Full wwPDB EM Validation Report ⓘ

Nov 13, 2022 – 07:42 PM EST

PDB ID	:	6WLW
EMDB ID	:	EMD-21844
Title	:	The Vo region of human V-ATPase in state 1 (focused refinement)
Authors	:	Wang, L.; Wu, H.; Fu, T.-M.
Deposited on	:	2020-04-20
Resolution	:	3.00 Å(reported)

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

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

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

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

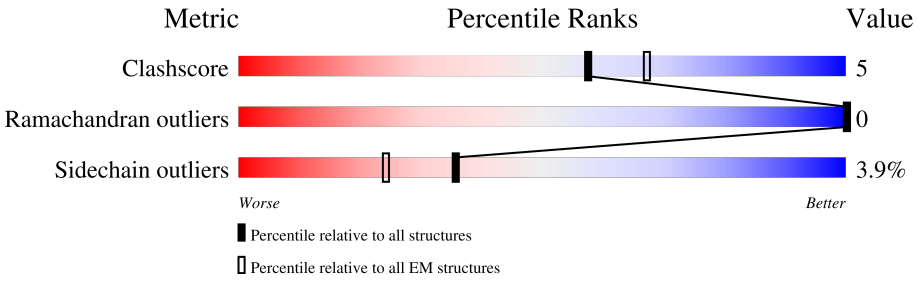
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 3.00 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
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	0	205	88% 11%
2	1	155	85% 12%
2	2	155	89% 8%
2	3	155	88% 8%
2	4	155	89% 7%
2	5	155	86% 11%
2	6	155	90% 6%
2	7	155	91% 6%

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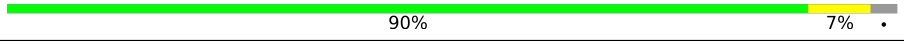
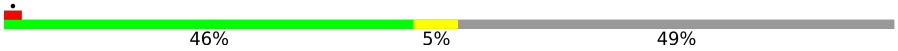
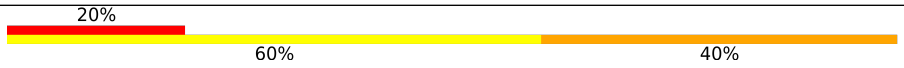
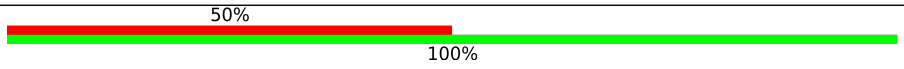
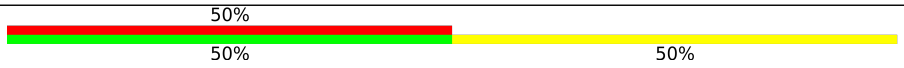
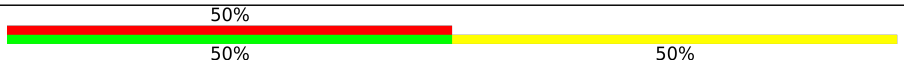
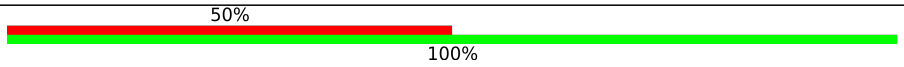
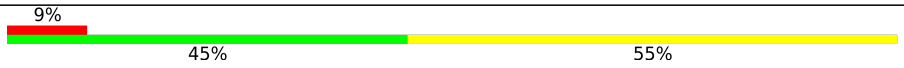
Mol	Chain	Length	Quality of chain
2	8	155	
2	9	155	
3	Q	351	
4	R	837	
5	S	81	
6	T	137	
7	U	470	
8	V	350	
9	W	5	
10	A	4	
11	B	2	
11	C	2	
11	D	2	
11	s	2	
11	u	2	
12	r	11	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	NGA	A	2	X	-	-	-
12	MAN	r	11	X	-	-	-
14	PTY	0	306	X	-	-	-
14	PTY	R	903	X	-	-	-

2 Entry composition

There are 19 unique types of molecules in this entry. The entry contains 22145 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 V-type proton ATPase 21 kDa proteolipid subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	204	Total	C	N	O	S	0	0
			1495	988	238	259	10		

- Molecule 2 is a protein called V-type proton ATPase 16 kDa proteolipid subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	150	Total	C	N	O	S	0	0
			1065	698	169	191	7		
2	2	150	Total	C	N	O	S	0	0
			1065	698	169	191	7		
2	3	150	Total	C	N	O	S	0	0
			1065	698	169	191	7		
2	4	150	Total	C	N	O	S	0	0
			1065	698	169	191	7		
2	5	150	Total	C	N	O	S	0	0
			1065	698	169	191	7		
2	6	150	Total	C	N	O	S	0	0
			1065	698	169	191	7		
2	7	150	Total	C	N	O	S	0	0
			1059	695	166	191	7		
2	8	150	Total	C	N	O	S	0	0
			1065	698	169	191	7		
2	9	150	Total	C	N	O	S	0	0
			1065	698	169	191	7		

- Molecule 3 is a protein called V-type proton ATPase subunit d 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	Q	350	Total	C	N	O	S	0	0
			2829	1825	461	530	13		

- Molecule 4 is a protein called V-type proton ATPase 116 kDa subunit a isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	R	428	Total	C	N	O	S	0	0
			3477	2335	542	578	22		

- Molecule 5 is a protein called V-type proton ATPase subunit e 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	S	77	Total	C	N	O	S	0	0
			631	436	97	93	5		

- Molecule 6 is a protein called Ribonuclease kappa.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	T	85	Total	C	N	O	S	0	0
			654	431	101	115	7		

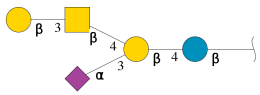
- Molecule 7 is a protein called V-type proton ATPase subunit S1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	U	205	Total	C	N	O	S	0	0
			1664	1089	265	300	10		

- Molecule 8 is a protein called Renin receptor.

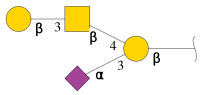
Mol	Chain	Residues	Atoms					AltConf	Trace
8	V	50	Total	C	N	O	S	0	0
			417	283	58	73	3		

- Molecule 9 is an oligosaccharide called beta-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-galactopyranose-(1-4)-[N-acetyl-alpha-neuraminic acid-(2-3)]beta-D-galactopyranose-(1-4)-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
9	W	5	Total	C	N	O	0	0
			68	37	2	29		

- Molecule 10 is an oligosaccharide called beta-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-galactopyranose-(1-4)-[N-acetyl-alpha-neuraminic acid-(2-3)]beta-D-galactopyranose.

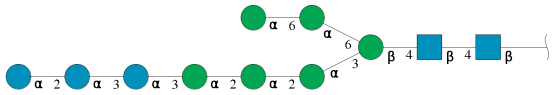


Mol	Chain	Residues	Atoms				AltConf	Trace
10	A	4	Total	C	N	O	0	0
			56	31	2	23		

- Molecule 11 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
11	s	2	Total	C	N	O	0	0
			28	16	2	10		
11	u	2	Total	C	N	O	0	0
			28	16	2	10		
11	B	2	Total	C	N	O	0	0
			28	16	2	10		
11	C	2	Total	C	N	O	0	0
			28	16	2	10		
11	D	2	Total	C	N	O	0	0
			28	16	2	10		

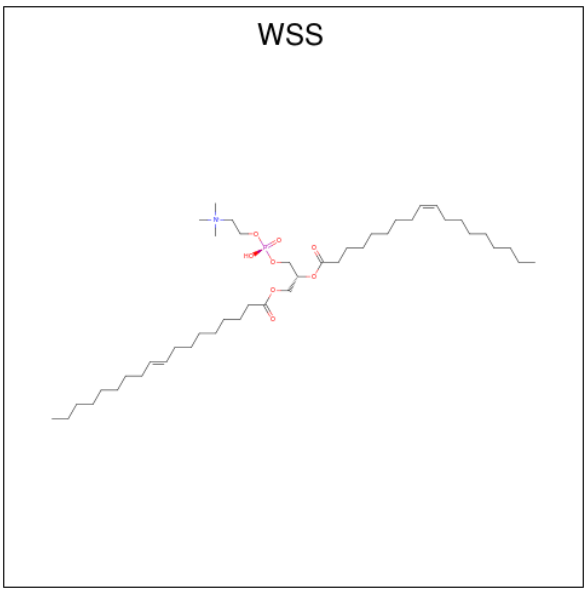
- Molecule 12 is an oligosaccharide called alpha-D-glucopyranose-(1-2)-alpha-D-glucopyranose-(1-3)-alpha-D-glucopyranose-(1-3)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
12	r	11	Total	C	N	O	0	0
			127	70	2	55		

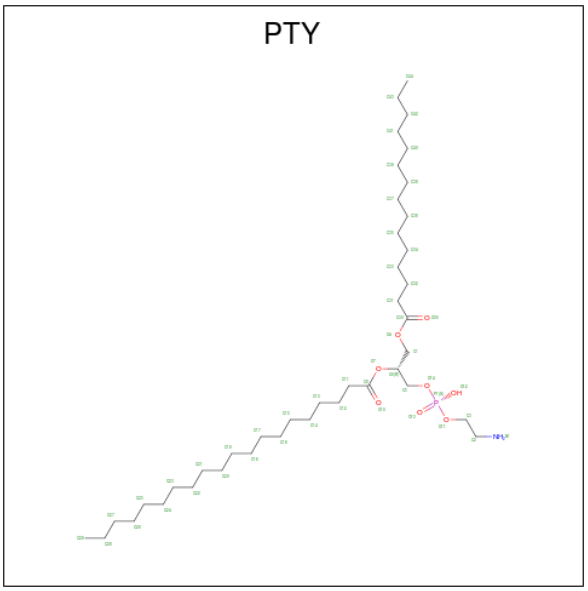
- Molecule 13 is tri(methyl)-[2-[[(2 {R})-2-[({Z})-octadec-9-enoyl]oxy-3-[({E})-1-oxidanylideneoctadec-9-enoxy]propoxy]-oxidanyl-phosphoryl]oxyethyl]azanium (three-letter code:

WSS) (formula: $C_{44}H_{85}NO_8P$).



Mol	Chain	Residues	Atoms	AltConf
13	0	1	Total C N O P 135 96 3 32 4	0
13	0	1	Total C N O P 135 96 3 32 4	0
13	0	1	Total C N O P 135 96 3 32 4	0
13	0	1	Total C N O P 135 96 3 32 4	0
13	1	1	Total C N O P 34 24 1 8 1	0
13	3	1	Total C O P 41 32 8 1	0
13	R	1	Total C N O P 40 30 1 8 1	0
13	U	1	Total C N O P 83 63 2 16 2	0
13	U	1	Total C N O P 83 63 2 16 2	0
13	V	1	Total C N O P 37 27 1 8 1	0

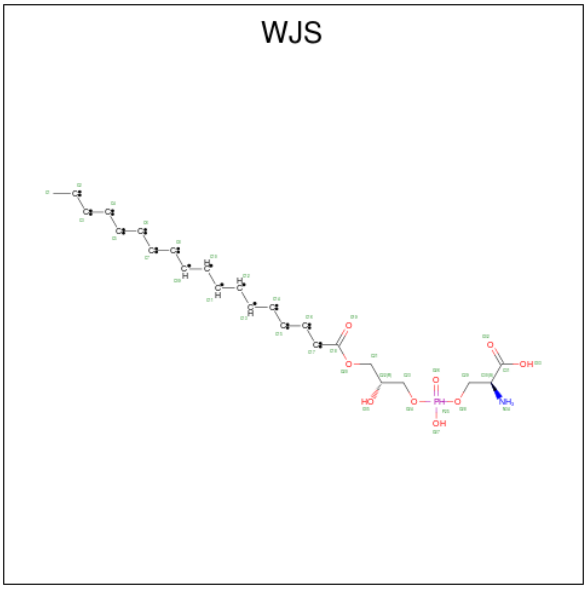
- Molecule 14 is PHOSPHATIDYLETHANOLAMINE (three-letter code: PTY) (formula: $C_{40}H_{80}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
14	0	1	Total	C	N	O	P	0
			65	47	1	15	2	
14	0	1	Total	C	N	O	P	0
			65	47	1	15	2	
14	2	1	Total	C	N	O	P	0
			29	20	1	7	1	
14	5	1	Total	C	N	O	P	0
			35	25	1	8	1	
14	6	1	Total	C	N	O	P	0
			63	45	1	15	2	
14	6	1	Total	C	N	O	P	0
			63	45	1	15	2	
14	8	1	Total	C	N	O	P	0
			83	68	1	13	1	
14	8	1	Total	C	N	O	P	0
			83	68	1	13	1	
14	R	1	Total	C	N	O	P	0
			29	20	1	7	1	
14	S	1	Total	C	O			0
			32	27	5			
14	U	1	Total	C	N	O	P	0
			56	41	1	13	1	
14	U	1	Total	C	N	O	P	0
			56	41	1	13	1	
14	V	1	Total	C	N	O	P	0
			29	20	1	7	1	

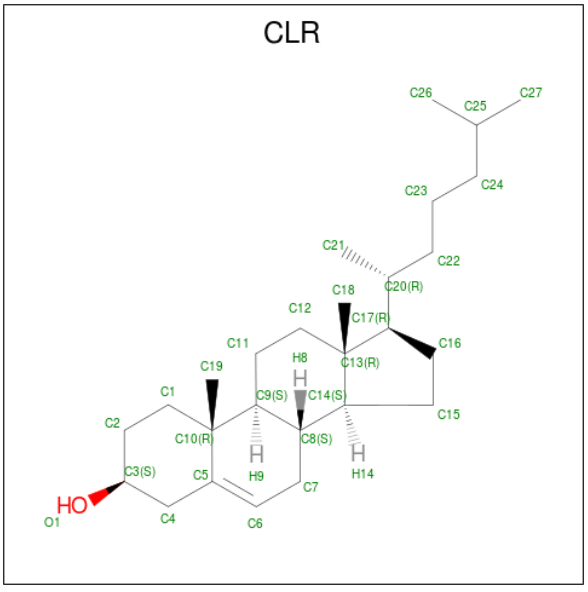
- Molecule 15 is (2 {S})-2-$l^{4}-azanyl-3-[[(2 {R})-3-octadecanoyloxy-2-oxidanyl-propoxy

]-oxidanyl-oxidanylidene-$l^{6}-phosphanyl]oxy-propanoic acid (three-letter code: WJS) (formula: $C_{24}H_{20}NO_9P$).



Mol	Chain	Residues	Atoms					AltConf
15	3	1	Total	C	N	O	P	0
			27	16	1	9	1	

- Molecule 16 is CHOLESTEROL (three-letter code: CLR) (formula: $C_{27}H_{46}O$).



Mol	Chain	Residues	Atoms			AltConf
16	5	1	Total	C	O	0
			28	27	1	

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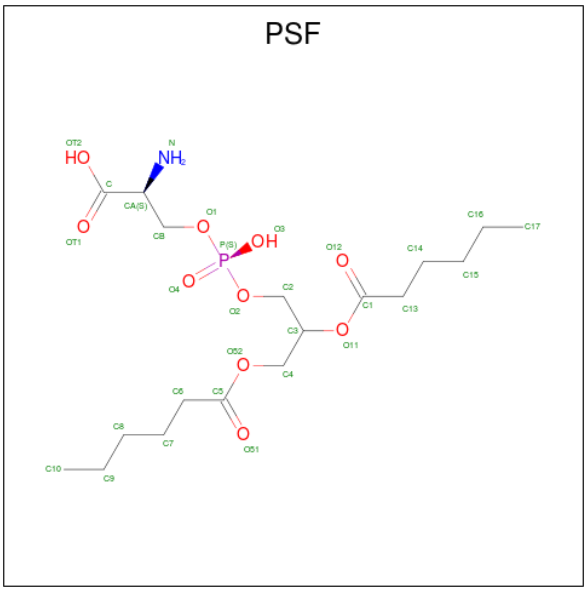
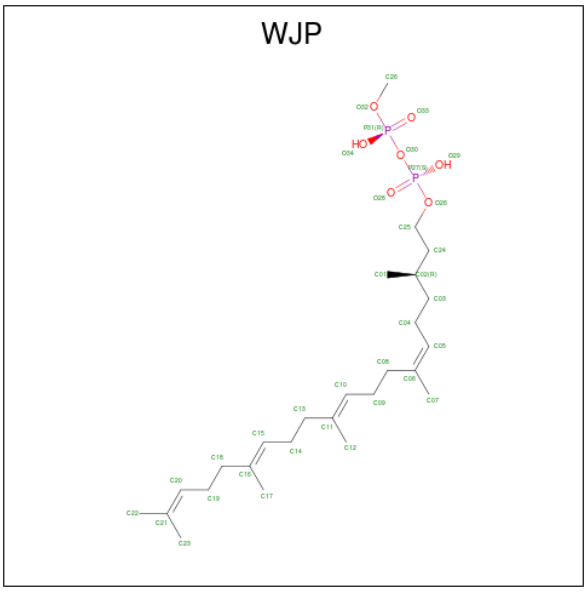
Mol	Chain	Residues	Atoms	AltConf
16	R	1	Total C O 28 27 1	0
16	V	1	Total C O 56 54 2	0
16	V	1	Total C O 56 54 2	0

- Molecule 17 is 1,2-DICAPROYL-SN-PHOSPHATIDYL-L-SERINE (three-letter code: PSF) (formula: $C_{18}H_{34}NO_{10}P$).



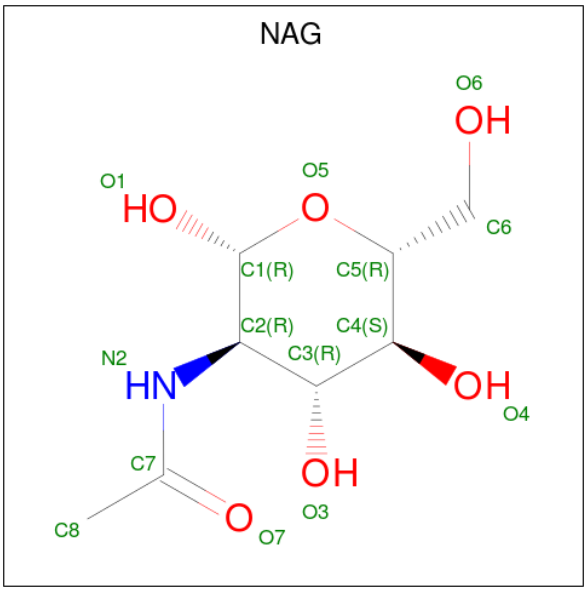
Mol	Chain	Residues	Atoms	AltConf
17	R	1	Total C N O P 30 18 1 10 1	0

- Molecule 18 is methyl (3R,6Z,10E,14E)-3,7,11,15,19-pentamethylicosa-6,10,14,18-tetraen-1-yl dihydrogen diphosphate (three-letter code: WJP) (formula: $C_{26}H_{48}O_7P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
18	R	1	Total	C	O	P	0
			34	25	7	2	

- Molecule 19 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



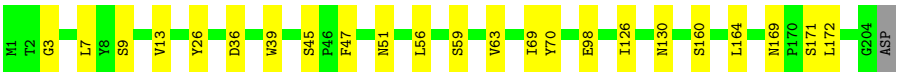
Mol	Chain	Residues	Atoms				AltConf
19	U	1	Total	C	N	O	0
			14	8	1	5	

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: V-type proton ATPase 21 kDa proteolipid subunit

Chain 0:

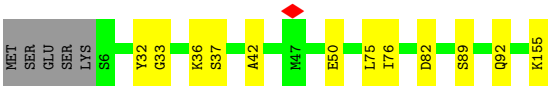


• Molecule 2: V-type proton ATPase 16 kDa proteolipid subunit

Chain 1:

• Molecule 2: V-type proton ATPase 16 kDa proteolipid subunit

Chain 2:

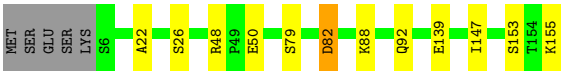


• Molecule 2: V-type proton ATPase 16 kDa proteolipid subunit

Chain 3:

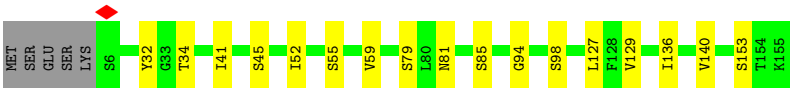
• Molecule 2: V-type proton ATPase 16 kDa proteolipid subunit

Chain 4:



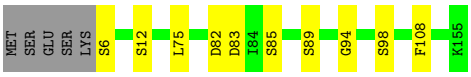
• Molecule 2: V-type proton ATPase 16 kDa proteolipid subunit

Chain 5:



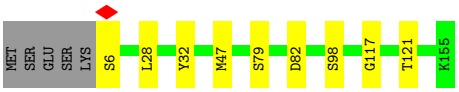
• Molecule 2: V-type proton ATPase 16 kDa proteolipid subunit

Chain 6:



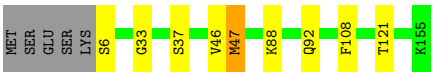
• Molecule 2: V-type proton ATPase 16 kDa proteolipid subunit

Chain 7:



• Molecule 2: V-type proton ATPase 16 kDa proteolipid subunit

Chain 8:

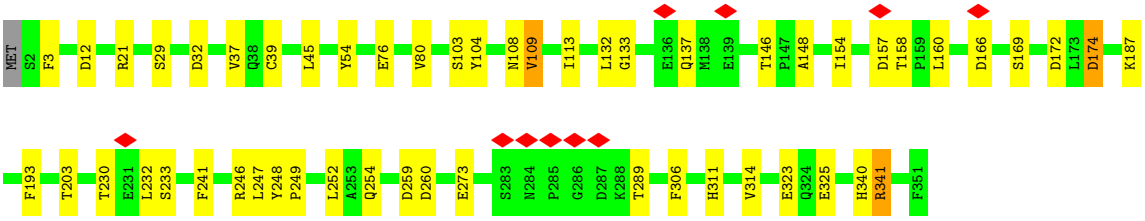


• Molecule 2: V-type proton ATPase 16 kDa proteolipid subunit

Chain 9:

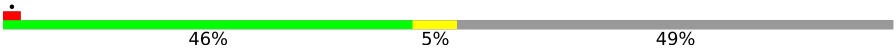
• Molecule 3: V-type proton ATPase subunit d 1

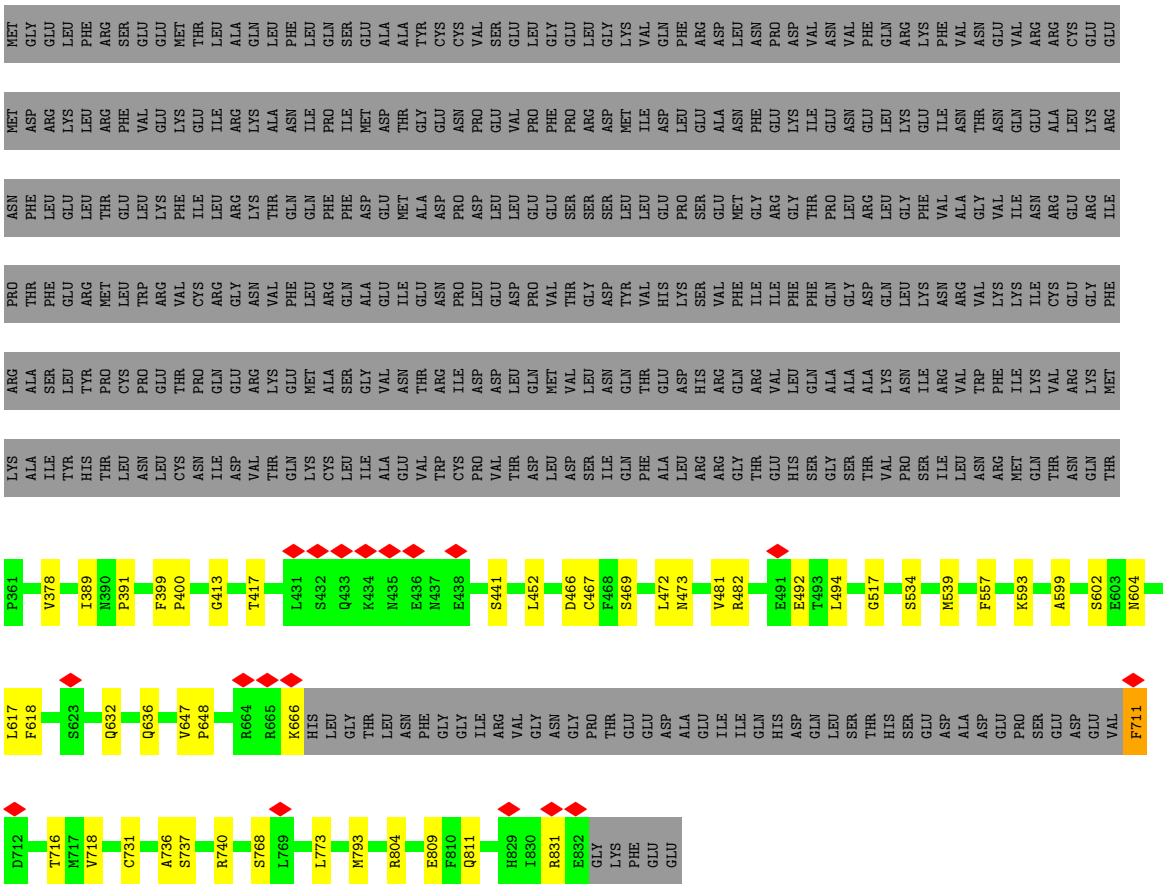
Chain Q:



• Molecule 4: V-type proton ATPase 116 kDa subunit a isoform 1

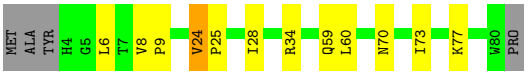
Chain R:





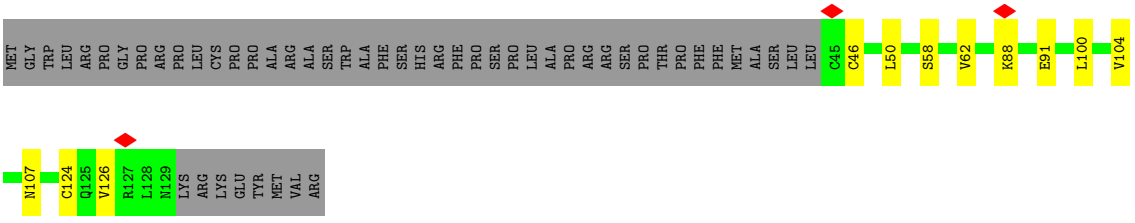
• Molecule 5: V-type proton ATPase subunit e 1

Chain S:



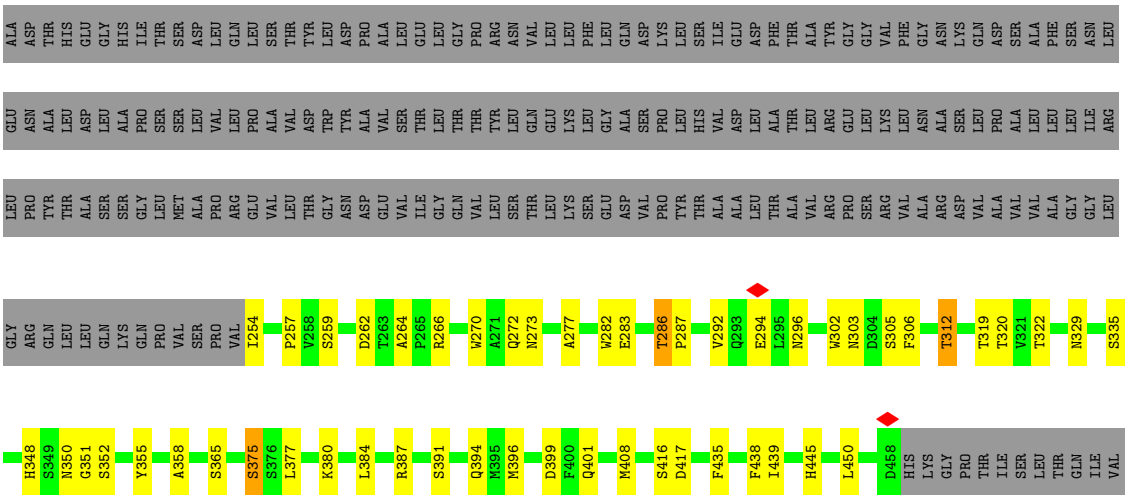
• Molecule 6: Ribonuclease kappa

Chain T:



• Molecule 7: V-type proton ATPase subunit S1

Chain U:

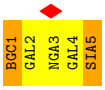


• Molecule 8: Renin receptor

Chain V:

• Molecule 9: beta-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-galactopyranose-(1-4)-[N-acetyl-alpha-neuraminic acid-(2-3)]beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain W:



• Molecule 10: beta-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-galactopyranose-(1-4)-[N-acetyl-alpha-neuraminic acid-(2-3)]beta-D-galactopyranose

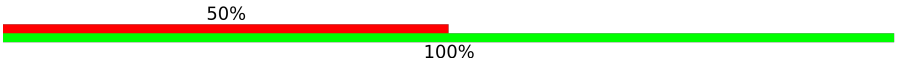
Chain A:

• Molecule 11: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain s:

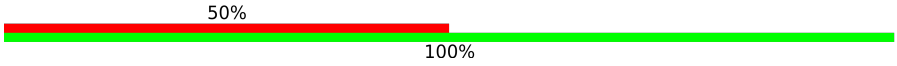
• Molecule 11: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain u:



• Molecule 11: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain B:



• Molecule 11: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:

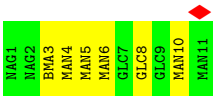
• Molecule 11: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:

• Molecule 12: alpha-D-glucopyranose-(1-2)-alpha-D-glucopyranose-(1-3)-alpha-D-glucopyranose-(1-3)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain r:


