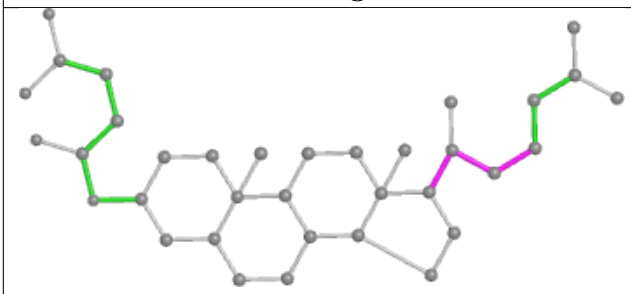
Ligand Y01 A 2032



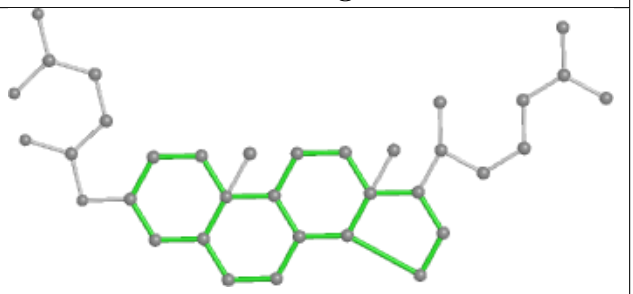
Bond lengths



Bond angles

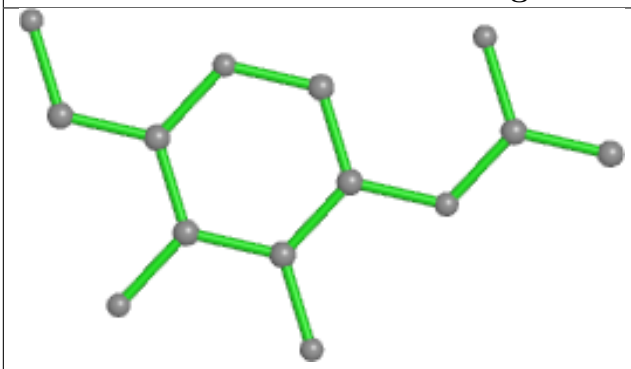


Torsions

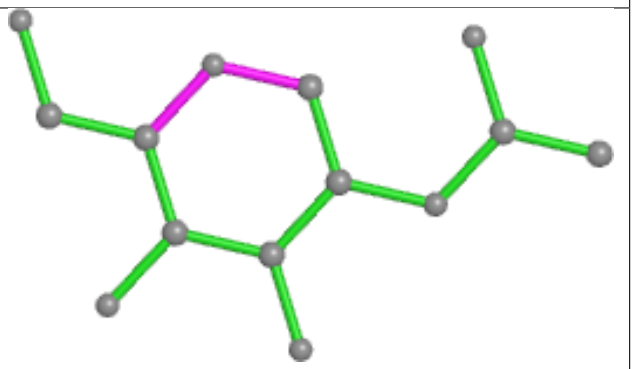


Rings

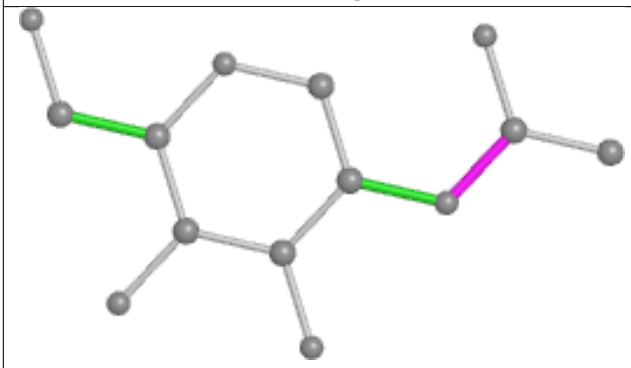
Ligand NAG A 2008



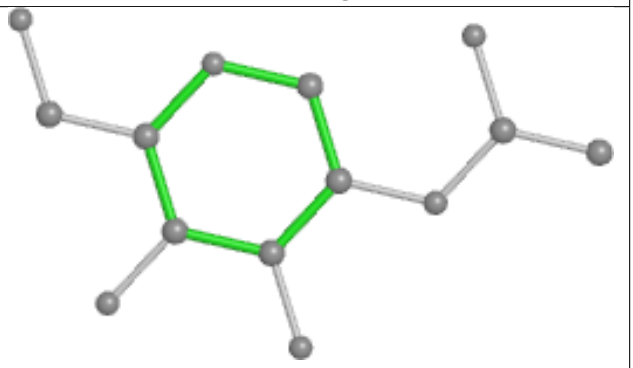
Bond lengths



Bond angles

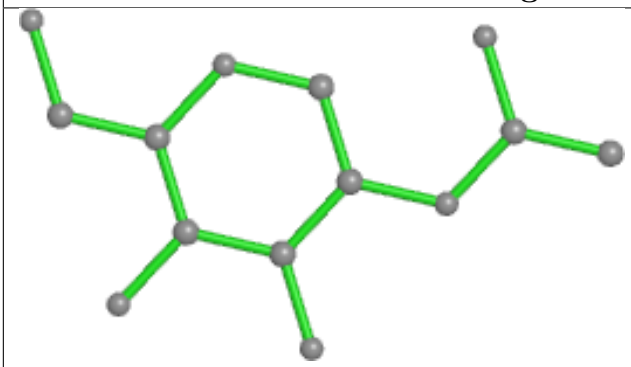


Torsions

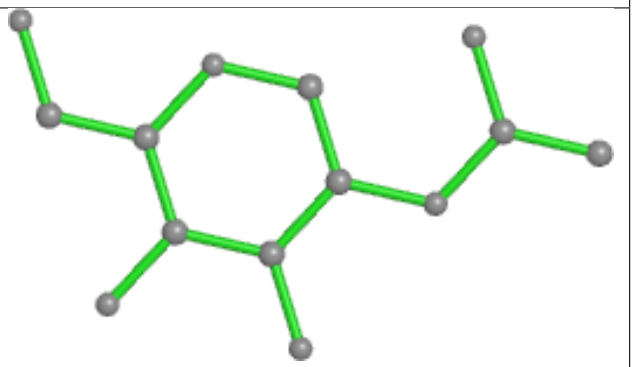


Rings

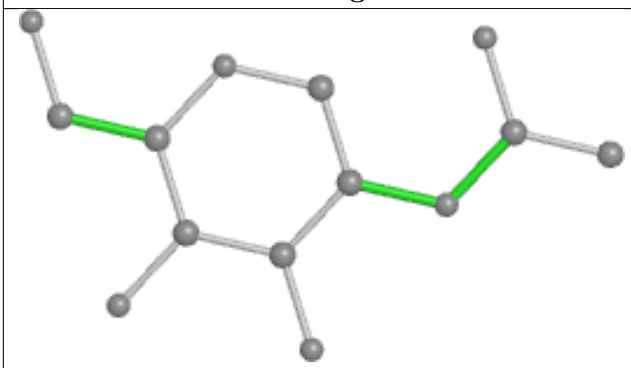
Ligand NAG B 301



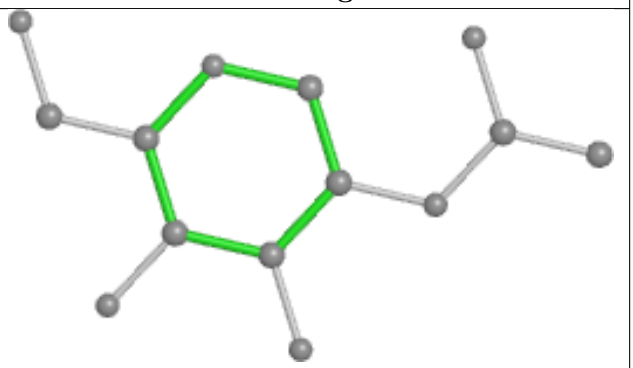
Bond lengths



Bond angles

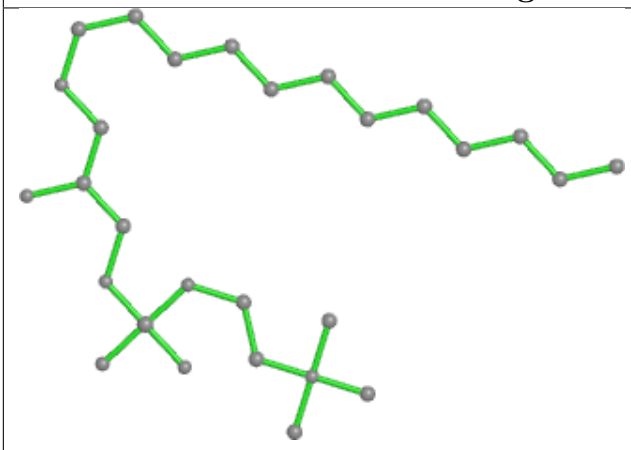


Torsions

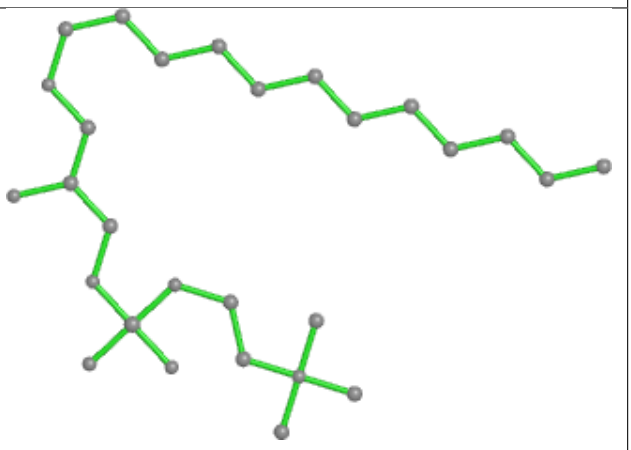


Rings

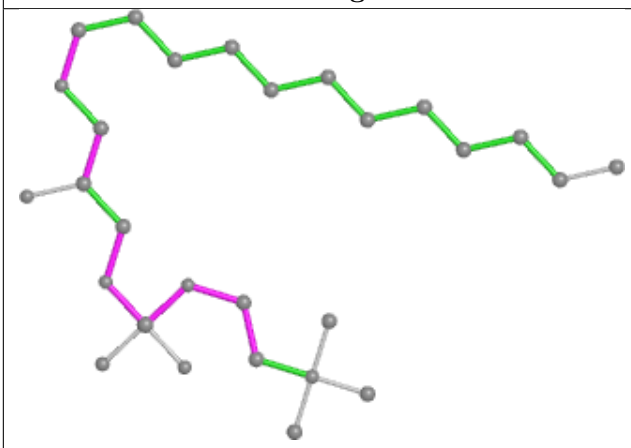
Ligand LPE A 2017



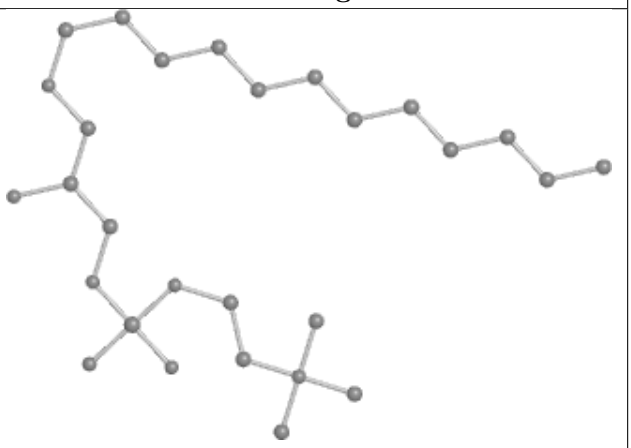
Bond lengths



Bond angles

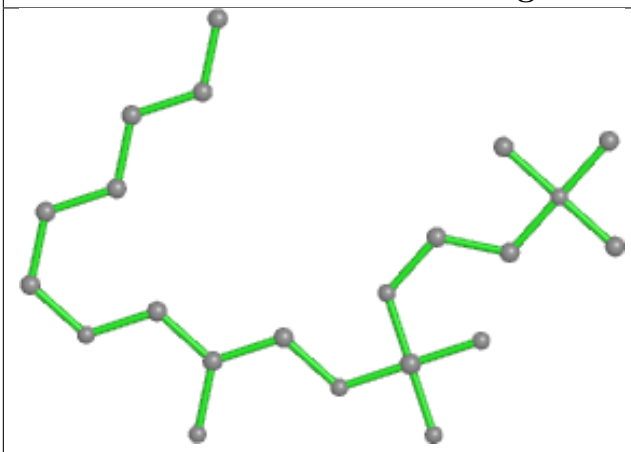


Torsions

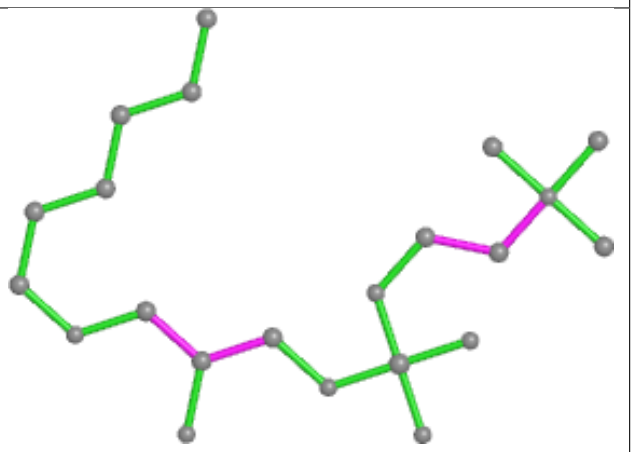


Rings

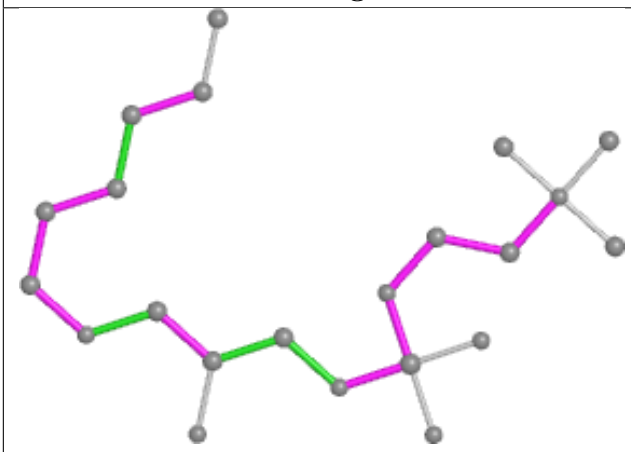
Ligand LPE A 2016



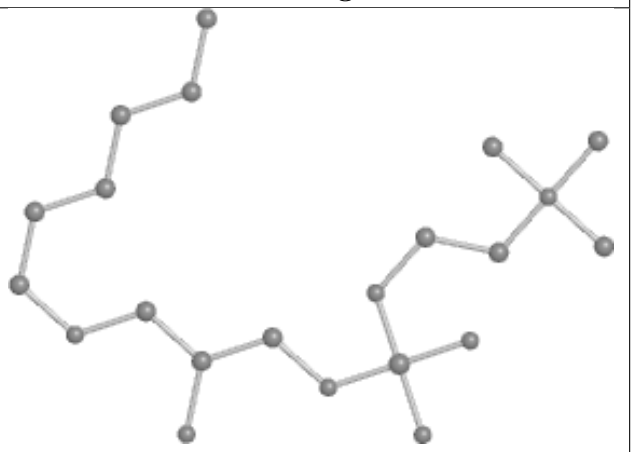
Bond lengths



Bond angles

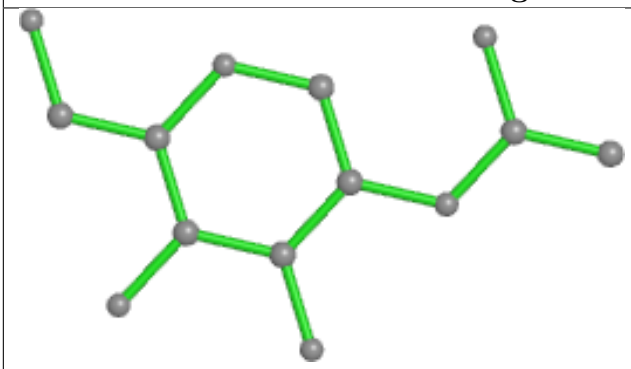


Torsions

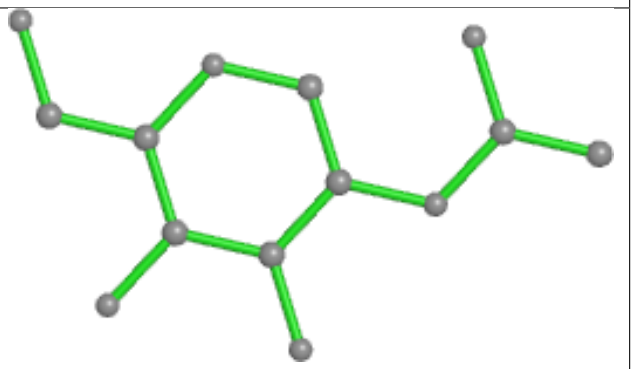


Rings

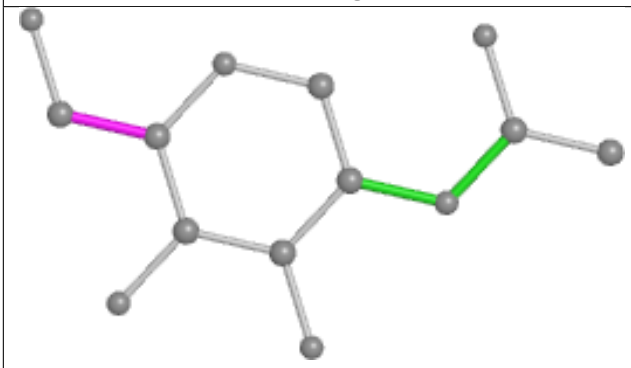
Ligand NAG A 2001



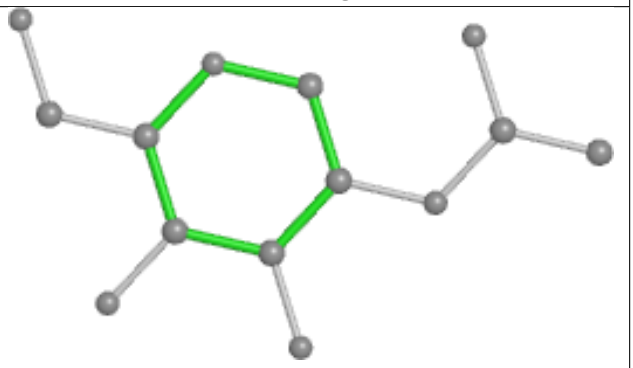
