wwPDB EM Validation Summary Report (i)

Feb 2, 2025 – 12:07 AM JST

PDB ID	:	8YT8
EMDB ID	:	EMD-39568
Title	:	Cryo-EM structure of the dystrophin glycoprotein complex
Authors	:	Wu, J.P.; Yan, Z.; Wan, L.
Deposited on	:	2024-03-25
Resolution	:	3.50 Å(reported)

This is a wwPDB EM Validation Summary 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 (i) 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 (i)) were used in the production of this report:

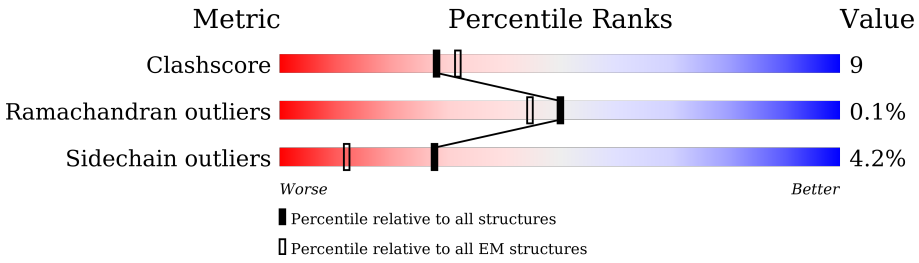
EMDB validation analysis	:	FAILED
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

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 3.50 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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%

Mol	Chain	Length	Quality of chain
1	A	291	86% 14%
2	B	263	80% 19%
3	C	206	97%
4	D	263	76% 23%
5	E	331	60% 37%
6	G	265	77% 22%
7	I	5	60% 40%
8	O	289	77% 22%
9	S	179	72% 27%

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Mol	Chain	Length	Quality of chain
10	F	3	100%
10	K	3	100%
10	L	3	100%
10	M	3	100%
10	N	3	100%
11	H	3	67% 33%
12	J	2	100%
12	Q	2	100%
13	P	3	100%

2 Entry composition (i)

There are 18 unique types of molecules in this entry. The entry contains 16309 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 Alpha-sarcoglycan.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	291	Total	C	N	O	S	0	0
			2296	1481	389	418	8		

- Molecule 2 is a protein called Beta-sarcoglycan.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	263	Total	C	N	O	S	0	0
			2009	1259	357	379	14		

- Molecule 3 is a protein called Dystrobrevin alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	206	Total	C	N	O	S	0	0
			1078	649	215	213	1		

- Molecule 4 is a protein called Delta-sarcoglycan.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	263	Total	C	N	O	S	0	0
			2045	1303	354	376	12		

- Molecule 5 is a protein called Dystrophin.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	331	Total	C	N	O	S	0	0
			2686	1705	479	478	24		

- Molecule 6 is a protein called Gamma-sarcoglycan.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	265	Total	C	N	O	S	0	0
			2031	1284	349	387	11		

- Molecule 7 is a protein called unknown segment.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	5	Total	C	N	O	S	0	0
			37	25	6	5	1		

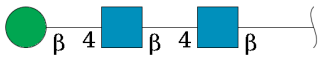
- Molecule 8 is a protein called Beta-dystroglycan.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	O	289	Total	C	N	O	S	0	0
			2247	1423	399	418	7		

- Molecule 9 is a protein called Sarcospan.

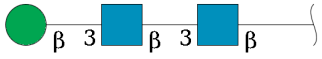
Mol	Chain	Residues	Atoms					AltConf	Trace
9	S	179	Total	C	N	O	S	0	0
			1390	921	217	233	19		

- Molecule 10 is an oligosaccharide called 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
10	F	3	Total	C	N	O	0	0
			39	22	2	15		
10	K	3	Total	C	N	O	0	0
			39	22	2	15		
10	L	3	Total	C	N	O	0	0
			39	22	2	15		
10	M	3	Total	C	N	O	0	0
			39	22	2	15		
10	N	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 11 is an oligosaccharide called beta-D-mannopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose.

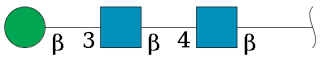


Mol	Chain	Residues	Atoms				AltConf	Trace
11	H	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 12 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

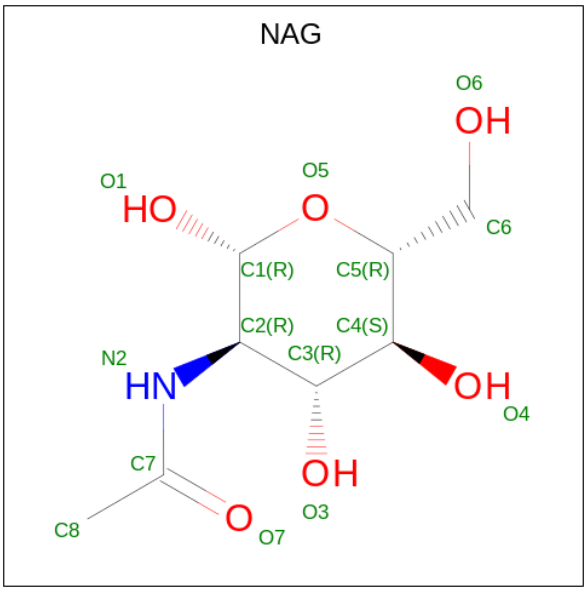
Mol	Chain	Residues	Atoms				AltConf	Trace
12	J	2	Total	C	N	O	0	0
			28	16	2	10		
12	Q	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 13 is an oligosaccharide called beta-D-mannopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