9%
45%
55%


NAG1
NAG2
BMA3
MAN4
MAN5
MAN6
GLC7
GLC8
GLC9
MAN10
MAN11

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	1000000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50.1	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	3.470	Depositor
Minimum map value	-1.625	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.068	Depositor
Recommended contour level	0.6	Depositor
Map size (Å)	388.80002, 388.80002, 388.80002	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.08, 1.08, 1.08	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GLC, BGC, MAN, WJP, PSF, NGA, WJS, NAG, PTY, CLR, GAL, WSS, BMA, SIA

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	0	0.28	0/1529	0.40	0/2079
2	1	0.28	0/1080	0.39	0/1461
2	2	0.27	0/1080	0.39	0/1461
2	3	0.28	0/1080	0.40	0/1461
2	4	0.28	0/1080	0.39	0/1461
2	5	0.28	0/1080	0.40	0/1461
2	6	0.27	0/1080	0.39	0/1461
2	7	0.28	0/1074	0.40	0/1454
2	8	0.28	0/1080	0.39	0/1461
2	9	0.28	0/1080	0.39	0/1461
3	Q	0.30	0/2895	0.40	0/3922
4	R	0.29	0/3591	0.39	0/4876
5	S	0.27	0/657	0.37	0/902
6	T	0.27	0/670	0.38	0/911
7	U	0.28	0/1718	0.44	0/2337
8	V	0.30	0/431	0.35	0/591
All	All	0.28	0/21205	0.40	0/28760

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	1495	0	1537	14	0
2	1	1065	0	1131	11	0
2	2	1065	0	1131	8	0
2	3	1065	0	1131	11	0
2	4	1065	0	1131	6	0
2	5	1065	0	1131	7	0
2	6	1065	0	1131	3	0
2	7	1059	0	1120	6	0
2	8	1065	0	1131	7	0
2	9	1065	0	1131	4	0
3	Q	2829	0	2757	24	0
4	R	3477	0	3478	32	0
5	S	631	0	646	8	0
6	T	654	0	641	4	0
7	U	1664	0	1583	41	0
8	V	417	0	405	7	0
9	W	68	0	58	6	0
10	A	56	0	47	5	0
11	B	28	0	25	0	0
11	C	28	0	25	0	0
11	D	28	0	25	2	0
11	s	28	0	25	0	0
11	u	28	0	25	0	0
12	r	127	0	106	0	0
13	0	135	0	0	1	0
13	1	34	0	0	0	0
13	3	41	0	0	0	0
13	R	40	0	0	6	0
13	U	83	0	0	3	0
13	V	37	0	0	0	0
14	0	65	0	85	4	0
14	2	29	0	40	4	0
14	5	35	0	46	7	0
14	6	63	0	79	10	0
14	8	83	0	129	11	0
14	R	29	0	37	1	0
14	S	32	0	48	0	0
14	U	56	0	66	18	0
14	V	29	0	40	9	0
15	3	27	0	0	5	0
16	5	28	0	46	16	0
16	R	28	0	46	2	0
16	V	56	0	92	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	R	30	0	32	0	0
18	R	34	0	0	1	0
19	U	14	0	13	0	0
All	All	22145	0	22350	222	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (222) 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)
7:U:273:ASN:ND2	11:D:1:NAG:C1	1.72	1.50
4:R:473:ASN:ND2	13:R:904:WSS:C4	1.80	1.45
4:R:473:ASN:HD22	13:R:904:WSS:C4	1.43	1.23
14:6:201:PTY:O13	14:6:202:PTY:C2	1.95	1.14
7:U:438:PHE:CE2	14:U:504:PTY:H181	1.86	1.10
4:R:618:PHE:O	9:W:5:SIA:O1A	1.71	1.09
16:5:201:CLR:C2	14:V:404:PTY:HC51	1.83	1.08
16:5:201:CLR:C1	14:V:404:PTY:HC51	1.83	1.08
14:6:201:PTY:O13	14:6:202:PTY:HC22	1.56	1.04
7:U:438:PHE:HE2	14:U:504:PTY:C18	1.70	1.02
14:U:503:PTY:H322	14:U:504:PTY:H321	1.37	1.02
2:8:108:PHE:HZ	14:8:202:PTY:H341	1.24	1.02
16:5:201:CLR:H21	14:V:404:PTY:C5	1.90	1.00
14:6:201:PTY:O13	14:6:202:PTY:HC21	1.61	1.00
14:5:202:PTY:O13	14:6:201:PTY:C3	2.11	0.98
14:5:202:PTY:H121	16:V:403:CLR:H193	1.45	0.95
2:8:108:PHE:HB3	14:8:201:PTY:O13	1.63	0.95
16:5:201:CLR:H21	14:V:404:PTY:HC51	1.41	0.94
14:U:503:PTY:H112	14:U:504:PTY:O10	1.65	0.94
7:U:438:PHE:CE2	14:U:504:PTY:C18	2.50	0.91
14:U:503:PTY:C32	14:U:504:PTY:H321	2.00	0.90
4:R:473:ASN:ND2	13:R:904:WSS:C5	2.35	0.89
16:5:201:CLR:H11	14:V:404:PTY:HC51	1.55	0.88
2:8:108:PHE:CZ	14:8:202:PTY:H341	2.10	0.86
4:R:473:ASN:HD22	13:R:904:WSS:C5	1.89	0.86
7:U:273:ASN:ND2	11:D:1:NAG:O5	2.11	0.84
7:U:438:PHE:HE2	14:U:504:PTY:H182	1.44	0.83
4:R:473:ASN:HD21	13:R:904:WSS:C4	1.88	0.83
2:3:108:PHE:CE2	15:3:202:WJS:O27	2.32	0.82
14:5:202:PTY:H121	16:V:403:CLR:C19	2.11	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:39:CYS:O	3:Q:341:ARG:NH2	2.20	0.75
16:5:201:CLR:C2	14:V:404:PTY:C5	2.57	0.71
7:U:438:PHE:CD2	14:U:504:PTY:H181	2.25	0.71
7:U:435:PHE:HE1	14:U:504:PTY:C20	2.04	0.70
2:3:108:PHE:CD2	15:3:202:WJS:O27	2.45	0.70
1:0:13:VAL:HG11	14:0:305:PTY:H312	1.75	0.69
2:7:47:MET:SD	3:Q:254:GLN:NE2	2.67	0.68
2:3:98:SER:O	2:3:102:SER:OG	2.10	0.67
9:W:1:BGC:O4	9:W:1:BGC:O2	2.10	0.67
3:Q:174:ASP:N	3:Q:174:ASP:OD1	2.28	0.67
2:3:108:PHE:HE2	15:3:202:WJS:O27	1.77	0.66
14:5:202:PTY:H312	14:5:202:PTY:H122	1.76	0.66
4:R:617:LEU:HB3	10:A:2:NGA:H81	1.78	0.65
2:6:108:PHE:HE2	14:6:201:PTY:HC6	1.62	0.65
14:2:201:PTY:O12	15:3:202:WJS:C29	2.45	0.64
10:A:4:SIA:H112	10:A:4:SIA:O4	1.98	0.63
16:5:201:CLR:H193	16:V:403:CLR:C19	2.29	0.62
2:7:28:LEU:HD22	14:8:201:PTY:HC11	1.80	0.62
2:1:36:LYS:HE2	2:1:112:ILE:HD13	1.79	0.62
3:Q:146:THR:HG22	3:Q:148:ALA:H	1.65	0.61
4:R:494:LEU:O	5:S:70:ASN:ND2	2.33	0.61
2:1:33:GLY:O	2:1:37:SER:OG	2.18	0.61
16:5:201:CLR:H193	16:V:403:CLR:H191	1.83	0.61
7:U:435:PHE:CE1	14:U:504:PTY:C20	2.83	0.61
14:5:202:PTY:H111	16:V:403:CLR:H22	1.82	0.60
3:Q:108:ASN:ND2	3:Q:133:GLY:O	2.34	0.59
2:6:94:GLY:O	2:6:98:SER:OG	2.19	0.59
7:U:296:ASN:O	7:U:312:THR:OG1	2.19	0.59
1:0:3:GLY:HA3	13:0:304:WSS:C1	2.32	0.59
3:Q:12:ASP:OD1	3:Q:12:ASP:N	2.36	0.59
3:Q:203:THR:HB	3:Q:311:HIS:HB3	1.85	0.59
7:U:377:LEU:HB2	7:U:380:LYS:HB2	1.84	0.59
7:U:445:HIS:CE1	14:U:504:PTY:H311	2.38	0.59
7:U:329:ASN:ND2	7:U:365:SER:OG	2.37	0.58
7:U:303:ASN:HB3	7:U:305:SER:H	1.66	0.58
4:R:452:LEU:HD11	16:R:901:CLR:H121	1.85	0.58
7:U:401:GLN:HE22	8:V:296:ALA:H	1.50	0.57
14:U:503:PTY:C32	14:U:504:PTY:C32	2.79	0.57
7:U:272:GLN:NE2	7:U:399:ASP:OD2	2.37	0.57
4:R:593:LYS:NZ	18:R:905:WJP:O29	2.34	0.57
14:U:503:PTY:H321	14:U:504:PTY:H312	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:158:THR:HG23	3:Q:160:LEU:H	1.71	0.55
16:5:201:CLR:H121	16:V:403:CLR:H181	1.89	0.55
7:U:375:SER:HB2	7:U:396:MET:HA	1.88	0.55
2:5:32:TYR:CE1	14:5:202:PTY:HC31	2.42	0.55
2:6:108:PHE:CE2	14:6:201:PTY:HC6	2.42	0.55
14:8:201:PTY:H122	14:8:201:PTY:HC12	1.88	0.55
16:5:201:CLR:H212	16:V:403:CLR:H181	1.88	0.54
2:2:36:LYS:HG2	14:2:201:PTY:HC22	1.88	0.54
2:8:33:GLY:O	2:8:37:SER:OG	2.25	0.54
7:U:319:THR:HG22	7:U:320:THR:H	1.73	0.53
8:V:329:TRP:CE3	14:V:404:PTY:O30	2.61	0.53
1:0:56:LEU:HD21	7:U:435:PHE:HZ	1.74	0.53
7:U:335:SER:CB	13:U:502:WSS:O2P	2.57	0.53
1:0:56:LEU:HD21	7:U:435:PHE:CZ	2.44	0.52
2:1:6:SER:OG	2:1:7:GLY:N	2.42	0.52
4:R:618:PHE:C	9:W:5:SIA:O1A	2.46	0.52
2:4:82:ASP:OD1	2:4:82:ASP:N	2.41	0.51
6:T:46:CYS:HB3	6:T:50:LEU:HD22	1.93	0.51
7:U:257:PRO:HB3	7:U:270:TRP:HB2	1.93	0.51
7:U:335:SER:HB3	13:U:502:WSS:O2P	2.11	0.51
2:4:139:GLU:OE1	4:R:740:ARG:NH2	2.44	0.51
2:7:28:LEU:CD2	14:8:201:PTY:HC11	2.41	0.51
4:R:481:VAL:HG11	5:S:73:ILE:HG23	1.93	0.50
7:U:439:ILE:HG12	14:U:504:PTY:H192	1.92	0.50
15:3:202:WJS:O26	8:V:327:ASN:OD1	2.29	0.50
16:5:201:CLR:H261	16:V:403:CLR:H261	1.92	0.50
14:8:202:PTY:H332	14:8:202:PTY:C17	2.41	0.50
7:U:254:ILE:HG21	8:V:292:PRO:HG2	1.92	0.50
2:3:47:MET:HG2	2:3:48:ARG:HG3	1.94	0.50
2:7:82:ASP:OD1	2:7:82:ASP:N	2.40	0.50
7:U:438:PHE:CE1	14:U:504:PTY:C36	2.95	0.50
2:4:48:ARG:NH2	2:4:50:GLU:OE2	2.45	0.49
3:Q:248:TYR:HB3	3:Q:249:PRO:HD3	1.94	0.49
2:5:94:GLY:O	2:5:98:SER:OG	2.27	0.49
16:5:201:CLR:H11	14:V:404:PTY:HC12	1.93	0.49
3:Q:230:THR:HG22	3:Q:232:LEU:H	1.77	0.49
10:A:4:SIA:H6	10:A:4:SIA:O1A	2.12	0.49
2:4:22:ALA:O	2:4:26:SER:OG	2.20	0.48
4:R:413:GLY:O	4:R:417:THR:HG23	2.14	0.48
4:R:517:GLY:O	5:S:59:GLN:NE2	2.46	0.48
3:Q:260:ASP:N	3:Q:260:ASP:OD1	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:5:201:CLR:H11	14:V:404:PTY:C1	2.44	0.48
3:Q:187:LYS:NZ	3:Q:241:PHE:O	2.47	0.48
6:T:58:SER:O	6:T:62:VAL:HG23	2.14	0.48
7:U:319:THR:HG21	7:U:350:ASN:HA	1.96	0.48
4:R:737:SER:OG	4:R:809:GLU:OE1	2.32	0.48
7:U:445:HIS:ND1	14:U:504:PTY:C30	2.77	0.47
2:3:136:ILE:O	2:3:140:VAL:HG23	2.15	0.47
1:0:69:ILE:HD12	2:1:141:LEU:HD11	1.96	0.47
4:R:632:GLN:HE21	4:R:636:GLN:NE2	2.12	0.47
2:7:117:GLY:O	2:7:121:THR:OG1	2.28	0.47
2:9:8:PRO:HD2	2:9:11:ALA:HB2	1.96	0.47
2:2:82:ASP:OD1	2:2:82:ASP:N	2.48	0.46
2:5:136:ILE:O	2:5:140:VAL:HG23	2.14	0.46
2:2:155:LYS:HB2	2:2:155:LYS:HE3	1.67	0.46
9:W:5:SIA:C11	10:A:4:SIA:H31	2.44	0.46
2:3:117:GLY:O	2:3:121:THR:HG22	2.15	0.46
7:U:335:SER:OG	13:U:502:WSS:O2P	2.25	0.46
16:R:901:CLR:H213	14:R:903:PTY:H191	1.97	0.46
7:U:350:ASN:OD1	7:U:351:GLY:N	2.49	0.46
2:1:45:SER:HB2	2:1:52:ILE:HG12	1.98	0.46
7:U:303:ASN:HD22	7:U:306:PHE:HB3	1.81	0.46
7:U:266:ARG:HD2	7:U:302:TRP:CE3	2.50	0.46
7:U:292:VAL:HG12	7:U:294:GLU:H	1.80	0.46
1:0:59:SER:HB2	2:1:101:LEU:HB3	1.97	0.45
14:5:202:PTY:O10	14:6:201:PTY:HC12	2.16	0.45
14:6:202:PTY:O10	14:6:202:PTY:HC12	2.16	0.45
1:0:63:VAL:HG22	2:1:105:ALA:HB2	1.99	0.45
4:R:399:PHE:HB3	4:R:400:PRO:HD3	1.97	0.45
3:Q:247:LEU:O	3:Q:252:LEU:N	2.49	0.45
7:U:286:THR:HG23	7:U:287:PRO:HD3	1.99	0.45
1:0:36:ASP:HB3	1:0:39:TRP:HB3	1.99	0.45
2:3:32:TYR:O	2:3:36:LYS:HB2	2.17	0.45
7:U:355:TYR:HB2	7:U:387:ARG:HG3	1.98	0.45
2:5:140:VAL:HG21	4:R:793:MET:HE2	1.96	0.45
6:T:100:LEU:O	6:T:104:VAL:HG22	2.16	0.45
2:8:46:VAL:HG23	2:8:47:MET:HG3	1.98	0.45
7:U:277:ALA:HB2	7:U:282:TRP:CD2	2.52	0.45
2:2:32:TYR:CD1	14:2:201:PTY:HC32	2.51	0.44
3:Q:76:GLU:O	3:Q:80:VAL:HG23	2.16	0.44
2:1:108:PHE:O	2:1:112:ILE:HG12	2.18	0.44
2:9:6:SER:OG	2:9:7:GLY:N	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:831:ARG:HB2	4:R:831:ARG:CZ	2.47	0.44
2:1:114:GLY:O	2:1:118:VAL:HG22	2.18	0.43
2:1:136:ILE:O	2:1:140:VAL:HG23	2.18	0.43
7:U:303:ASN:HB2	7:U:306:PHE:HB3	2.00	0.43
7:U:358:ALA:HB2	7:U:384:LEU:HD23	2.01	0.43
1:0:7:LEU:HD13	8:V:323:ILE:HD11	2.00	0.43
16:5:201:CLR:H121	16:V:403:CLR:C18	2.47	0.43
3:Q:29:SER:OG	3:Q:32:ASP:OD1	2.32	0.43
3:Q:246:ARG:NH2	3:Q:273:GLU:OE2	2.52	0.43
5:S:24:VAL:HG12	5:S:25:PRO:HD3	2.01	0.43
7:U:322:THR:HB	7:U:348:HIS:HB2	2.00	0.43
14:0:306:PTY:H161	14:0:306:PTY:H412	2.00	0.43
4:R:473:ASN:HD21	13:R:904:WSS:C5	2.22	0.43
4:R:482:ARG:NH1	5:S:77:LYS:O	2.51	0.43
14:0:306:PTY:C30	14:0:306:PTY:H112	2.48	0.43
14:8:202:PTY:HC6	14:8:202:PTY:H111	1.70	0.43
1:0:126:ILE:O	1:0:130:ASN:ND2	2.39	0.43
2:8:88:LYS:O	2:8:92:GLN:HG2	2.18	0.43
8:V:321:VAL:O	8:V:325:SER:OG	2.24	0.43
9:W:5:SIA:H111	10:A:4:SIA:H31	2.01	0.43
4:R:389:ILE:HD11	4:R:557:PHE:HB2	2.01	0.43
14:U:503:PTY:H361	14:U:503:PTY:H332	1.72	0.43
2:4:147:ILE:HD11	4:R:736:ALA:HB1	2.00	0.42
2:1:143:LEU:HD12	2:1:146:LEU:HD23	2.02	0.42
2:5:34:THR:HG23	2:5:59:VAL:HG13	2.00	0.42
3:Q:109:VAL:O	3:Q:113:ILE:HG13	2.18	0.42
4:R:378:VAL:HG11	4:R:391:PRO:HG2	2.01	0.42
4:R:467:CYS:HB2	4:R:472:LEU:HD11	2.01	0.42
1:0:47:PHE:O	1:0:51:ASN:ND2	2.42	0.42
2:4:88:LYS:O	2:4:92:GLN:HG2	2.19	0.42
3:Q:154:ILE:O	3:Q:158:THR:HG22	2.19	0.42
2:2:33:GLY:O	2:2:37:SER:OG	2.33	0.42
4:R:711:PHE:HE1	4:R:716:THR:HG21	1.85	0.42
5:S:8:VAL:HB	5:S:9:PRO:HD3	2.02	0.42
2:5:41:ILE:O	2:5:45:SER:HB3	2.20	0.42
2:2:32:TYR:CE1	14:2:201:PTY:HC32	2.55	0.42
16:5:201:CLR:H261	16:V:403:CLR:C26	2.49	0.42
14:6:202:PTY:H432	14:8:201:PTY:H261	2.01	0.42
4:R:768:SER:HA	6:T:107:ASN:HD21	1.85	0.42
2:5:45:SER:HB2	2:5:52:ILE:HG12	2.02	0.42
3:Q:54:TYR:OH	3:Q:325:GLU:OE1	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:164:LEU:HD13	3:Q:21:ARG:HD2	2.03	0.41
14:0:306:PTY:HC11	14:U:504:PTY:H141	2.01	0.41
14:6:202:PTY:H392	14:8:201:PTY:H252	2.02	0.41
8:V:322:ILE:HD13	16:V:403:CLR:H161	2.02	0.41
4:R:599:ALA:O	4:R:602:SER:OG	2.27	0.41
5:S:6:LEU:HD22	5:S:60:LEU:HD11	2.01	0.41
1:0:169:ASN:HB3	1:0:172:LEU:HG	2.03	0.41
2:2:42:ALA:HA	2:3:127:LEU:HD21	2.01	0.41
16:5:201:CLR:C26	16:V:403:CLR:C26	2.98	0.41
4:R:378:VAL:HG13	4:R:811:GLN:HE22	1.86	0.41
2:3:47:MET:SD	2:3:47:MET:N	2.91	0.41
2:7:32:TYR:CD1	14:8:201:PTY:HC32	2.56	0.41
9:W:5:SIA:O7	9:W:5:SIA:H113	2.21	0.41
2:8:47:MET:HE2	2:8:47:MET:HB2	1.96	0.41
4:R:666:LYS:HE3	4:R:666:LYS:HB3	1.91	0.41
7:U:277:ALA:HB3	7:U:394:GLN:HB2	2.03	0.41
3:Q:169:SER:OG	3:Q:172:ASP:OD2	2.37	0.41
5:S:28:ILE:O	5:S:34:ARG:NH1	2.52	0.41
3:Q:104:TYR:OH	3:Q:323:GLU:OE2	2.24	0.40
2:2:76:ILE:HG23	2:2:92:GLN:HB3	2.03	0.40
2:9:48:ARG:HB3	2:9:51:GLN:HG2	2.03	0.40
2:9:128:PHE:O	2:9:132:ILE:HG12	2.21	0.40
3:Q:132:LEU:HA	3:Q:132:LEU:HD23	1.87	0.40
1:0:9:SER:O	1:0:13:VAL:HG12	2.21	0.40
2:3:86:LEU:HD12	2:3:86:LEU:HA	1.92	0.40
3:Q:306:PHE:CE1	3:Q:314:VAL:HG13	2.57	0.40
4:R:647:VAL:HB	4:R:648:PRO:HD3	2.04	0.40
7:U:262:ASP:C	7:U:264:ALA:H	2.23	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	0	202/205 (98%)	202 (100%)	0	0	100	100
2	1	148/155 (96%)	147 (99%)	1 (1%)	0	100	100
2	2	148/155 (96%)	147 (99%)	1 (1%)	0	100	100
2	3	148/155 (96%)	147 (99%)	1 (1%)	0	100	100
2	4	148/155 (96%)	148 (100%)	0	0	100	100
2	5	148/155 (96%)	147 (99%)	1 (1%)	0	100	100
2	6	148/155 (96%)	146 (99%)	2 (1%)	0	100	100
2	7	148/155 (96%)	147 (99%)	1 (1%)	0	100	100
2	8	148/155 (96%)	145 (98%)	3 (2%)	0	100	100
2	9	148/155 (96%)	147 (99%)	1 (1%)	0	100	100
3	Q	348/351 (99%)	338 (97%)	10 (3%)	0	100	100
4	R	424/837 (51%)	409 (96%)	15 (4%)	0	100	100
5	S	75/81 (93%)	72 (96%)	3 (4%)	0	100	100
6	T	83/137 (61%)	80 (96%)	3 (4%)	0	100	100
7	U	203/470 (43%)	192 (95%)	11 (5%)	0	100	100
8	V	48/350 (14%)	45 (94%)	3 (6%)	0	100	100
All	All	2715/3826 (71%)	2659 (98%)	56 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	0	153/155 (99%)	147 (96%)	6 (4%)	32	69
2	1	107/112 (96%)	105 (98%)	2 (2%)	57	84
2	2	107/112 (96%)	104 (97%)	3 (3%)	43	77
2	3	107/112 (96%)	105 (98%)	2 (2%)	57	84
2	4	107/112 (96%)	103 (96%)	4 (4%)	34	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	5	107/112 (96%)	100 (94%)	7 (6%)	17 50
2	6	107/112 (96%)	100 (94%)	7 (6%)	17 50
2	7	106/112 (95%)	103 (97%)	3 (3%)	43 77
2	8	107/112 (96%)	104 (97%)	3 (3%)	43 77
2	9	107/112 (96%)	104 (97%)	3 (3%)	43 77
3	Q	303/306 (99%)	288 (95%)	15 (5%)	24 60
4	R	376/746 (50%)	364 (97%)	12 (3%)	39 74
5	S	69/72 (96%)	68 (99%)	1 (1%)	67 88
6	T	70/116 (60%)	66 (94%)	4 (6%)	20 56
7	U	182/397 (46%)	171 (94%)	11 (6%)	19 53
8	V	45/308 (15%)	43 (96%)	2 (4%)	28 65
All	All	2160/3108 (70%)	2075 (96%)	85 (4%)	36 69

All (85) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	26	TYR
1	0	45	SER
1	0	70	TYR
1	0	98	GLU
1	0	160	SER
1	0	171	SER
2	1	45	SER
2	1	129	VAL
2	2	50	GLU
2	2	75	LEU
2	2	89	SER
2	3	47	MET
2	3	75	LEU
2	4	79	SER
2	4	82	ASP
2	4	153	SER
2	4	155	LYS
2	5	55	SER
2	5	79	SER
2	5	81	ASN
2	5	85	SER
2	5	127	LEU

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Mol	Chain	Res	Type
2	5	129	VAL
2	5	153	SER
2	6	6	SER
2	6	12	SER
2	6	75	LEU
2	6	82	ASP
2	6	83	ASP
2	6	85	SER
2	6	89	SER
2	7	6	SER
2	7	79	SER
2	7	98	SER
2	8	6	SER
2	8	47	MET
2	8	121	THR
2	9	20	SER
2	9	82	ASP
2	9	115	ASP
3	Q	3	PHE
3	Q	37	VAL
3	Q	45	LEU
3	Q	103	SER
3	Q	109	VAL
3	Q	137	GLN
3	Q	157	ASP
3	Q	166	ASP
3	Q	174	ASP
3	Q	193	PHE
3	Q	233	SER
3	Q	259	ASP
3	Q	289	THR
3	Q	340	HIS
3	Q	341	ARG
4	R	441	SER
4	R	466	ASP
4	R	469	SER
4	R	492	GLU
4	R	534	SER
4	R	539	MET
4	R	604	ASN
4	R	711	PHE
4	R	718	VAL

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Mol	Chain	Res	Type
4	R	731	CYS
4	R	773	LEU
4	R	804	ARG
5	S	24	VAL
6	T	88	LYS
6	T	91	GLU
6	T	124	CYS
6	T	126	VAL
7	U	259	SER
7	U	283	GLU
7	U	286	THR
7	U	312	THR
7	U	352	SER
7	U	375	SER
7	U	391	SER
7	U	408	MET
7	U	416	SER
7	U	417	ASP
7	U	450	LEU
8	V	304	SER
8	V	337	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
2	1	78	ASN
2	4	78	ASN
2	5	51	GLN
2	5	81	ASN
2	5	123	GLN
2	6	78	ASN
3	Q	50	GLN
4	R	433	GLN
4	R	473	ASN
4	R	497	ASN
4	R	547	HIS
4	R	600	HIS
4	R	604	ASN
4	R	636	GLN
4	R	734	ASN
4	R	761	HIS
4	R	811	GLN

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Mol	Chain	Res	Type
5	S	33	ASN
5	S	67	GLN
6	T	107	ASN
7	U	272	GLN
7	U	293	GLN
7	U	329	ASN
7	U	348	HIS
7	U	398	GLN
7	U	401	GLN
7	U	403	GLN
7	U	411	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

30 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	$\#\|Z\| > 2$
10	GAL	A	1	10	11,11,12	0.59	0	15,15,17	1.40	2 (13%)
10	NGA	A	2	10	14,14,15	0.71	0	17,19,21	1.86	4 (23%)
10	GAL	A	3	10	11,11,12	0.60	0	15,15,17	1.78	2 (13%)
10	SIA	A	4	10	20,20,21	0.73	1 (5%)	24,28,31	1.13	2 (8%)
11	NAG	B	1	7,11	14,14,15	0.18	0	17,19,21	0.48	0
11	NAG	B	2	11	14,14,15	0.26	0	17,19,21	0.44	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
11	NAG	C	1	7,11	14,14,15	0.30	0	17,19,21	0.77	1 (5%)
11	NAG	C	2	11	14,14,15	0.18	0	17,19,21	0.58	0
11	NAG	D	1	11	14,14,15	0.34	0	17,19,21	0.38	0
11	NAG	D	2	11	14,14,15	0.23	0	17,19,21	0.39	0
9	BGC	W	1	9	12,12,12	0.55	0	17,17,17	1.39	4 (23%)
9	GAL	W	2	9	11,11,12	0.77	0	15,15,17	1.44	2 (13%)
9	NGA	W	3	9	14,14,15	0.43	0	17,19,21	1.94	6 (35%)
9	GAL	W	4	9	11,11,12	0.32	0	15,15,17	0.86	1 (6%)
9	SIA	W	5	9	20,20,21	0.60	0	24,28,31	1.37	2 (8%)
12	NAG	r	1	12	14,14,15	0.18	0	17,19,21	0.45	0
12	MAN	r	10	12	11,11,12	0.57	0	15,15,17	1.04	2 (13%)
12	MAN	r	11	12	11,11,12	0.37	0	15,15,17	0.79	0
12	NAG	r	2	12	14,14,15	0.22	0	17,19,21	0.44	0
12	BMA	r	3	12	11,11,12	0.54	0	15,15,17	0.88	1 (6%)
12	MAN	r	4	12	11,11,12	0.61	0	15,15,17	1.01	2 (13%)
12	MAN	r	5	12	11,11,12	0.63	0	15,15,17	1.15	2 (13%)
12	MAN	r	6	12	11,11,12	0.73	0	15,15,17	0.90	1 (6%)
12	GLC	r	7	12	11,11,12	0.67	0	15,15,17	0.73	0
12	GLC	r	8	12	11,11,12	0.62	0	15,15,17	0.89	1 (6%)
12	GLC	r	9	12	11,11,12	0.62	0	15,15,17	0.82	0
11	NAG	s	1	5,11	14,14,15	0.32	0	17,19,21	0.69	1 (5%)
11	NAG	s	2	11	14,14,15	0.28	0	17,19,21	0.51	0
11	NAG	u	1	7,11	14,14,15	0.27	0	17,19,21	0.48	0
11	NAG	u	2	11	14,14,15	0.33	0	17,19,21	0.48	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	GAL	A	1	10	-	0/2/19/22	0/1/1/1
10	NGA	A	2	10	1/1/5/7	3/6/23/26	0/1/1/1
10	GAL	A	3	10	-	1/2/19/22	0/1/1/1
10	SIA	A	4	10	-	13/18/34/38	0/1/1/1
11	NAG	B	1	7,11	-	1/6/23/26	0/1/1/1
11	NAG	B	2	11	-	4/6/23/26	0/1/1/1
11	NAG	C	1	7,11	-	3/6/23/26	0/1/1/1
11	NAG	C	2	11	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	NAG	D	1	11	-	2/6/23/26	0/1/1/1
11	NAG	D	2	11	-	3/6/23/26	0/1/1/1
9	BGC	W	1	9	-	1/2/22/22	0/1/1/1
9	GAL	W	2	9	-	0/2/19/22	0/1/1/1
9	NGA	W	3	9	-	2/6/23/26	0/1/1/1
9	GAL	W	4	9	-	1/2/19/22	0/1/1/1
9	SIA	W	5	9	-	2/18/34/38	0/1/1/1
12	NAG	r	1	12	-	2/6/23/26	0/1/1/1
12	MAN	r	10	12	-	2/2/19/22	0/1/1/1
12	MAN	r	11	12	1/1/4/5	0/2/19/22	0/1/1/1
12	NAG	r	2	12	-	0/6/23/26	0/1/1/1
12	BMA	r	3	12	-	0/2/19/22	0/1/1/1
12	MAN	r	4	12	-	2/2/19/22	0/1/1/1
12	MAN	r	5	12	-	2/2/19/22	0/1/1/1
12	MAN	r	6	12	-	2/2/19/22	0/1/1/1
12	GLC	r	7	12	-	1/2/19/22	0/1/1/1
12	GLC	r	8	12	-	0/2/19/22	0/1/1/1
12	GLC	r	9	12	-	0/2/19/22	0/1/1/1
11	NAG	s	1	5,11	-	2/6/23/26	0/1/1/1
11	NAG	s	2	11	-	3/6/23/26	0/1/1/1
11	NAG	u	1	7,11	-	2/6/23/26	0/1/1/1
11	NAG	u	2	11	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	4	SIA	O1B-C1	-2.84	1.21	1.30