Bond lengths



Bond angles

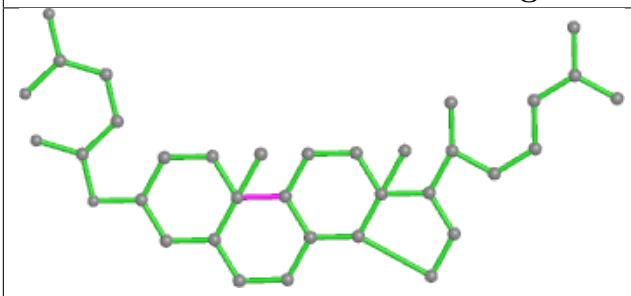


Torsions

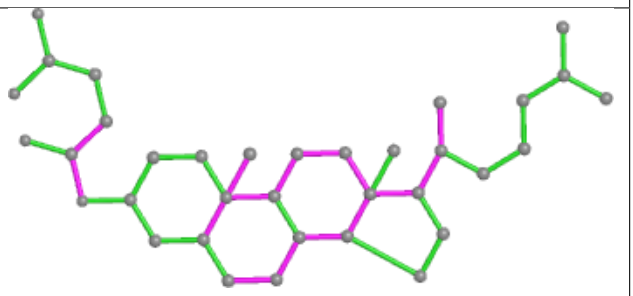


Rings

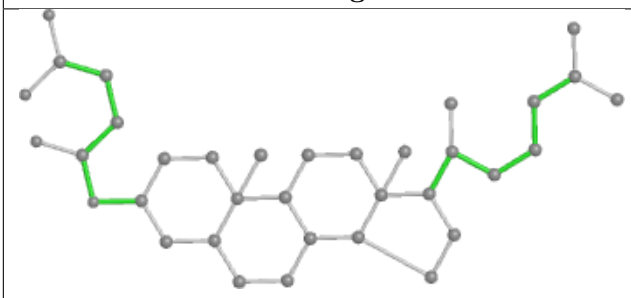
Ligand Y01 A 2007



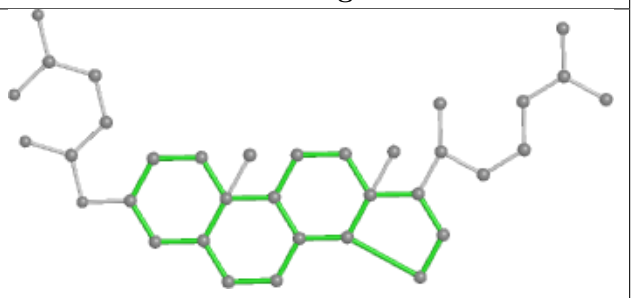
Bond lengths



Bond angles

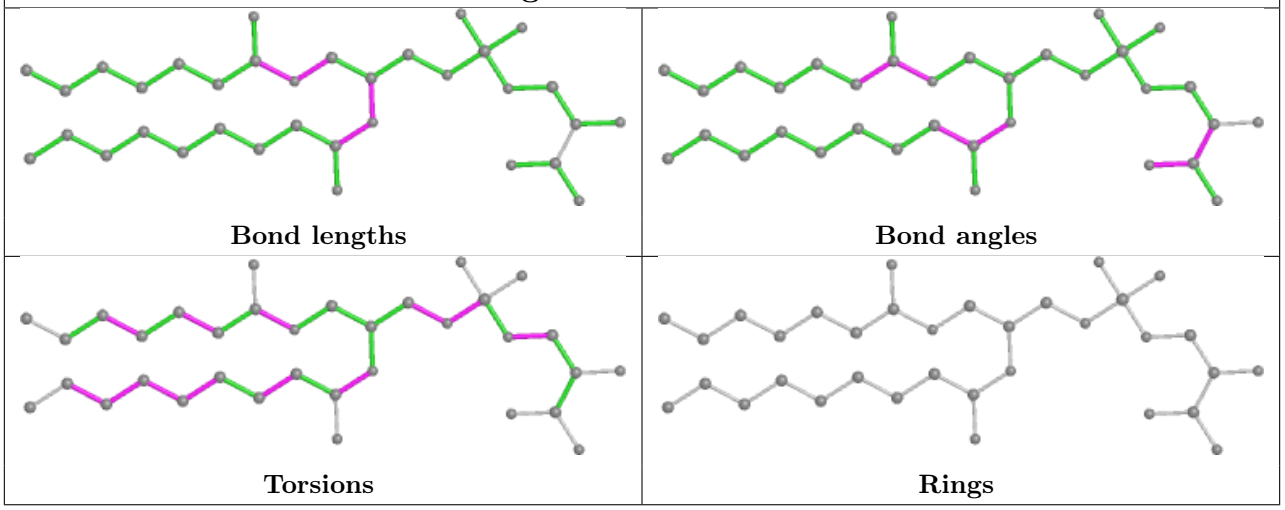


Torsions

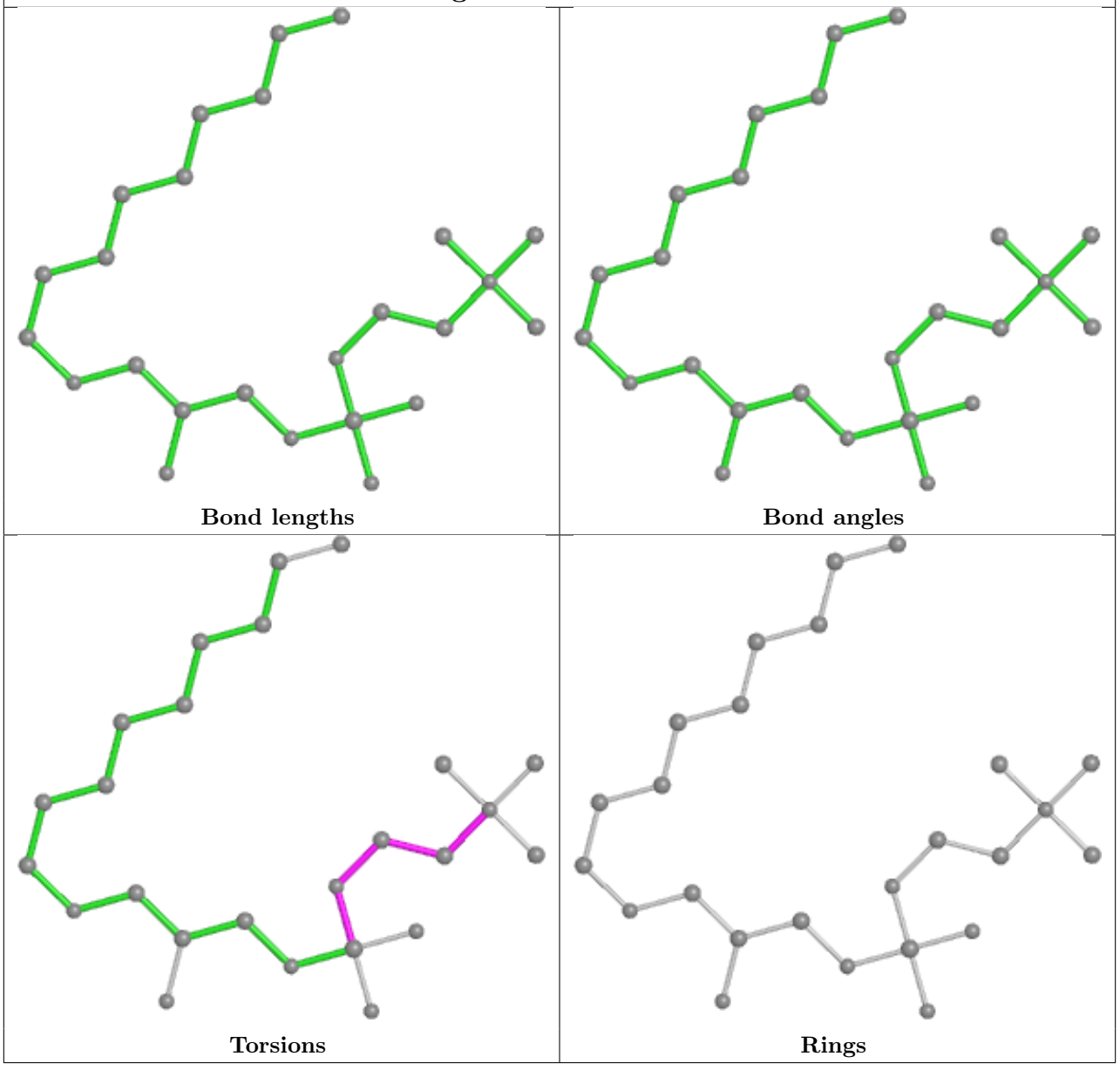


Rings

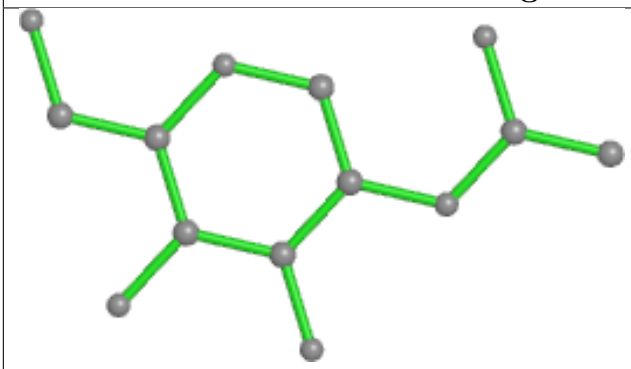
Ligand P5S A 2031



Ligand LPE A 2025



Ligand NAG B 302



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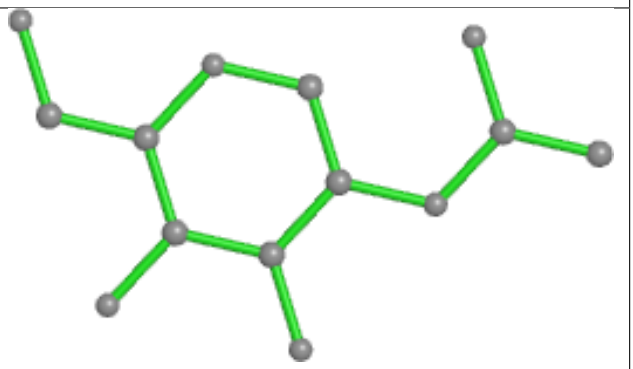
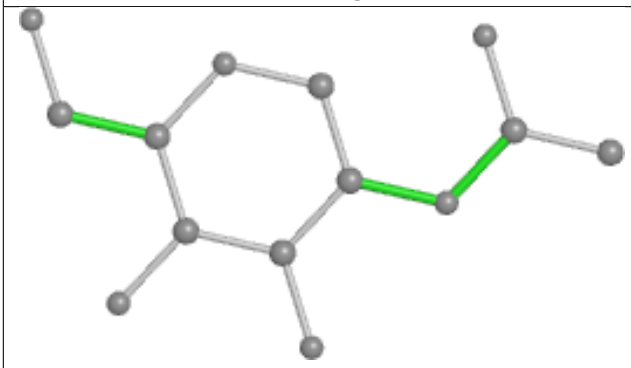


Bond angles



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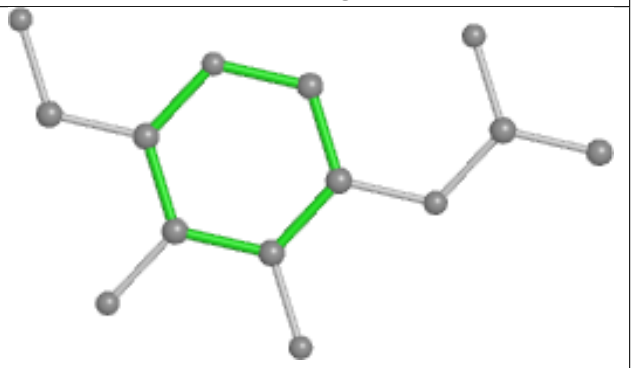
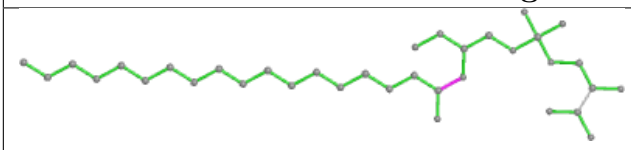


Rings

Ligand P5S A 2002



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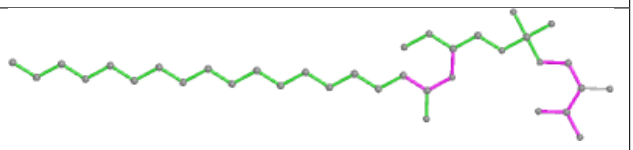
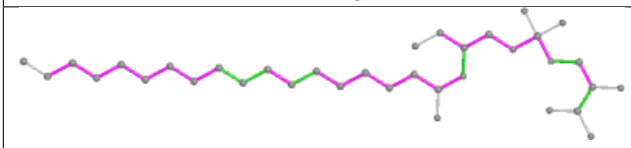


Bond angles



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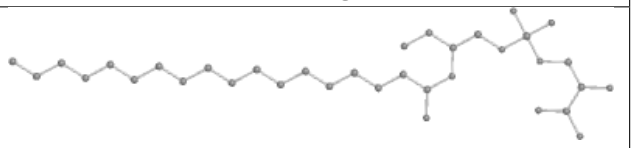
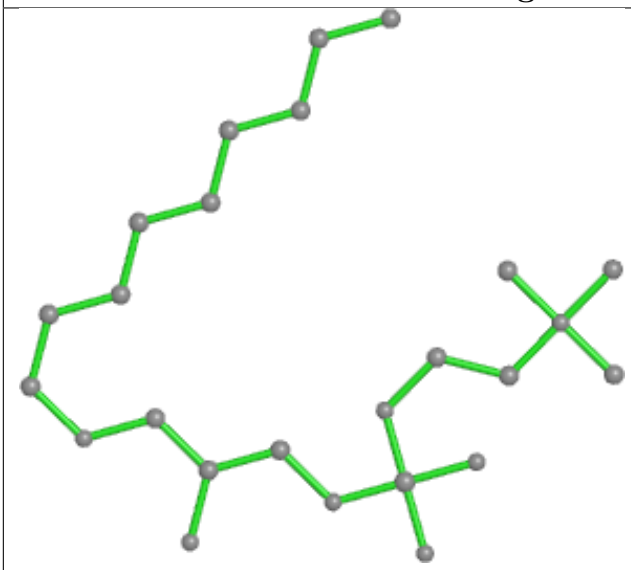


Rings

Ligand LPE A 2021



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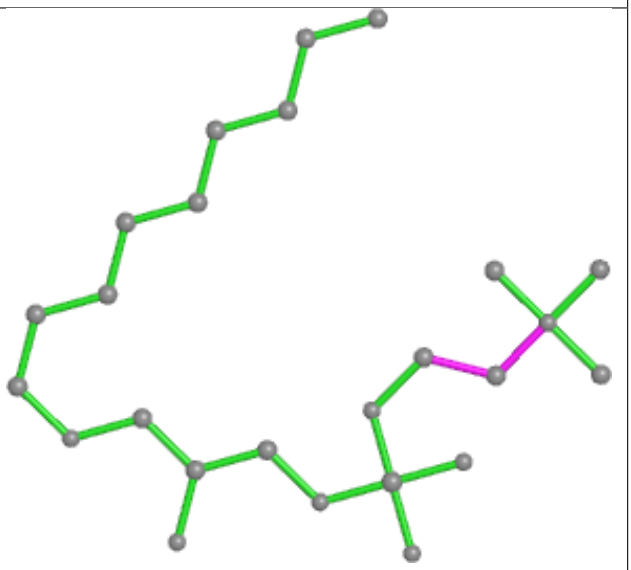
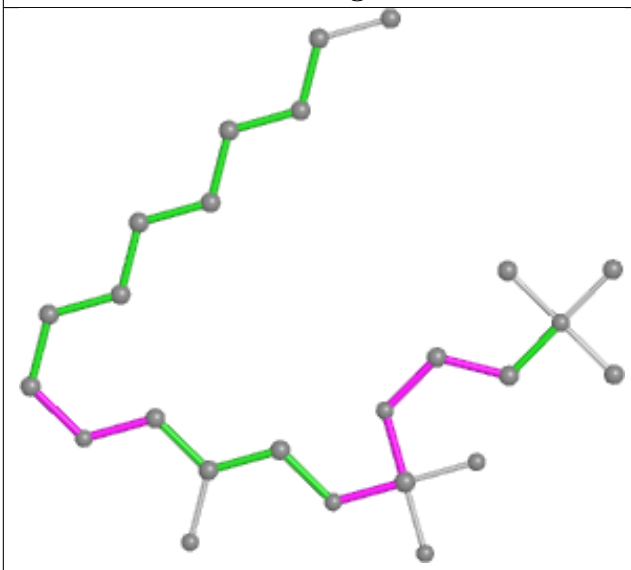