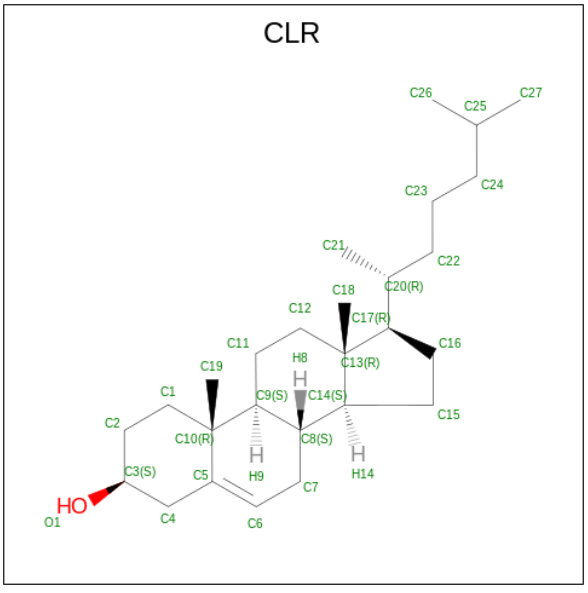
Mol	Chain	Residues	Atoms				AltConf	Trace
13	P	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 14 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 15 is CHOLESTEROL (three-letter code: CLR) (formula: $C_{27}H_{46}O$).



Mol	Chain	Residues	Atoms	AltConf
15	D	1	Total C O 28 27 1	0

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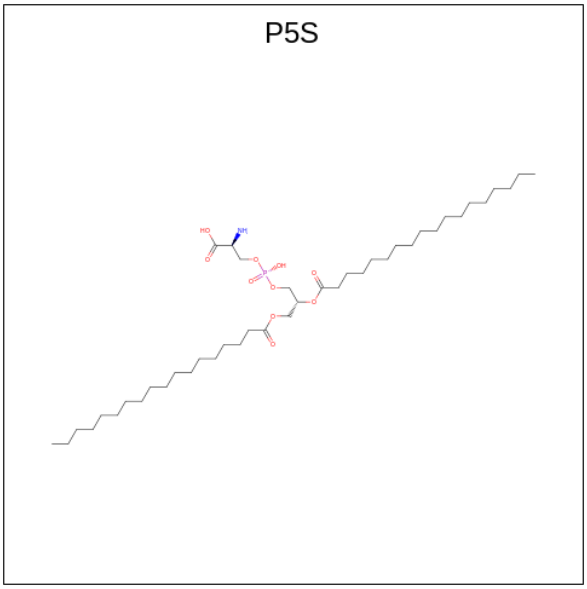
Mol	Chain	Residues	Atoms	AltConf
15	D	1	Total C O 28 27 1	0
15	S	1	Total C O 28 27 1	0

- Molecule 16 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
16	E	1	Total Zn 1 1	0

- Molecule 17 is O-[(R)-{[(2R)-2,3-bis(octadecanoyloxy)propyl]oxy}(hydroxy)phosphoryl]-L-serine (three-letter code: P5S) (formula: $C_{42}H_{82}NO_{10}P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
17	G	1	Total C N O P 33 21 1 10 1	0

- Molecule 18 is CALCIUM ION (three-letter code: CA) (formula: Ca).

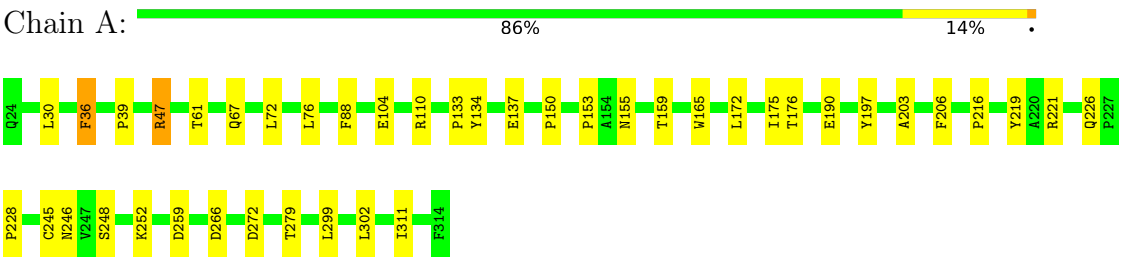
Mol	Chain	Residues	Atoms	AltConf
18	O	1	Total Ca 1 1	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

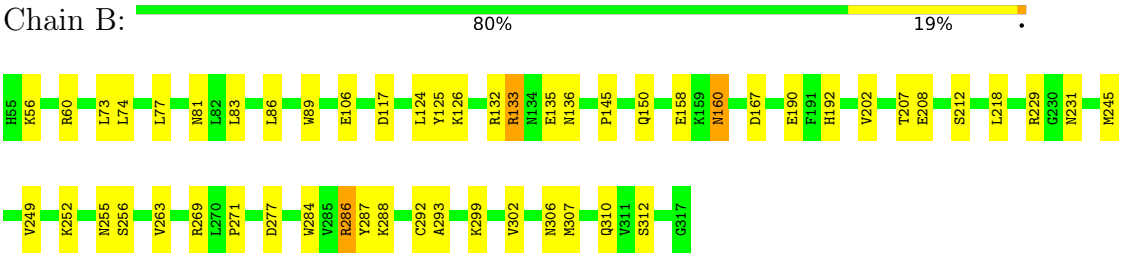
• Molecule 1: Alpha-sarcoglycan

Chain A:



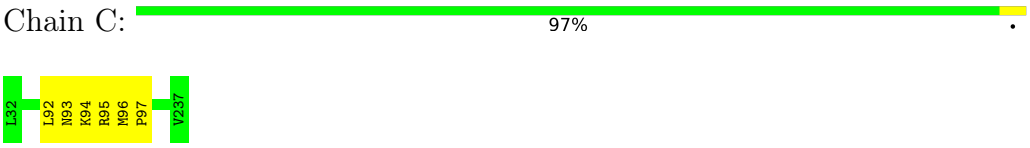
• Molecule 2: Beta-sarcoglycan

Chain B:



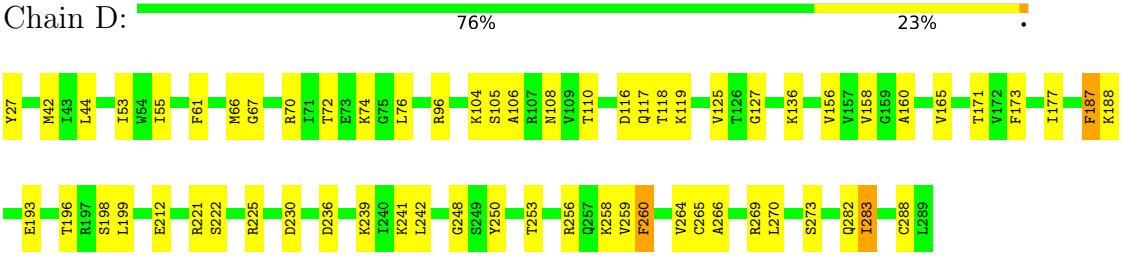
• Molecule 3: Dystrobrevin alpha

Chain C:



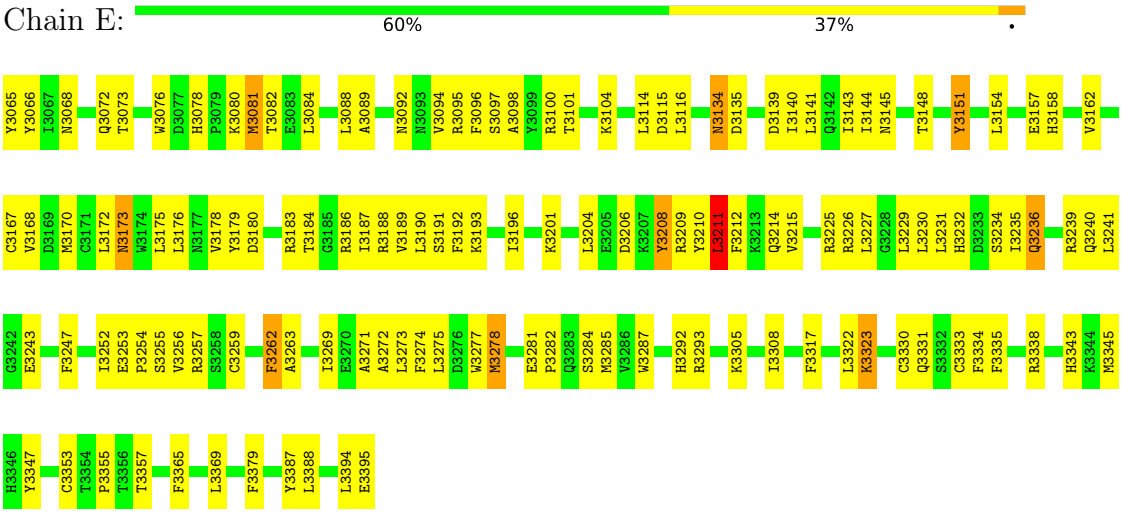
• Molecule 4: Delta-sarcoglycan

Chain D:



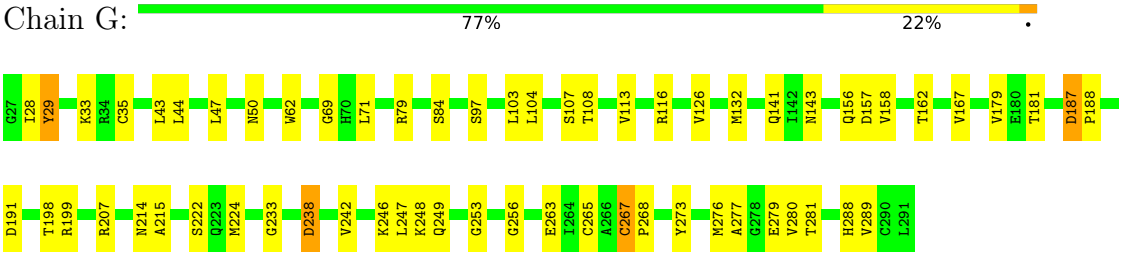
• Molecule 5: Dystrophin

Chain E:



• Molecule 6: Gamma-sarcoglycan

Chain G:

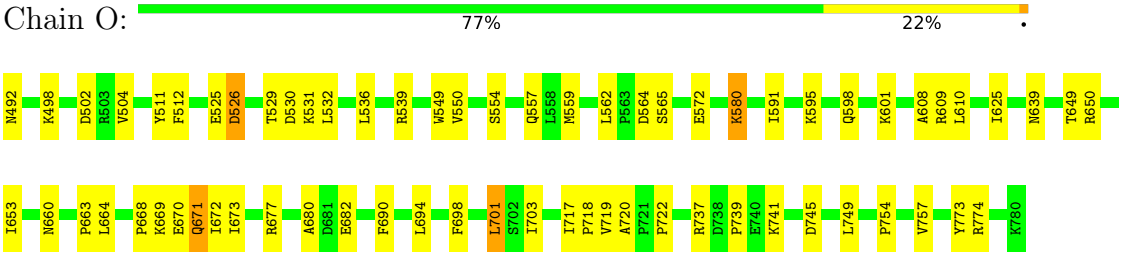


• Molecule 7: unknown segment

Chain I:

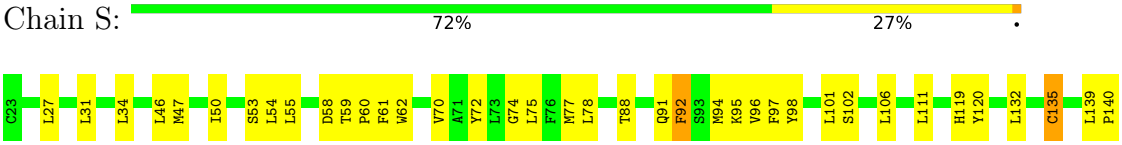
• Molecule 8: Beta-dystroglycan

Chain O:

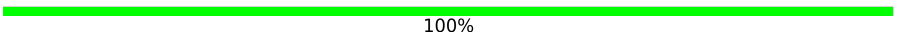


• Molecule 9: Sarcospan

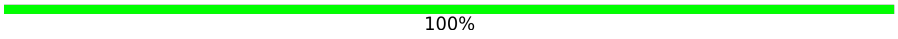
Chain S:



• Molecule 10: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F: 

• Molecule 10: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K: 

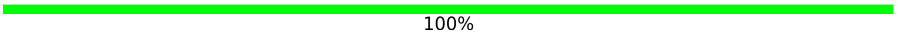
• Molecule 10: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L: 

• Molecule 10: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M: 

• Molecule 10: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N: 

• Molecule 11: beta-D-mannopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose

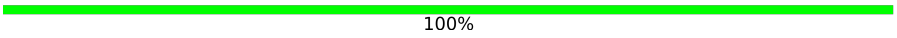
Chain H: 

• Molecule 12: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:

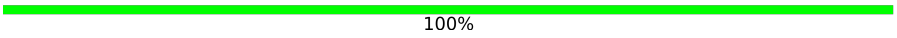
• Molecule 12: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q:



• Molecule 13: beta-D-mannopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	499658	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	Depositor
Minimum defocus (nm)	1400	Depositor
Maximum defocus (nm)	1900	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CLR, P5S, CA, NAG, ZN, BMA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.26	0/2366	0.51	0/3248
2	B	0.27	0/2042	0.51	0/2758
3	C	0.24	0/1082	0.37	0/1503
4	D	0.27	0/2076	0.53	0/2799
5	E	0.26	0/2747	0.58	1/3713 (0.0%)
6	G	0.28	0/2067	0.53	0/2799
7	I	0.21	0/37	0.45	0/48
8	O	0.26	0/2299	0.49	0/3119
9	S	0.27	0/1422	0.53	0/1934
All	All	0.26	0/16138	0.52	1/21921 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	E	3211	LEU	CA-CB-CG	5.61	128.20	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	311	ILE	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2296	0	2269	29	0
2	B	2009	0	2022	44	0
3	C	1078	0	556	4	0
4	D	2045	0	2129	43	0
5	E	2686	0	2678	99	0
6	G	2031	0	2039	53	0
7	I	37	0	44	1	0
8	O	2247	0	2257	46	0
9	S	1390	0	1434	32	0
10	F	39	0	34	0	0
10	K	39	0	34	0	0
10	L	39	0	34	0	0
10	M	39	0	34	0	0
10	N	39	0	34	0	0
11	H	39	0	34	2	0
12	J	28	0	25	0	0
12	Q	28	0	25	0	0
13	P	39	0	34	0	0
14	A	28	0	26	2	0
14	O	14	0	13	1	0
15	D	56	0	92	3	0
15	S	28	0	46	4	0
16	E	1	0	0	0	0
17	G	33	0	32	3	0
18	O	1	0	0	0	0
All	All	16309	0	15925	303	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 9.

The worst 5 of 303 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)
6:G:35:CYS:SG	17:G:301:P5S:H21A	2.11	0.90
5:E:3275:LEU:HA	5:E:3278:MET:HE2	1.60	0.83
6:G:187:ASP:HB2	6:G:188:PRO:HD2	1.61	0.81
5:E:3104:LYS:HD3	5:E:3241:LEU:HD21	1.67	0.76
4:D:265:CYS:SG	4:D:266:ALA:N	2.57	0.76

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	289/291 (99%)	275 (95%)	14 (5%)	0	100	100
2	B	261/263 (99%)	241 (92%)	19 (7%)	1 (0%)	30	64
3	C	204/206 (99%)	201 (98%)	3 (2%)	0	100	100
4	D	261/263 (99%)	230 (88%)	30 (12%)	1 (0%)	30	64
5	E	329/331 (99%)	307 (93%)	22 (7%)	0	100	100
6	G	263/265 (99%)	249 (95%)	13 (5%)	1 (0%)	30	64
7	I	3/5 (60%)	2 (67%)	1 (33%)	0	100	100
8	O	287/289 (99%)	272 (95%)	15 (5%)	0	100	100
9	S	177/179 (99%)	171 (97%)	6 (3%)	0	100	100
All	All	2074/2092 (99%)	1948 (94%)	123 (6%)	3 (0%)	50	79

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	G	187	ASP
2	B	160	ASN
4	D	283	ILE