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	A	2	NGA	C1-O5-C5	4.83	118.74	112.19
10	A	3	GAL	C1-C2-C3	4.46	115.15	109.67
10	A	3	GAL	C1-O5-C5	4.04	117.67	112.19
10	A	2	NGA	C2-N2-C7	-3.71	117.61	122.90
9	W	5	SIA	C11-C10-N5	3.69	122.34	116.10
9	W	3	NGA	C1-C2-N2	3.69	116.78	110.49
9	W	3	NGA	O5-C1-C2	-3.66	105.50	111.29
9	W	3	NGA	C4-C3-C2	-3.33	106.14	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	A	4	SIA	O6-C2-C3	-3.12	106.16	110.46
12	r	5	MAN	O2-C2-C3	-2.98	104.17	110.14
9	W	3	NGA	C1-O5-C5	2.93	116.17	112.19
10	A	1	GAL	C1-C2-C3	2.77	113.06	109.67
9	W	2	GAL	O4-C4-C3	2.61	116.38	110.35
9	W	4	GAL	C1-C2-C3	2.56	112.81	109.67
12	r	4	MAN	O2-C2-C3	-2.51	105.11	110.14
12	r	5	MAN	C1-O5-C5	2.50	115.58	112.19
9	W	1	BGC	O5-C5-C6	2.50	112.64	106.44
9	W	1	BGC	C4-C3-C2	-2.49	106.48	110.82
9	W	5	SIA	O9-C9-C8	-2.48	105.66	111.07
10	A	1	GAL	C1-O5-C5	-2.48	108.83	112.19
10	A	2	NGA	C1-C2-N2	2.45	114.67	110.49
10	A	2	NGA	O3-C3-C2	-2.37	104.55	109.47
11	s	1	NAG	C1-O5-C5	2.35	115.37	112.19
9	W	3	NGA	O3-C3-C2	2.34	114.30	109.47
11	C	1	NAG	C1-O5-C5	2.33	115.35	112.19
12	r	10	MAN	O2-C2-C3	-2.32	105.48	110.14
12	r	6	MAN	O2-C2-C3	-2.30	105.53	110.14
12	r	4	MAN	C1-O5-C5	2.29	115.29	112.19
12	r	10	MAN	C1-O5-C5	2.26	115.25	112.19
9	W	1	BGC	O2-C2-C1	-2.24	103.97	109.16
9	W	2	GAL	C1-C2-C3	2.23	112.41	109.67
10	A	4	SIA	O1B-C1-C2	2.20	119.31	113.03
12	r	3	BMA	O2-C2-C3	-2.17	105.79	110.14
12	r	8	GLC	C1-C2-C3	2.15	112.31	109.67
9	W	3	NGA	O3-C3-C4	-2.04	105.63	110.35
9	W	1	BGC	O2-C2-C3	-2.02	105.69	110.35

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
10	A	2	NGA	C1
12	r	11	MAN	C1

All (58) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	W	3	NGA	C8-C7-N2-C2
9	W	3	NGA	O7-C7-N2-C2
10	A	4	SIA	C5-C6-C7-C8
10	A	4	SIA	C5-C6-C7-O7

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Mol	Chain	Res	Type	Atoms
10	A	4	SIA	O6-C6-C7-C8
10	A	4	SIA	O6-C6-C7-O7
10	A	4	SIA	C6-C7-C8-C9
10	A	4	SIA	C7-C8-C9-O9
12	r	4	MAN	O5-C5-C6-O6
11	B	2	NAG	O5-C5-C6-O6
11	s	2	NAG	C4-C5-C6-O6
10	A	4	SIA	O8-C8-C9-O9
12	r	1	NAG	O5-C5-C6-O6
11	s	2	NAG	O5-C5-C6-O6
12	r	10	MAN	O5-C5-C6-O6
11	B	2	NAG	C4-C5-C6-O6
11	D	1	NAG	O5-C5-C6-O6
10	A	4	SIA	O7-C7-C8-O8
12	r	4	MAN	C4-C5-C6-O6
10	A	4	SIA	C6-C7-C8-O8
11	s	1	NAG	O5-C5-C6-O6
10	A	4	SIA	C11-C10-N5-C5
10	A	4	SIA	O10-C10-N5-C5
11	C	2	NAG	O5-C5-C6-O6
12	r	6	MAN	O5-C5-C6-O6
10	A	4	SIA	O7-C7-C8-C9
11	u	1	NAG	C4-C5-C6-O6
11	C	2	NAG	C4-C5-C6-O6
11	D	1	NAG	C4-C5-C6-O6
12	r	1	NAG	C4-C5-C6-O6
12	r	10	MAN	C4-C5-C6-O6
9	W	5	SIA	C11-C10-N5-C5
9	W	5	SIA	O10-C10-N5-C5
10	A	2	NGA	C8-C7-N2-C2
11	B	2	NAG	C8-C7-N2-C2
11	B	2	NAG	O7-C7-N2-C2
11	D	2	NAG	C8-C7-N2-C2
11	D	2	NAG	O7-C7-N2-C2
11	s	1	NAG	C4-C5-C6-O6
11	C	1	NAG	O5-C5-C6-O6
12	r	6	MAN	C4-C5-C6-O6
11	u	1	NAG	O5-C5-C6-O6
10	A	2	NGA	O7-C7-N2-C2
11	C	1	NAG	C4-C5-C6-O6
12	r	7	GLC	O5-C5-C6-O6
9	W	4	GAL	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
11	u	2	NAG	O5-C5-C6-O6
11	B	1	NAG	O5-C5-C6-O6
10	A	2	NGA	C4-C5-C6-O6
12	r	5	MAN	O5-C5-C6-O6
12	r	5	MAN	C4-C5-C6-O6
10	A	3	GAL	O5-C5-C6-O6
10	A	4	SIA	O1A-C1-C2-O6
11	s	2	NAG	C3-C2-N2-C7
11	u	2	NAG	C3-C2-N2-C7
11	C	1	NAG	C3-C2-N2-C7
9	W	1	BGC	O5-C5-C6-O6
11	D	2	NAG	C4-C5-C6-O6

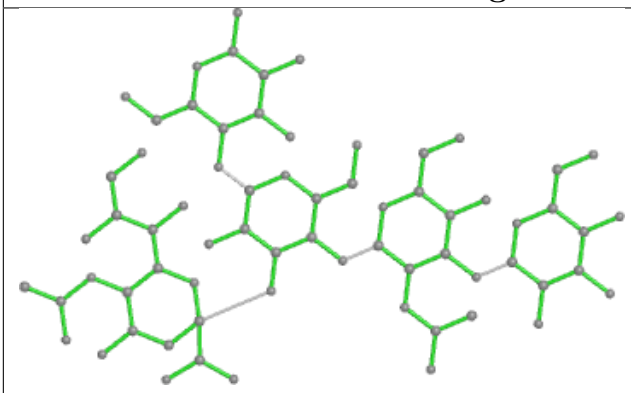
There are no ring outliers.

5 monomers are involved in 11 short contacts:

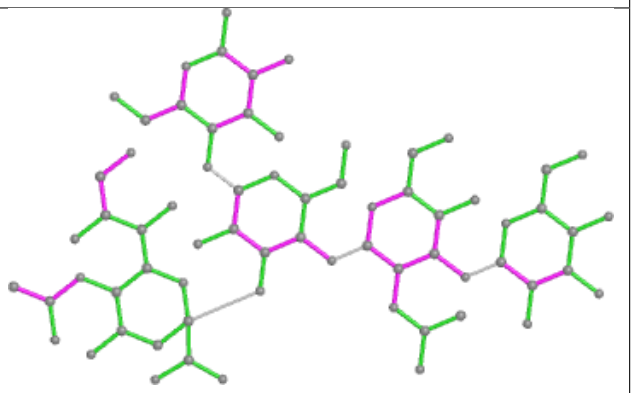
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	D	1	NAG	2	0
9	W	1	BGC	1	0
10	A	2	NGA	1	0
9	W	5	SIA	5	0
10	A	4	SIA	4	0