Bond angles



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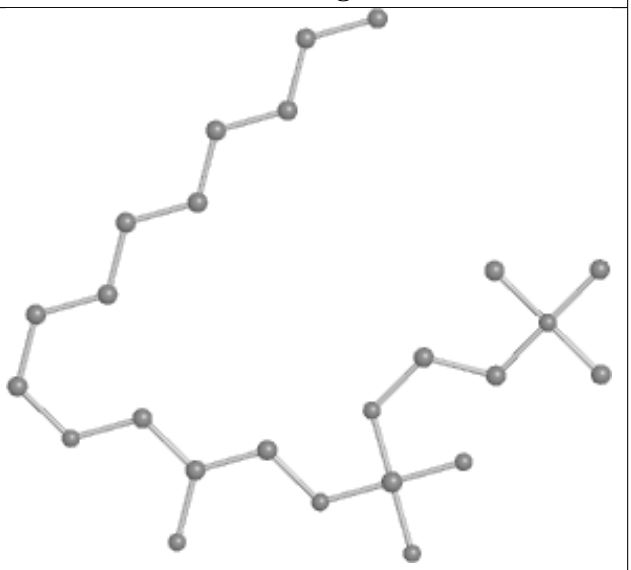
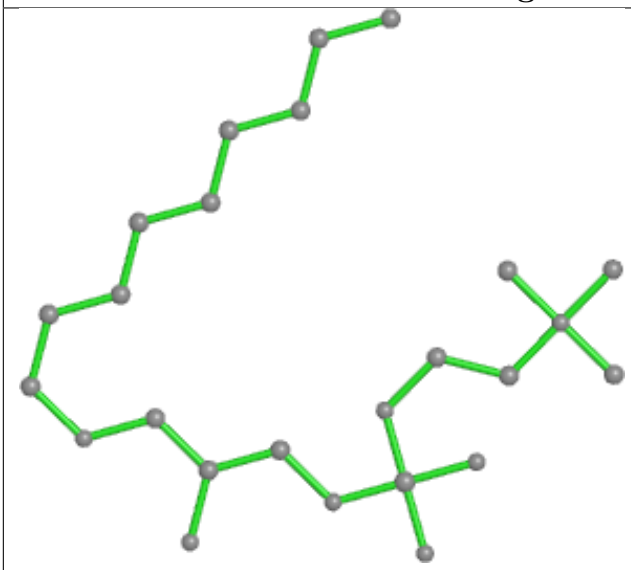


Rings

Ligand LPE A 2024



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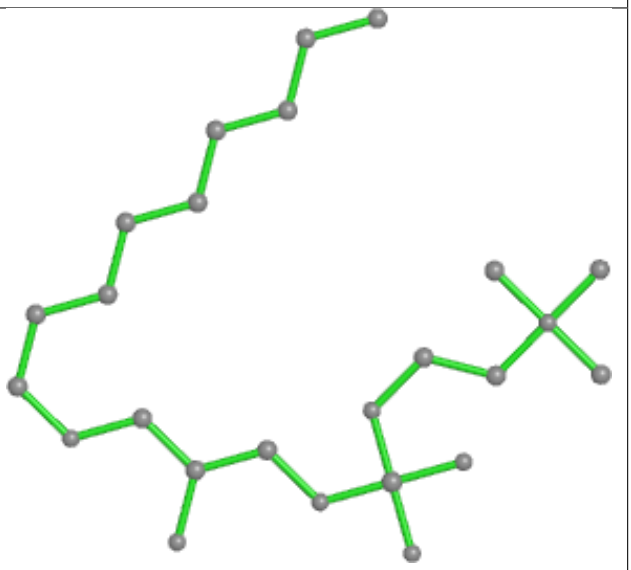
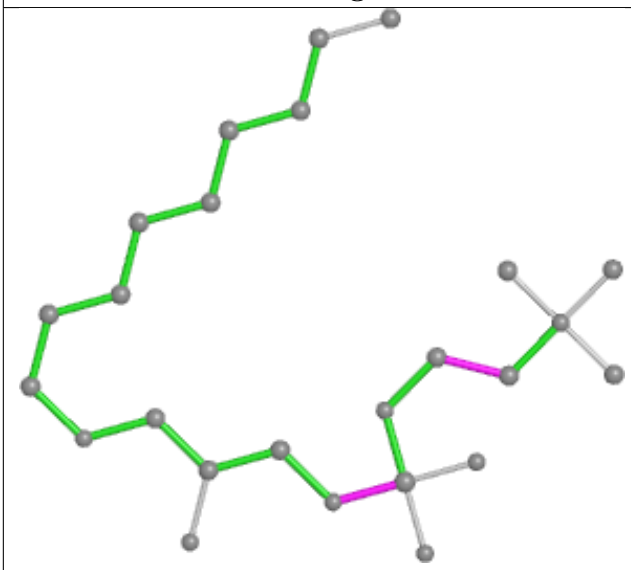


Bond angles



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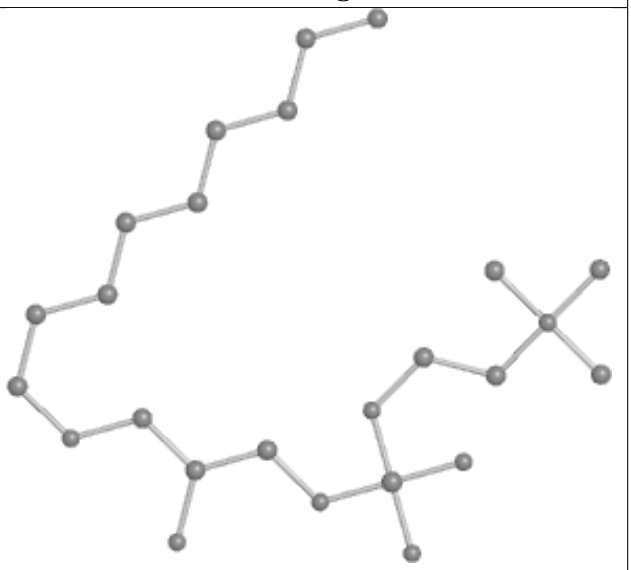
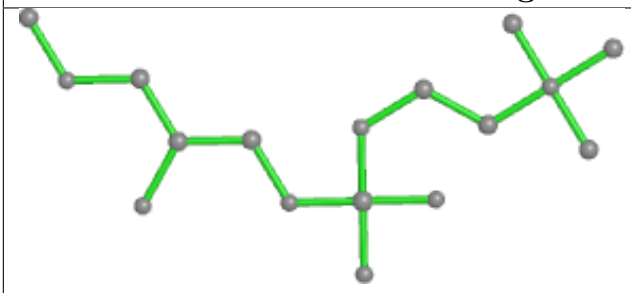


Rings

Ligand LPE A 2033



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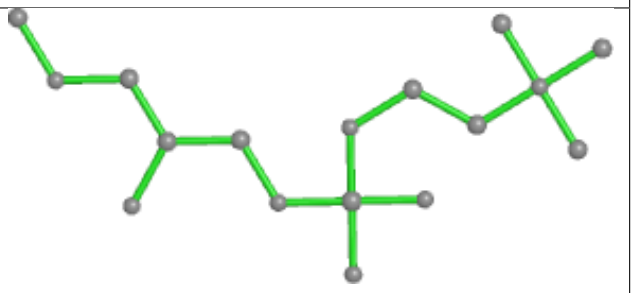
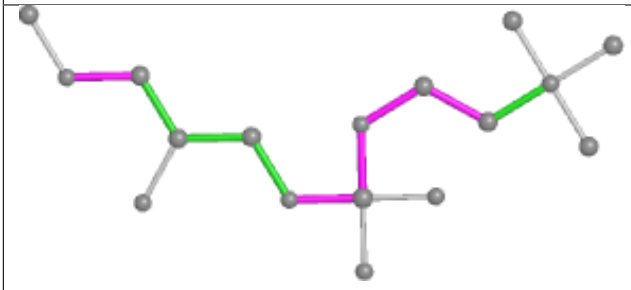


Bond angles



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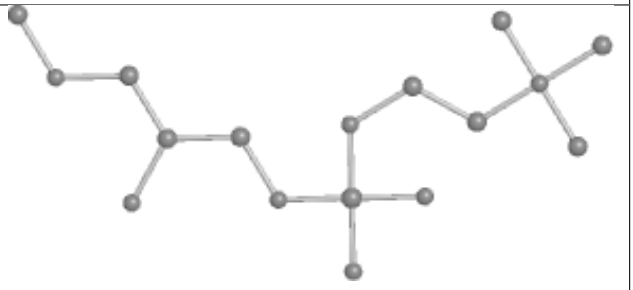
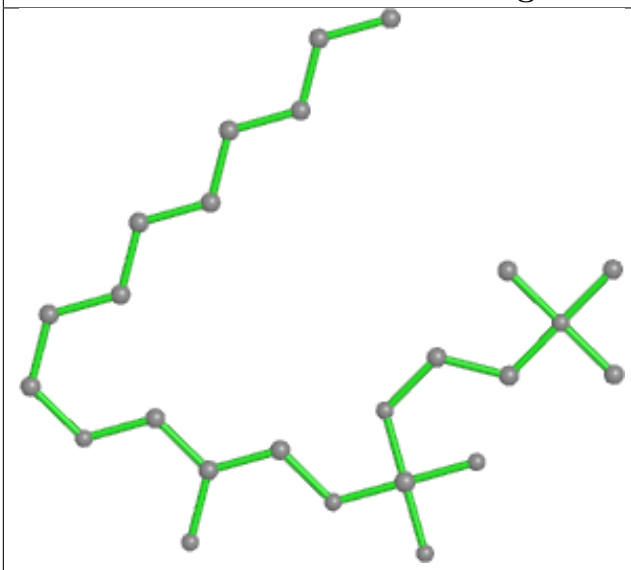


Rings

Ligand LPE A 2023



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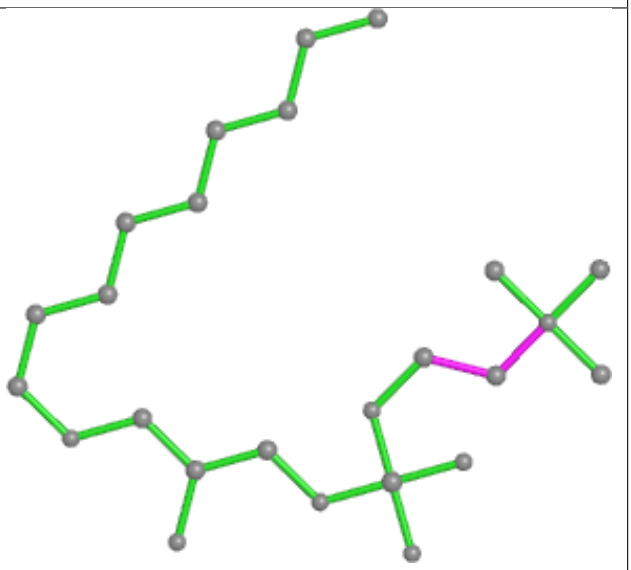
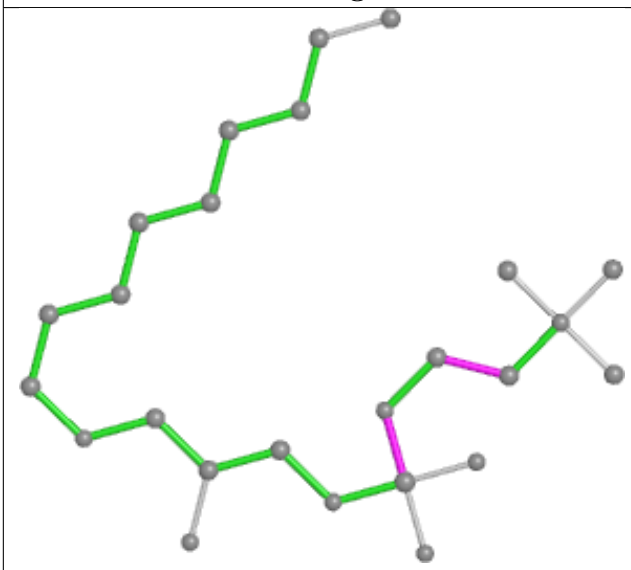


Bond angles



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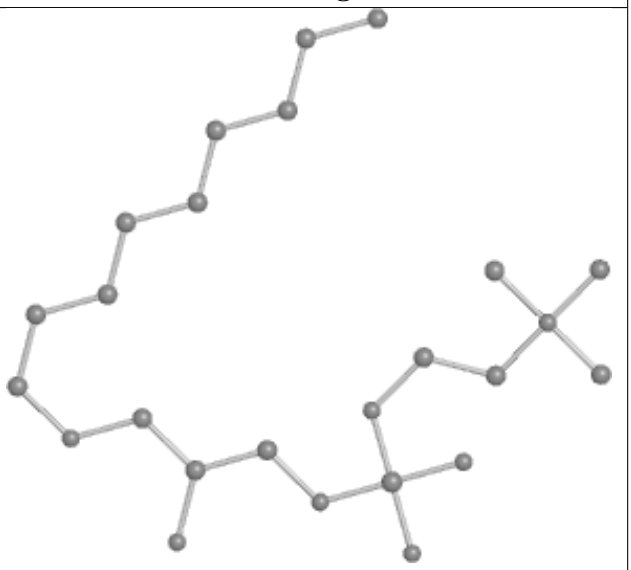
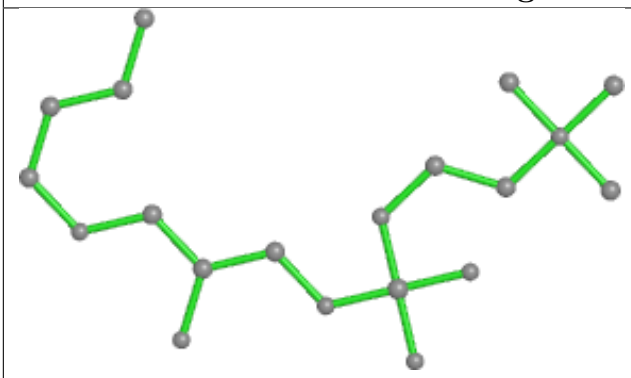


Rings

Ligand LPE A 2014



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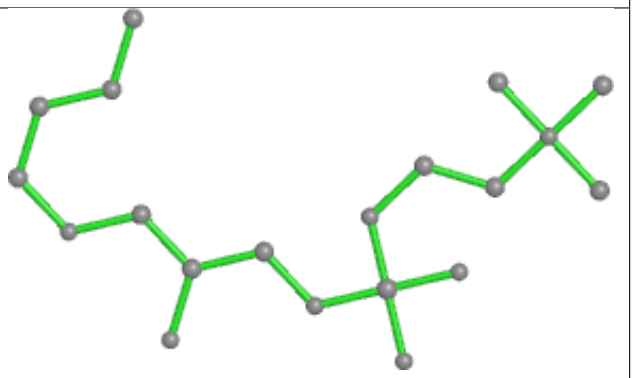
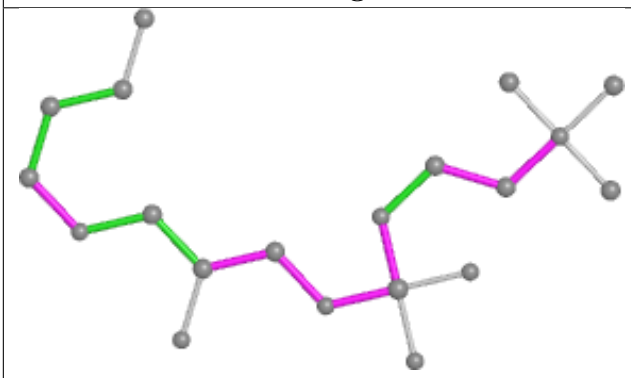


Bond angles



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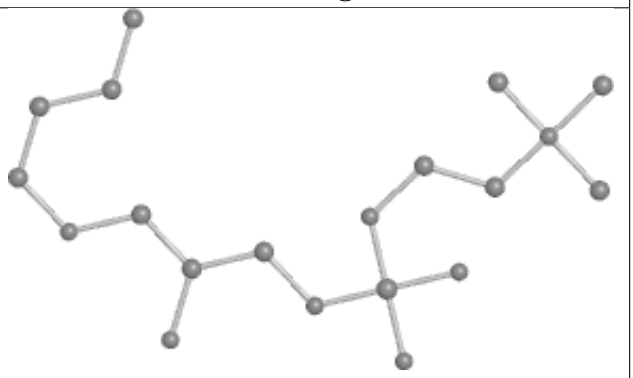
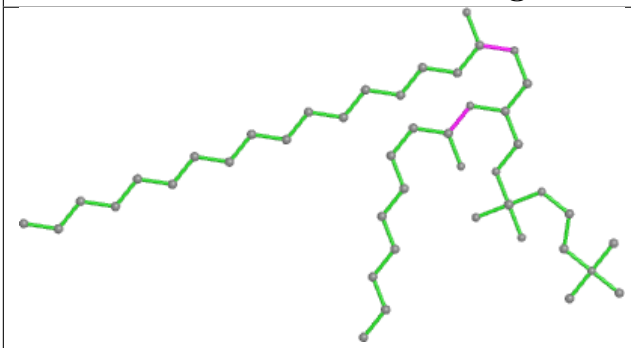