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	256/256 (100%)	252 (98%)	4 (2%)	58 76
2	B	228/228 (100%)	220 (96%)	8 (4%)	31 59
3	C	16/184 (9%)	16 (100%)	0	100 100
4	D	225/225 (100%)	213 (95%)	12 (5%)	19 46
5	E	297/297 (100%)	276 (93%)	21 (7%)	12 38
6	G	224/224 (100%)	216 (96%)	8 (4%)	30 59
7	I	4/4 (100%)	3 (75%)	1 (25%)	0 3
8	O	246/246 (100%)	236 (96%)	10 (4%)	26 55
9	S	157/157 (100%)	151 (96%)	6 (4%)	28 57
All	All	1653/1821 (91%)	1583 (96%)	70 (4%)	27 54

5 of 70 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	O	554	SER
8	O	580	LYS
9	S	92	PHE
5	E	3066	TYR
4	D	288	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
5	E	3145	ASN
6	G	141	GLN
6	G	143	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

25 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	NAG	F	1	1,10	14,14,15	0.25	0	17,19,21	0.43	0
10	NAG	F	2	10	14,14,15	0.24	0	17,19,21	0.43	0
10	BMA	F	3	10	11,11,12	0.66	0	15,15,17	0.72	0
11	NAG	H	1	1,11	14,14,15	0.36	0	17,19,21	0.37	0
11	NAG	H	2	11	14,14,15	0.28	0	17,19,21	0.37	0
11	BMA	H	3	11	11,11,12	0.63	0	15,15,17	0.72	0
12	NAG	J	1	2,12	14,14,15	0.16	0	17,19,21	0.44	0
12	NAG	J	2	12	14,14,15	0.21	0	17,19,21	0.43	0
10	NAG	K	1	2,10	14,14,15	0.32	0	17,19,21	0.41	0
10	NAG	K	2	10	14,14,15	0.22	0	17,19,21	0.34	0
10	BMA	K	3	10	11,11,12	0.59	0	15,15,17	0.77	0
10	NAG	L	1	2,10	14,14,15	0.22	0	17,19,21	0.41	0
10	NAG	L	2	10	14,14,15	0.21	0	17,19,21	0.41	0
10	BMA	L	3	10	11,11,12	0.58	0	15,15,17	0.74	0
10	NAG	M	1	4,10	14,14,15	0.30	0	17,19,21	0.41	0
10	NAG	M	2	10	14,14,15	0.18	0	17,19,21	0.44	0
10	BMA	M	3	10	11,11,12	0.57	0	15,15,17	0.76	0
10	NAG	N	1	6,10	14,14,15	0.19	0	17,19,21	0.40	0
10	NAG	N	2	10	14,14,15	0.19	0	17,19,21	0.39	0
10	BMA	N	3	10	11,11,12	0.60	0	15,15,17	0.73	0
13	NAG	P	1	8,13	14,14,15	0.20	0	17,19,21	0.44	0
13	NAG	P	2	13	14,14,15	0.22	0	17,19,21	0.45	0
13	BMA	P	3	13	11,11,12	0.56	0	15,15,17	0.84	0
12	NAG	Q	1	12,8	14,14,15	0.21	0	17,19,21	0.48	0
12	NAG	Q	2	12	14,14,15	0.28	0	17,19,21	0.42	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	NAG	F	1	1,10	-	1/6/23/26	0/1/1/1
10	NAG	F	2	10	-	0/6/23/26	0/1/1/1
10	BMA	F	3	10	-	1/2/19/22	0/1/1/1
11	NAG	H	1	1,11	-	2/6/23/26	0/1/1/1
11	NAG	H	2	11	-	2/6/23/26	0/1/1/1
11	BMA	H	3	11	-	1/2/19/22	0/1/1/1
12	NAG	J	1	2,12	-	0/6/23/26	0/1/1/1
12	NAG	J	2	12	-	2/6/23/26	0/1/1/1
10	NAG	K	1	2,10	-	2/6/23/26	0/1/1/1
10	NAG	K	2	10	-	2/6/23/26	0/1/1/1
10	BMA	K	3	10	-	0/2/19/22	0/1/1/1
10	NAG	L	1	2,10	-	2/6/23/26	0/1/1/1
10	NAG	L	2	10	-	2/6/23/26	0/1/1/1
10	BMA	L	3	10	-	0/2/19/22	0/1/1/1
10	NAG	M	1	4,10	-	0/6/23/26	0/1/1/1
10	NAG	M	2	10	-	2/6/23/26	0/1/1/1
10	BMA	M	3	10	-	0/2/19/22	0/1/1/1
10	NAG	N	1	6,10	-	2/6/23/26	0/1/1/1
10	NAG	N	2	10	-	2/6/23/26	0/1/1/1
10	BMA	N	3	10	-	1/2/19/22	0/1/1/1
13	NAG	P	1	8,13	-	2/6/23/26	0/1/1/1
13	NAG	P	2	13	-	2/6/23/26	0/1/1/1
13	BMA	P	3	13	-	0/2/19/22	0/1/1/1
12	NAG	Q	1	12,8	-	2/6/23/26	0/1/1/1
12	NAG	Q	2	12	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 34 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	H	1	NAG	O5-C5-C6-O6
12	Q	1	NAG	O5-C5-C6-O6
10	K	2	NAG	O5-C5-C6-O6