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

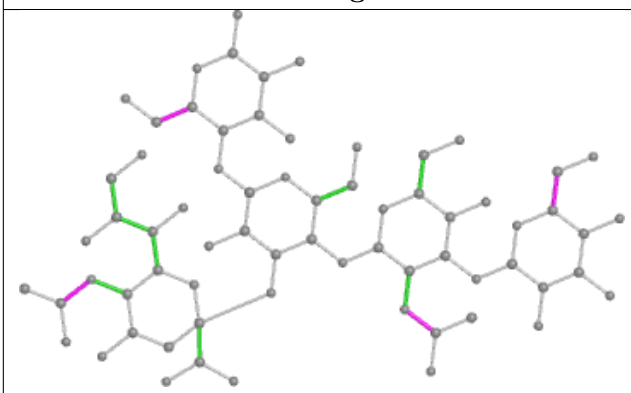
Oligosaccharide Chain W



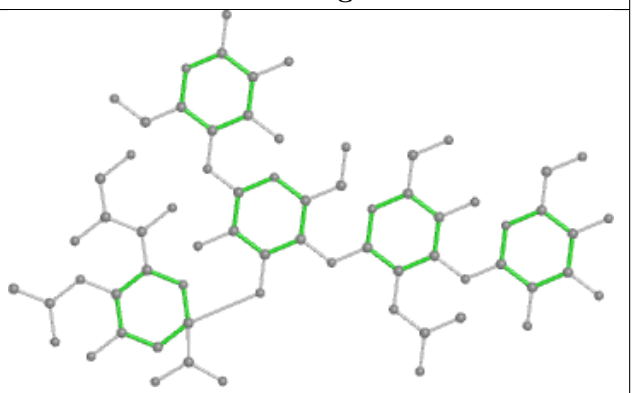
Bond lengths



Bond angles

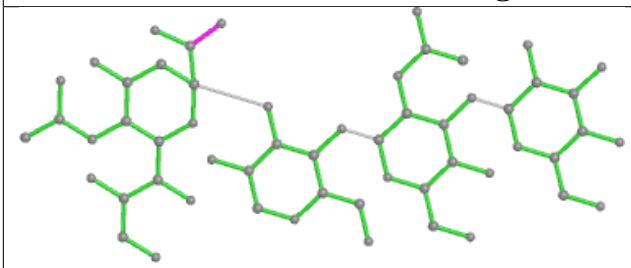


Torsions

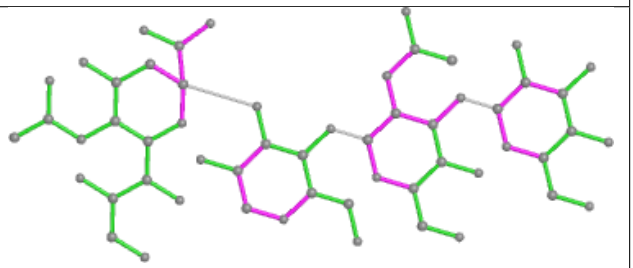


Rings

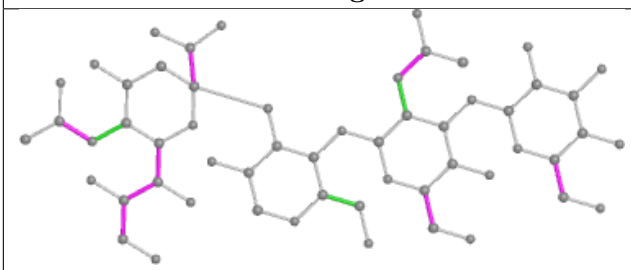
Oligosaccharide Chain A



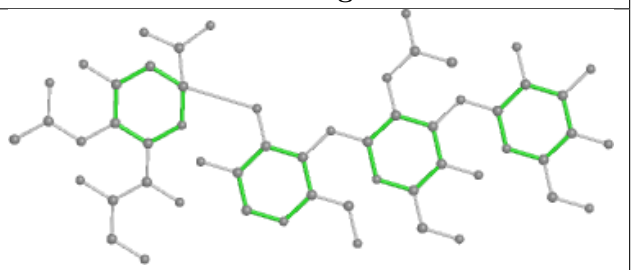
Bond lengths



Bond angles

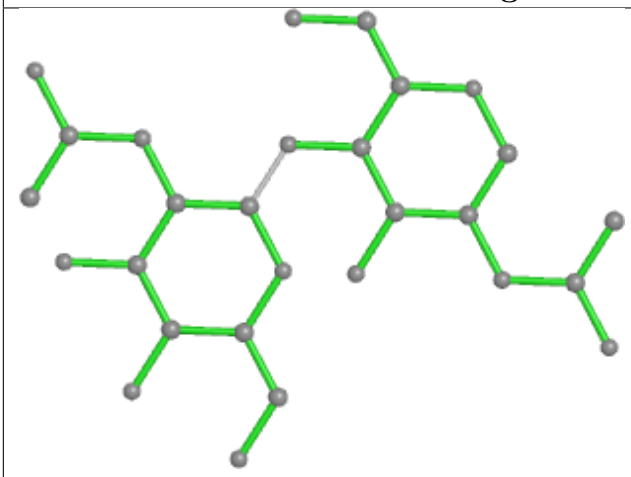


Torsions

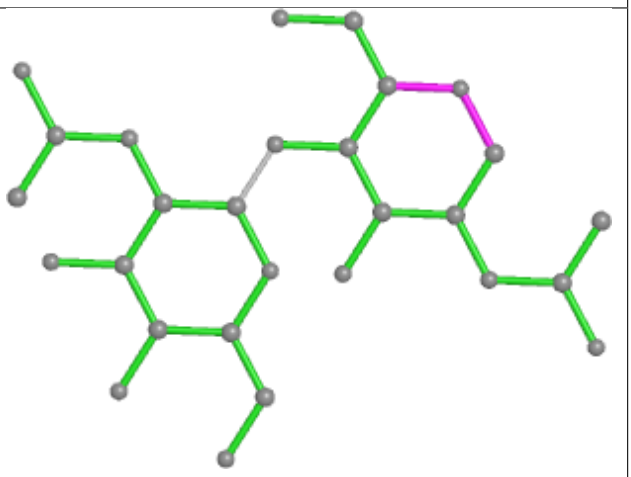


Rings

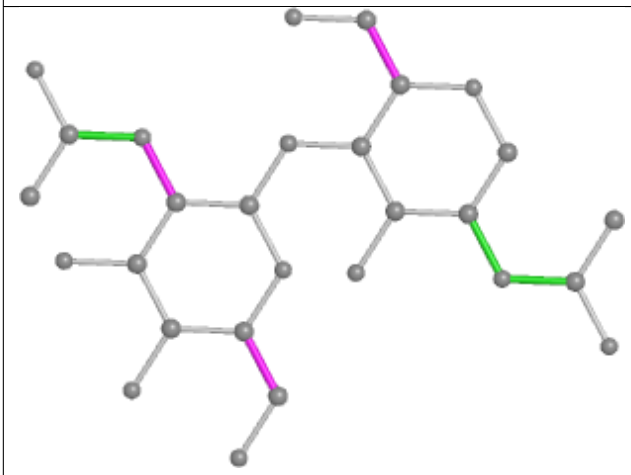
Oligosaccharide Chain s



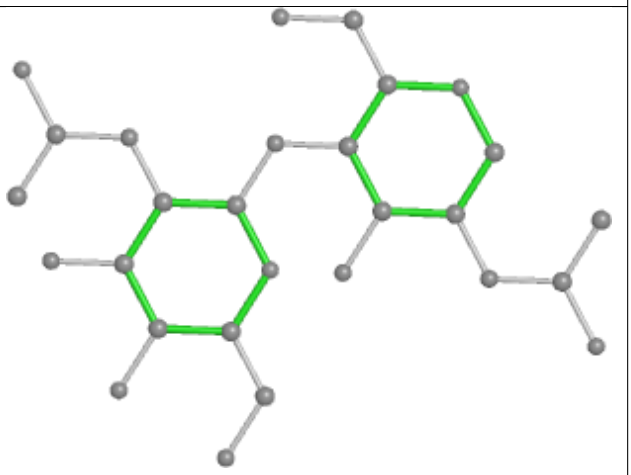
Bond lengths



Bond angles

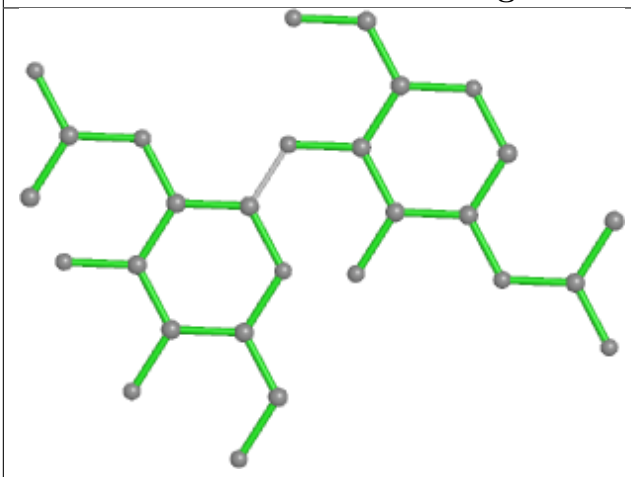


Torsions

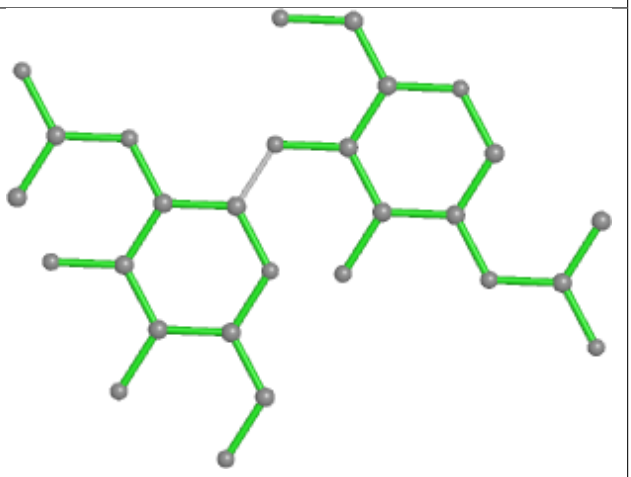


Rings

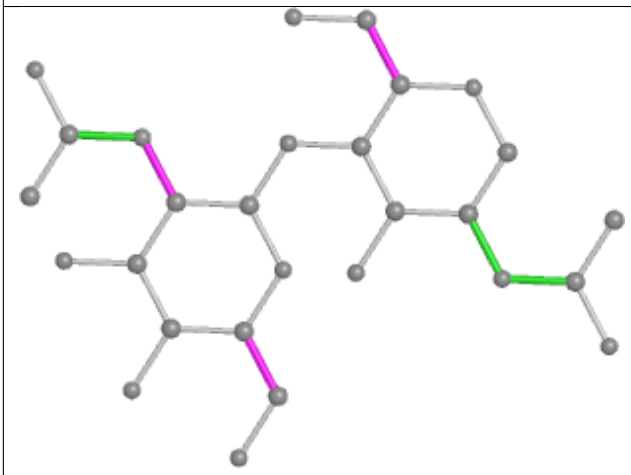
Oligosaccharide Chain u



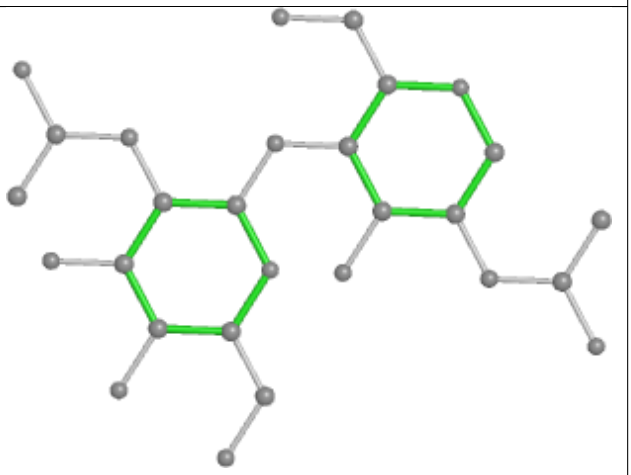
Bond lengths



Bond angles

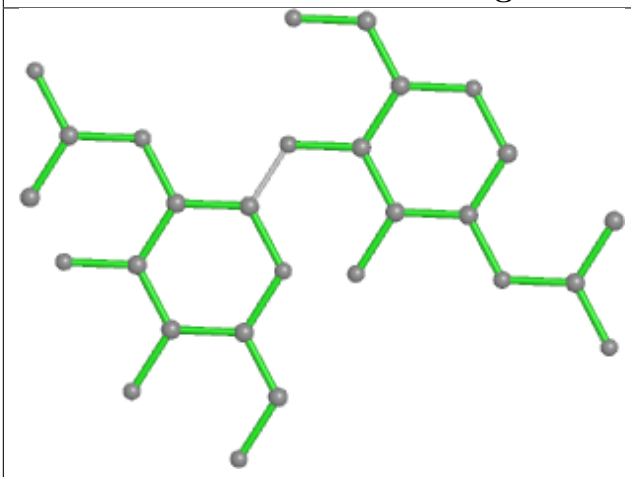


Torsions

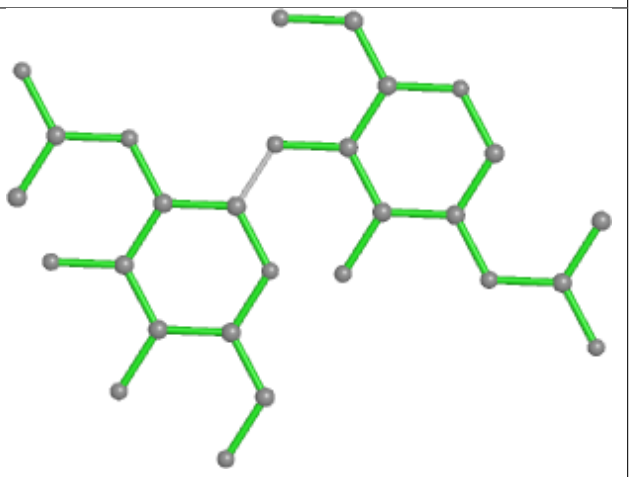


Rings

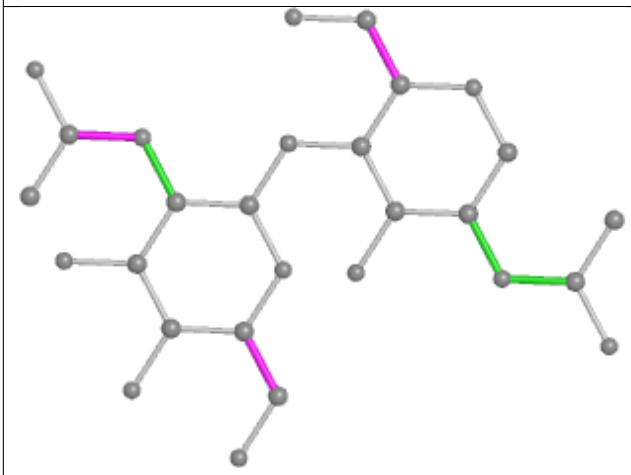
Oligosaccharide Chain B



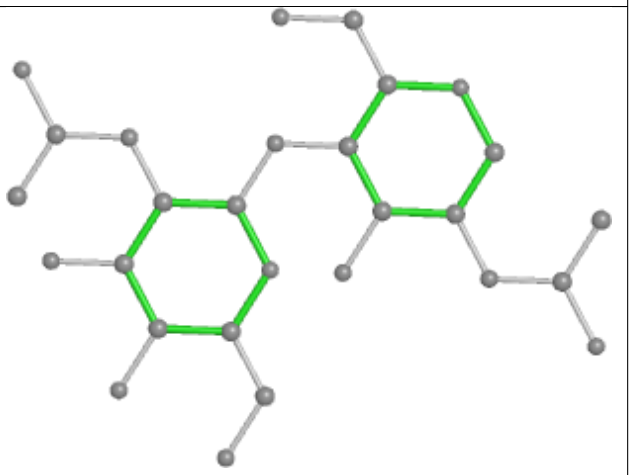
Bond lengths



Bond angles

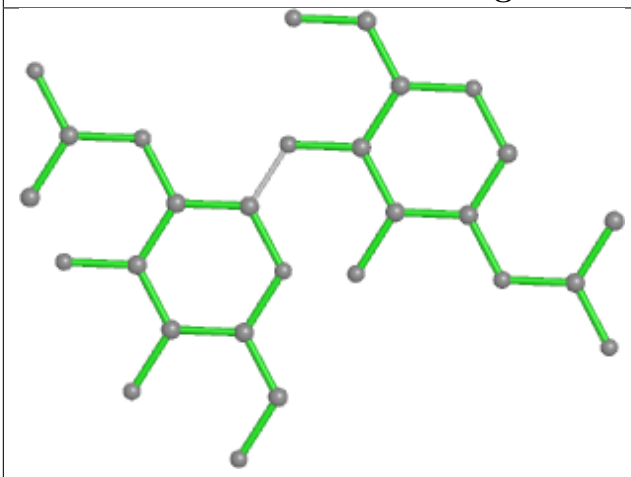


Torsions

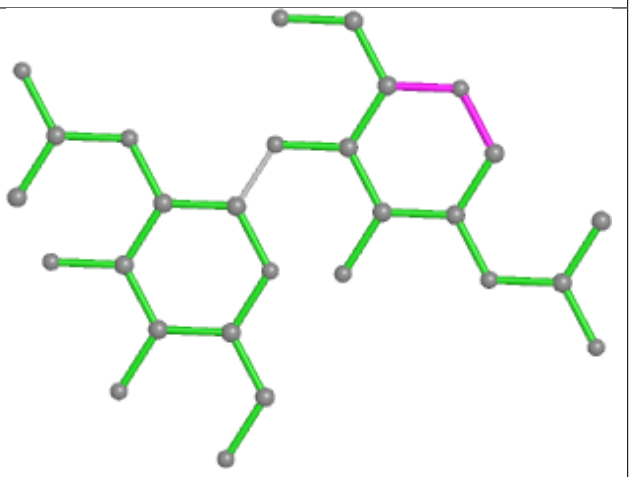


Rings

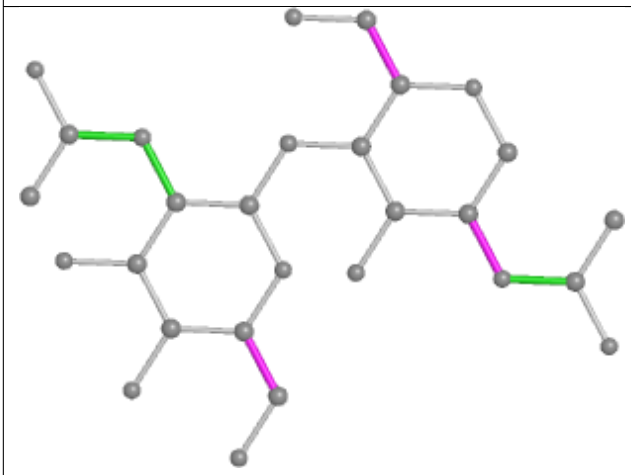
Oligosaccharide Chain C



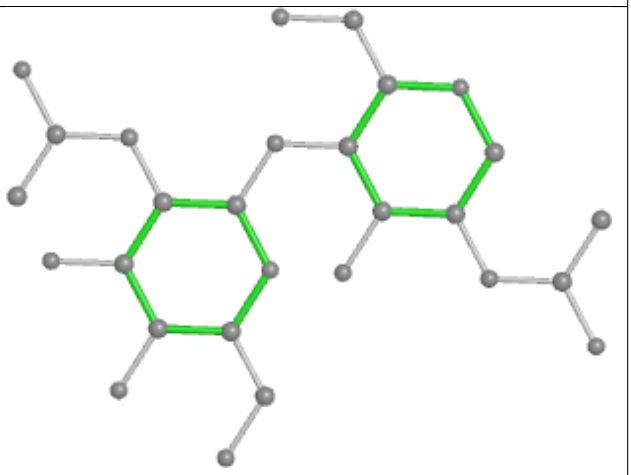
Bond lengths



Bond angles

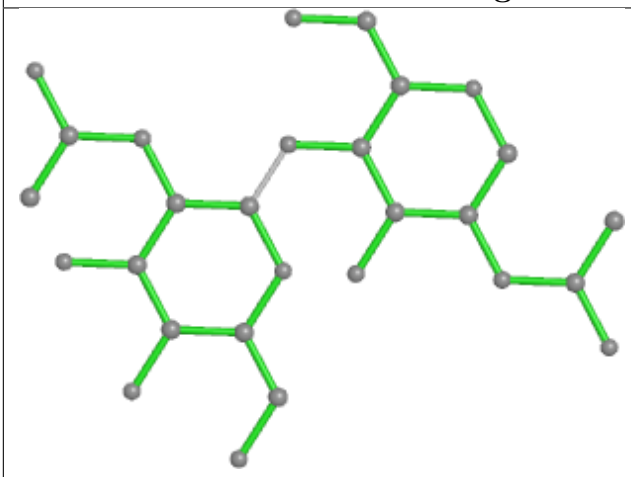


Torsions

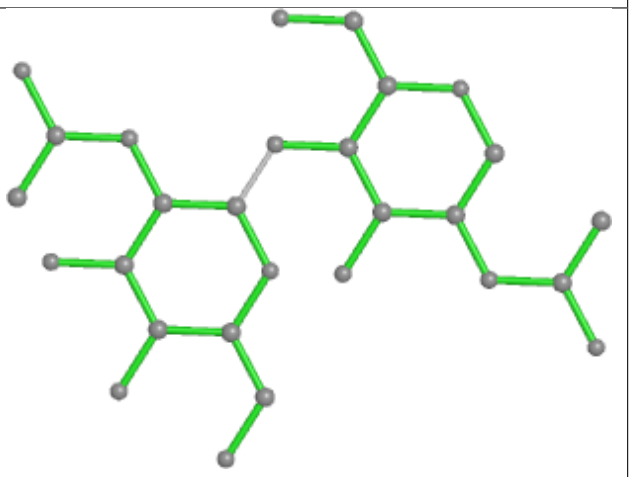


Rings

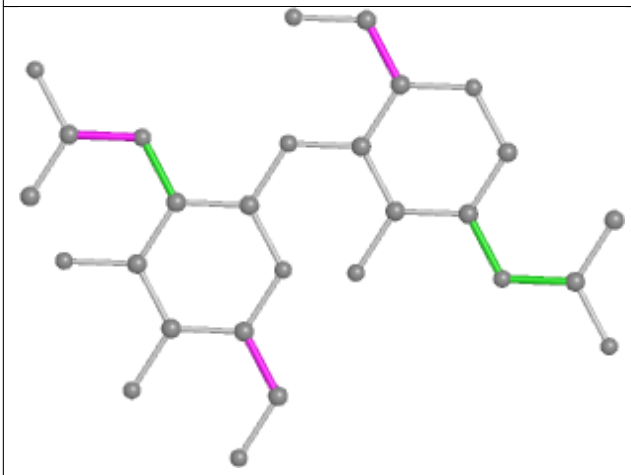
Oligosaccharide Chain D



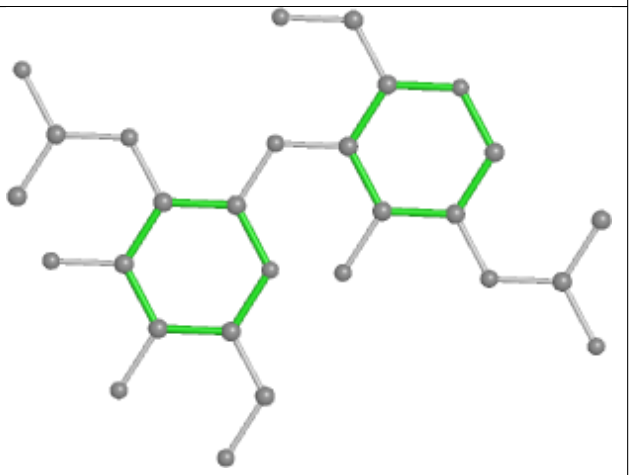
Bond lengths



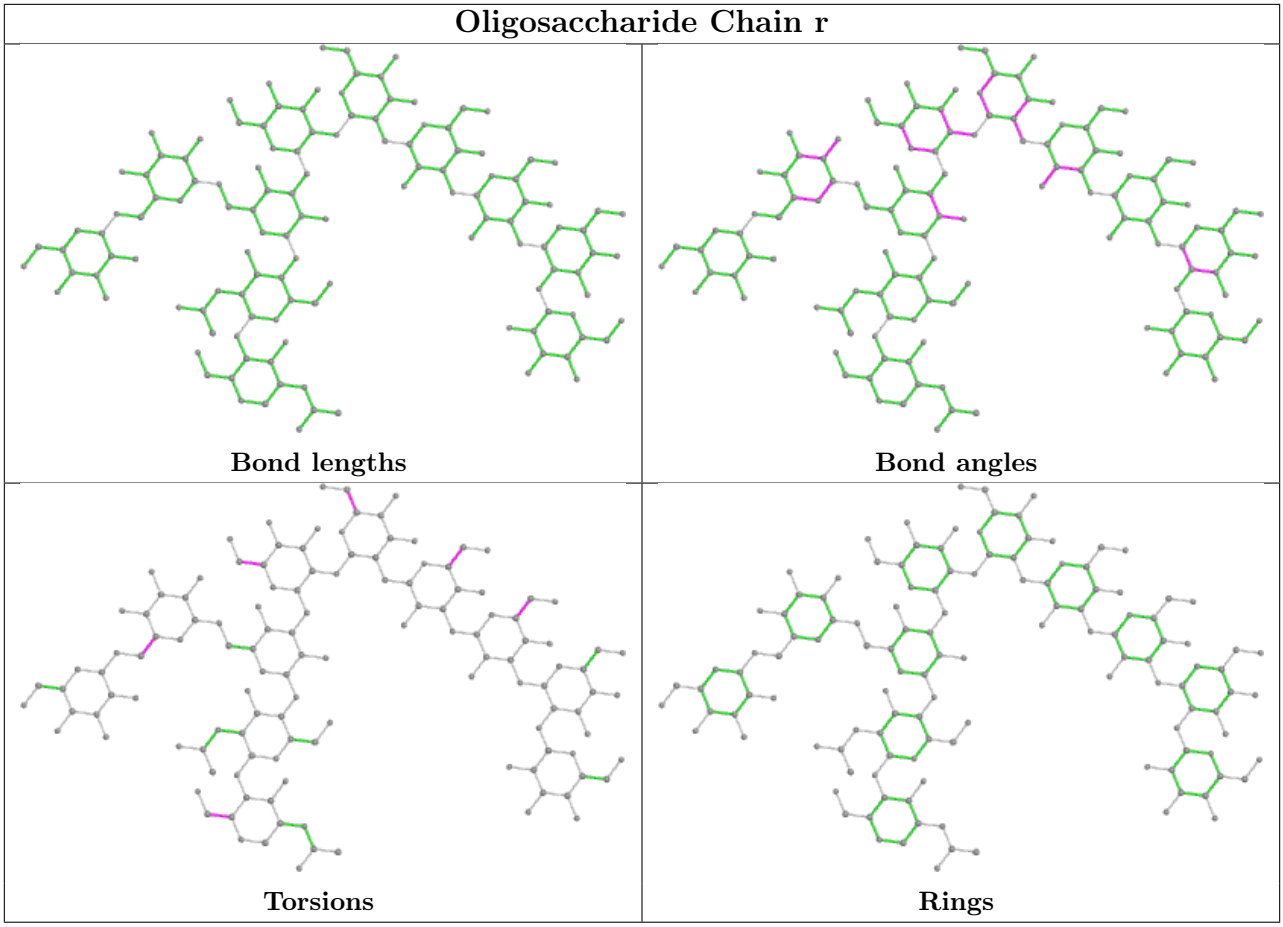
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

31 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
14	PTY	U	504	-	25,25,49	0.34	0	27,27,54	0.32	0
14	PTY	6	201	-	20,20,49	0.42	0	22,24,54	0.42	0
16	CLR	V	403	-	31,31,31	0.51	0	48,48,48	0.61	0
13	WSS	1	201	-	33,33,53	0.37	0	39,41,61	0.66	1 (2%)
13	WSS	0	304	-	30,30,53	0.47	0	33,35,61	0.63	1 (3%)
14	PTY	0	305	-	16,16,49	0.57	0	19,20,54	0.72	1 (5%)
16	CLR	V	402	-	31,31,31	0.31	0	48,48,48	0.41	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
13	WSS	R	904	-	39,39,53	0.35	0	45,47,61	0.39	0
13	WSS	3	201	-	40,40,53	0.46	0	43,45,61	0.69	1 (2%)
14	PTY	0	306	-	47,47,49	0.28	0	50,52,54	0.34	0
13	WSS	0	301	-	40,40,53	0.34	0	45,48,61	0.41	0
13	WSS	U	501	-	43,43,53	0.36	0	48,51,61	0.81	1 (2%)
14	PTY	5	202	-	34,34,49	0.36	0	37,39,54	0.43	0
13	WSS	0	303	-	25,25,53	0.39	0	31,33,61	0.81	1 (3%)
15	WJS	3	202	-	25,26,34	1.40	2 (8%)	28,32,40	1.54	2 (7%)
16	CLR	5	201	-	31,31,31	0.29	0	48,48,48	0.64	1 (2%)
16	CLR	R	901	-	31,31,31	0.27	0	48,48,48	0.49	0
13	WSS	0	302	-	36,36,53	0.39	0	42,44,61	0.54	0
14	PTY	S	101	-	31,31,49	0.31	0	33,33,54	0.32	0
18	WJP	R	905	-	31,33,34	1.65	4 (12%)	39,43,44	1.96	12 (30%)
13	WSS	U	502	-	38,38,53	0.37	0	43,46,61	0.34	0
14	PTY	R	903	-	28,28,49	0.32	0	30,32,54	0.45	0
14	PTY	8	202	-	32,32,49	0.29	0	34,34,54	0.43	0
14	PTY	8	201	-	49,49,49	0.29	0	52,54,54	0.31	0
17	PSF	R	902	-	28,29,29	0.51	0	32,36,36	0.57	0
14	PTY	V	404	-	28,28,49	0.34	0	30,32,54	0.40	0
14	PTY	U	503	-	29,29,49	0.36	0	32,34,54	0.45	0
14	PTY	6	202	-	41,41,49	0.30	0	44,46,54	0.38	0
19	NAG	U	505	7	14,14,15	0.19	0	17,19,21	0.43	0
13	WSS	V	401	-	36,36,53	0.35	0	42,44,61	0.47	0
14	PTY	2	201	-	28,28,49	0.34	0	30,32,54	0.48	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	PTY	U	504	-	-	10/27/27/53	-
14	PTY	6	201	-	-	11/22/22/53	-
16	CLR	V	403	-	-	0/10/68/68	0/4/4/4
13	WSS	1	201	-	-	5/37/37/57	-
13	WSS	0	304	-	-	9/32/32/57	-
14	PTY	0	305	-	-	6/16/16/53	-
16	CLR	V	402	-	-	0/10/68/68	0/4/4/4
13	WSS	R	904	-	-	18/43/43/57	-
13	WSS	3	201	-	-	10/44/44/57	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	PTY	0	306	-	1/1/4/4	35/51/51/53	-
13	WSS	0	301	-	-	12/44/44/57	-
13	WSS	U	501	-	-	15/47/47/57	-
14	PTY	5	202	-	-	23/38/38/53	-
13	WSS	0	303	-	-	7/29/29/57	-
15	WJS	3	202	-	-	13/30/30/38	-
16	CLR	5	201	-	-	0/10/68/68	0/4/4/4
16	CLR	R	901	-	-	6/10/68/68	0/4/4/4
13	WSS	0	302	-	-	4/40/40/57	-
14	PTY	S	101	-	-	20/33/33/53	-
18	WJP	R	905	-	-	12/37/37/40	-
13	WSS	U	502	-	-	4/42/42/57	-
14	PTY	R	903	-	1/1/3/4	20/31/31/53	-
14	PTY	8	202	-	-	18/34/34/53	-
14	PTY	8	201	-	-	29/53/53/53	-
17	PSF	R	902	-	-	18/35/35/35	-
14	PTY	V	404	-	-	18/30/30/53	-
14	PTY	U	503	-	-	15/33/33/53	-
14	PTY	6	202	-	-	22/45/45/53	-
19	NAG	U	505	7	-	2/6/23/26	0/1/1/1
13	WSS	V	401	-	-	6/40/40/57	-
14	PTY	2	201	-	-	11/30/30/53	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	R	905	WJP	P31-O34	5.06	1.74	1.54
15	3	202	WJS	P25-O24	4.31	1.76	1.59
18	R	905	WJP	P27-O26	3.96	1.75	1.59
18	R	905	WJP	C15-C16	3.12	1.40	1.33
18	R	905	WJP	C10-C11	3.04	1.40	1.33
15	3	202	WJS	C29-C30	2.07	1.58	1.52

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	3	202	WJS	O28-C29-C30	6.17	113.44	108.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	R	905	WJP	C12-C11-C13	5.44	124.42	115.27
18	R	905	WJP	C04-C05-C06	-4.75	116.23	127.66
18	R	905	WJP	C17-C16-C18	4.18	122.31	115.27
13	U	501	WSS	O2-C31-C32	4.06	120.25	111.50
13	0	303	WSS	O2-C31-C32	3.32	118.67	111.50
13	3	201	WSS	O2-C31-C32	3.08	118.13	111.50
18	R	905	WJP	C03-C04-C05	2.82	119.67	112.23
13	1	201	WSS	O2-C31-C32	2.71	117.35	111.50
18	R	905	WJP	C17-C16-C15	-2.65	116.88	123.68
13	0	304	WSS	O2P-P-O1P	2.44	120.22	110.68
14	0	305	PTY	O12-P1-O13	2.42	120.16	110.68
18	R	905	WJP	O34-P31-O30	2.41	112.72	104.64
15	3	202	WJS	O27-P25-O26	2.34	123.80	112.24
18	R	905	WJP	C13-C14-C15	2.33	119.53	111.88
16	5	201	CLR	C15-C14-C13	2.31	106.62	103.84
18	R	905	WJP	O26-P27-O28	-2.27	100.22	109.07
18	R	905	WJP	C08-C06-C05	-2.19	116.69	121.12
18	R	905	WJP	C12-C11-C10	-2.12	118.23	123.68
18	R	905	WJP	C07-C06-C05	2.12	129.10	123.68
18	R	905	WJP	O34-P31-O33	-2.11	102.44	110.68

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
14	0	306	PTY	C6
14	R	903	PTY	C6

All (379) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	0	301	WSS	C5-C4-O4P-P
13	0	303	WSS	C32-C31-O2-C2
13	0	303	WSS	O31-C31-O2-C2
13	0	304	WSS	C39-C40-C41-C42
13	1	201	WSS	O31-C31-O2-C2
13	3	201	WSS	C32-C31-O2-C2
13	3	201	WSS	O31-C31-O2-C2
13	U	501	WSS	C32-C31-O2-C2
13	U	501	WSS	O31-C31-O2-C2
13	U	501	WSS	C39-C40-C41-C42
13	U	501	WSS	C1-O3P-P-O1P
13	U	501	WSS	C4-O4P-P-O1P

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Mol	Chain	Res	Type	Atoms
13	U	501	WSS	C4-O4P-P-O3P
13	V	401	WSS	C1-O3P-P-O2P
14	0	305	PTY	C5-O14-P1-O11
14	0	306	PTY	O4-C1-C6-O7
14	0	306	PTY	O10-C8-O7-C6
14	0	306	PTY	C11-C8-O7-C6
14	0	306	PTY	C3-O11-P1-O14
14	2	201	PTY	N1-C2-C3-O11
14	2	201	PTY	O14-C5-C6-C1
14	2	201	PTY	C5-O14-P1-O11
14	2	201	PTY	C5-O14-P1-O12
14	2	201	PTY	C5-O14-P1-O13
14	5	202	PTY	N1-C2-C3-O11
14	5	202	PTY	C3-O11-P1-O12
14	5	202	PTY	C3-O11-P1-O13
14	5	202	PTY	C5-O14-P1-O12
14	6	201	PTY	C5-O14-P1-O12
14	6	202	PTY	N1-C2-C3-O11
14	6	202	PTY	C3-O11-P1-O12
14	6	202	PTY	C5-O14-P1-O12
14	8	201	PTY	N1-C2-C3-O11
14	8	202	PTY	O10-C8-O7-C6
14	8	202	PTY	C11-C8-O7-C6
14	R	903	PTY	C11-C8-O7-C6
14	R	903	PTY	C5-O14-P1-O11
14	R	903	PTY	C5-O14-P1-O12
14	R	903	PTY	C5-O14-P1-O13
14	S	101	PTY	C11-C8-O7-C6
14	U	503	PTY	O30-C30-O4-C1
14	U	504	PTY	O14-C5-C6-C1
14	U	504	PTY	O14-C5-C6-O7
14	V	404	PTY	O4-C1-C6-O7
14	V	404	PTY	C3-O11-P1-O12
14	V	404	PTY	C5-O14-P1-O13
15	3	202	WJS	C29-O28-P25-O24
15	3	202	WJS	C29-O28-P25-O26
15	3	202	WJS	C30-C29-O28-P25
15	3	202	WJS	O28-C29-C30-C31
15	3	202	WJS	O28-C29-C30-N34
17	R	902	PSF	C2-O2-P-O4
17	R	902	PSF	C2-O2-P-O3
17	R	902	PSF	C13-C1-O11-C3

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Mol	Chain	Res	Type	Atoms
18	R	905	WJP	C02-C03-C04-C05
18	R	905	WJP	C25-O26-P27-O30
18	R	905	WJP	P27-O30-P31-O34
14	8	201	PTY	O30-C30-O4-C1
14	R	903	PTY	O10-C8-O7-C6
14	S	101	PTY	O10-C8-O7-C6
17	R	902	PSF	O12-C1-O11-C3
14	8	201	PTY	C31-C30-O4-C1
14	U	503	PTY	C31-C30-O4-C1
13	1	201	WSS	C32-C31-O2-C2
17	R	902	PSF	OT2-C-CA-N
14	8	202	PTY	O30-C30-O4-C1
14	S	101	PTY	O30-C30-O4-C1
15	3	202	WJS	O20-C21-C22-O35
13	R	904	WSS	C32-C31-O2-C2
14	0	306	PTY	C33-C34-C35-C36
15	3	202	WJS	C12-C13-C14-C15
14	0	306	PTY	C17-C18-C19-C20
16	R	901	CLR	C13-C17-C20-C22
14	8	202	PTY	C31-C30-O4-C1
14	S	101	PTY	C31-C30-O4-C1
14	0	306	PTY	C36-C37-C38-C39
14	V	404	PTY	O14-C5-C6-C1
14	8	202	PTY	C32-C33-C34-C35
14	6	201	PTY	C31-C30-O4-C1
15	3	202	WJS	C10-C11-C12-C13
19	U	505	NAG	C8-C7-N2-C2
19	U	505	NAG	O7-C7-N2-C2
14	0	305	PTY	C30-C31-C32-C33
14	V	404	PTY	C30-C31-C32-C33
18	R	905	WJP	C01-C02-C03-C04
16	R	901	CLR	C13-C17-C20-C21
14	0	306	PTY	C30-C31-C32-C33
14	8	201	PTY	C8-C11-C12-C13
14	8	202	PTY	C8-C11-C12-C13
14	8	202	PTY	C30-C31-C32-C33
13	R	904	WSS	O31-C31-O2-C2
16	R	901	CLR	C22-C23-C24-C25
14	6	202	PTY	C30-C31-C32-C33
14	6	201	PTY	O30-C30-O4-C1
14	2	201	PTY	O14-C5-C6-O7
14	V	404	PTY	O14-C5-C6-O7

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Mol	Chain	Res	Type	Atoms
14	U	504	PTY	C31-C30-O4-C1
13	0	301	WSS	C1-O3P-P-O4P
13	0	301	WSS	C4-O4P-P-O3P
13	U	501	WSS	C1-O3P-P-O4P
13	U	502	WSS	C1-O3P-P-O4P
13	V	401	WSS	C1-O3P-P-O4P
14	0	306	PTY	C5-O14-P1-O11
14	5	202	PTY	C3-O11-P1-O14
14	5	202	PTY	C5-O14-P1-O11
14	6	202	PTY	C3-O11-P1-O14
14	6	202	PTY	C5-O14-P1-O11
14	V	404	PTY	C3-O11-P1-O14
14	V	404	PTY	C5-O14-P1-O11
17	R	902	PSF	C2-O2-P-O1
13	V	401	WSS	C31-C32-C33-C34
14	8	201	PTY	C11-C8-O7-C6
13	0	304	WSS	C34-C35-C36-C37
14	0	306	PTY	C14-C15-C16-C17
14	8	201	PTY	C18-C19-C20-C21
13	R	904	WSS	C32-C33-C34-C35
14	0	306	PTY	C23-C24-C25-C26
14	6	202	PTY	C37-C38-C39-C40
14	8	201	PTY	O10-C8-O7-C6
14	2	201	PTY	C31-C32-C33-C34
14	6	202	PTY	C34-C35-C36-C37
14	8	201	PTY	C39-C40-C41-C42
14	S	101	PTY	C36-C37-C38-C39
14	U	503	PTY	C35-C36-C37-C38
14	R	903	PTY	C20-C21-C22-C23
14	8	201	PTY	C31-C32-C33-C34
14	8	202	PTY	C40-C41-C42-C43
15	3	202	WJS	C13-C14-C15-C16
14	U	504	PTY	O30-C30-O4-C1
14	0	306	PTY	C35-C36-C37-C38
14	5	202	PTY	C39-C40-C41-C42
14	R	903	PTY	C19-C20-C21-C22
14	S	101	PTY	C14-C15-C16-C17
14	0	306	PTY	C31-C32-C33-C34
14	8	201	PTY	C12-C13-C14-C15
14	8	201	PTY	C32-C33-C34-C35
14	8	202	PTY	C34-C35-C36-C37
14	S	101	PTY	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
14	U	504	PTY	C32-C33-C34-C35
13	R	904	WSS	C42-C43-C44-C45
14	0	306	PTY	C16-C17-C18-C19
14	8	201	PTY	C30-C31-C32-C33
14	0	306	PTY	C12-C13-C14-C15
14	R	903	PTY	C18-C19-C20-C21
14	S	101	PTY	O4-C1-C6-C5
14	R	903	PTY	C11-C12-C13-C14
17	R	902	PSF	C6-C5-O52-C4
13	R	904	WSS	C43-C44-C45-C46
14	V	404	PTY	C31-C32-C33-C34
13	R	904	WSS	C11-C12-C13-C14
14	2	201	PTY	C31-C30-O4-C1
14	0	306	PTY	C21-C22-C23-C24
14	5	202	PTY	C32-C33-C34-C35
14	S	101	PTY	C32-C33-C34-C35
16	R	901	CLR	C16-C17-C20-C21
14	0	306	PTY	C19-C20-C21-C22
14	0	305	PTY	C31-C32-C33-C34
14	5	202	PTY	C11-C12-C13-C14
13	R	904	WSS	C38-C39-C40-C41
16	R	901	CLR	C16-C17-C20-C22
14	5	202	PTY	C31-C30-O4-C1
14	6	202	PTY	C31-C30-O4-C1
14	V	404	PTY	C39-C40-C41-C42
14	5	202	PTY	C40-C41-C42-C43
17	R	902	PSF	O51-C5-O52-C4
14	V	404	PTY	C31-C30-O4-C1
14	6	202	PTY	C36-C37-C38-C39
14	U	503	PTY	C11-C8-O7-C6
14	6	202	PTY	C13-C14-C15-C16
14	S	101	PTY	C35-C36-C37-C38
14	R	903	PTY	C15-C16-C17-C18
14	U	503	PTY	O10-C8-O7-C6
14	R	903	PTY	C13-C14-C15-C16
14	V	404	PTY	C36-C37-C38-C39
14	6	202	PTY	C12-C13-C14-C15
14	8	201	PTY	C23-C24-C25-C26
14	U	504	PTY	C11-C12-C13-C14
14	0	306	PTY	C20-C21-C22-C23
14	6	202	PTY	C39-C40-C41-C42
16	R	901	CLR	C20-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
14	6	201	PTY	C5-O14-P1-O11
14	R	903	PTY	C3-O11-P1-O14
14	0	306	PTY	C6-C5-O14-P1
14	5	202	PTY	O30-C30-O4-C1
13	U	501	WSS	O3P-C1-C2-C3
14	R	903	PTY	O14-C5-C6-C1
14	0	306	PTY	C32-C33-C34-C35
14	2	201	PTY	O30-C30-O4-C1
14	0	306	PTY	C38-C39-C40-C41
14	8	201	PTY	C22-C23-C24-C25
13	0	304	WSS	C1-C2-C3-O3
14	0	306	PTY	O4-C1-C6-C5
14	S	101	PTY	C15-C16-C17-C18
14	0	306	PTY	C15-C16-C17-C18
13	R	904	WSS	C35-C36-C37-C38
14	U	503	PTY	C11-C12-C13-C14
14	2	201	PTY	C30-C31-C32-C33
14	6	202	PTY	C41-C42-C43-C44
14	U	503	PTY	C36-C37-C38-C39
14	8	202	PTY	C36-C37-C38-C39
14	8	202	PTY	C41-C42-C43-C44
17	R	902	PSF	C7-C8-C9-C10
14	0	305	PTY	C32-C33-C34-C35
14	6	202	PTY	O30-C30-O4-C1
14	8	202	PTY	C15-C16-C17-C18
13	U	501	WSS	C1-C2-O2-C31
14	0	305	PTY	C5-O14-P1-O13
14	6	201	PTY	C31-C32-C33-C34
14	S	101	PTY	C37-C38-C39-C40
14	V	404	PTY	O30-C30-O4-C1
13	R	904	WSS	C41-C42-C43-C44
17	R	902	PSF	C1-C13-C14-C15
14	R	903	PTY	C21-C22-C23-C24
13	0	303	WSS	O2-C2-C3-O3
14	5	202	PTY	O4-C1-C6-O7
18	R	905	WJP	C24-C02-C03-C04
14	8	201	PTY	C25-C26-C27-C28
14	0	306	PTY	O14-C5-C6-C1
14	5	202	PTY	C30-C31-C32-C33
14	8	202	PTY	C33-C34-C35-C36
14	8	201	PTY	C17-C18-C19-C20
13	0	301	WSS	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
14	6	201	PTY	C30-C31-C32-C33
14	8	201	PTY	C24-C25-C26-C27
14	U	503	PTY	C33-C34-C35-C36
14	6	202	PTY	C6-C5-O14-P1
14	8	202	PTY	C14-C15-C16-C17
13	3	201	WSS	C1-C2-C3-O3
14	5	202	PTY	O4-C1-C6-C5
14	6	202	PTY	O4-C1-C6-C5
14	V	404	PTY	O4-C1-C6-C5
14	8	202	PTY	C11-C12-C13-C14
17	R	902	PSF	C13-C14-C15-C16
13	0	301	WSS	C33-C34-C35-C36
15	3	202	WJS	C23-O24-P25-O28
14	8	201	PTY	C26-C27-C28-C29
13	0	303	WSS	O3P-C1-C2-O2
13	U	501	WSS	O3P-C1-C2-O2
14	0	306	PTY	O14-C5-C6-O7
14	8	202	PTY	C37-C38-C39-C40
14	S	101	PTY	C41-C42-C43-C44
14	U	503	PTY	C31-C32-C33-C34
17	R	902	PSF	OT1-C-CA-N
14	8	201	PTY	C6-C5-O14-P1
14	6	201	PTY	C32-C33-C34-C35
14	5	202	PTY	C37-C38-C39-C40
14	0	306	PTY	C18-C19-C20-C21
13	0	301	WSS	C19-C20-C21-C22
18	R	905	WJP	P31-O30-P27-O26
14	5	202	PTY	O14-C5-C6-C1
14	U	503	PTY	O14-C5-C6-C1
13	0	304	WSS	C37-C38-C39-C40
14	8	201	PTY	C35-C36-C37-C38
14	5	202	PTY	C31-C32-C33-C34
14	5	202	PTY	C36-C37-C38-C39
13	3	201	WSS	C19-C20-C21-C22
14	8	201	PTY	C33-C34-C35-C36
14	U	503	PTY	C1-C6-O7-C8
13	U	501	WSS	C2-C1-O3P-P
13	U	502	WSS	C2-C1-O3P-P
14	U	503	PTY	O4-C1-C6-C5
14	R	903	PTY	O14-C5-C6-O7
14	U	503	PTY	O14-C5-C6-O7
13	0	302	WSS	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
13	3	201	WSS	O2-C2-C3-O3
14	S	101	PTY	O4-C1-C6-O7
13	0	301	WSS	C11-C12-C13-C14
13	R	904	WSS	C4-C5-N1-C8
14	S	101	PTY	C11-C12-C13-C14
17	R	902	PSF	N-CA-CB-O1
14	0	306	PTY	C31-C30-O4-C1
14	5	202	PTY	C34-C35-C36-C37
14	6	202	PTY	C40-C41-C42-C43
13	0	303	WSS	C1-O3P-P-O4P
13	0	301	WSS	C1-O3P-P-O2P
13	0	301	WSS	C4-O4P-P-O2P
13	U	501	WSS	C1-O3P-P-O2P
14	0	306	PTY	C3-O11-P1-O12
14	0	306	PTY	C5-O14-P1-O13
14	5	202	PTY	C5-O14-P1-O13
14	6	201	PTY	C5-O14-P1-O13
14	V	404	PTY	C5-O14-P1-O12
18	R	905	WJP	C25-O26-P27-O29
18	R	905	WJP	C16-C18-C19-C20
13	0	302	WSS	C5-C4-O4P-P
17	R	902	PSF	C5-C6-C7-C8
14	6	201	PTY	O14-C5-C6-C1
15	3	202	WJS	C21-C22-C23-O24
13	3	201	WSS	C17-C18-C19-C20
13	0	301	WSS	O4P-C4-C5-N1
13	0	302	WSS	O4P-C4-C5-N1
14	0	306	PTY	O30-C30-O4-C1
13	0	304	WSS	O2-C2-C3-O3
14	V	404	PTY	C41-C42-C43-C44
13	3	201	WSS	C36-C37-C38-C39
13	R	904	WSS	C4-C5-N1-C7
13	U	501	WSS	C12-C13-C14-C15
14	6	202	PTY	C14-C15-C16-C17
13	U	501	WSS	C17-C18-C19-C20
14	6	202	PTY	C1-C6-O7-C8
14	S	101	PTY	C5-C6-O7-C8
14	5	202	PTY	O14-C5-C6-O7
14	6	202	PTY	C33-C34-C35-C36
14	6	201	PTY	C33-C34-C35-C36
14	U	503	PTY	O4-C1-C6-O7
13	1	201	WSS	C4-O4P-P-O3P