Rings

Ligand PCW A 2020



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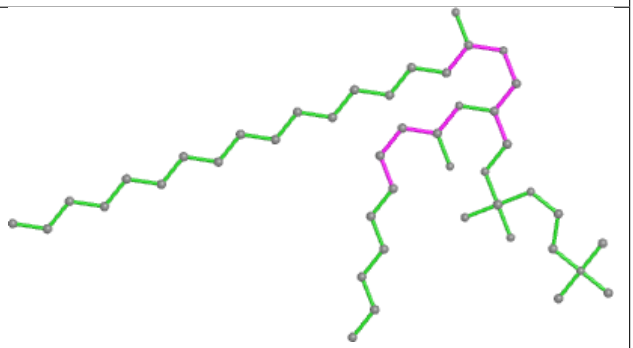
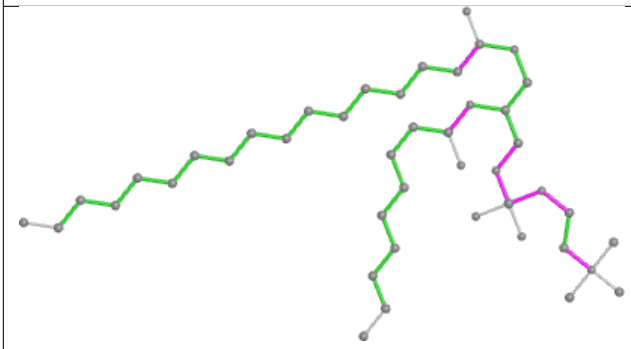


Bond angles



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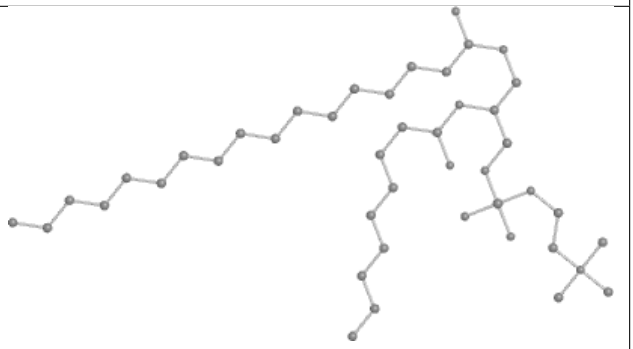
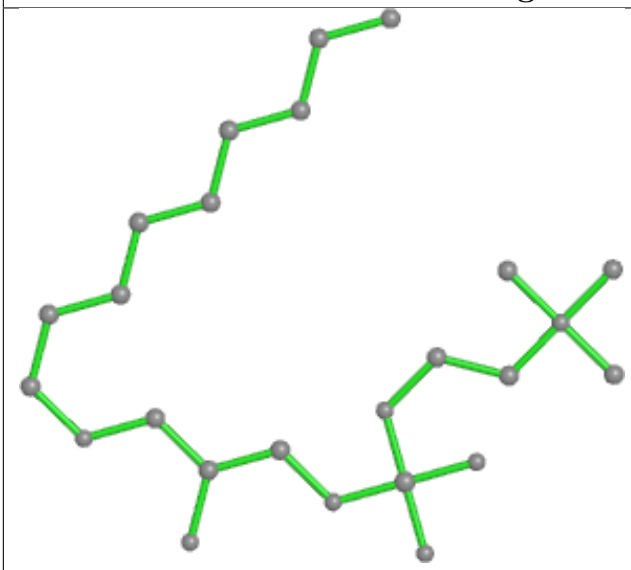


Rings

Ligand LPE A 2022



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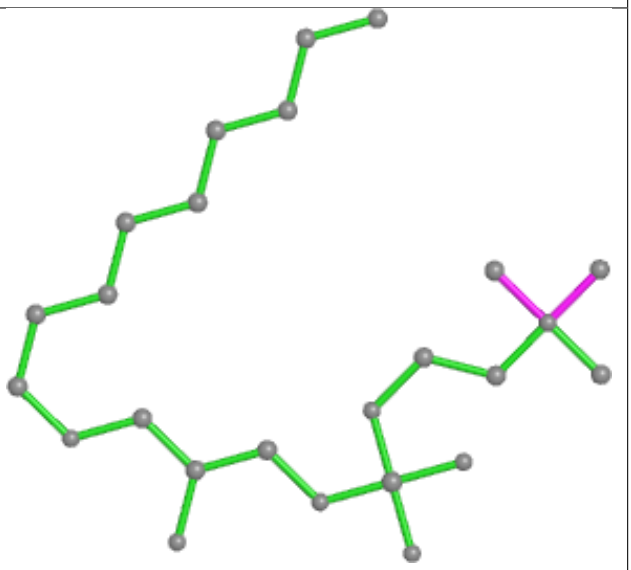

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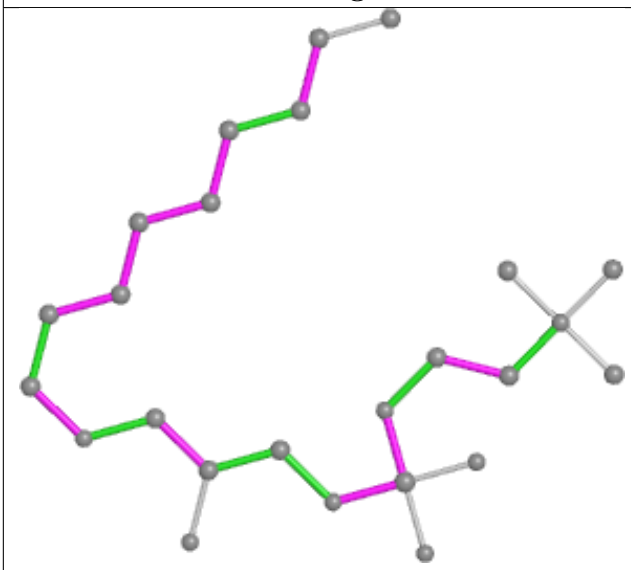
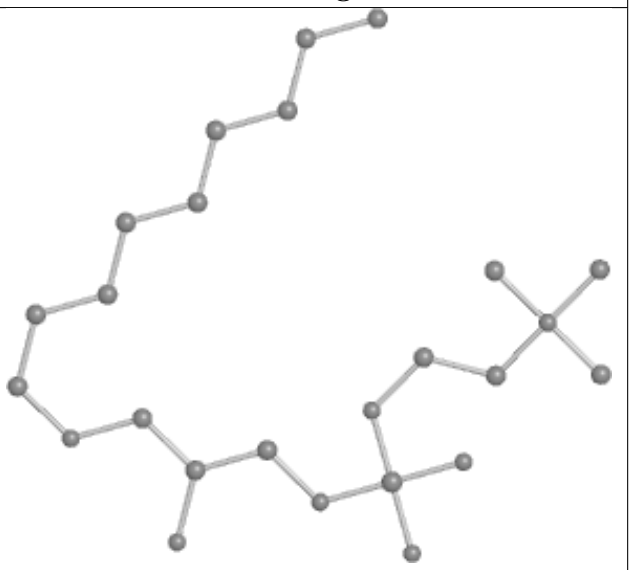
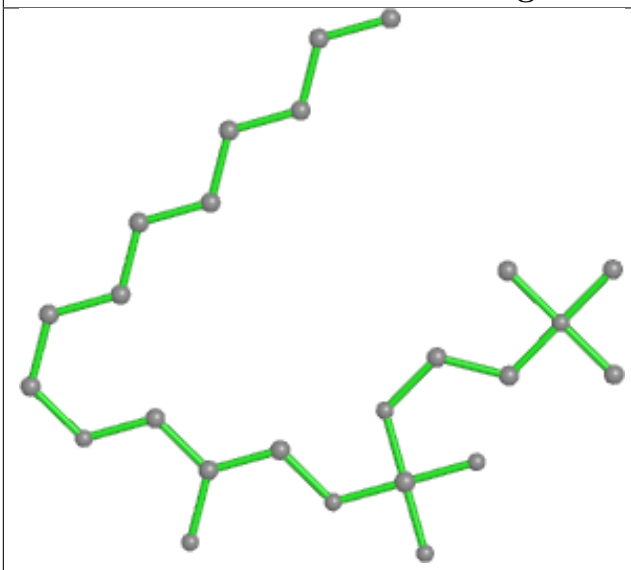


Torsions



Rings

Ligand LPE A 2011



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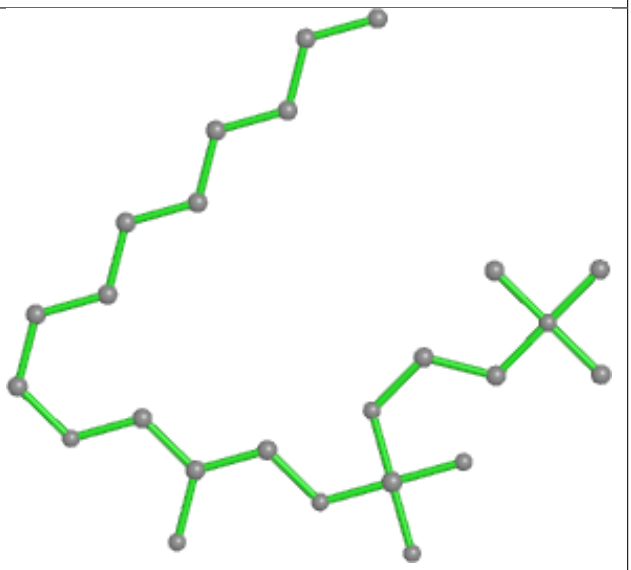
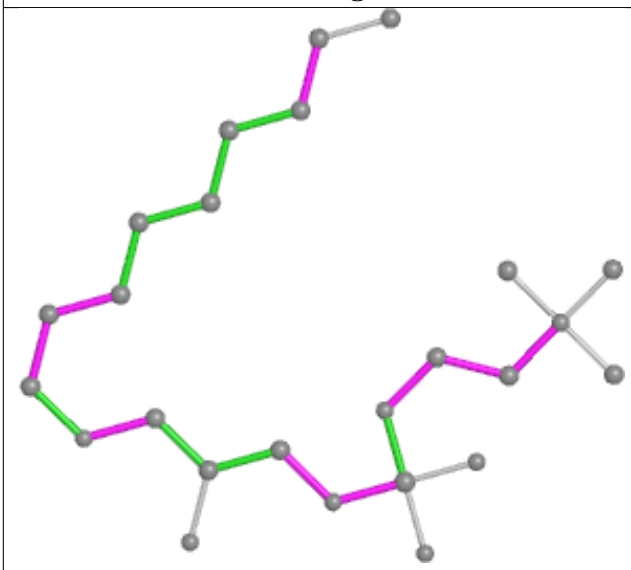


Bond angles



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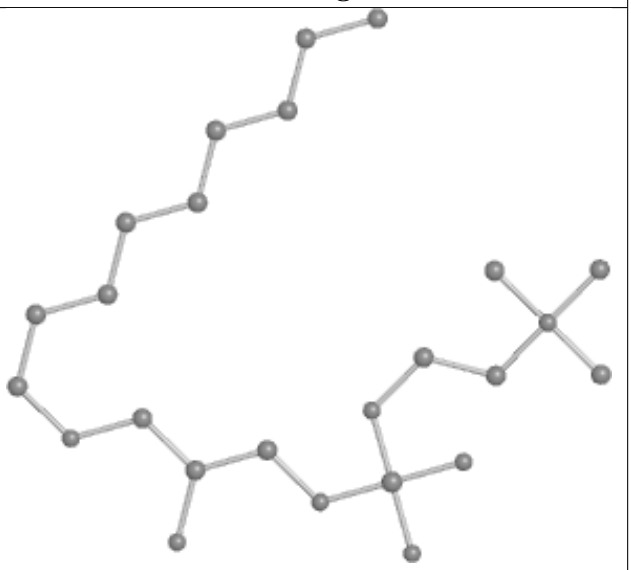
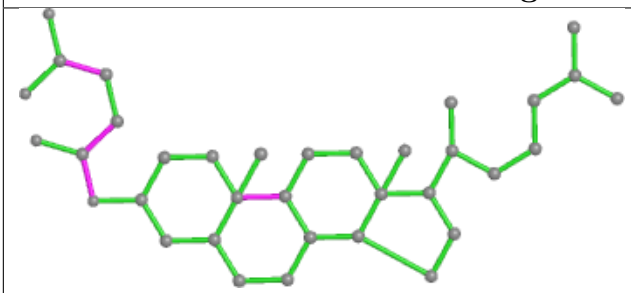


Rings

Ligand Y01 A 2005



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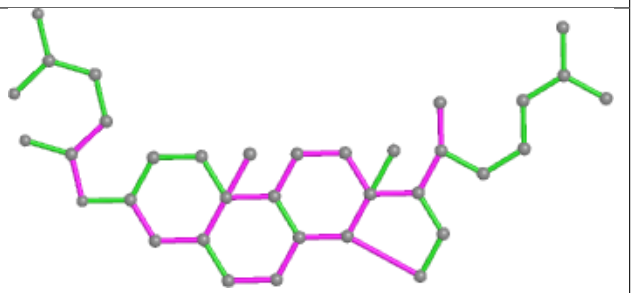
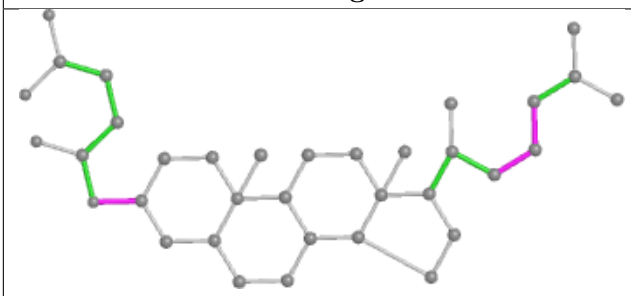


Bond angles



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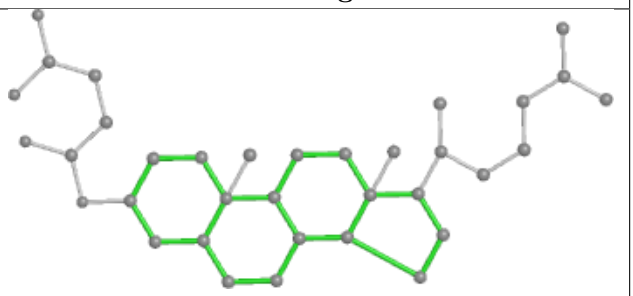
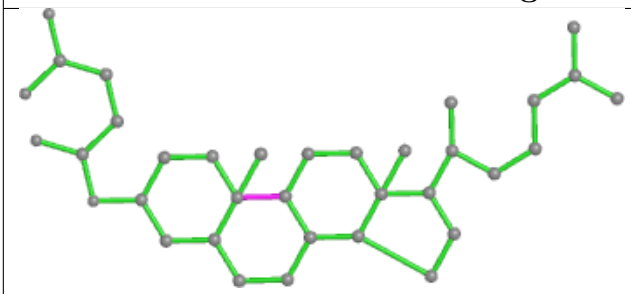


Rings

Ligand Y01 A 2003



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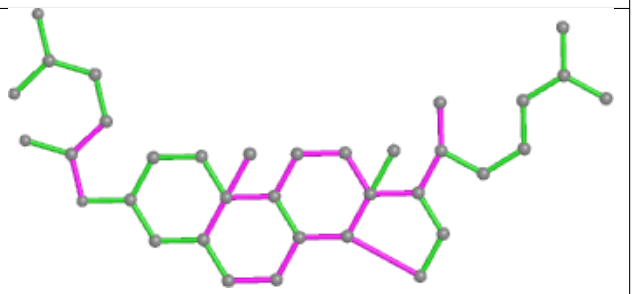
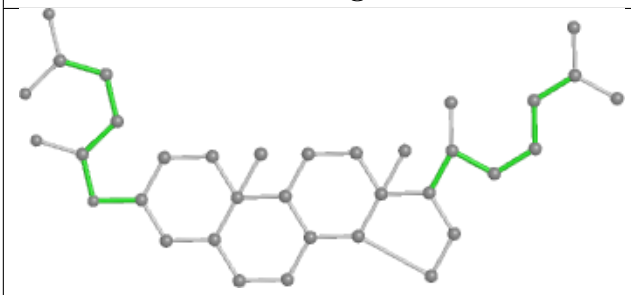


Bond angles



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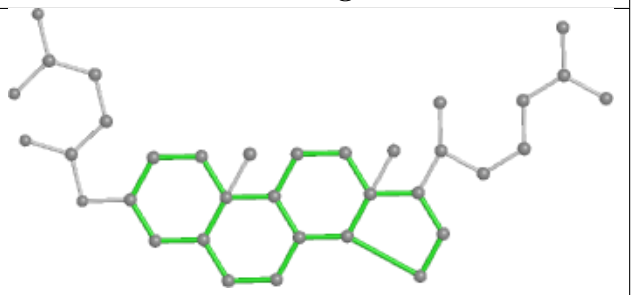
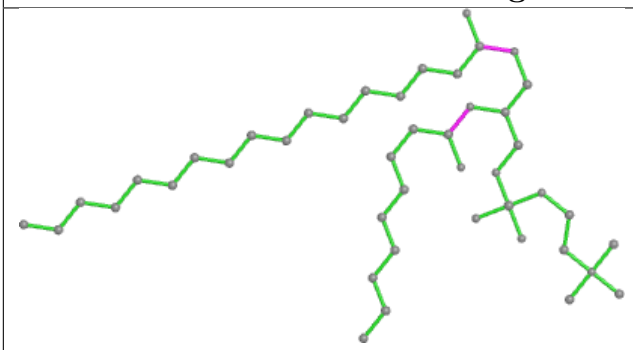
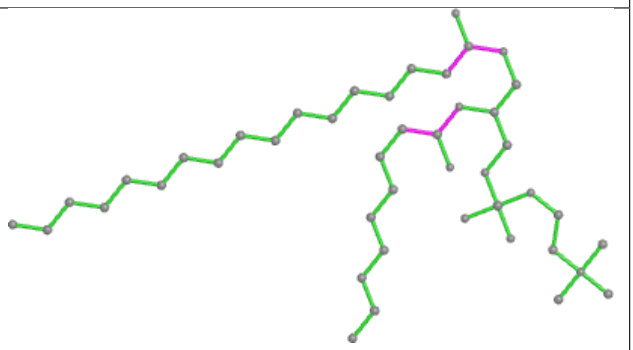