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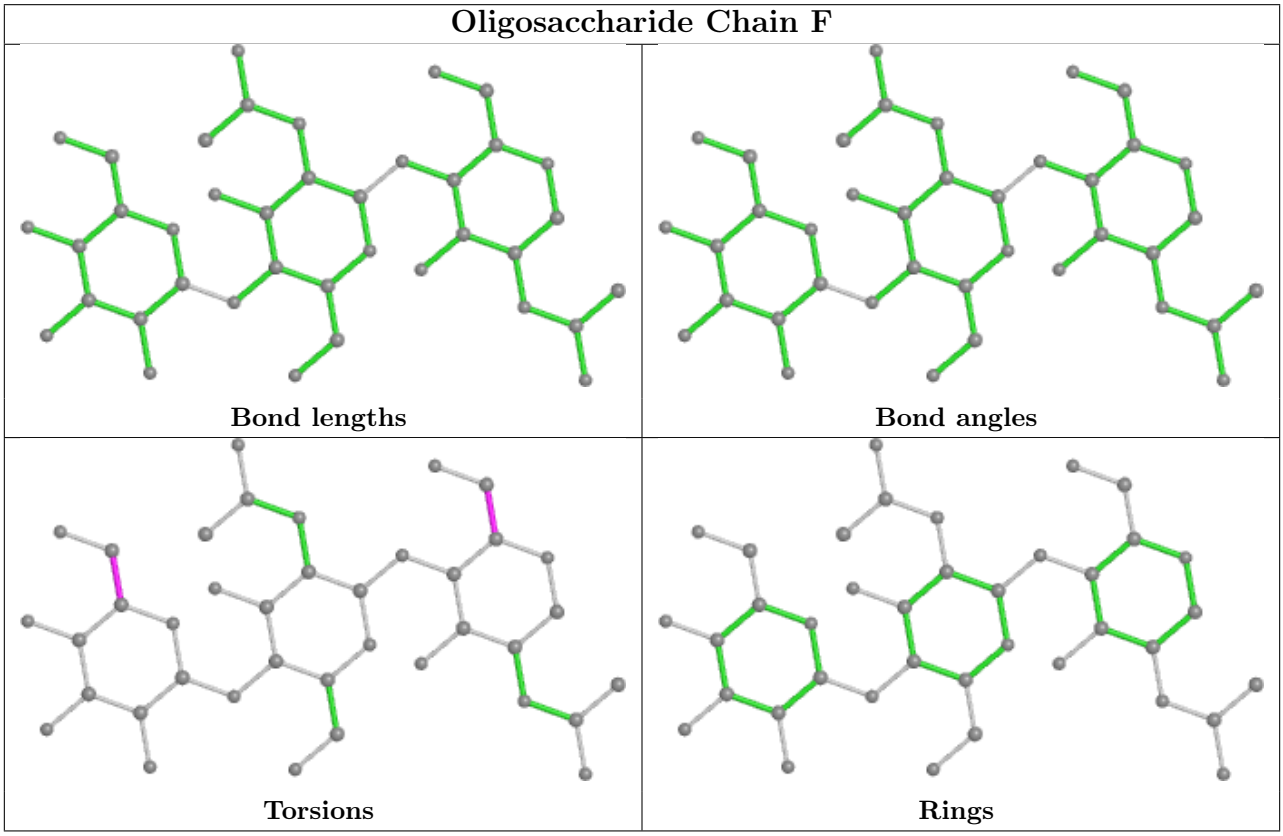
Mol	Chain	Res	Type	Atoms
12	Q	2	NAG	O5-C5-C6-O6
13	P	1	NAG	O5-C5-C6-O6

There are no ring outliers.

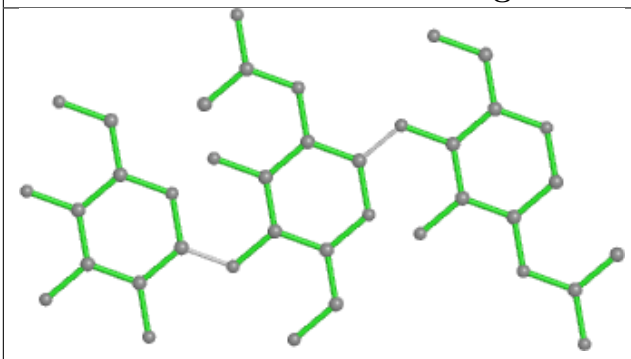
1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	H	1	NAG	2	0

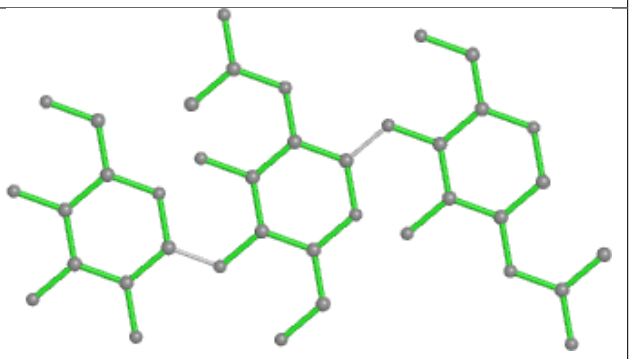
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