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Mol	Chain	Res	Type	Atoms
13	3	201	WSS	C4-O4P-P-O3P
14	8	201	PTY	C5-O14-P1-O11
17	R	902	PSF	CB-O1-P-O2
14	6	201	PTY	C3-O11-P1-O13
14	6	202	PTY	C35-C36-C37-C38
14	8	201	PTY	C20-C21-C22-C23
13	0	303	WSS	C1-C2-C3-O3
14	V	404	PTY	C37-C38-C39-C40
13	U	501	WSS	C19-C20-C21-C22
13	V	401	WSS	C13-C14-C15-C16
14	0	306	PTY	C37-C38-C39-C40
14	U	504	PTY	C12-C13-C14-C15
13	R	904	WSS	C34-C35-C36-C37
13	U	502	WSS	C17-C18-C19-C20
14	U	504	PTY	C6-C1-O4-C30
14	U	504	PTY	C13-C14-C15-C16
14	8	201	PTY	O4-C1-C6-O7
14	0	305	PTY	C6-C5-O14-P1
14	5	202	PTY	C35-C36-C37-C38
14	8	201	PTY	C34-C35-C36-C37
15	3	202	WJS	C29-C30-C31-O32
15	3	202	WJS	C29-C30-C31-O33
17	R	902	PSF	OT1-C-CA-CB
17	R	902	PSF	OT2-C-CA-CB
14	0	306	PTY	C40-C41-C42-C43
13	R	904	WSS	C4-C5-N1-C9
14	U	503	PTY	C34-C35-C36-C37
13	0	303	WSS	O3P-C1-C2-C3
14	R	903	PTY	O4-C1-C6-C5
14	S	101	PTY	C39-C40-C41-C42
18	R	905	WJP	P31-O30-P27-O28
13	R	904	WSS	O11-C11-O3-C3
18	R	905	WJP	C12-C11-C13-C14
13	0	301	WSS	C37-C38-C39-C40
13	3	201	WSS	C39-C40-C41-C42
18	R	905	WJP	C10-C11-C13-C14
13	R	904	WSS	C12-C11-O3-C3
14	0	306	PTY	C13-C14-C15-C16
14	R	903	PTY	O4-C1-C6-O7
14	R	903	PTY	C12-C13-C14-C15
13	0	301	WSS	C17-C18-C19-C20
18	R	905	WJP	P27-O30-P31-O33

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Mol	Chain	Res	Type	Atoms
14	2	201	PTY	C33-C34-C35-C36
13	0	304	WSS	O3-C11-C12-C13
14	0	306	PTY	C41-C42-C43-C44
13	0	302	WSS	C2-C1-O3P-P
14	8	201	PTY	O4-C1-C6-C5
13	R	904	WSS	C37-C38-C39-C40
13	3	201	WSS	C37-C38-C39-C40
14	S	101	PTY	C38-C39-C40-C41
14	S	101	PTY	C13-C14-C15-C16
13	V	401	WSS	C14-C15-C16-C17
13	R	904	WSS	C31-C32-C33-C34
14	V	404	PTY	C33-C34-C35-C36
13	1	201	WSS	C4-O4P-P-O1P
13	R	904	WSS	C1-O3P-P-O1P
13	U	502	WSS	C1-O3P-P-O1P
14	R	903	PTY	C3-O11-P1-O13
17	R	902	PSF	CB-O1-P-O4
14	0	306	PTY	N1-C2-C3-O11
14	8	202	PTY	C12-C11-C8-O7
14	8	201	PTY	C38-C39-C40-C41
13	0	304	WSS	O11-C11-C12-C13
14	8	201	PTY	C41-C42-C43-C44
14	R	903	PTY	C17-C18-C19-C20
13	1	201	WSS	O2-C31-C32-C33
14	S	101	PTY	C12-C11-C8-O7
13	V	401	WSS	O3P-C1-C2-O2
13	0	304	WSS	O2-C31-C32-C33
14	8	201	PTY	C12-C11-C8-O7
14	U	504	PTY	C15-C16-C17-C18
13	0	304	WSS	O31-C31-C32-C33
14	8	202	PTY	C12-C11-C8-O10

There are no ring outliers.

20 monomers are involved in 84 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	U	504	PTY	17	0
14	6	201	PTY	7	0
16	V	403	CLR	12	0
13	0	304	WSS	1	0
14	0	305	PTY	1	0
13	R	904	WSS	6	0

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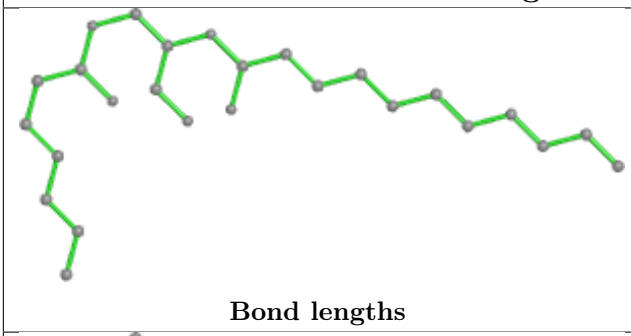
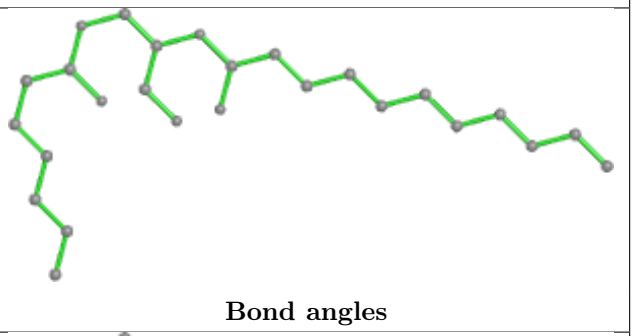
Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	0	306	PTY	3	0
14	5	202	PTY	7	0
15	3	202	WJS	5	0
16	5	201	CLR	16	0
16	R	901	CLR	2	0
18	R	905	WJP	1	0
13	U	502	WSS	3	0
14	R	903	PTY	1	0
14	8	202	PTY	4	0
14	8	201	PTY	7	0
14	V	404	PTY	9	0
14	U	503	PTY	6	0
14	6	202	PTY	6	0
14	2	201	PTY	4	0

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.

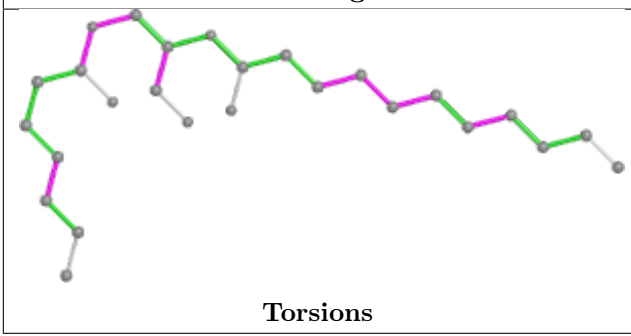
Ligand PTY U 504



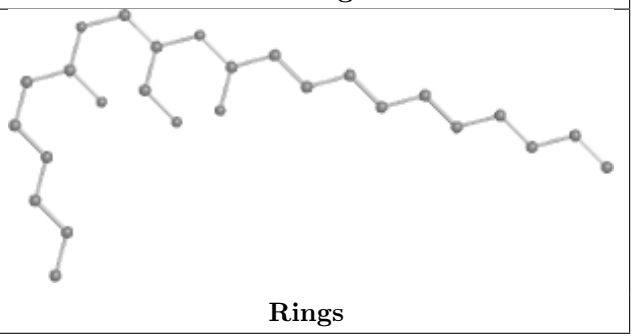
Bond lengths



Bond angles

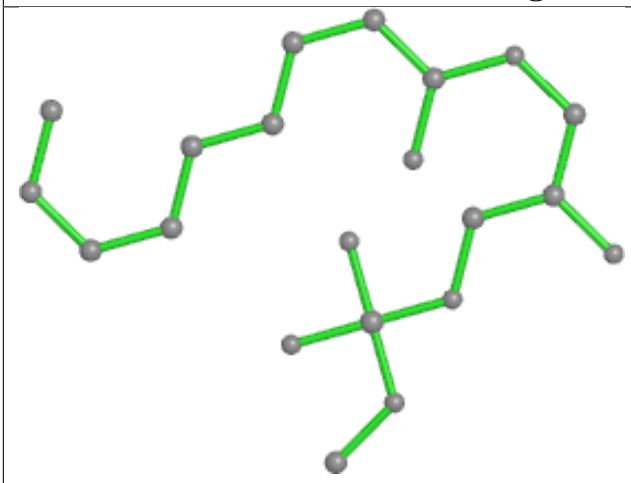


Torsions

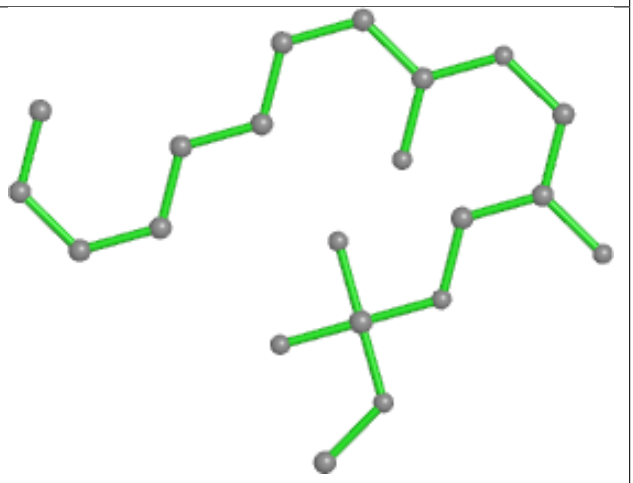


Rings

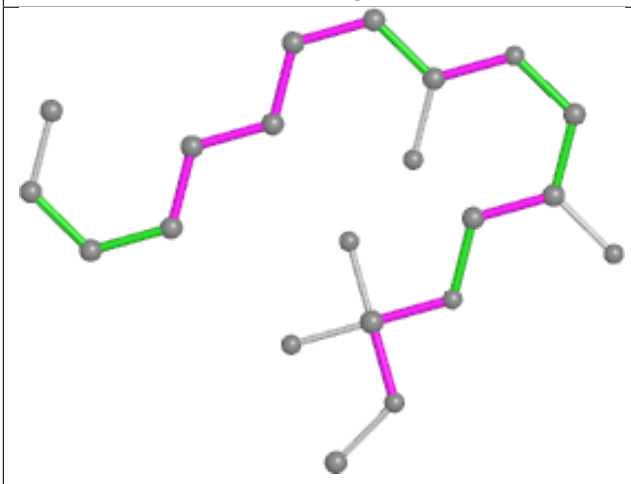
Ligand PTY 6 201



Bond lengths



Bond angles



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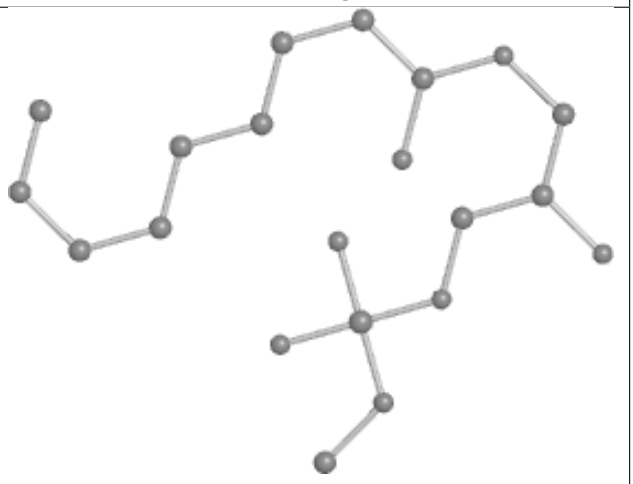
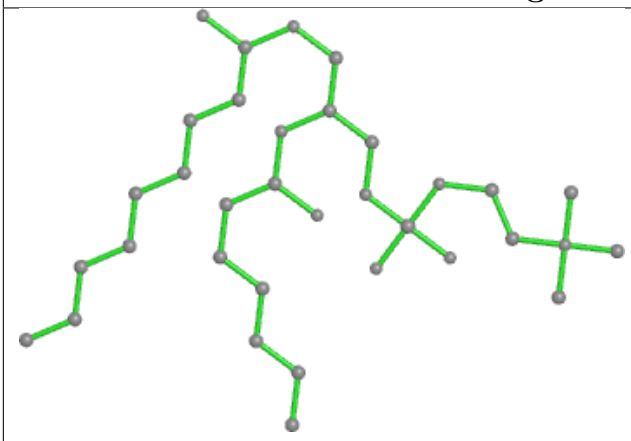
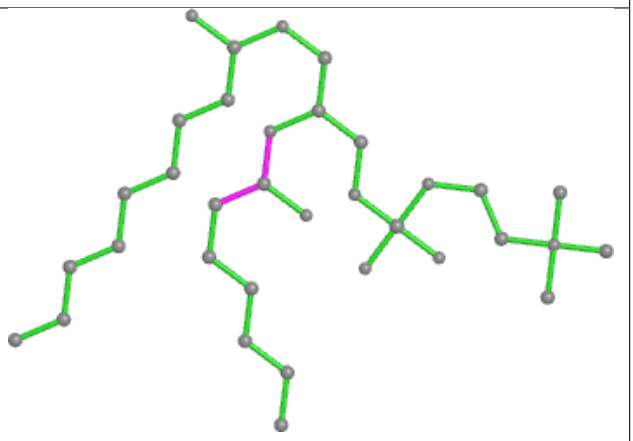


Rings

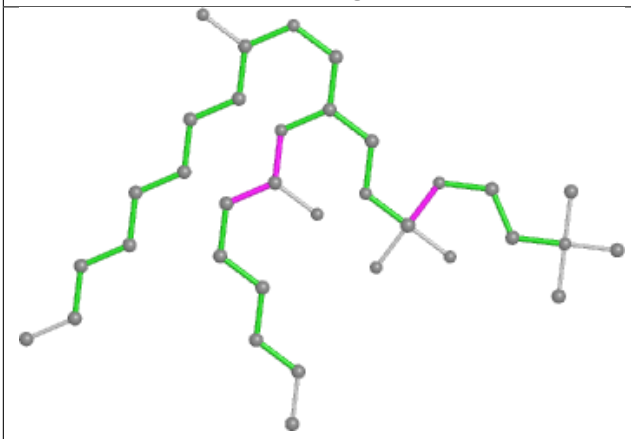
Ligand WSS 1 201



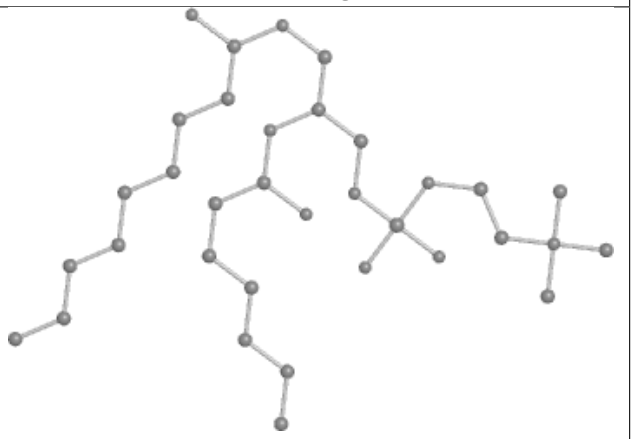
Bond lengths



Bond angles

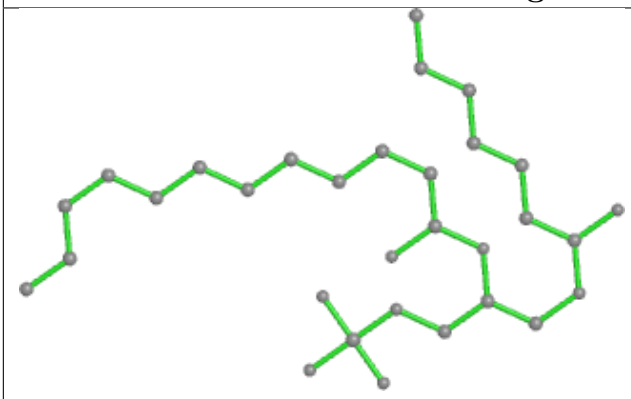


Torsions

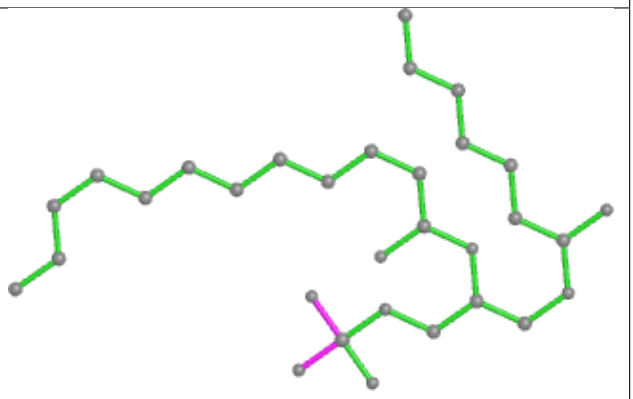


Rings

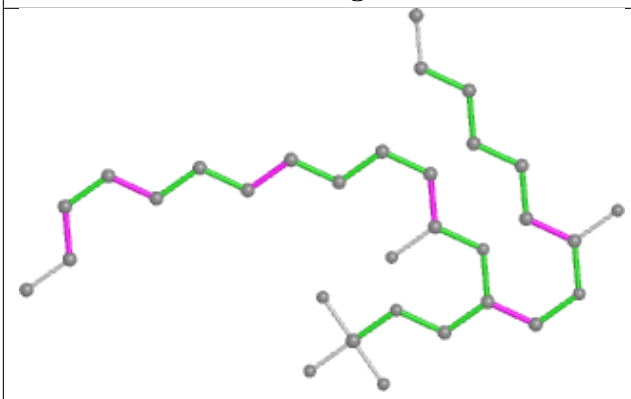
Ligand WSS 0 304



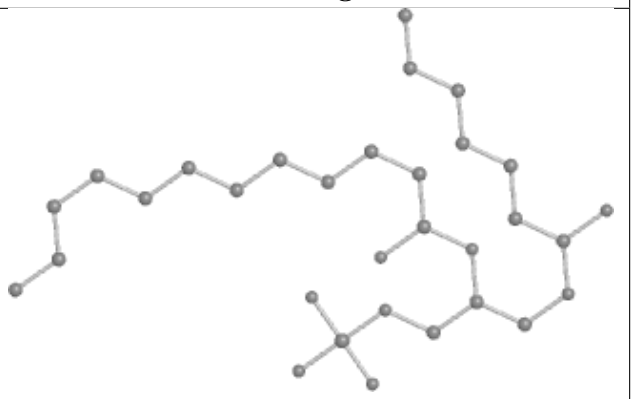
Bond lengths



Bond angles

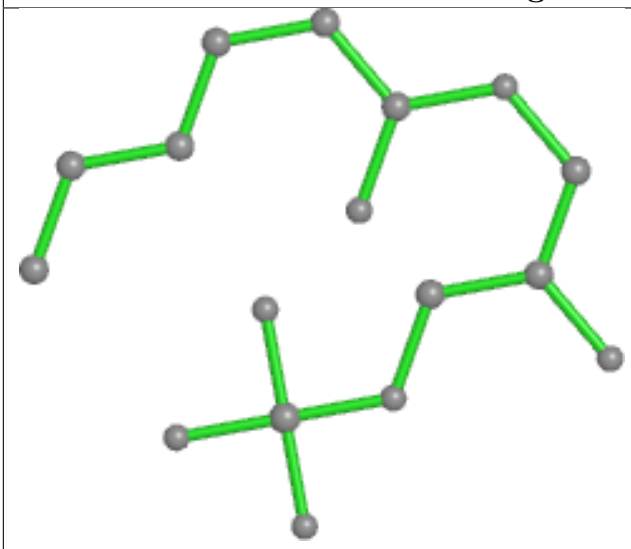


Torsions

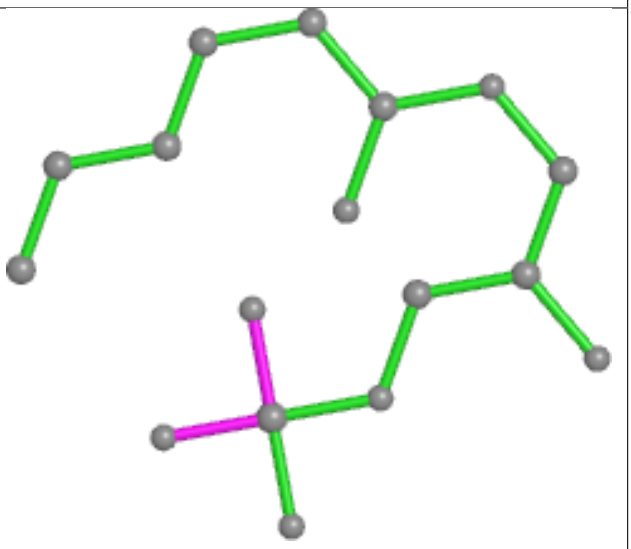


Rings

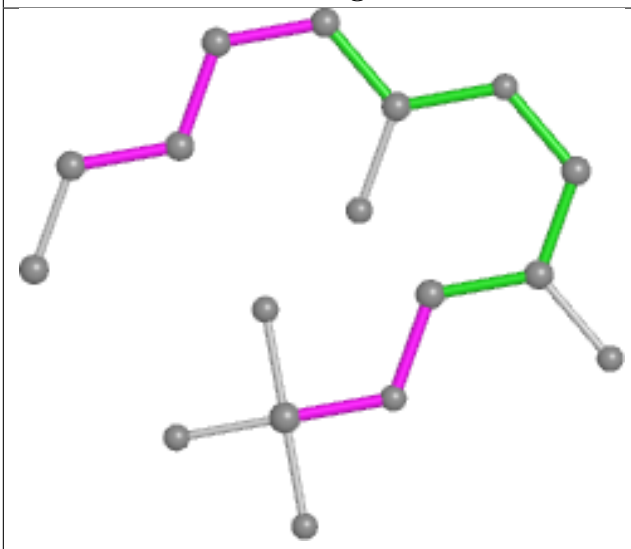
Ligand PTY 0 305



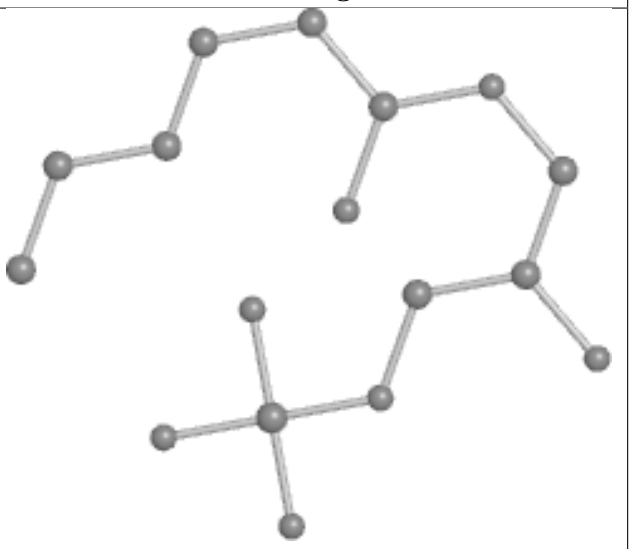
Bond lengths



Bond angles

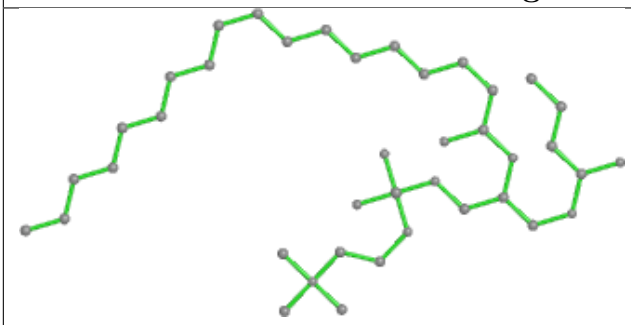


Torsions



Rings

Ligand WSS R 904



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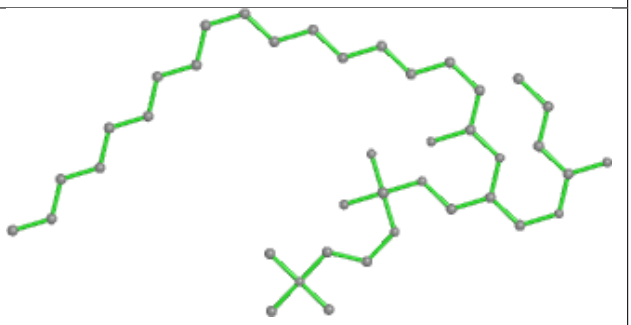
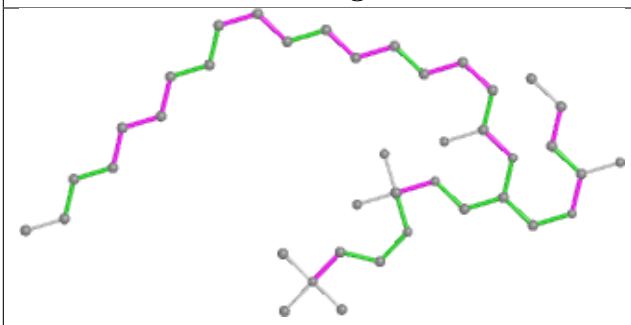


Bond angles



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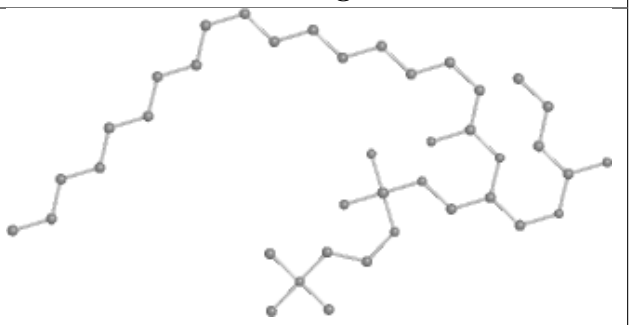
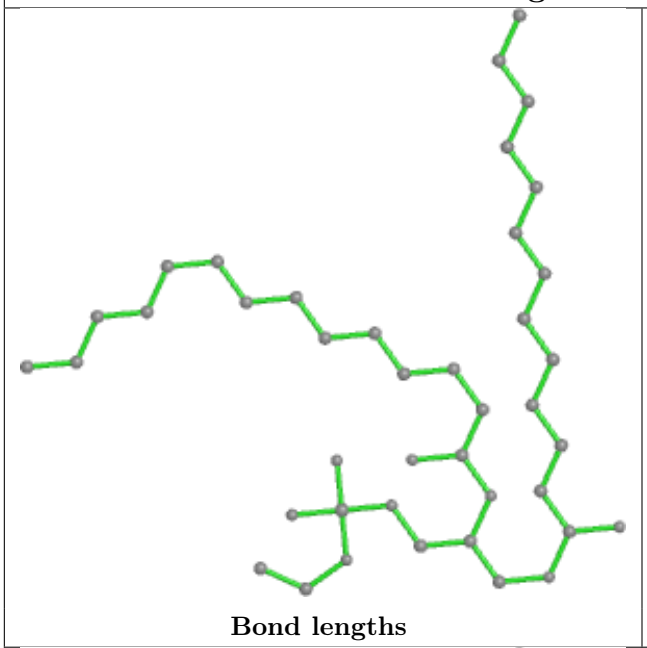
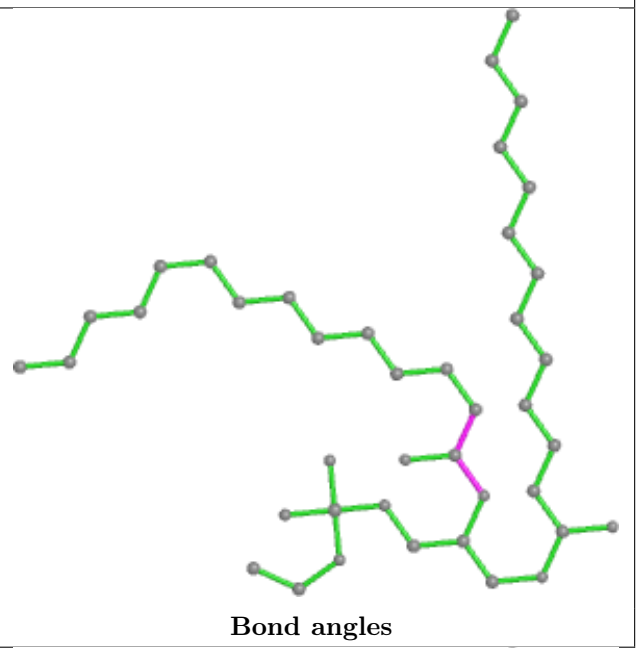