Rings

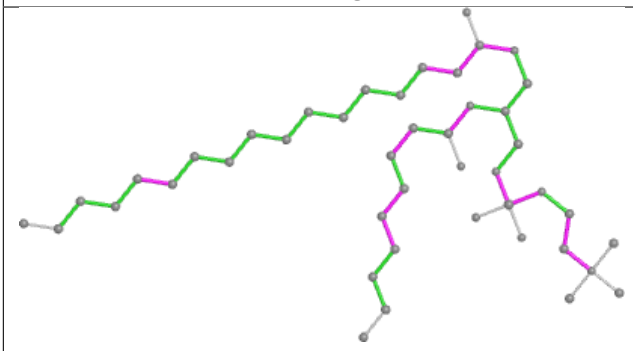
Ligand PCW A 2029



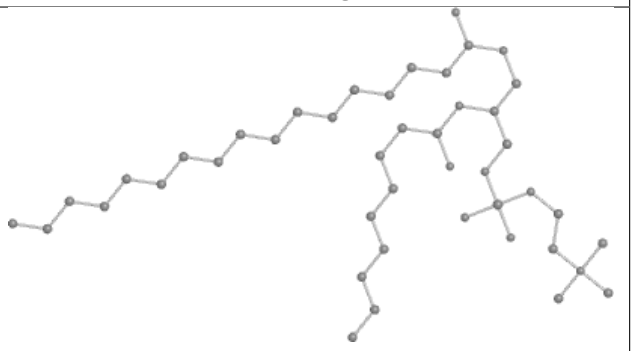
Bond lengths



Bond angles

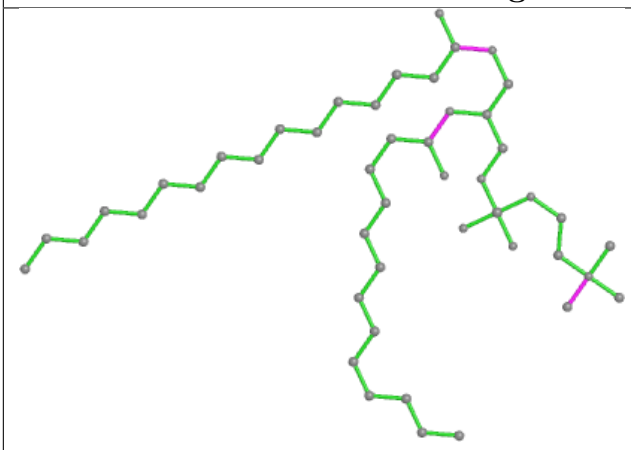


Torsions

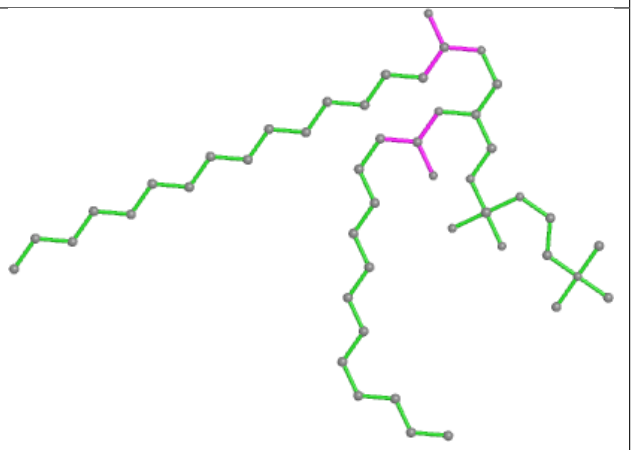


Rings

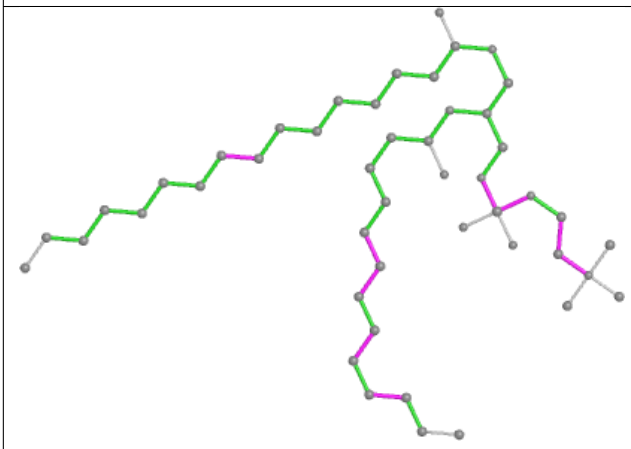
Ligand PCW A 2018



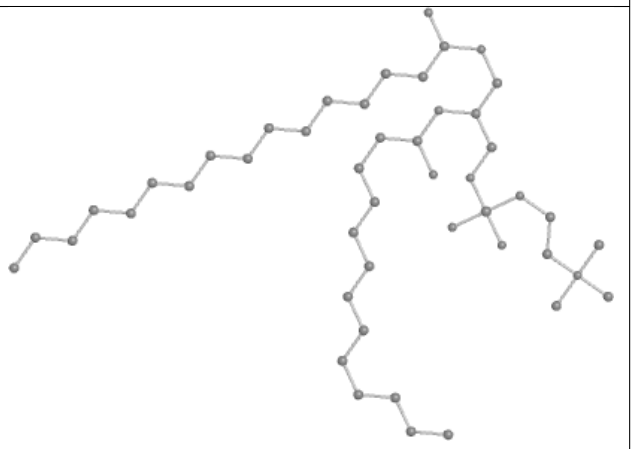
Bond lengths



Bond angles

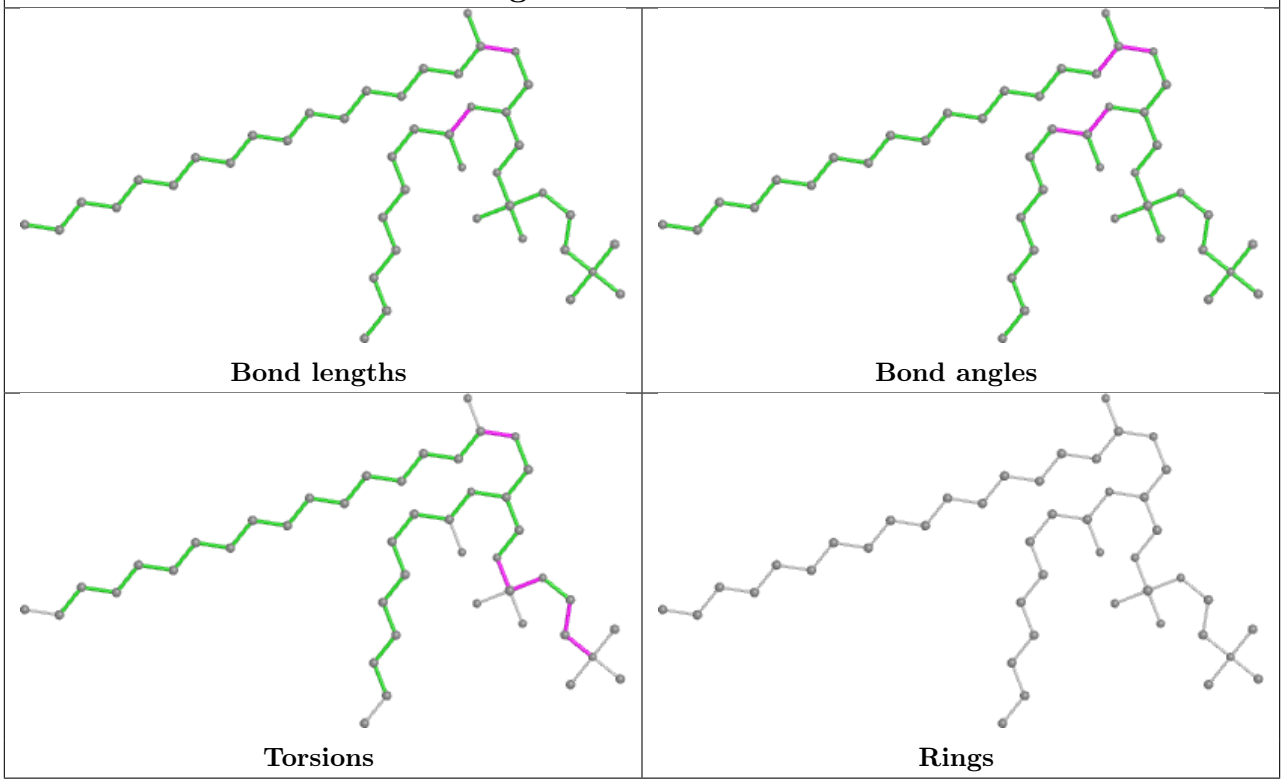


Torsions

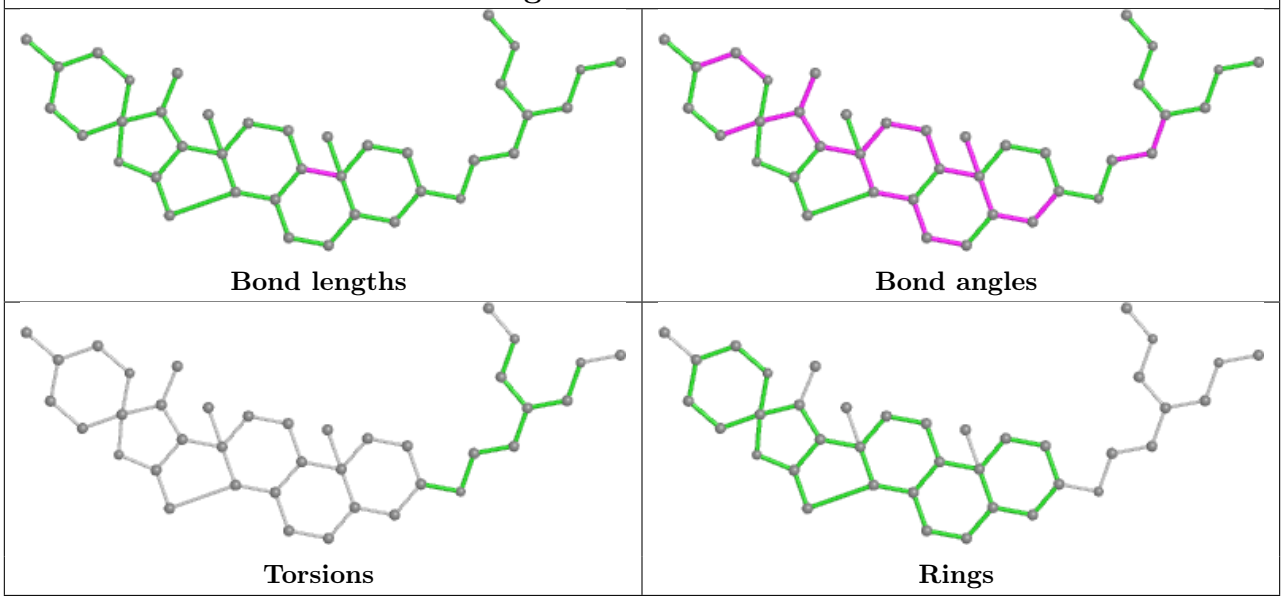


Rings

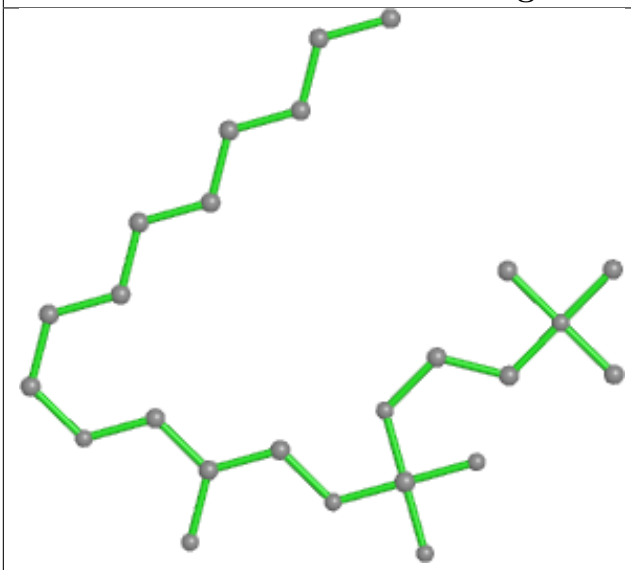
Ligand PCW A 2030



Ligand 9Z9 A 2006



Ligand LPE A 2026



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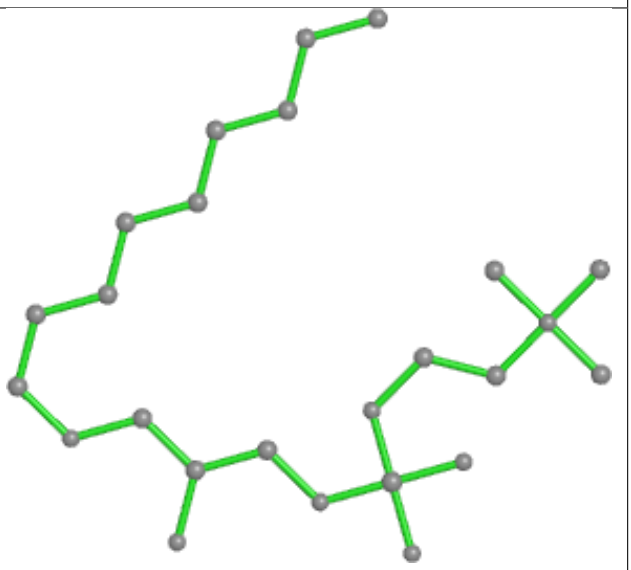
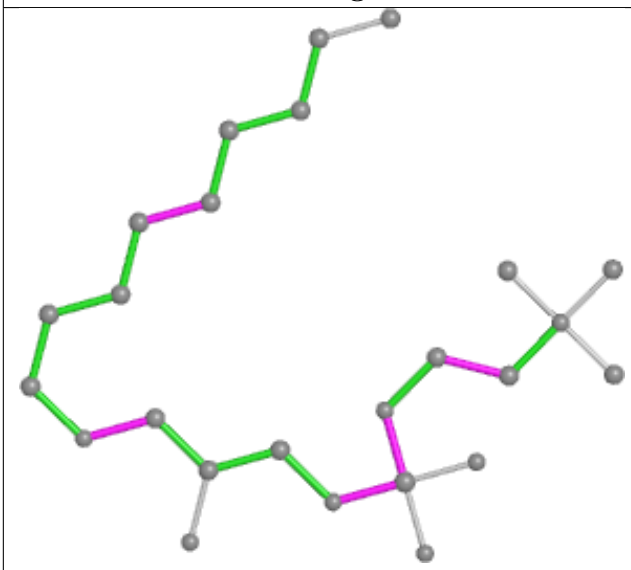


Bond angles



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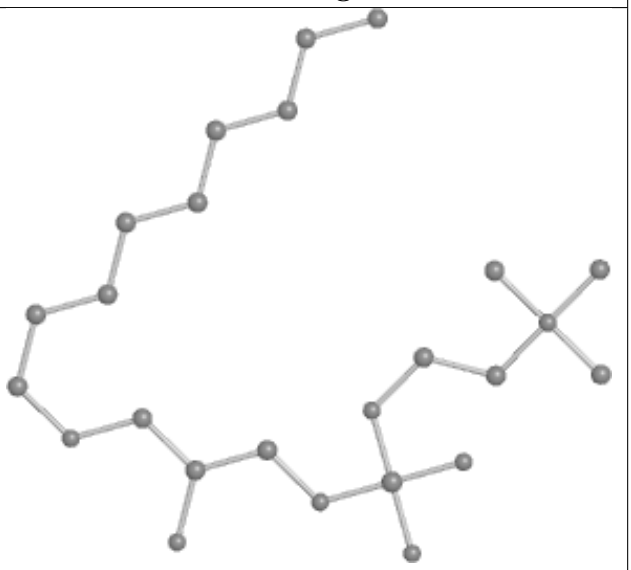
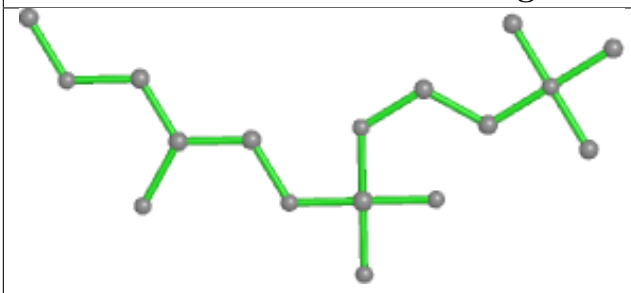
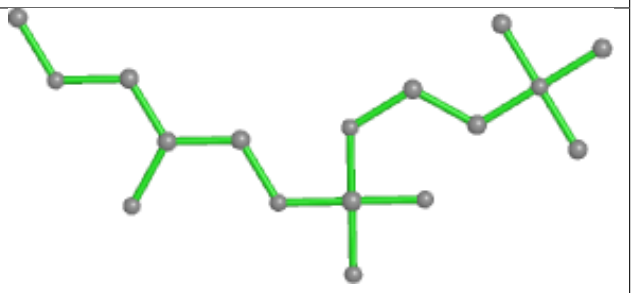