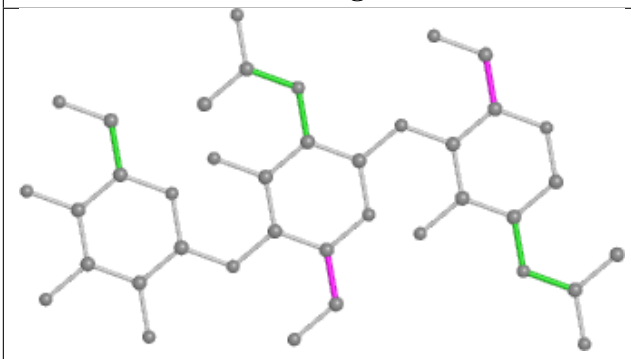
Oligosaccharide Chain K



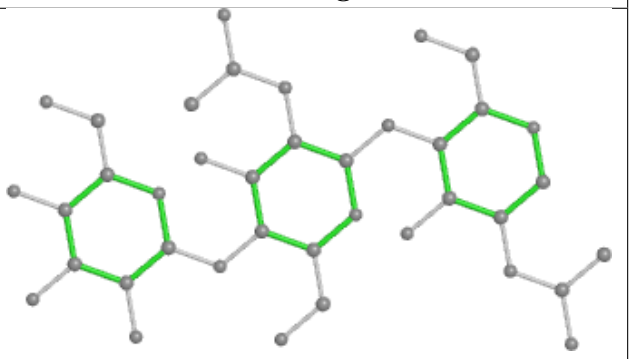
Bond lengths



Bond angles

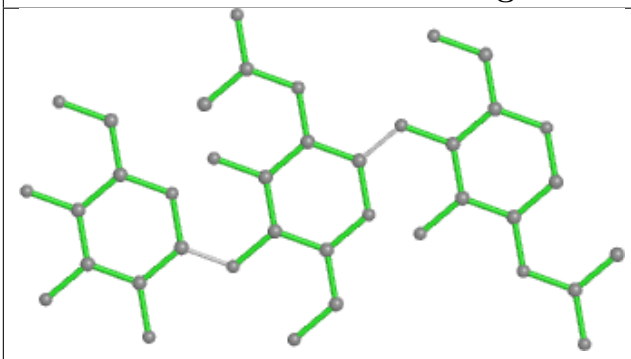


Torsions

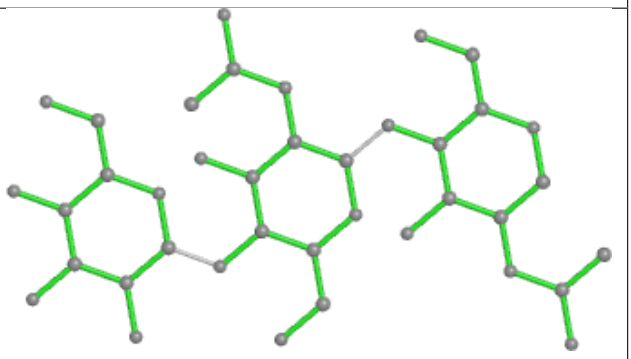


Rings

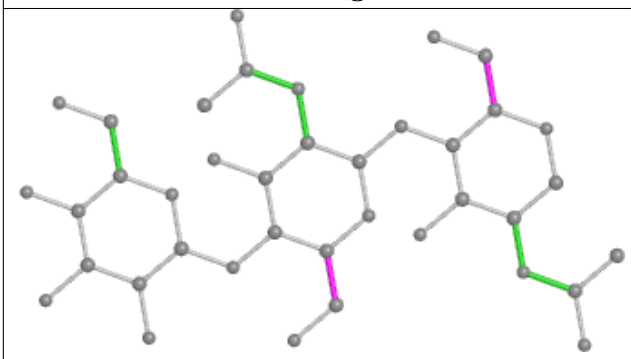
Oligosaccharide Chain L



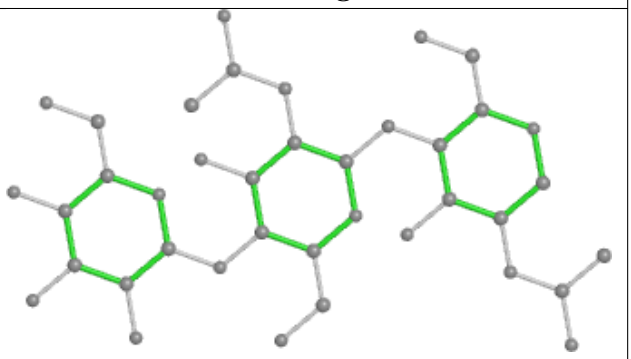
Bond lengths



Bond angles

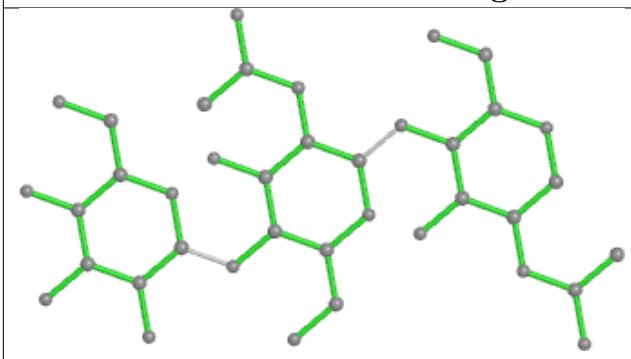


Torsions

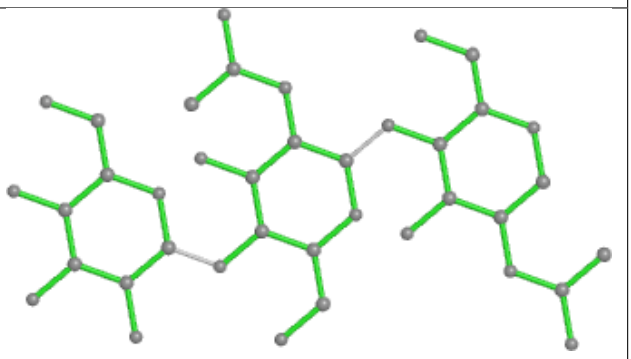