Rings

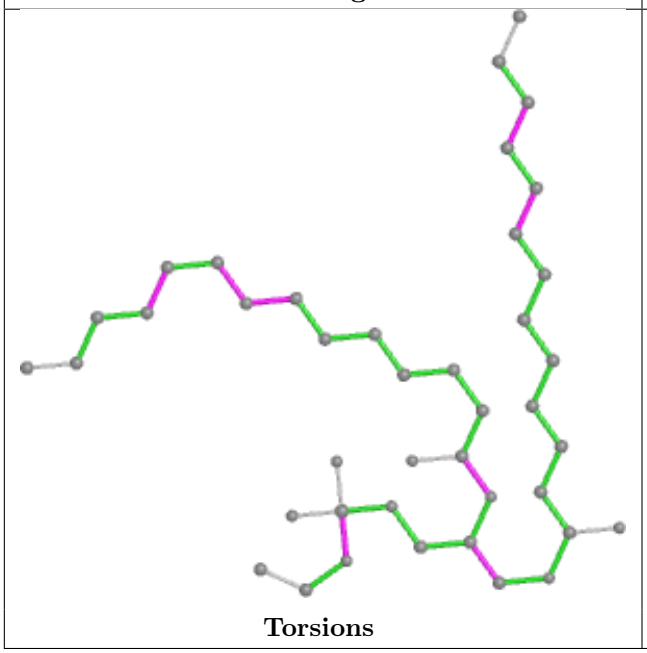
Ligand WSS 3 201



Bond lengths



Bond angles



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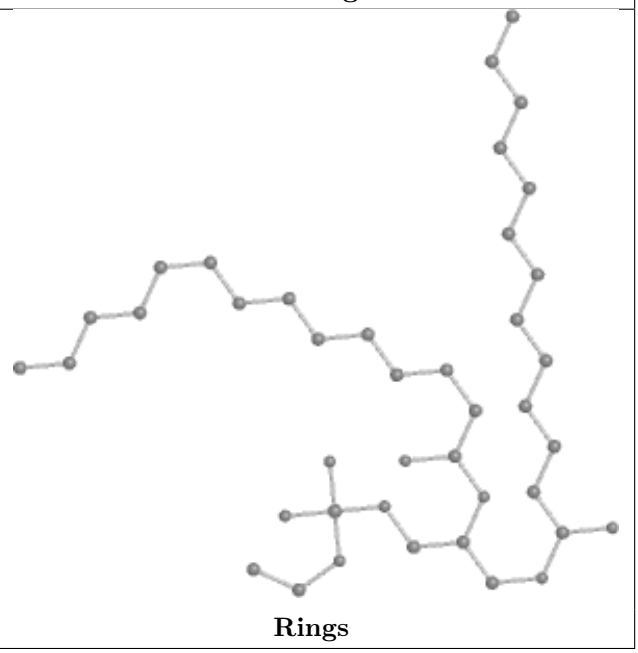
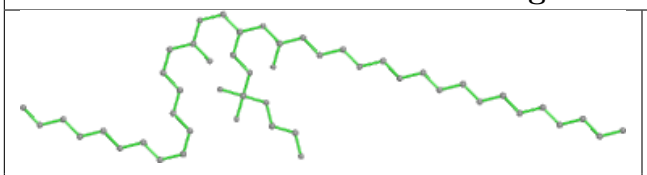
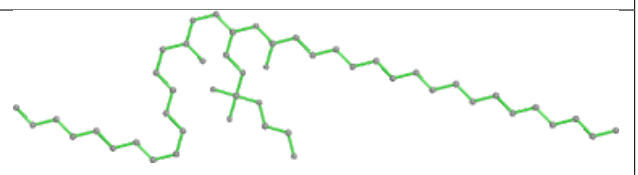


Rings

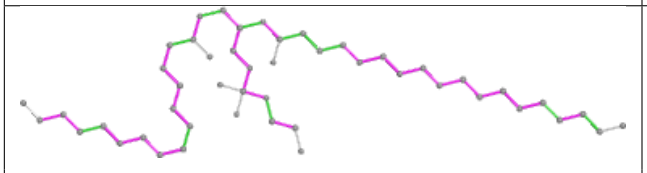
Ligand PTY 0 306



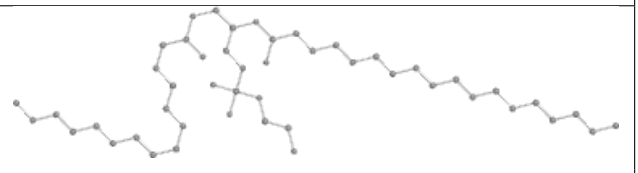
Bond lengths



Bond angles

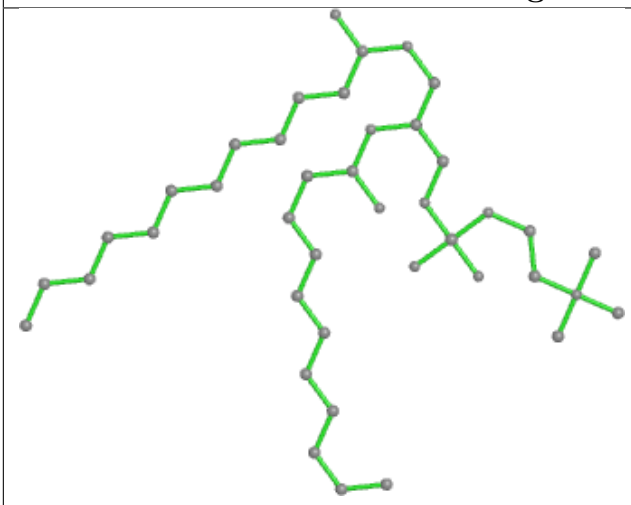


Torsions

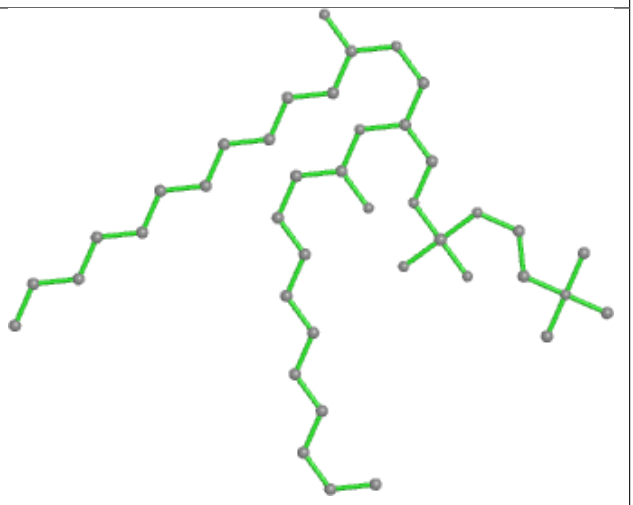


Rings

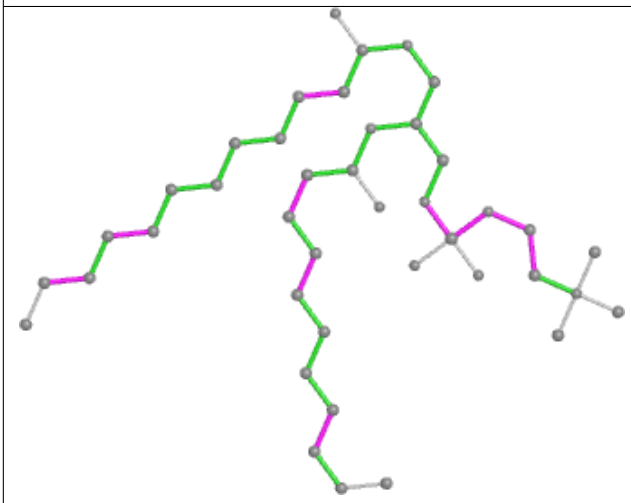
Ligand WSS 0 301



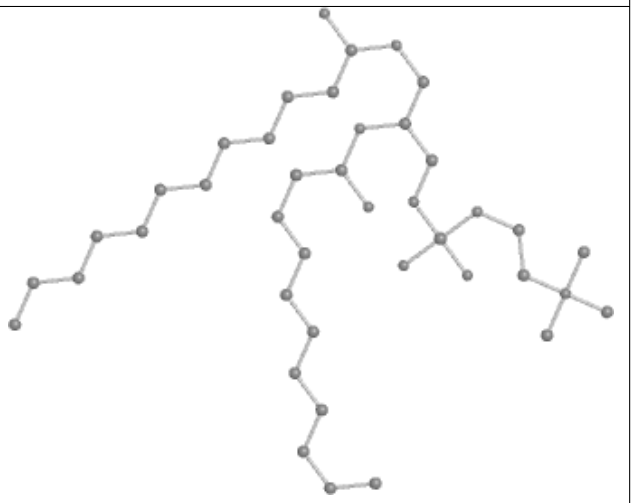
Bond lengths



Bond angles

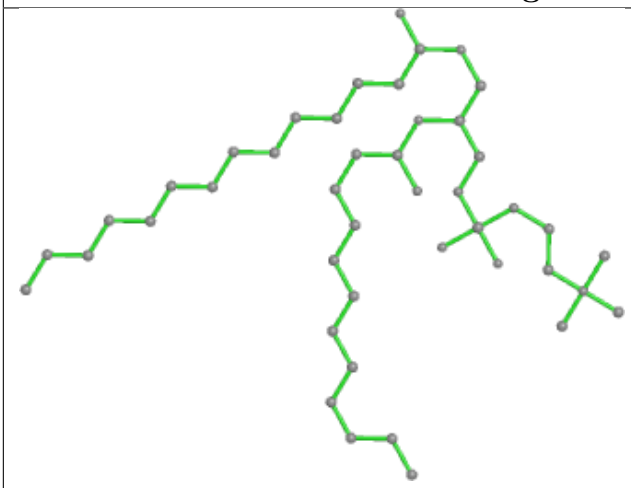


Torsions

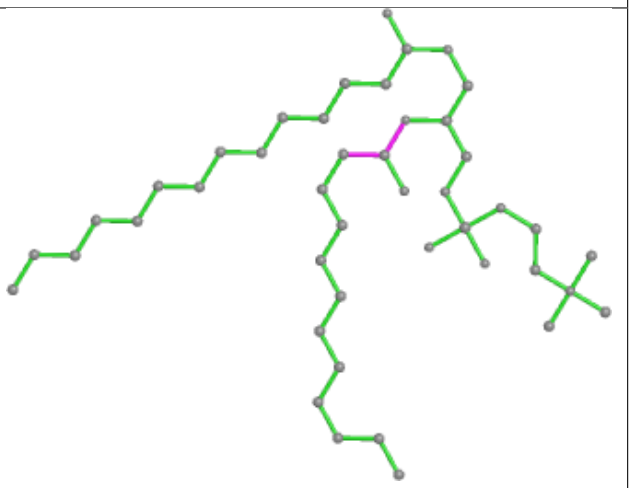


Rings

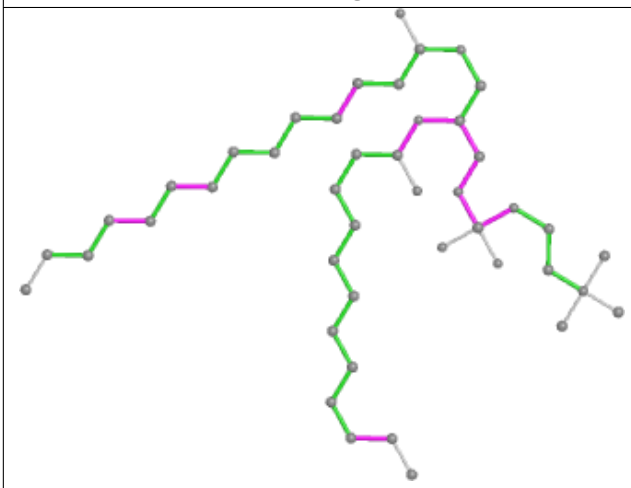
Ligand WSS U 501



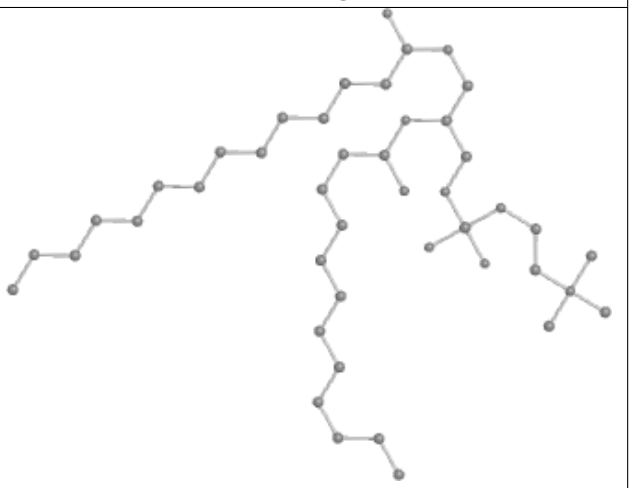
Bond lengths



Bond angles

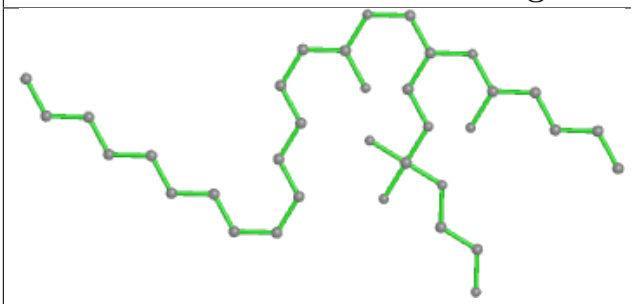


Torsions



Rings

Ligand PTY 5 202



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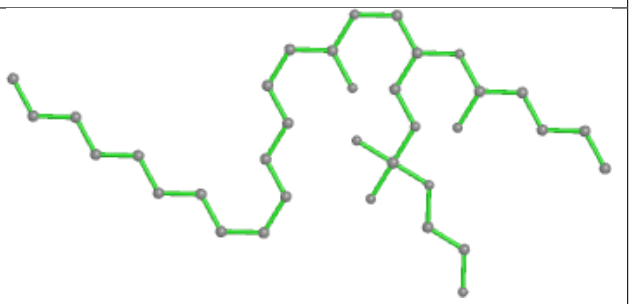
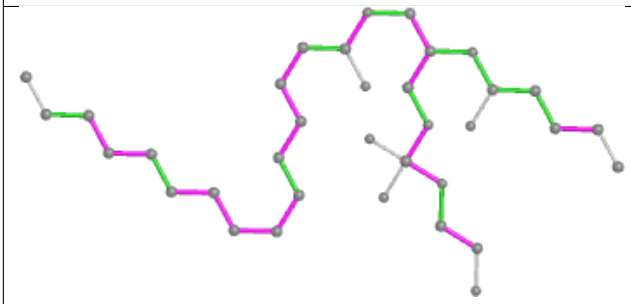
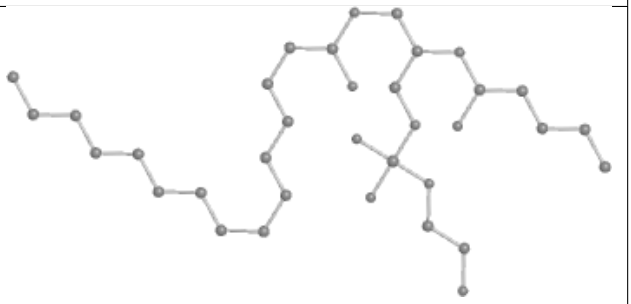


Bond angles

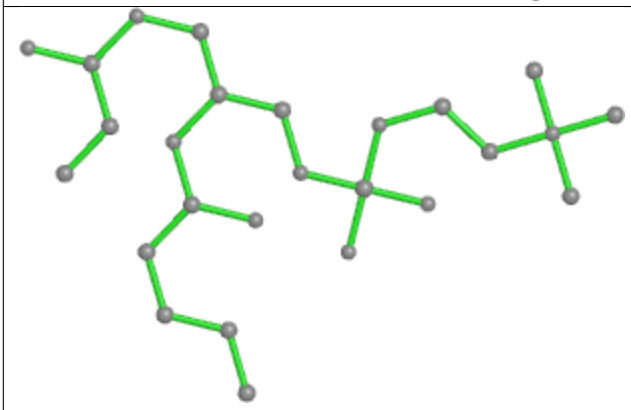


Torsions



Rings

Ligand WSS 0 303



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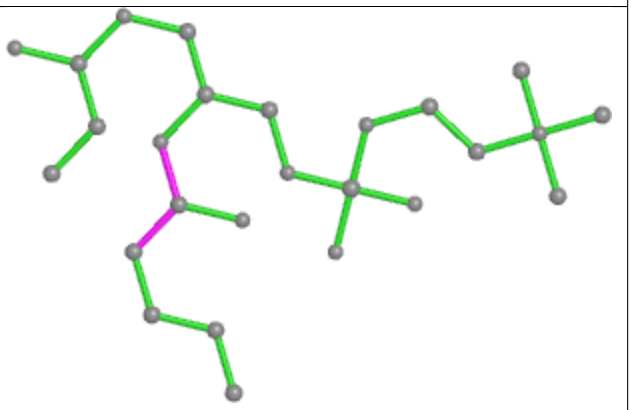
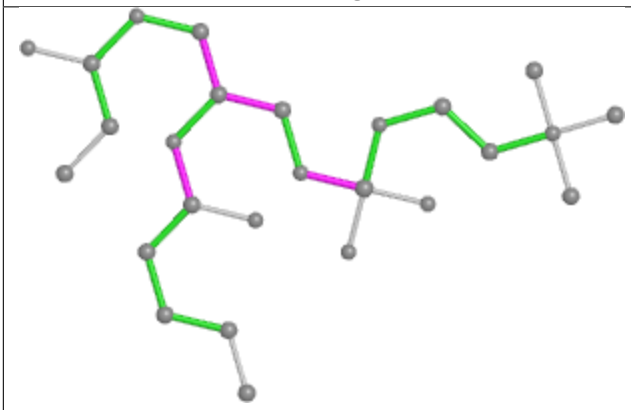


Bond angles



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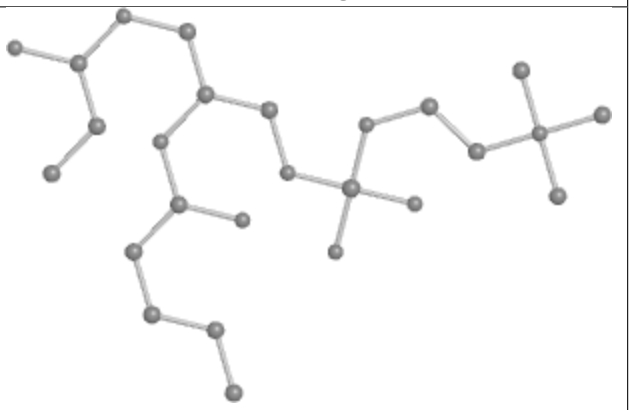
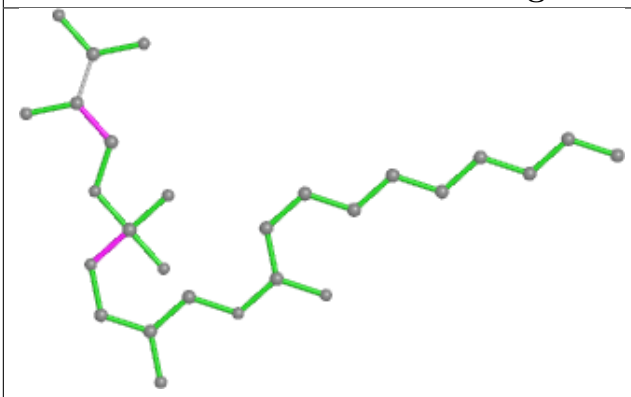


Rings

Ligand WJS 3 202



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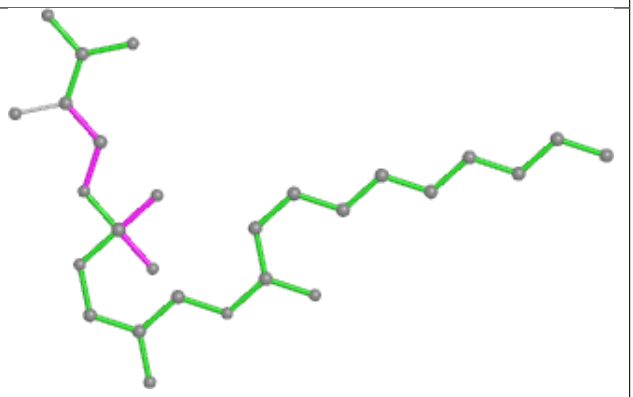
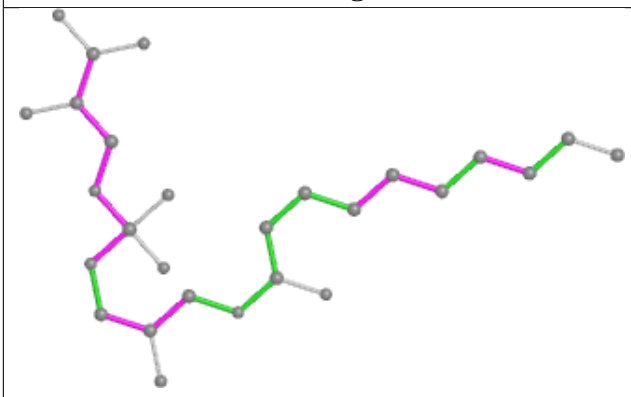


Bond angles



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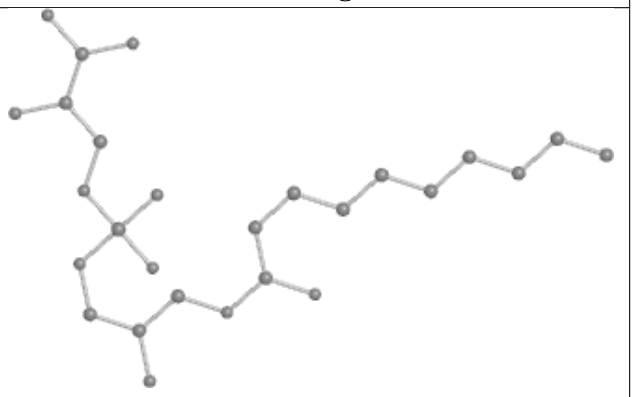
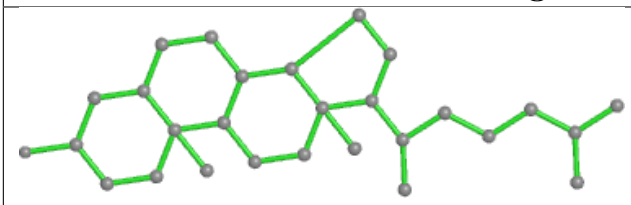


Rings

Ligand CLR 5 201



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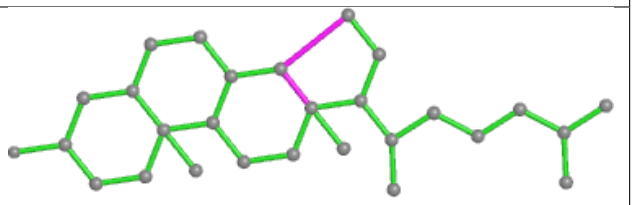
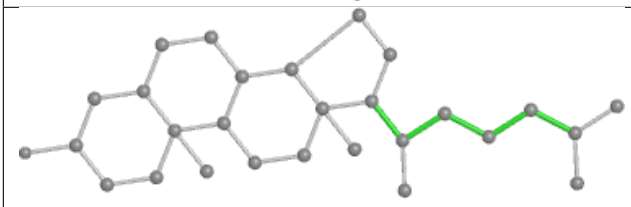
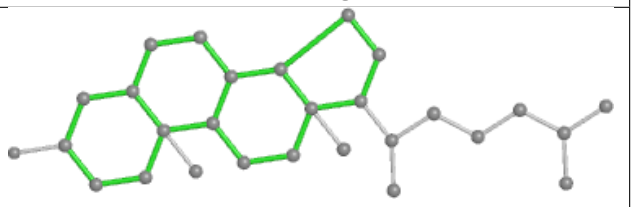


Bond angles

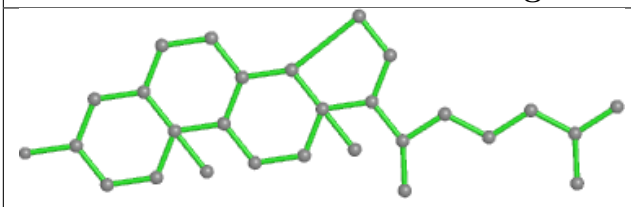


Torsions



Rings

Ligand CLR R 901



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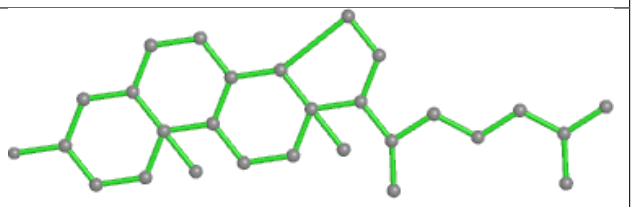
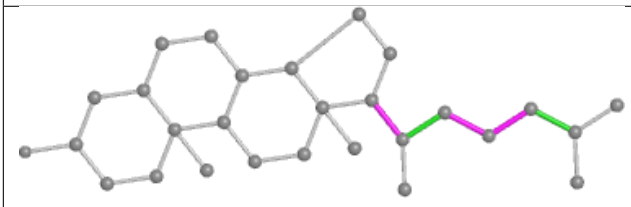
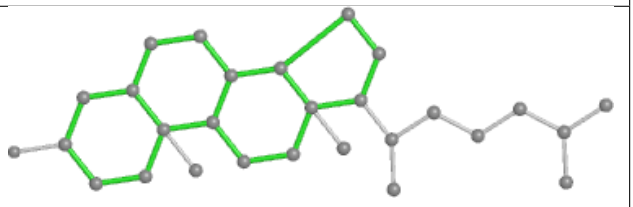


Bond angles

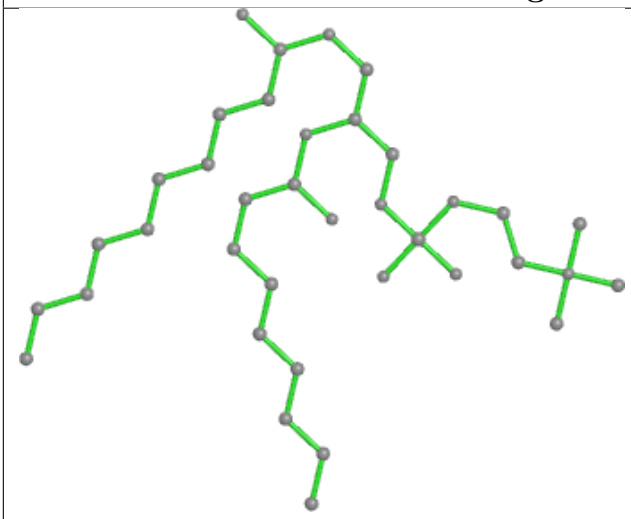


Torsions



Rings

Ligand WSS 0 302



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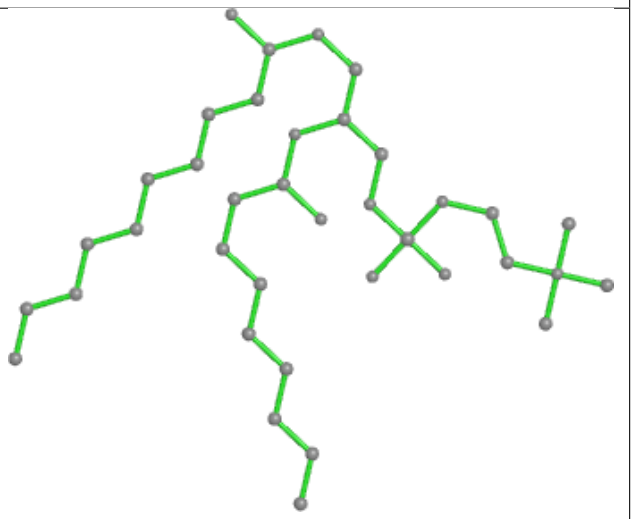
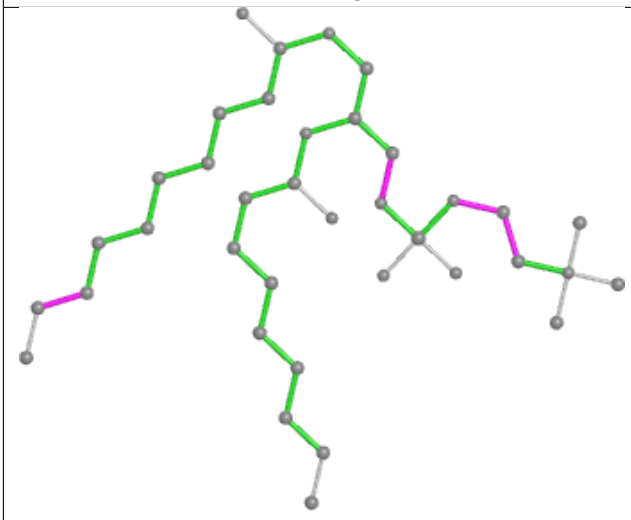


Bond angles



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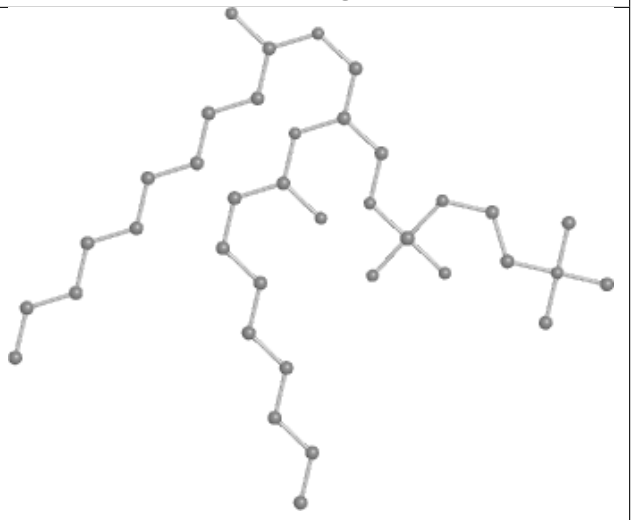
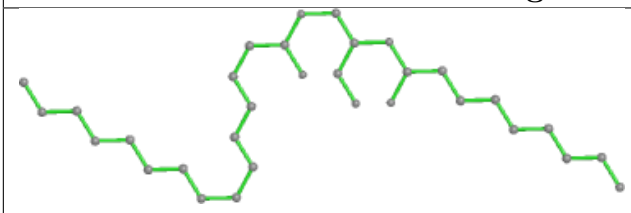