Rings

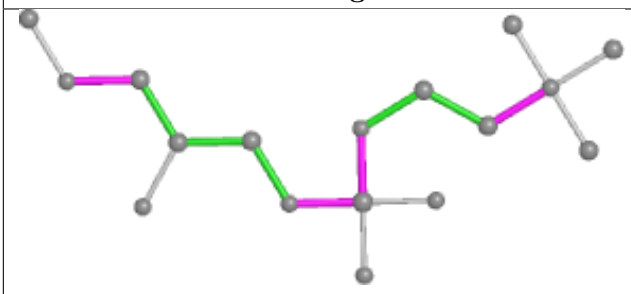
Ligand LPE A 2028



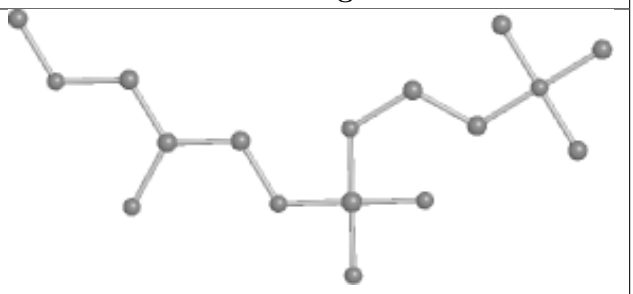
Bond lengths



Bond angles

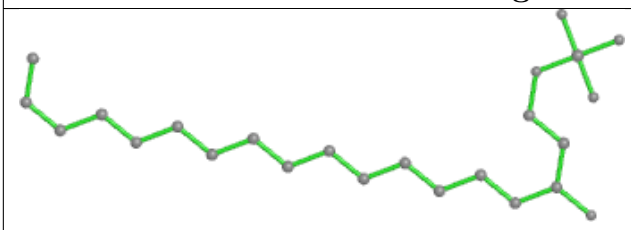


Torsions

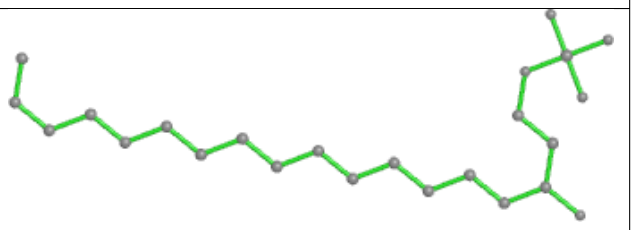


Rings

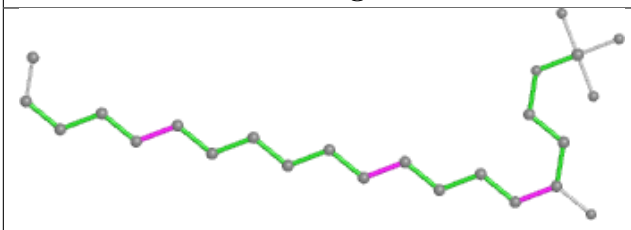
Ligand 1PW A 2013



Bond lengths



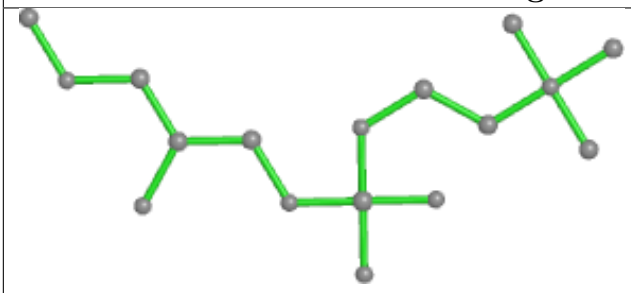
Bond angles



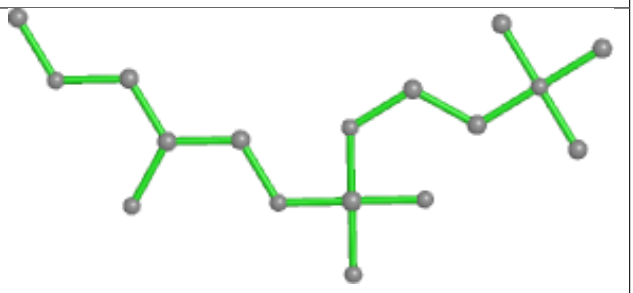
Torsions

Rings

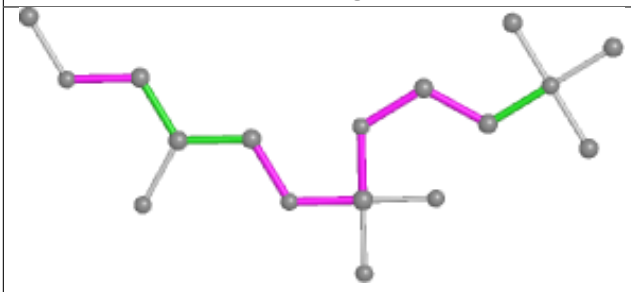
Ligand LPE B 304



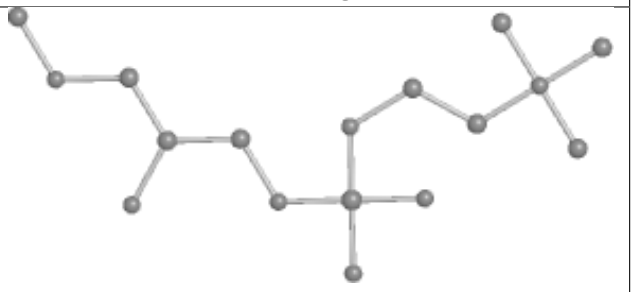
Bond lengths



Bond angles

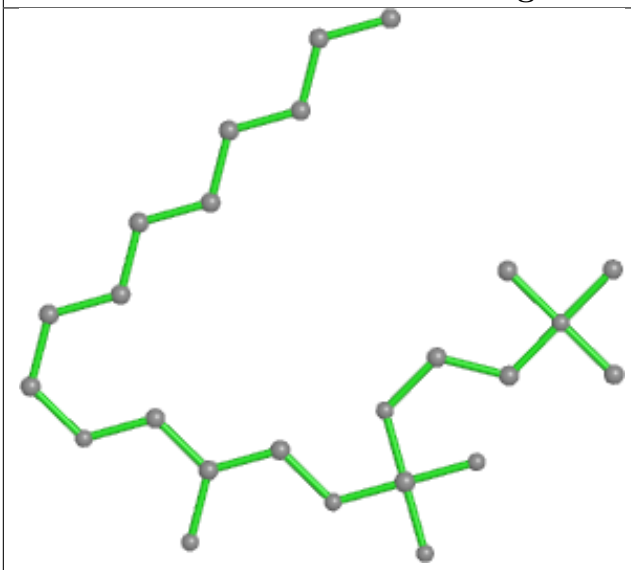


Torsions

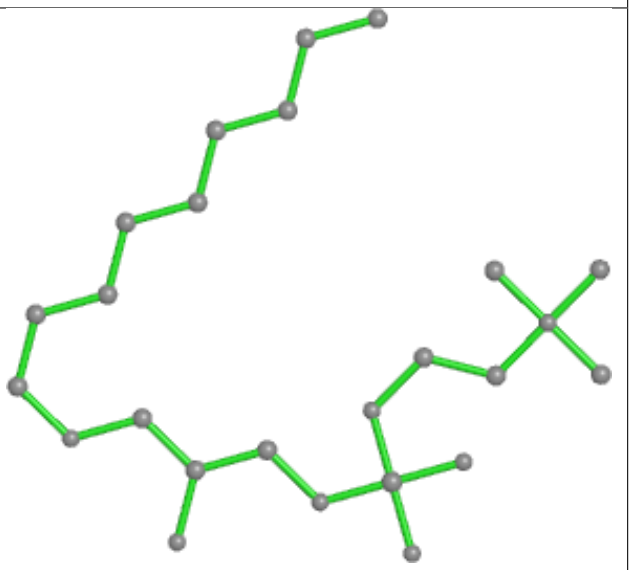


Rings

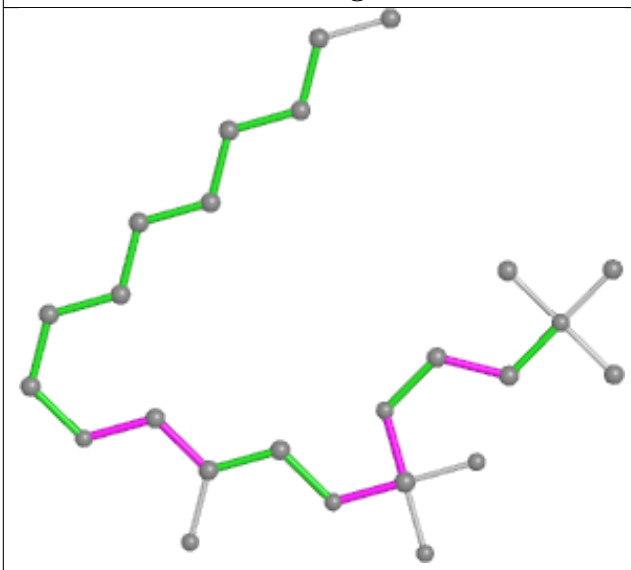
Ligand LPE A 2027



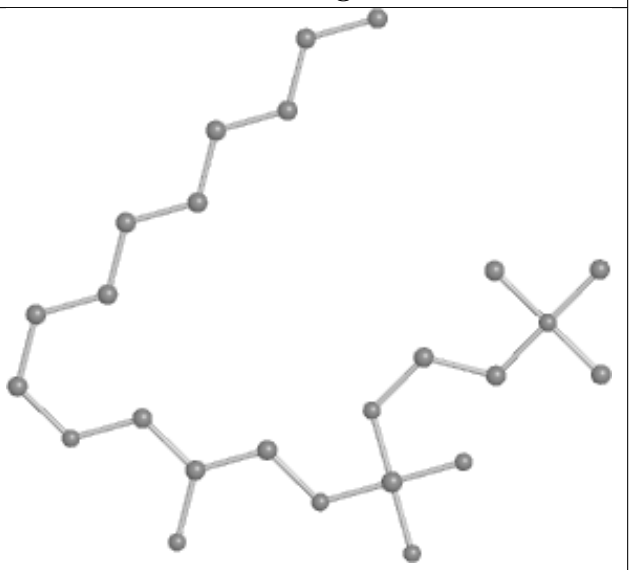
Bond lengths



Bond angles

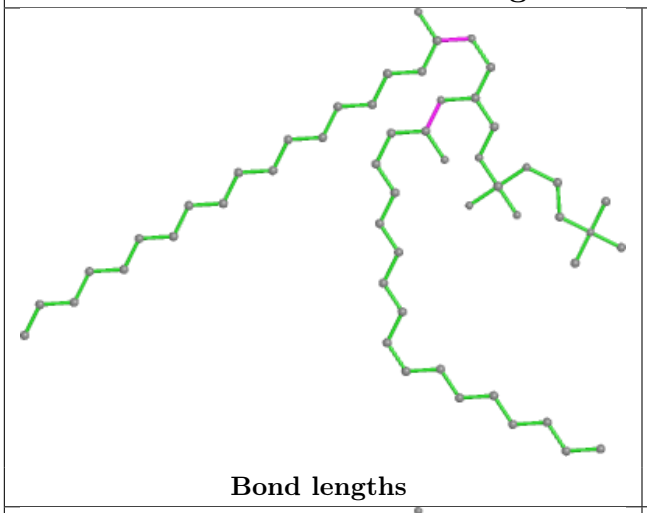


Torsions

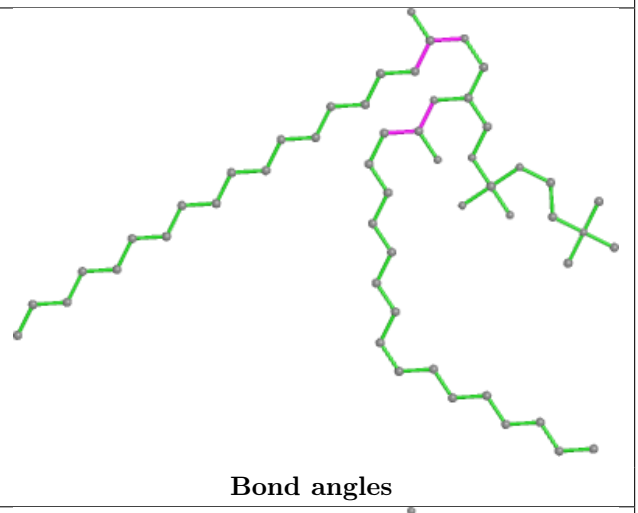


Rings

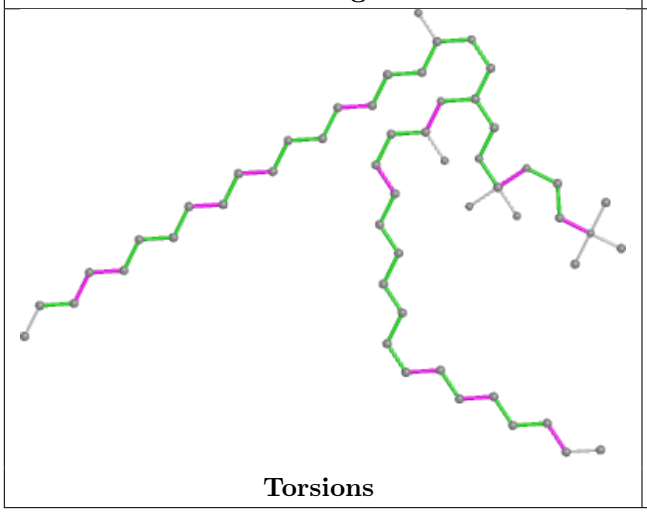
Ligand PCW A 2015



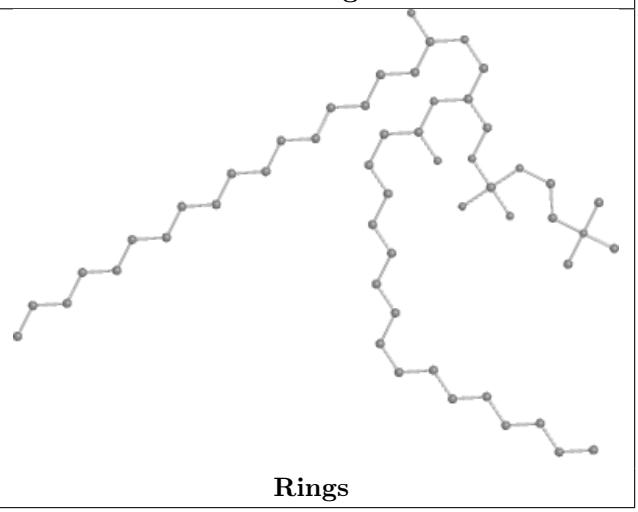
Bond lengths



Bond angles

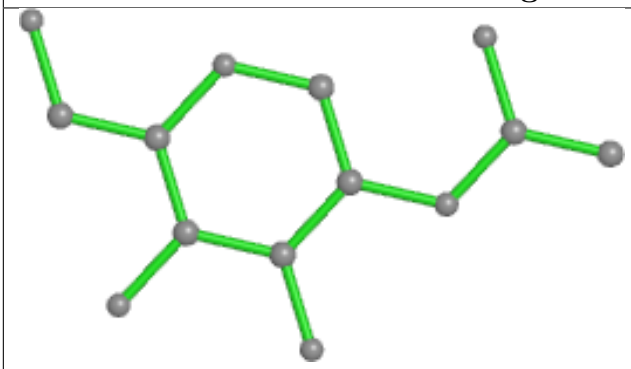


Torsions

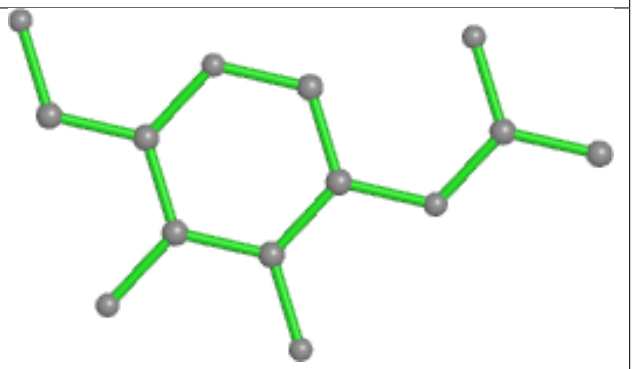


Rings

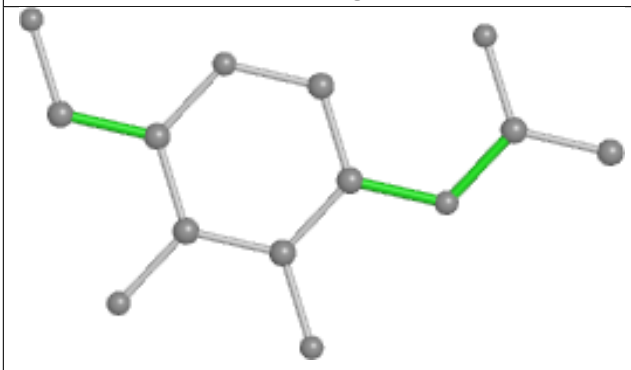
Ligand NAG B 303



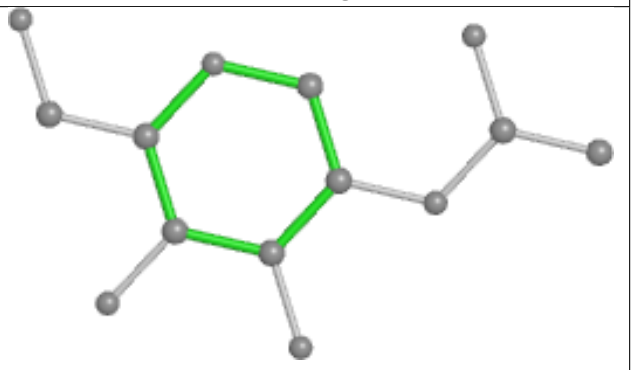
Bond lengths



Bond angles

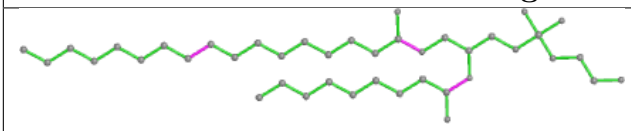


Torsions

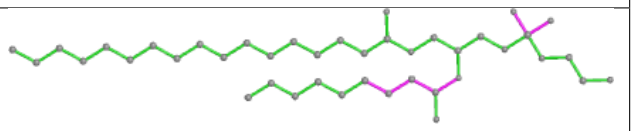


Rings

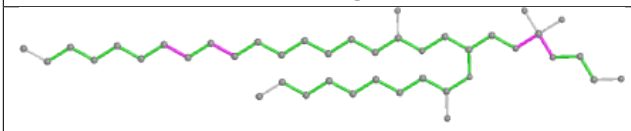
Ligand P5S A 2019



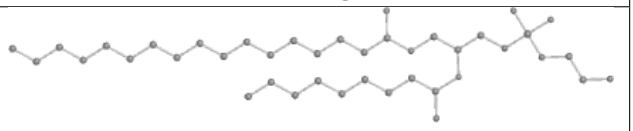
Bond lengths



Bond angles

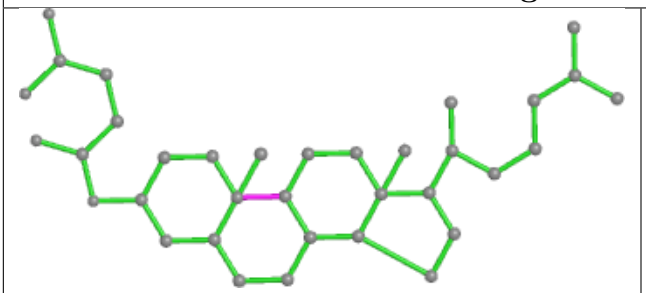


Torsions

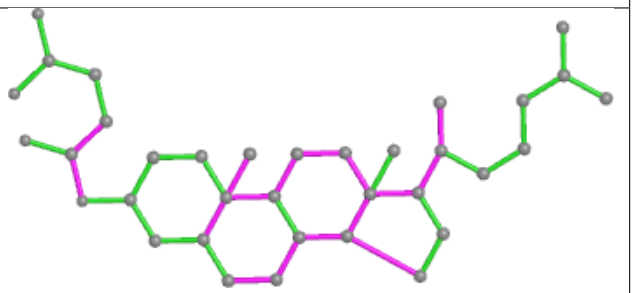


Rings

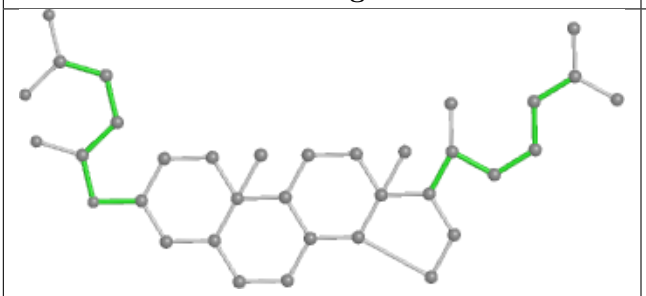
Ligand Y01 A 2004



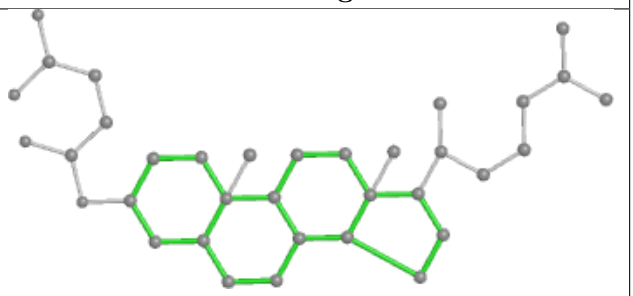
Bond lengths



Bond angles

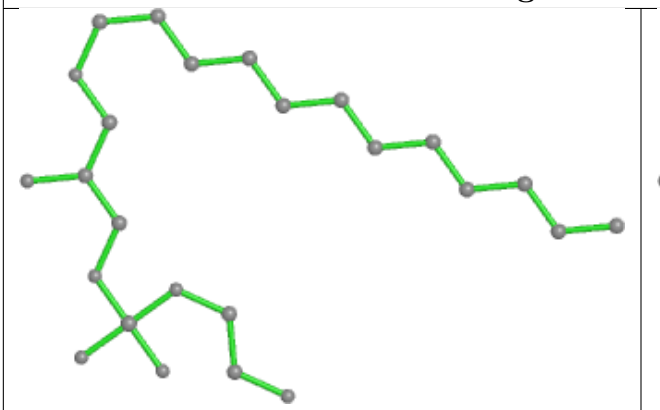


Torsions

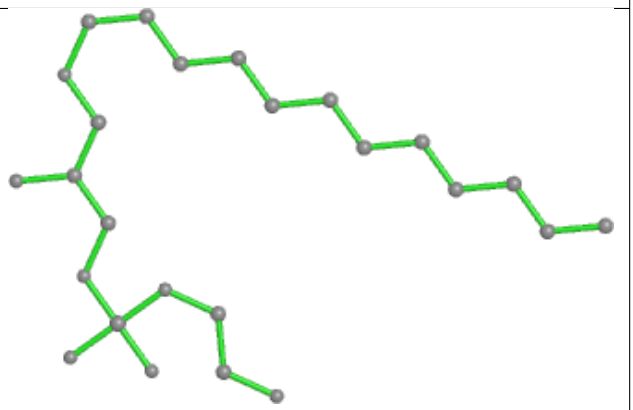


Rings

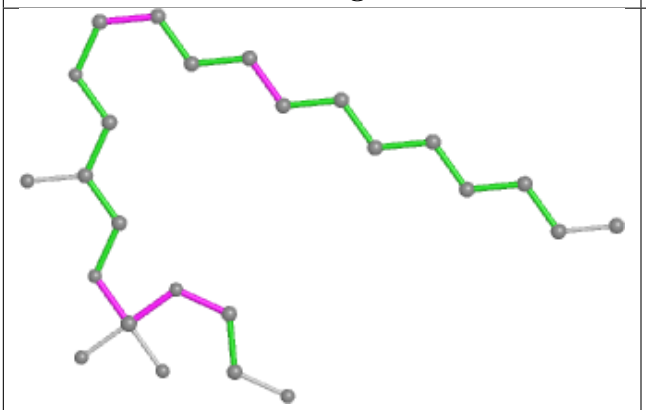
Ligand LPE A 2012



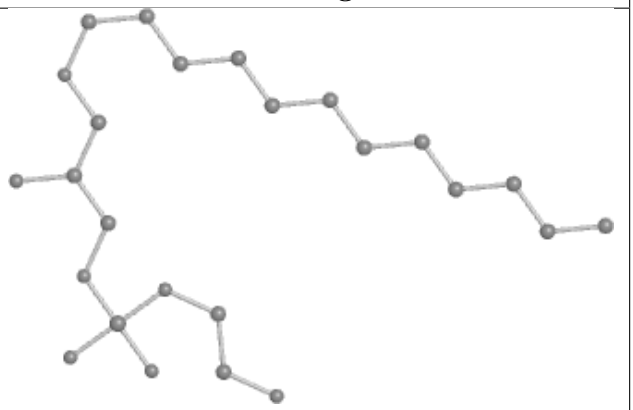
Bond lengths



Bond angles

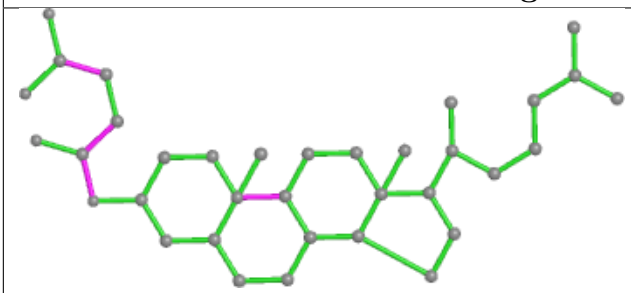


Torsions

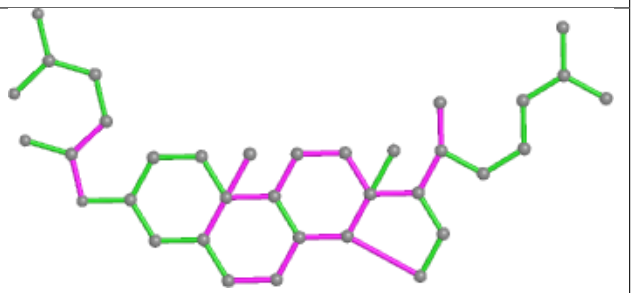


Rings

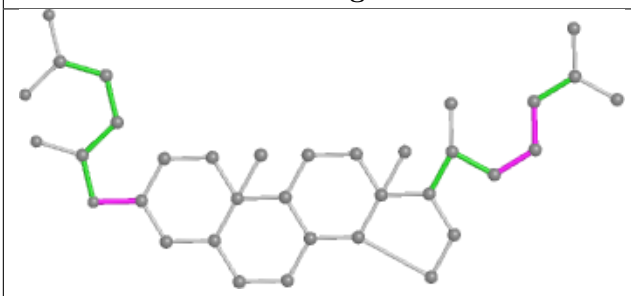
Ligand Y01 A 2009



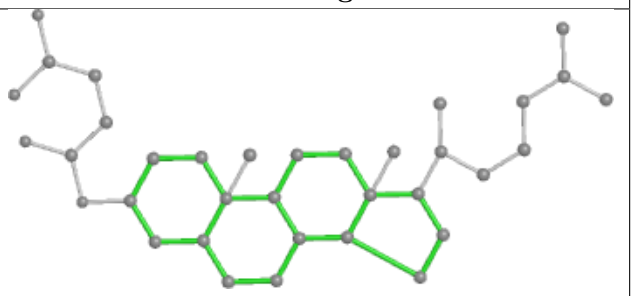
Bond lengths



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.

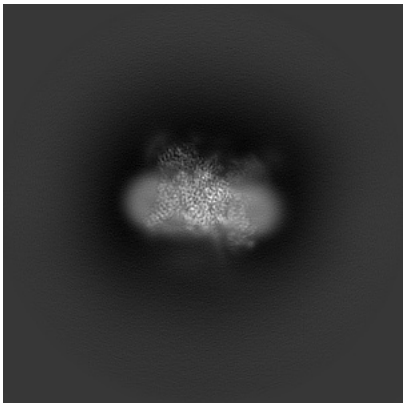
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-32368. These allow visual inspection of the internal detail of the map and identification of artifacts.

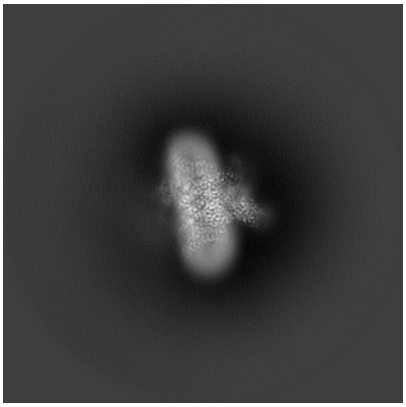
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

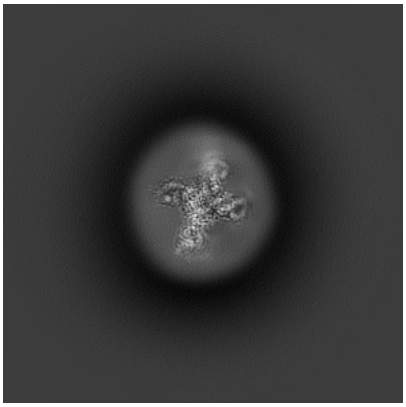
6.1.1 Primary map



X



Y

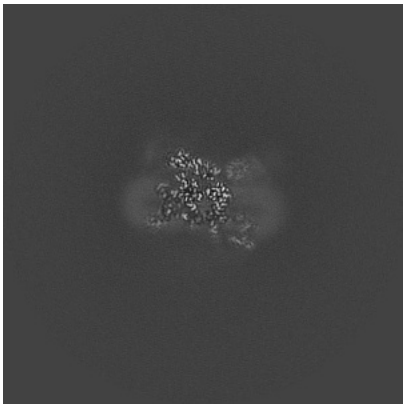


Z

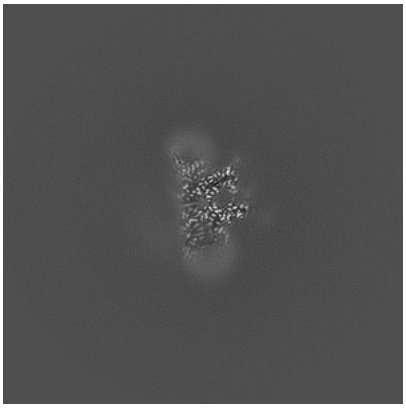
The images above show the map projected in three orthogonal directions.

6.2 Central slices

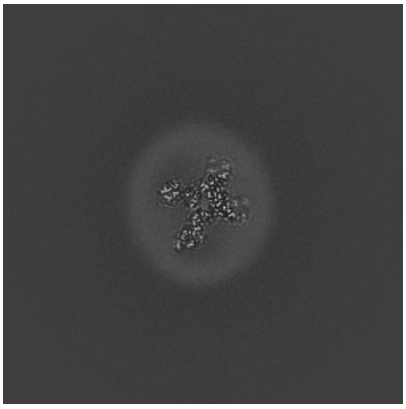
6.2.1 Primary map



X Index: 192



Y Index: 192

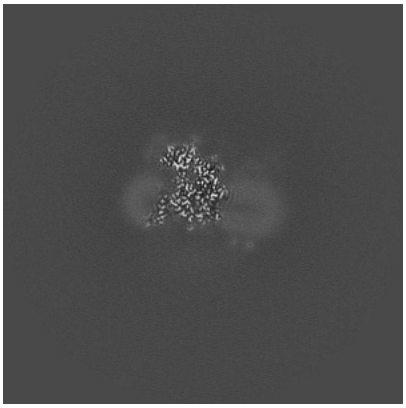


Z Index: 192

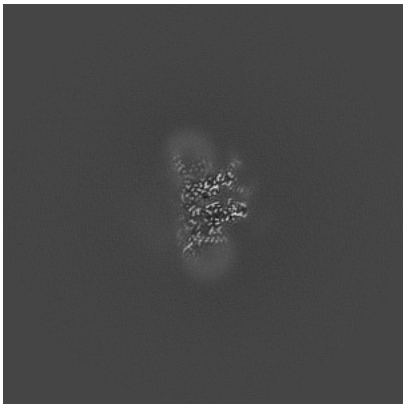
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

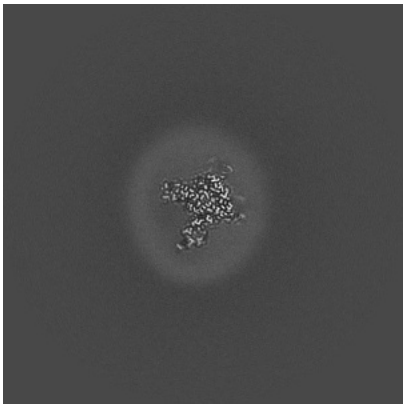
6.3.1 Primary map



X Index: 183



Y Index: 196



Z Index: 198

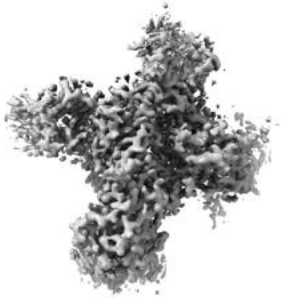
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

6.4.1 Primary map

X

Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.022. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

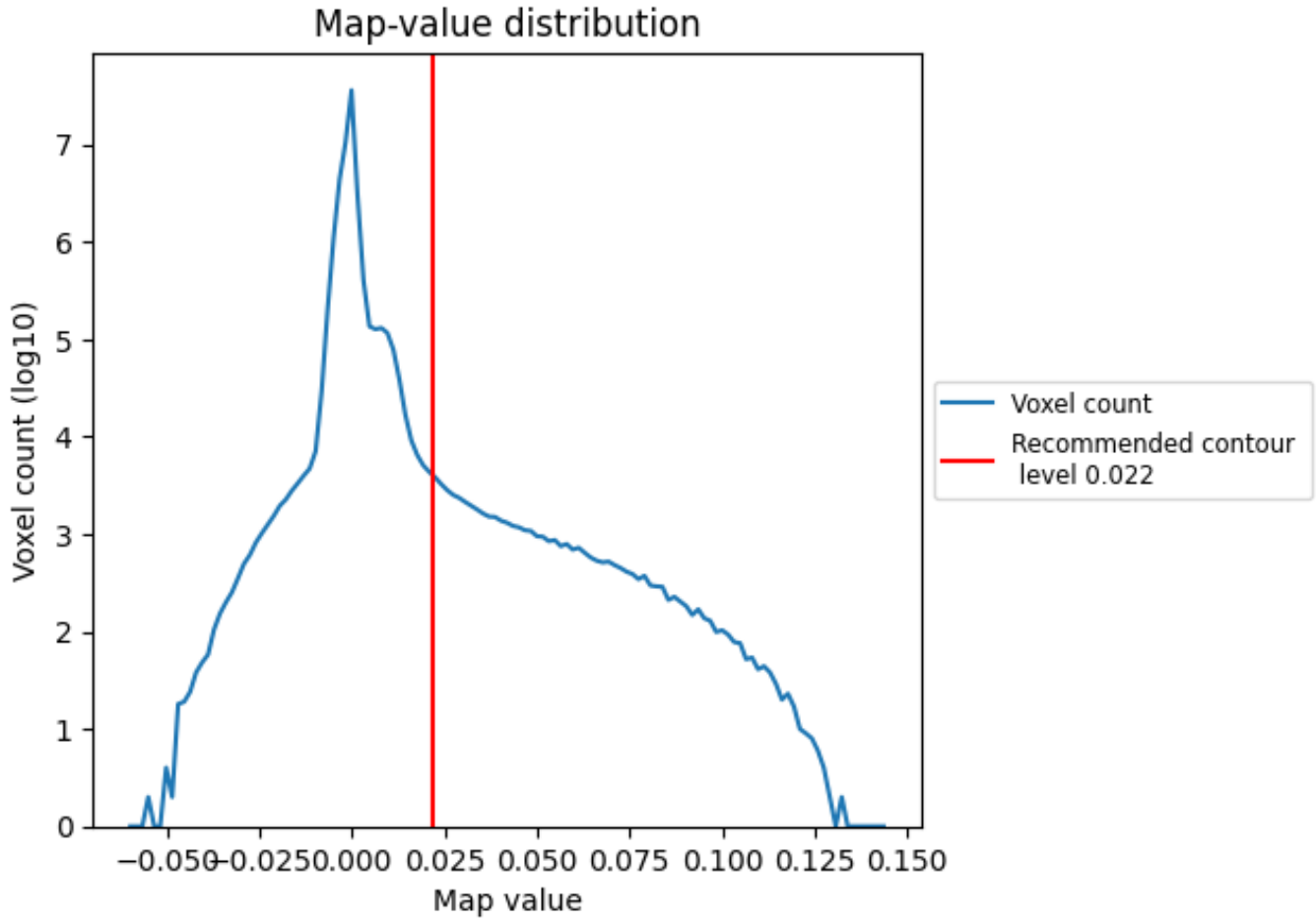
6.5 Mask visualisation (i)