Rings

Ligand PTY S 101



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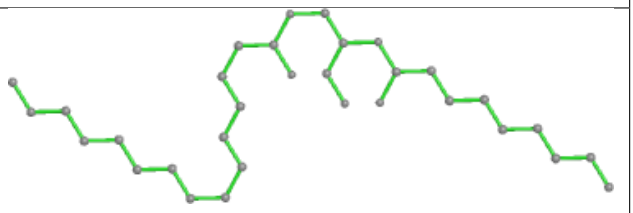
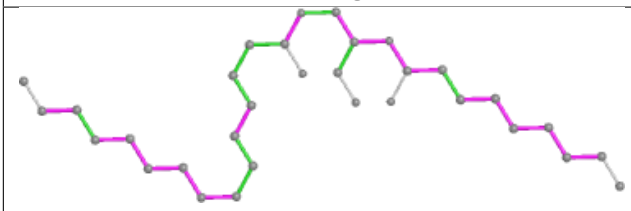


Bond angles



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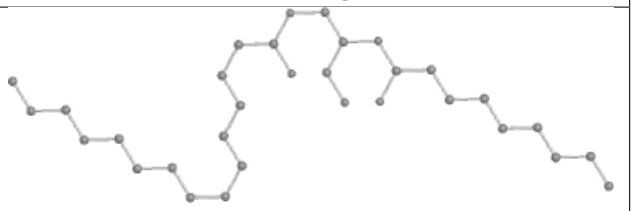
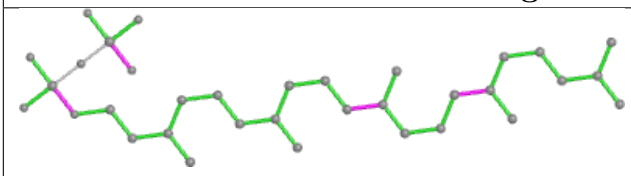


Rings

Ligand WJP R 905



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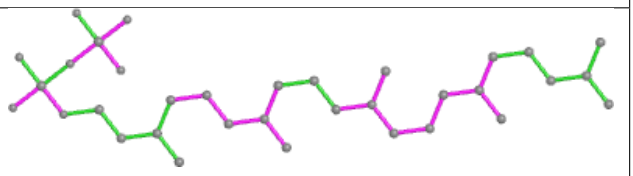
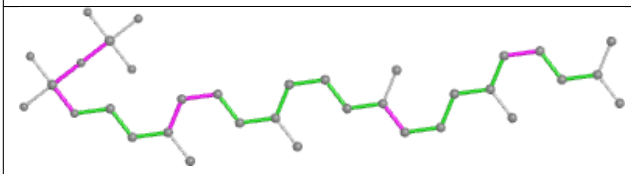
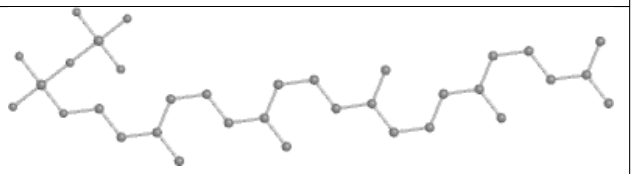


Bond angles

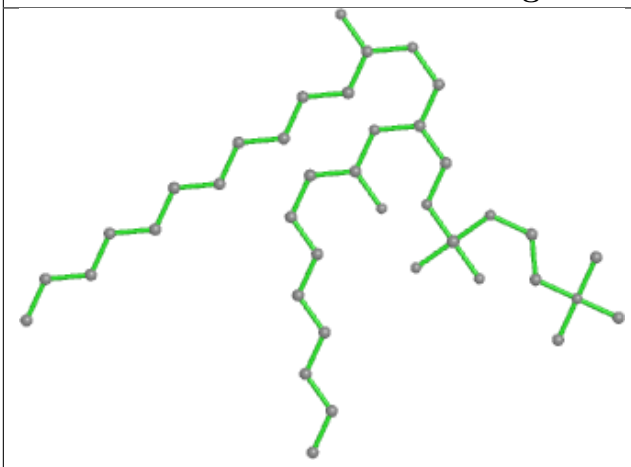


Torsions

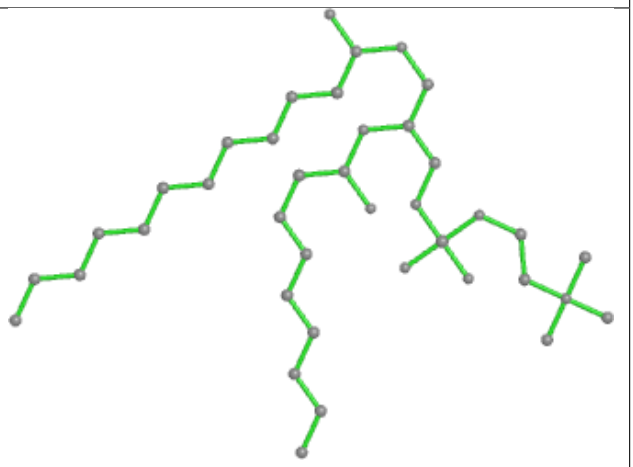


Rings

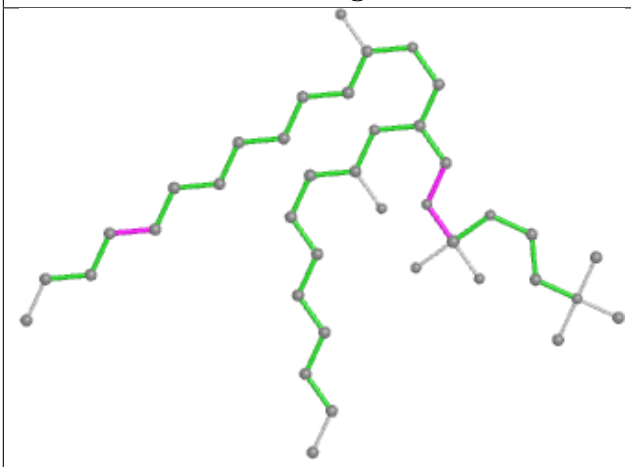
Ligand WSS U 502



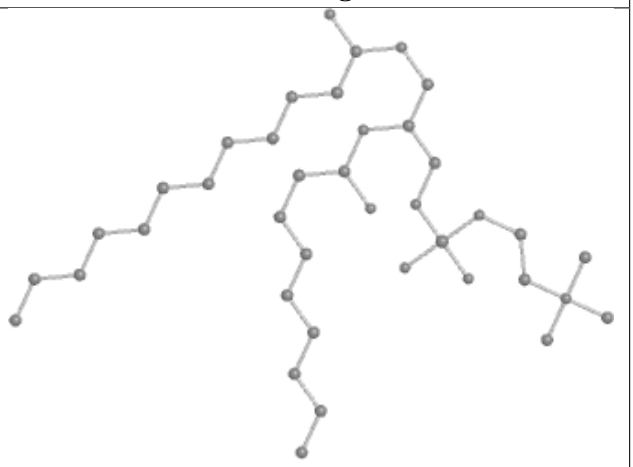
Bond lengths



Bond angles

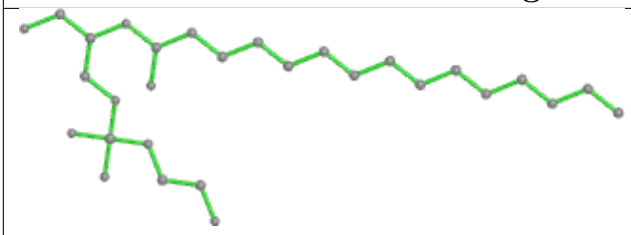


Torsions



Rings

Ligand PTY R 903



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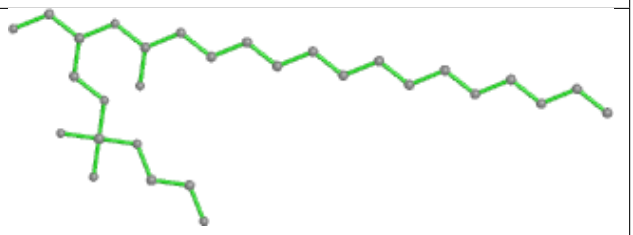
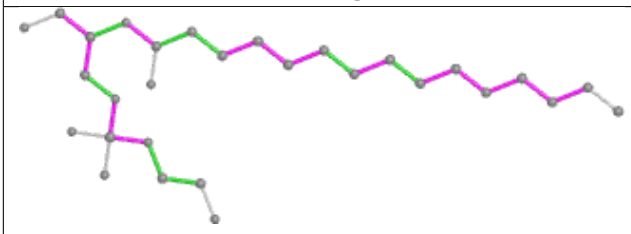


Bond angles



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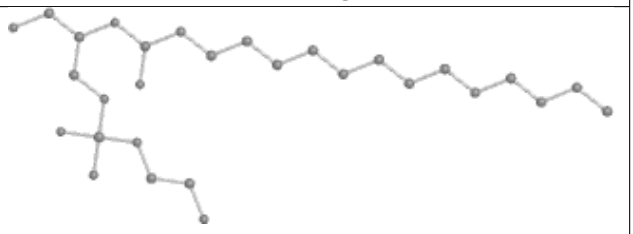
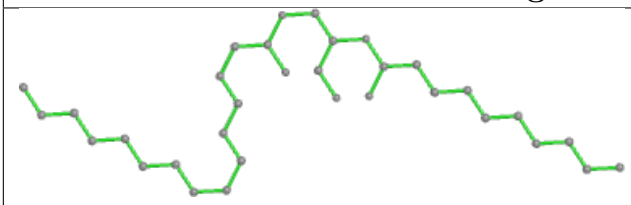


Rings

Ligand PTY 8 202



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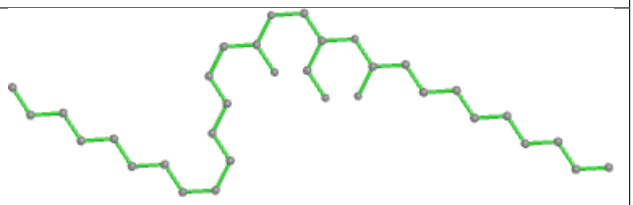
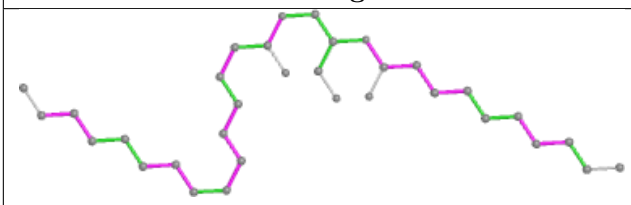
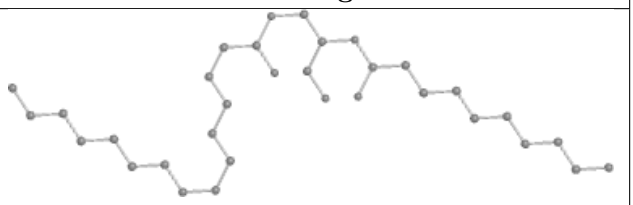


Bond angles

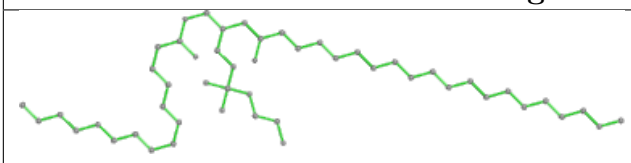


Torsions

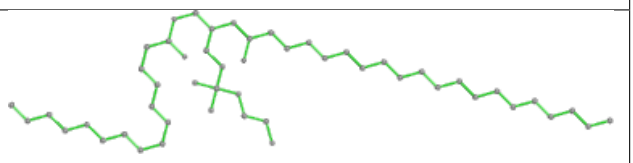


Rings

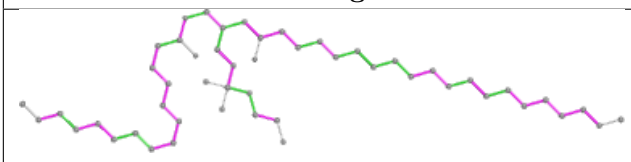
Ligand PTY 8 201



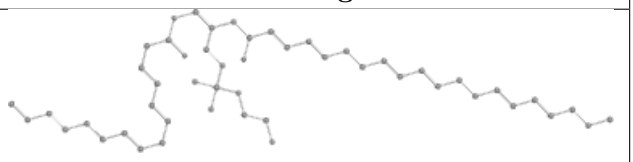
Bond lengths



Bond angles

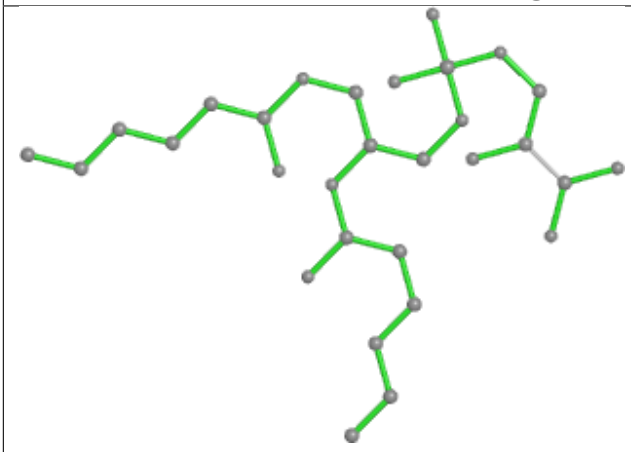


Torsions

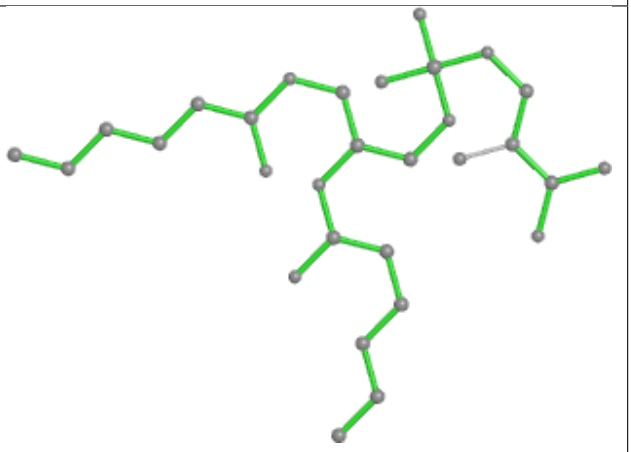


Rings

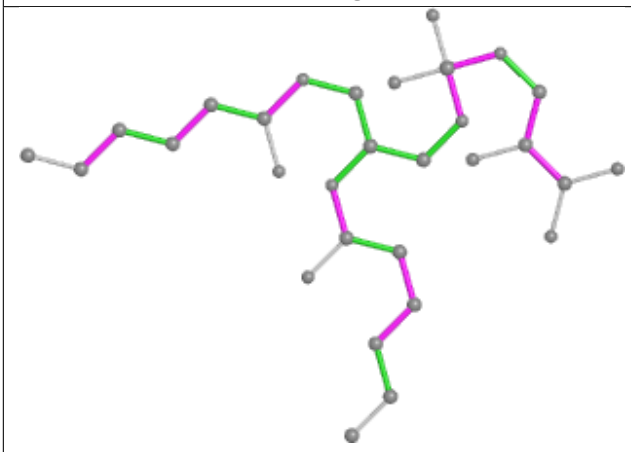
Ligand PSF R 902



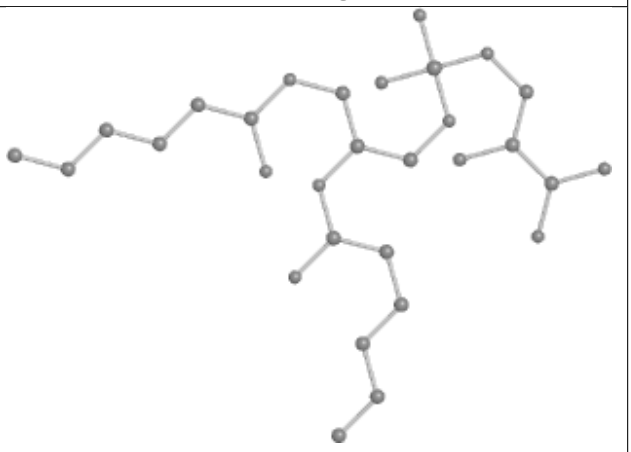
Bond lengths



Bond angles

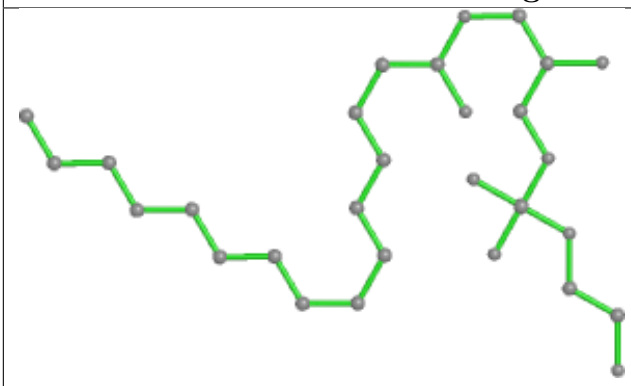


Torsions

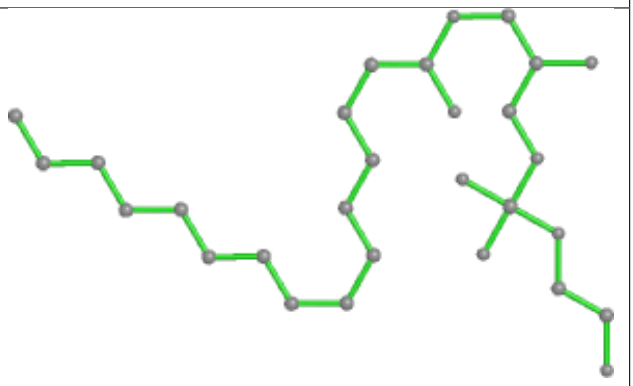


Rings

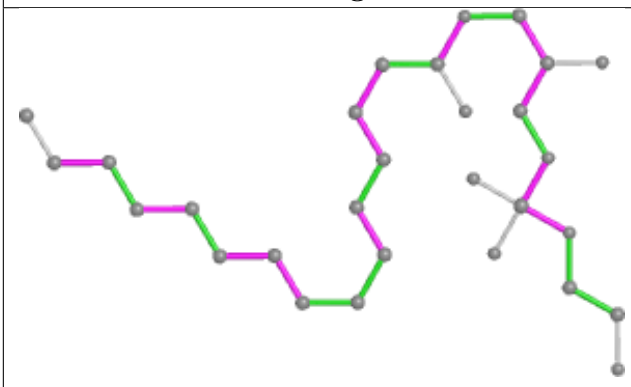
Ligand PTY V 404



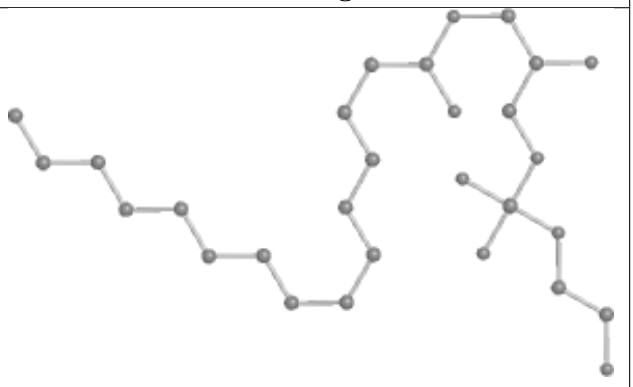
Bond lengths



Bond angles

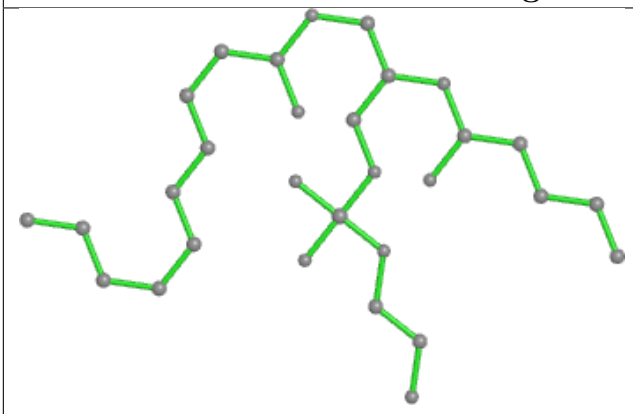


Torsions

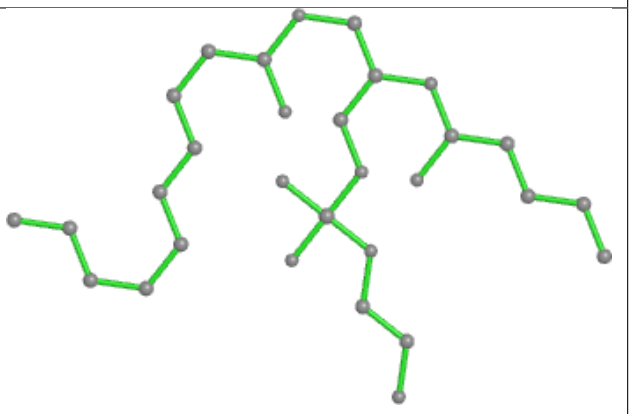


Rings

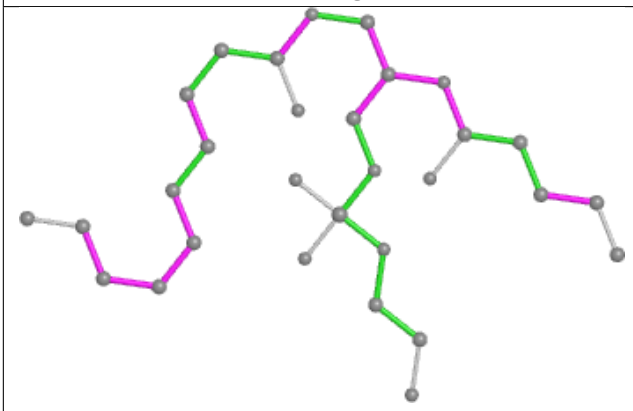
Ligand PTY U 503



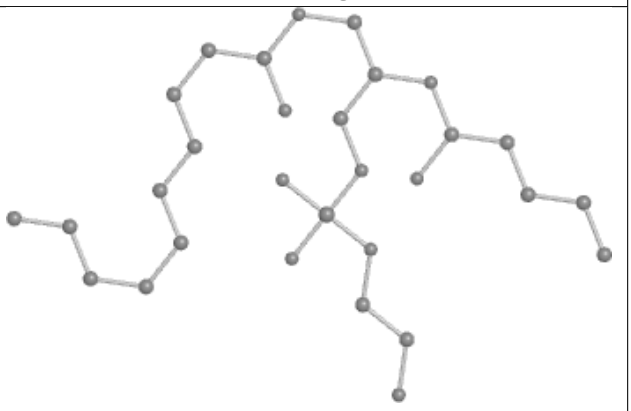
Bond lengths



Bond angles

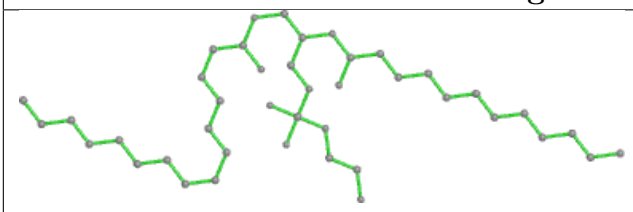


Torsions

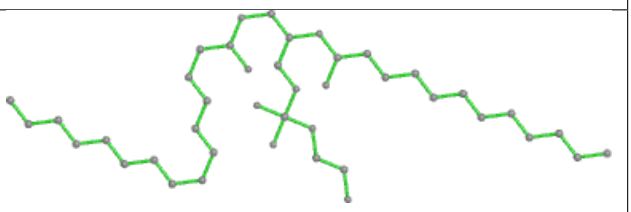


Rings

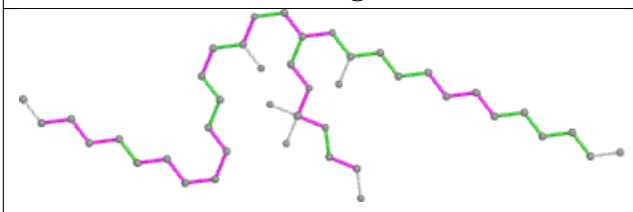
Ligand PTY 6 202



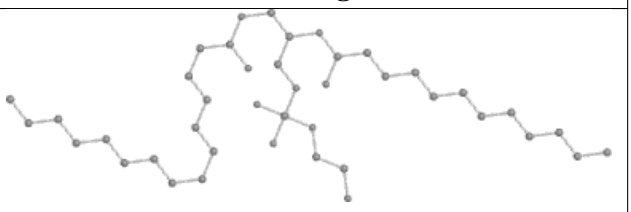
Bond lengths



Bond angles

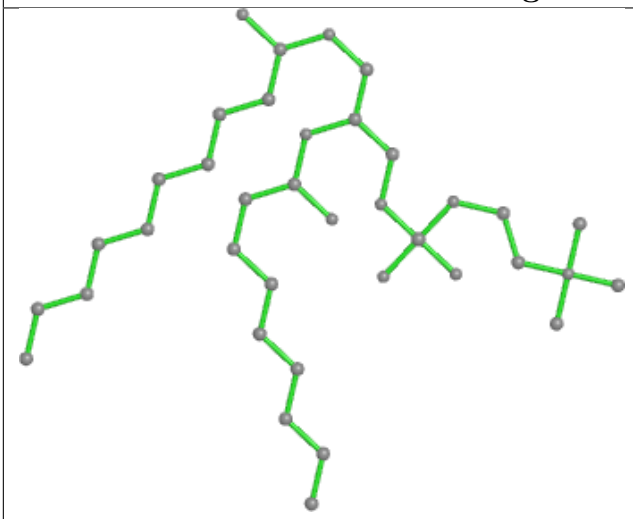


Torsions

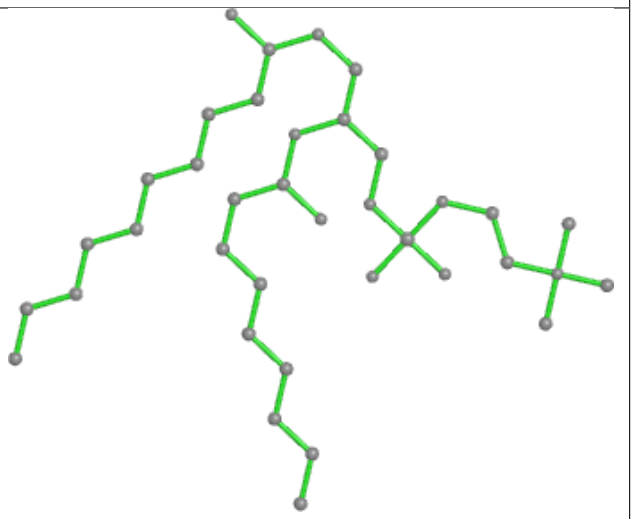


Rings

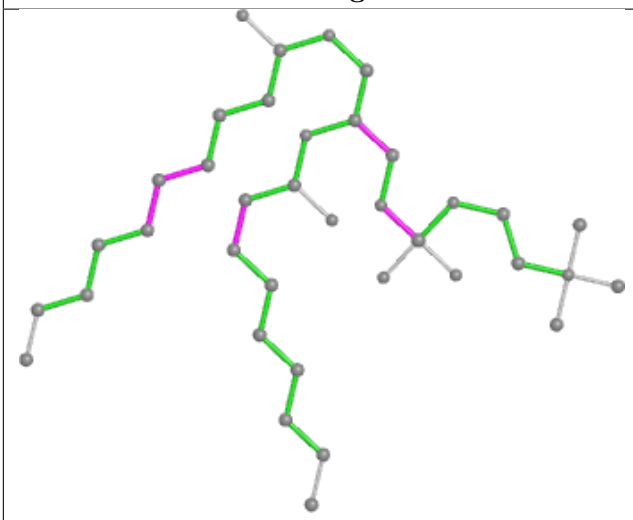
Ligand WSS V 401



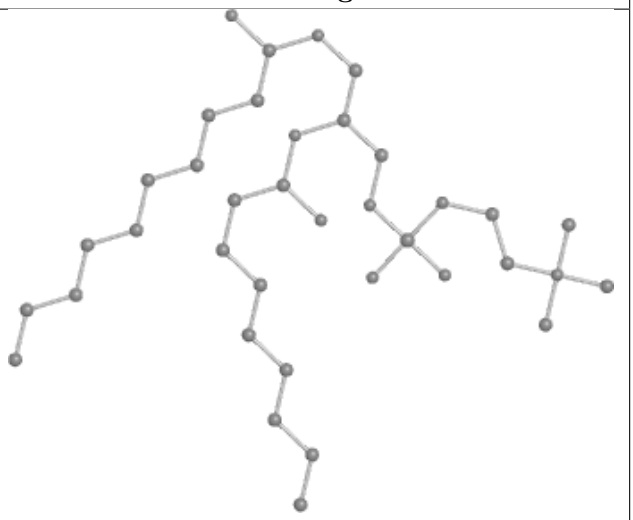
Bond lengths



Bond angles

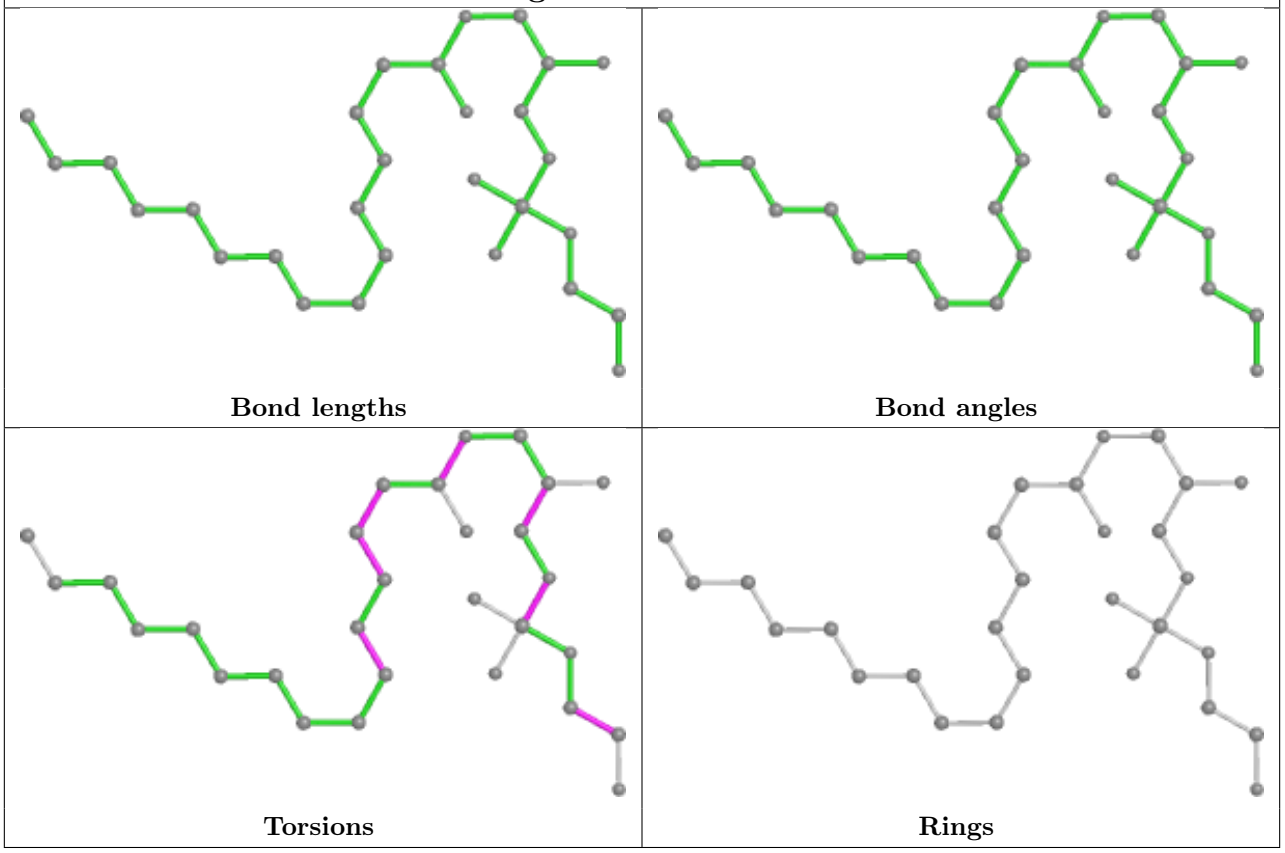


Torsions



Rings

Ligand PTY 2 201



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.