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

7 Map analysis

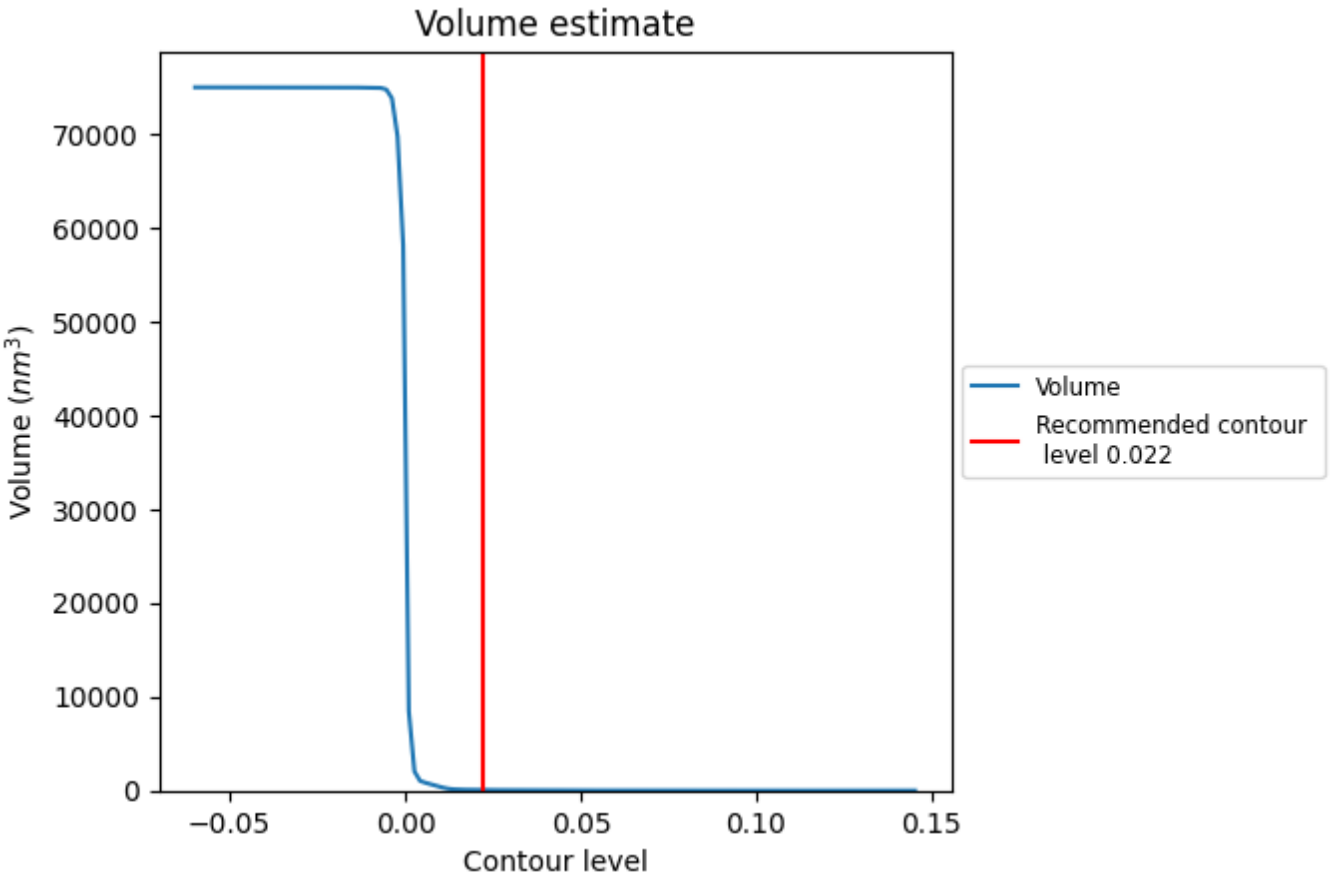
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

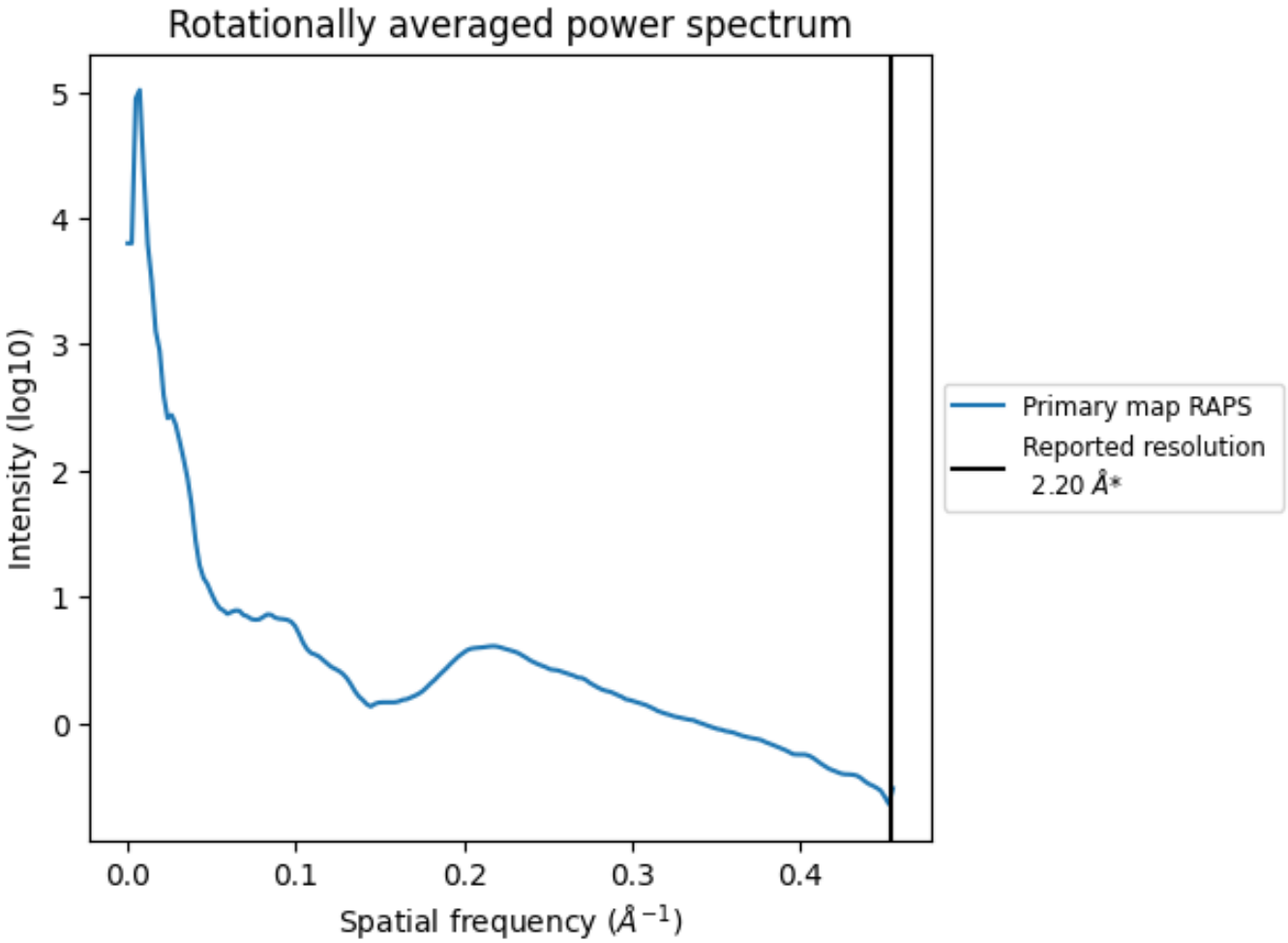
7.2 Volume estimate (i)



The volume at the recommended contour level is 65 nm^3; this corresponds to an approximate mass of 58 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)



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

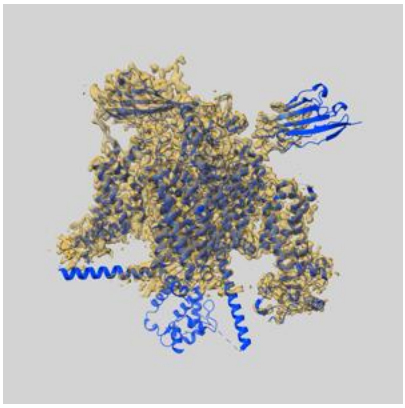
8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

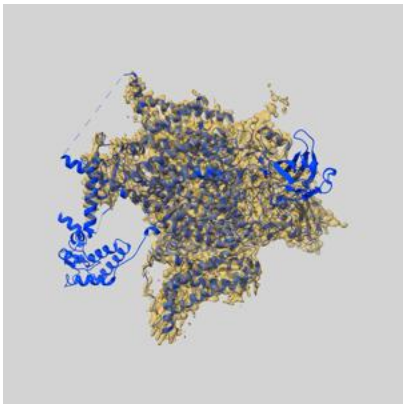
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-32368 and PDB model 7W9K. Per-residue inclusion information can be found in section 3 on page 11.

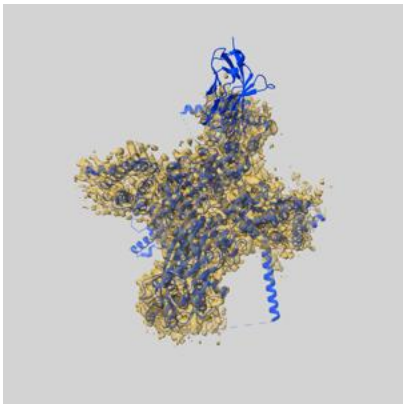
9.1 Map-model overlay



X



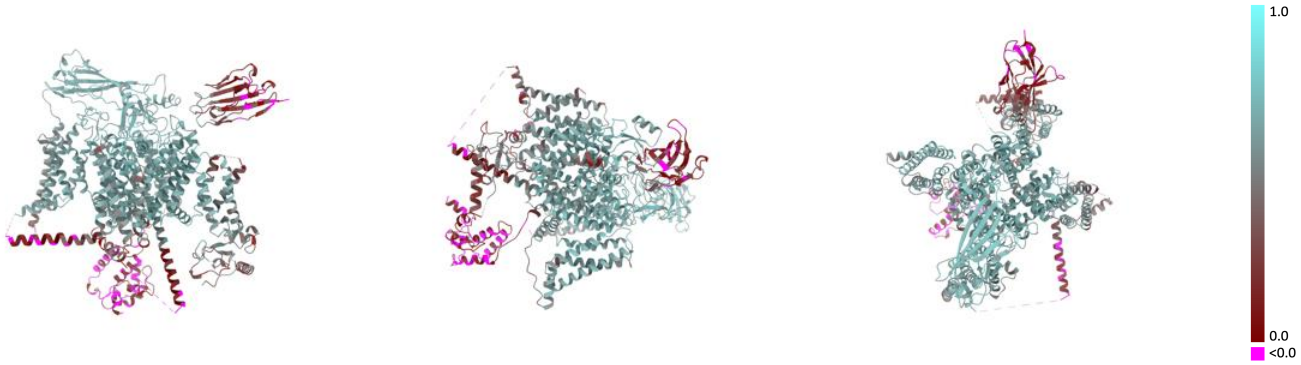
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.022 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

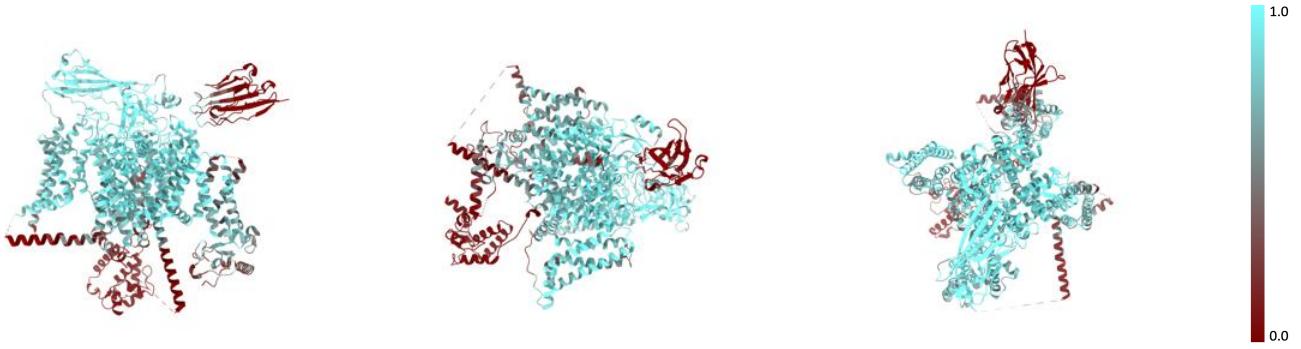
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

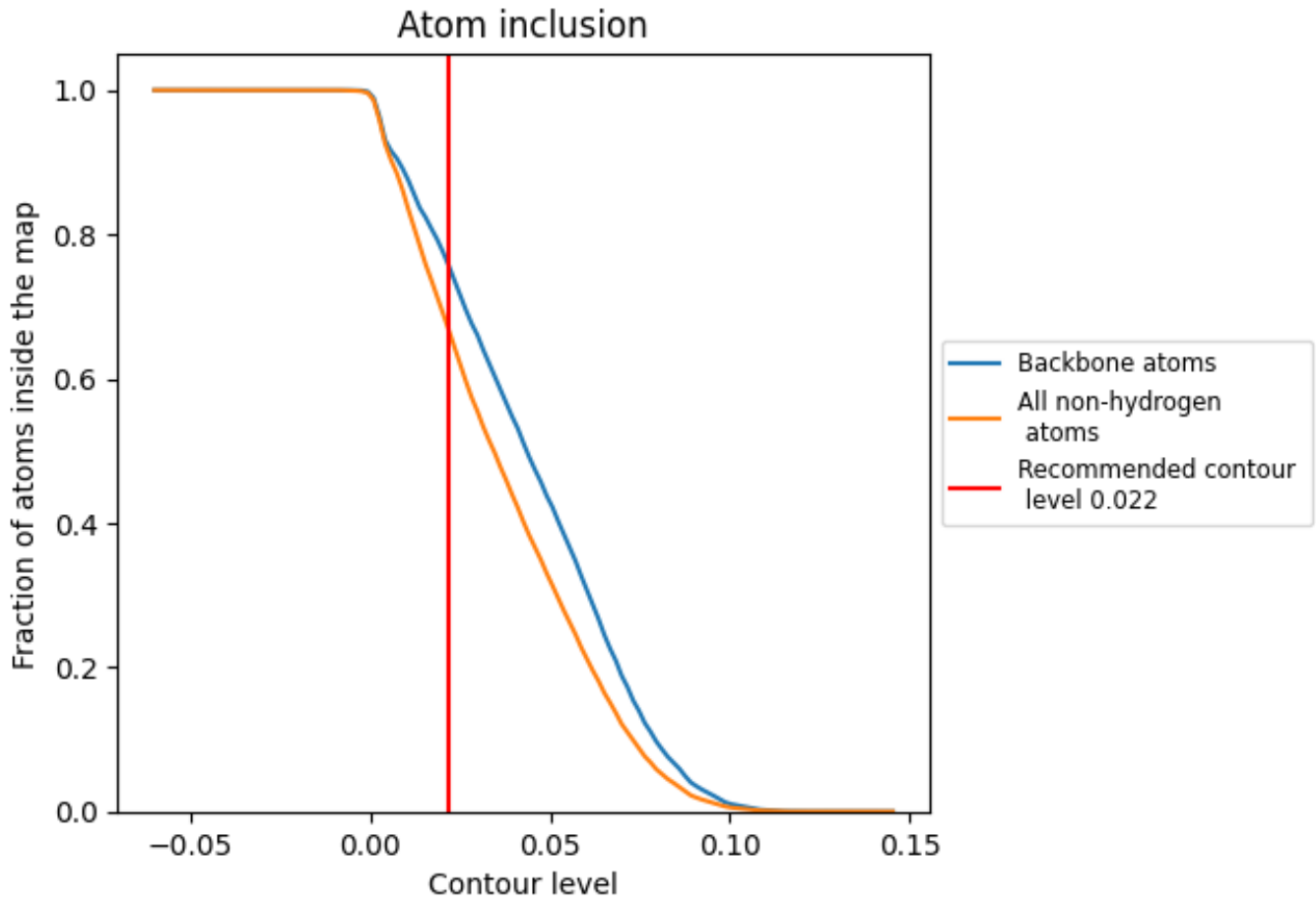
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.022).

9.4 Atom inclusion (i)



At the recommended contour level, 76% of all backbone atoms, 67% 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 (0.022) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6660	0.5070
A	0.6842	0.5180
B	0.8587	0.6100
C	0.1441	0.2110
D	0.5000	0.4100
E	0.7143	0.4790
F	0.9286	0.6380