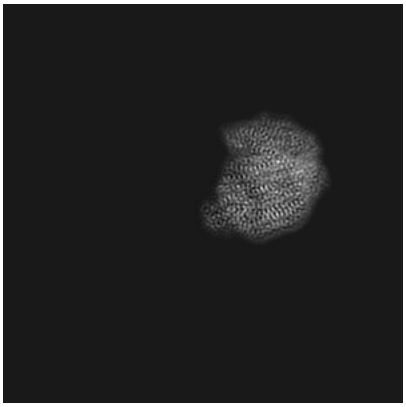
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-21844. These allow visual inspection of the internal detail of the map and identification of artifacts.

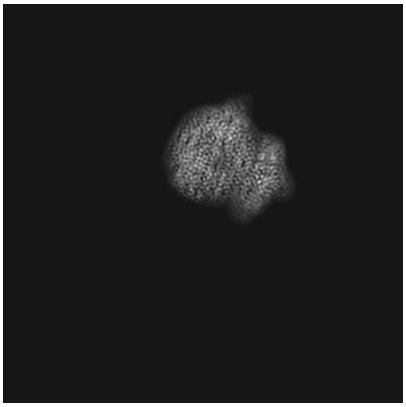
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

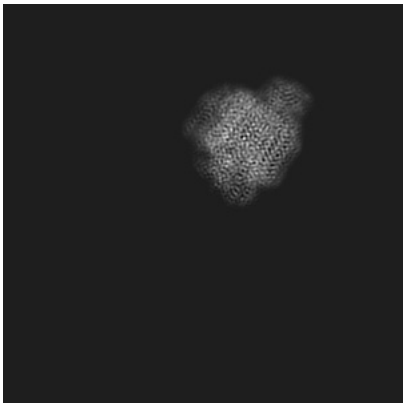
6.1.1 Primary map



X



Y

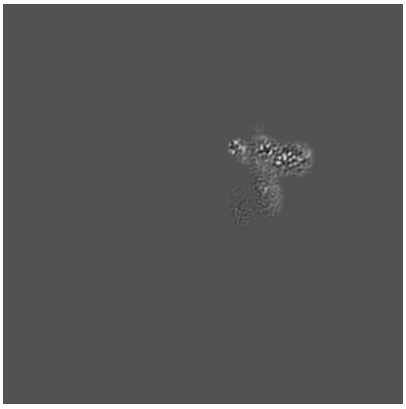


Z

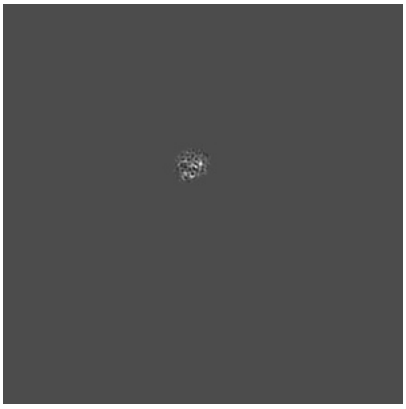
The images above show the map projected in three orthogonal directions.

6.2 Central slices

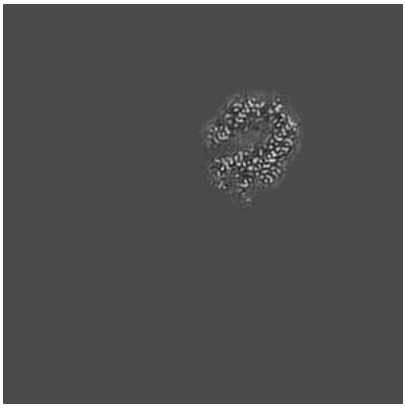
6.2.1 Primary map



X Index: 180



Y Index: 180

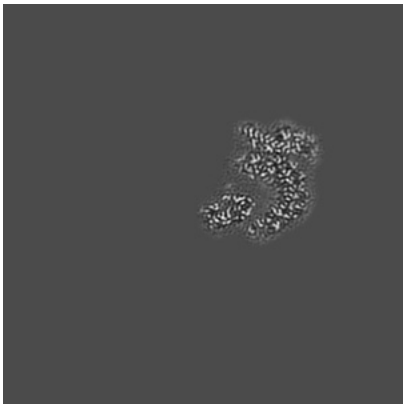


Z Index: 180

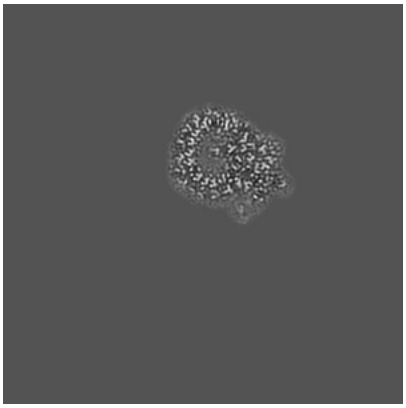
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map



X Index: 212



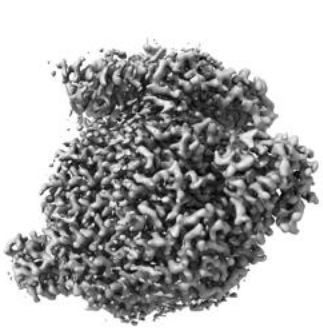
Y Index: 242

Z Index: 170

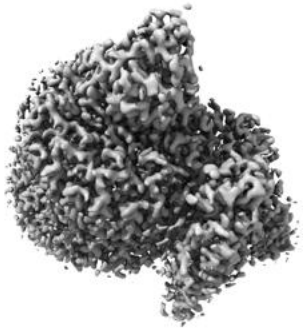
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

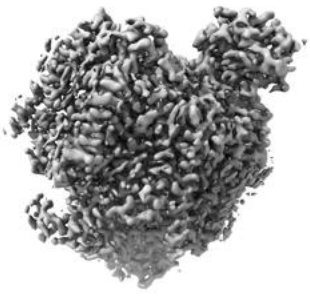
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.6. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

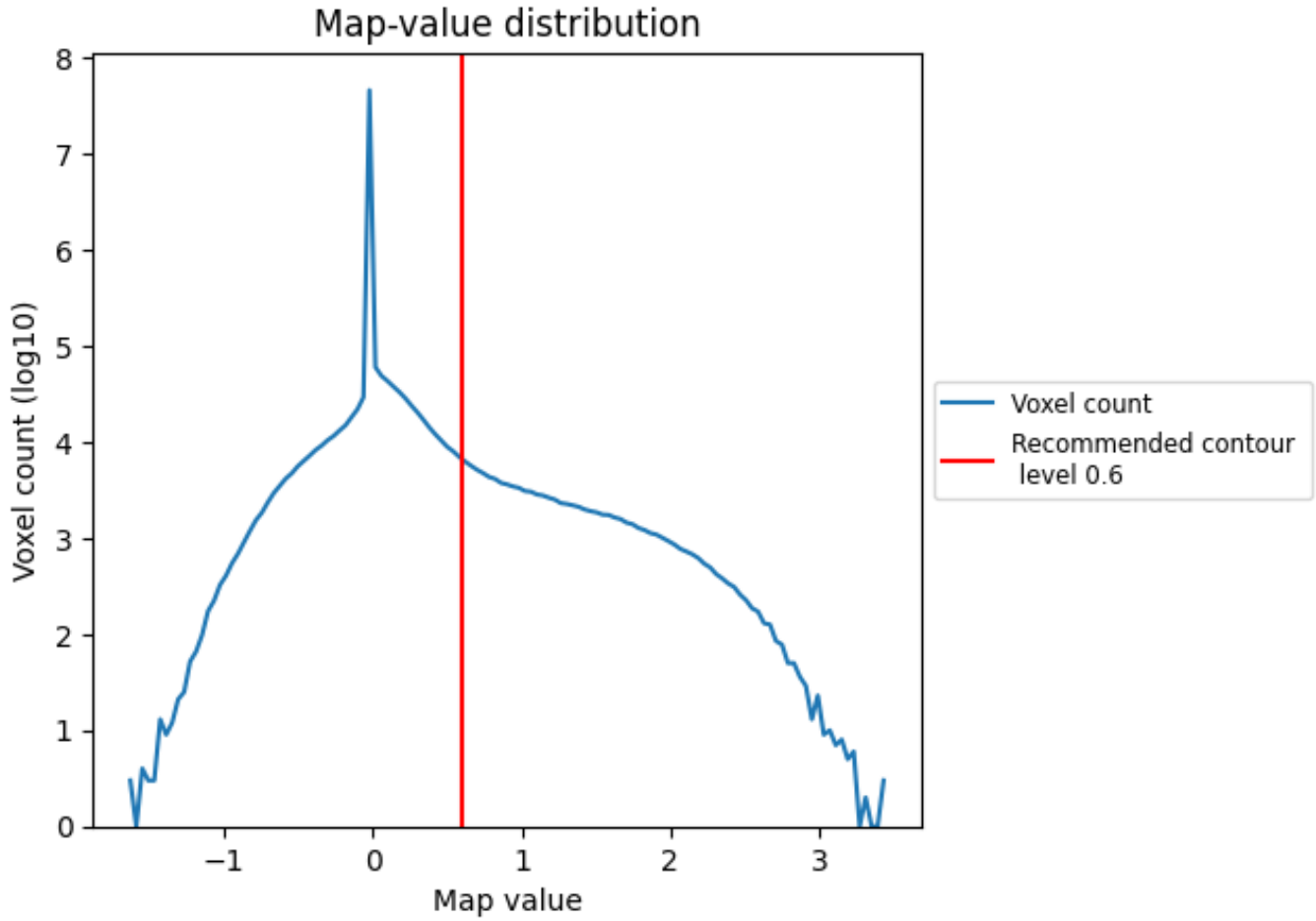
6.5 Mask visualisation (i)

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

7 Map analysis

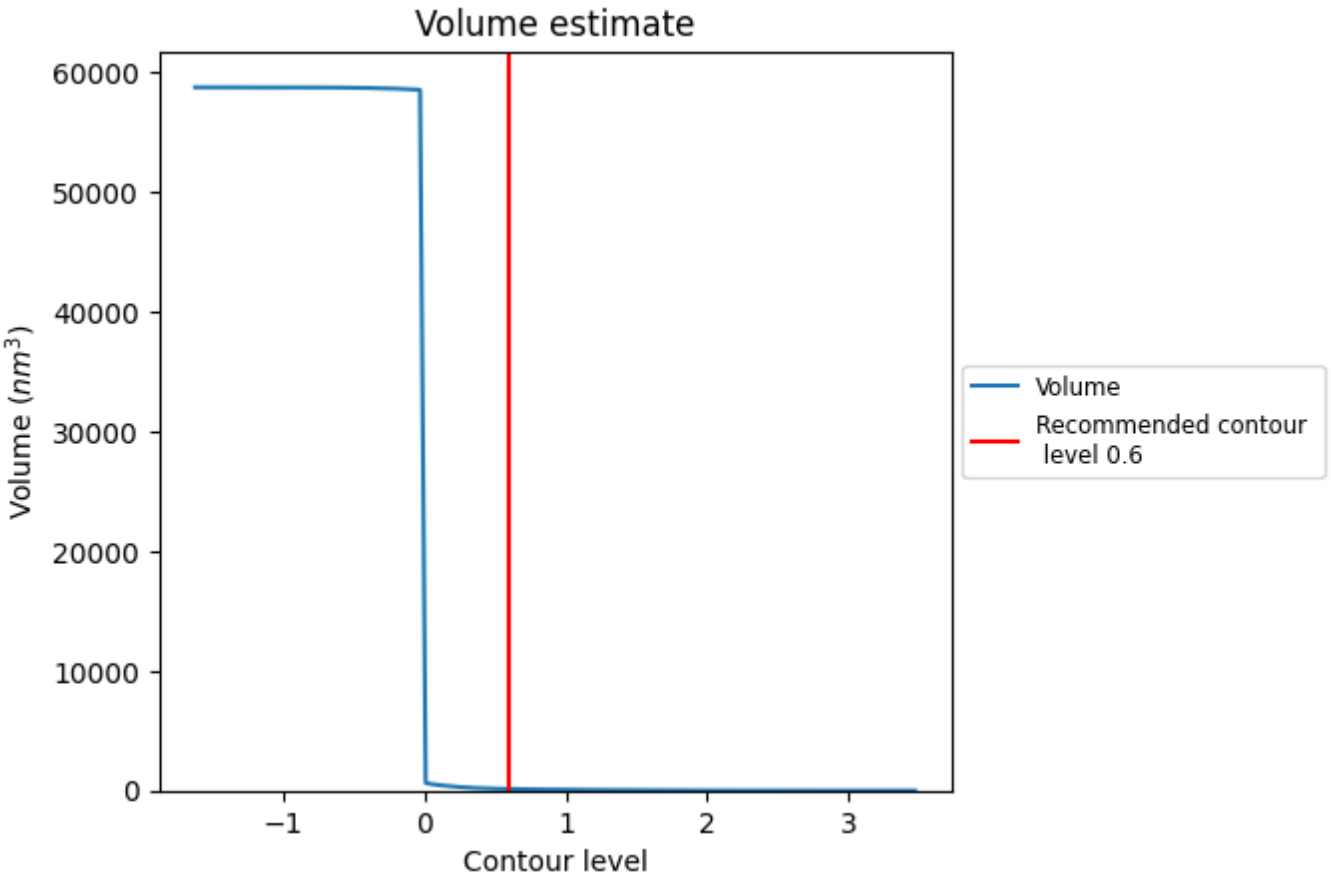
This section contains the results of statistical analysis of the map.

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.

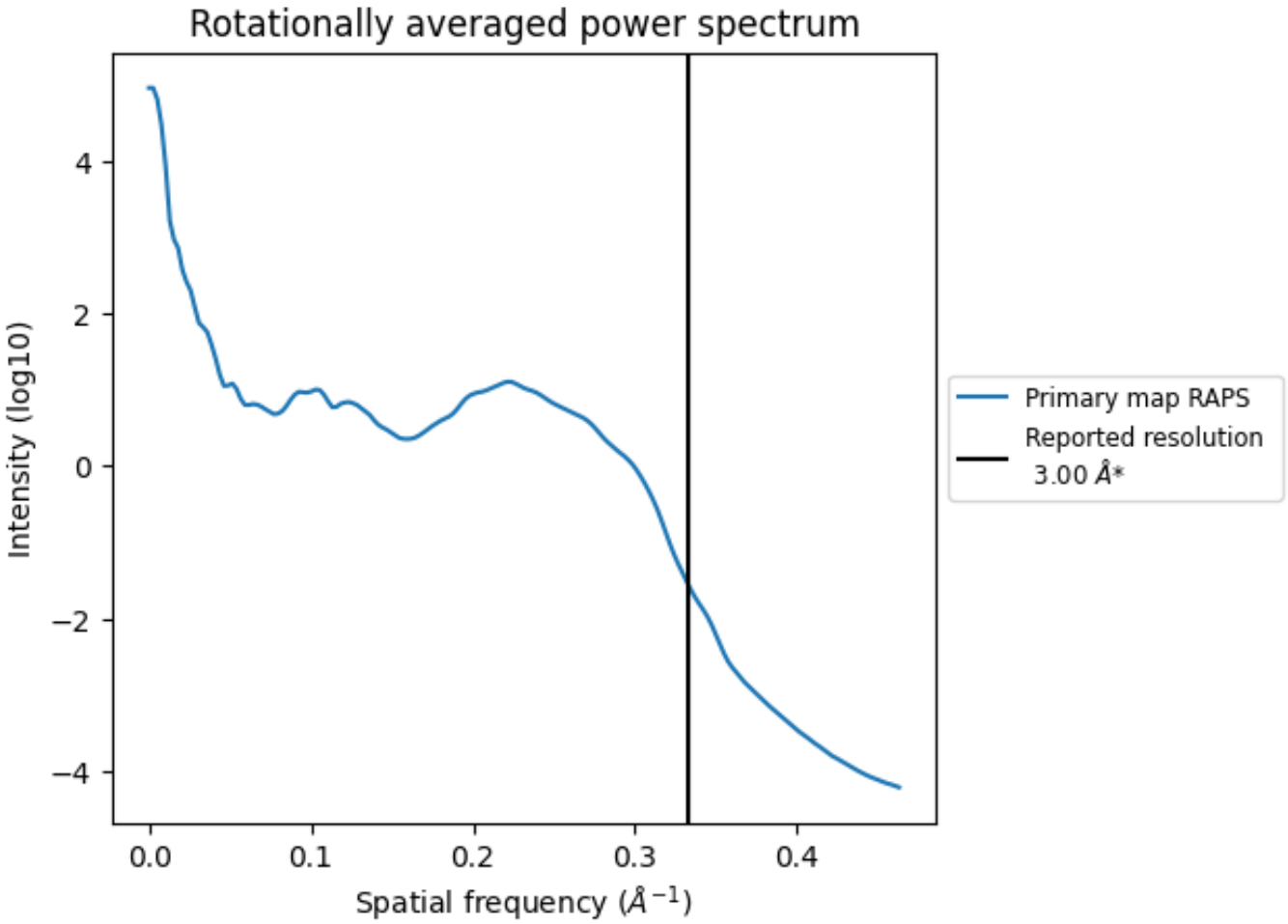
7.2 Volume estimate



The volume at the recommended contour level is 130 nm^3; this corresponds to an approximate mass of 118 kDa.

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

7.3 Rotationally averaged power spectrum (i)



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

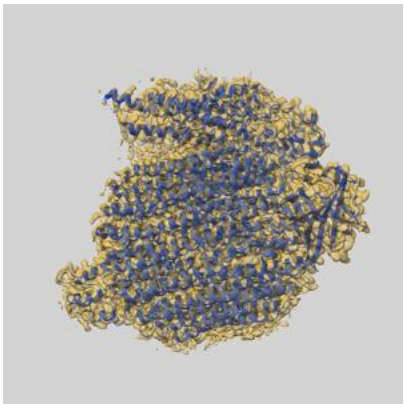
8 Fourier-Shell correlation (i)

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

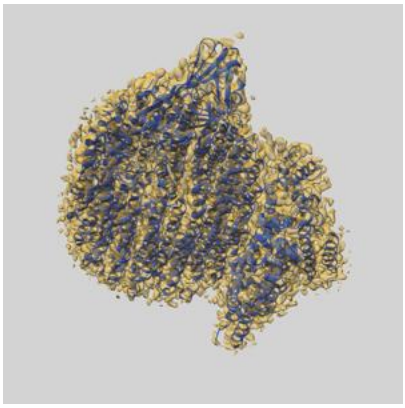
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-21844 and PDB model 6WLW. Per-residue inclusion information can be found in section 3 on page 12.

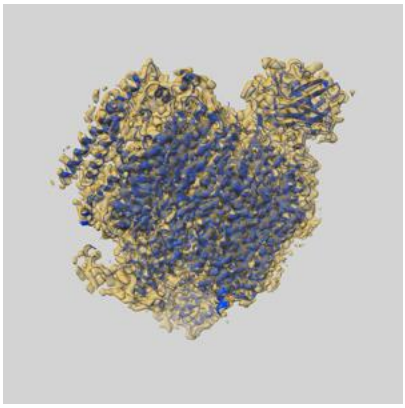
9.1 Map-model overlay



X



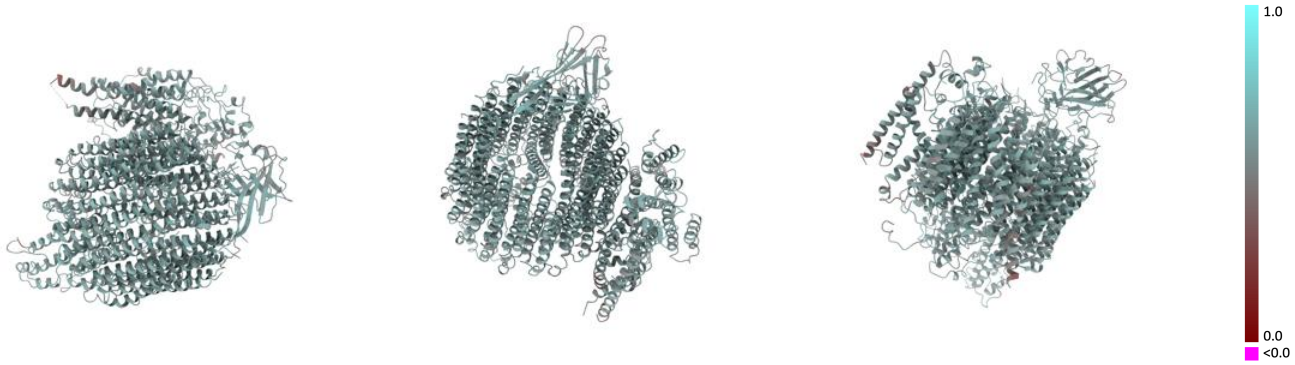
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.6 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.

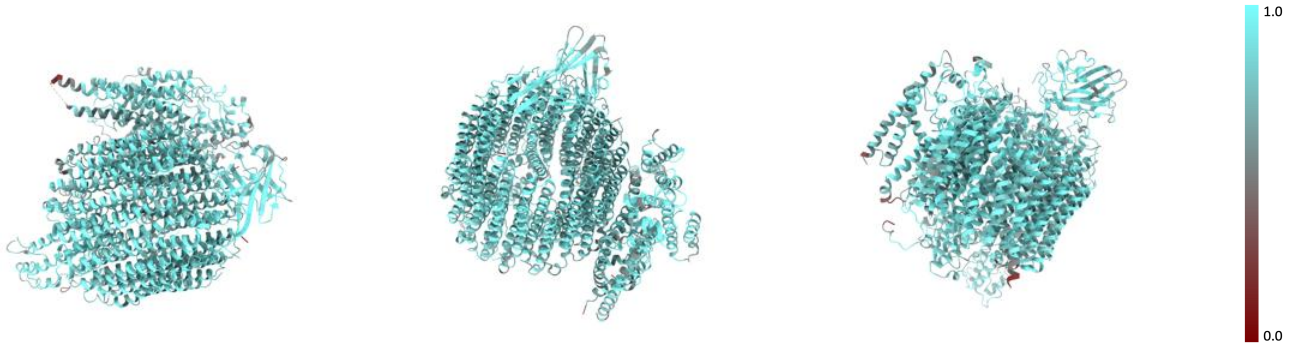
9.2 Q-score mapped to coordinate model (i)



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.

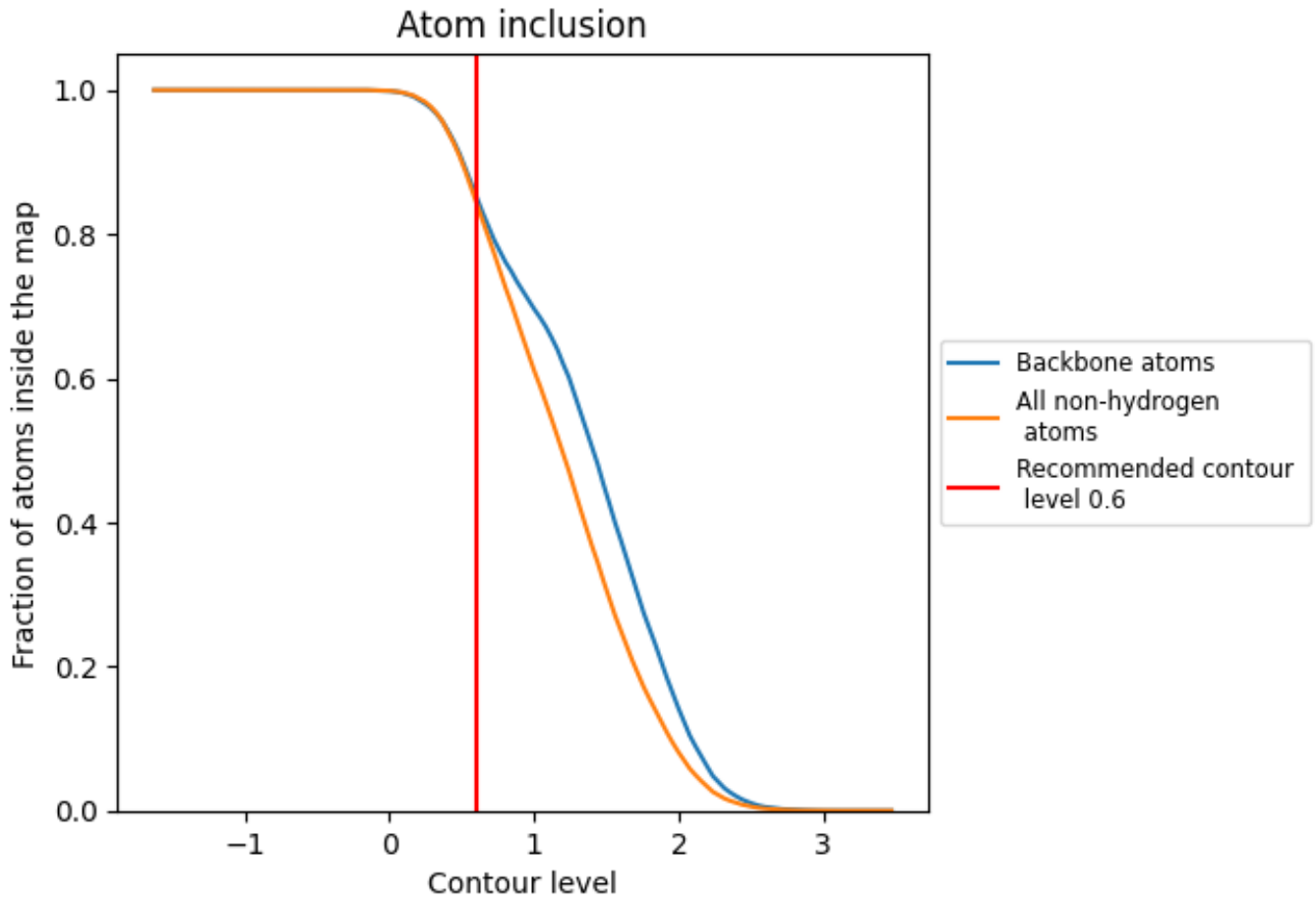
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.6).

9.4 Atom inclusion (i)



At the recommended contour level, 85% of all backbone atoms, 84% 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 (0.6) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8441	0.5790
0	0.8879	0.5940
1	0.8869	0.5900
2	0.8661	0.5850
3	0.8619	0.5920
4	0.8634	0.5860
5	0.8380	0.5830
6	0.8433	0.5860
7	0.8543	0.5860
8	0.8434	0.5860
9	0.8776	0.5880
A	0.5357	0.4410
B	0.5000	0.4410
C	0.3929	0.2610
D	0.3571	0.4090
Q	0.8446	0.5860
R	0.8323	0.5700
S	0.8285	0.5660
T	0.7496	0.5380
U	0.8400	0.5770
V	0.8453	0.5810
W	0.5000	0.4060
r	0.8031	0.5450
s	0.6786	0.4850
u	0.2500	0.3750