Rings

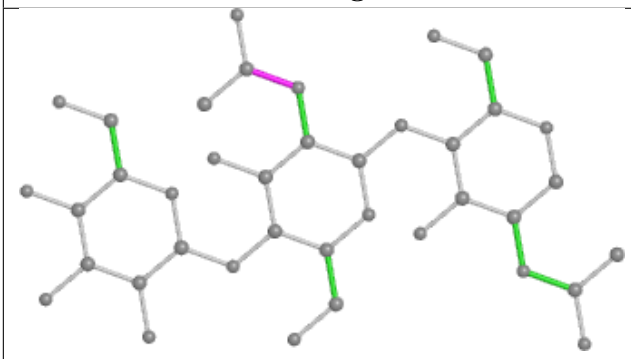
Oligosaccharide Chain M



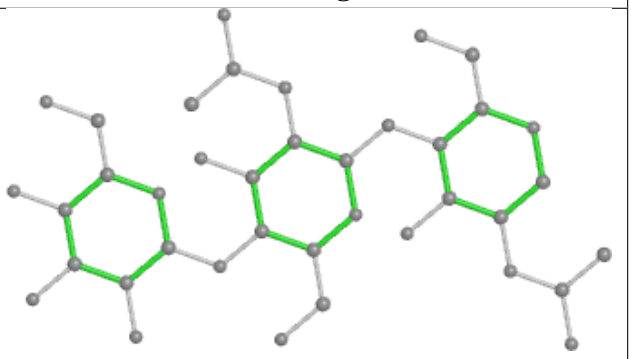
Bond lengths



Bond angles

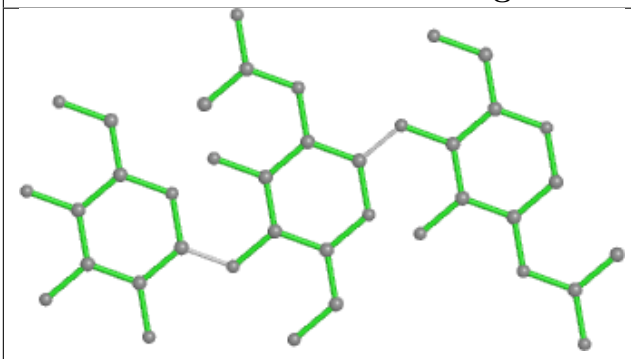


Torsions

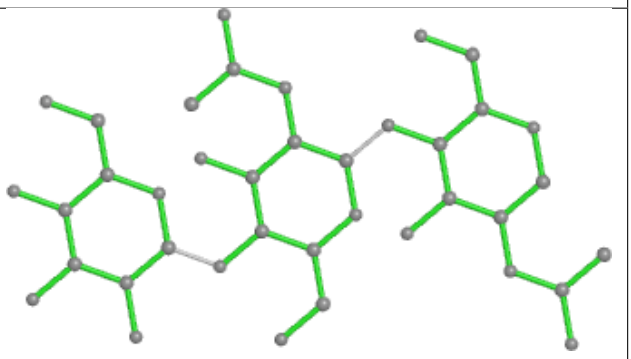


Rings

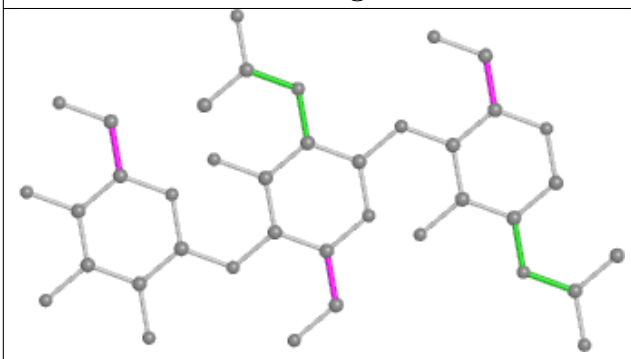
Oligosaccharide Chain N



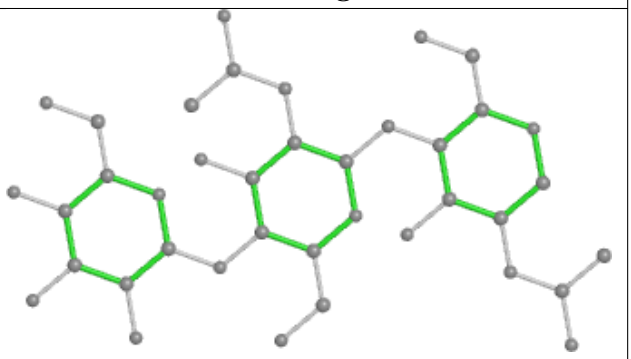
Bond lengths



Bond angles

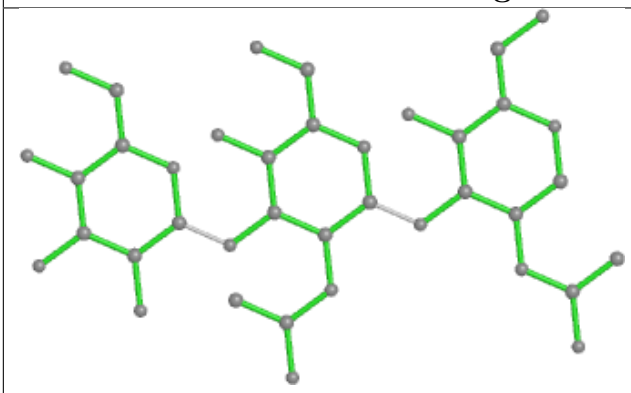


Torsions

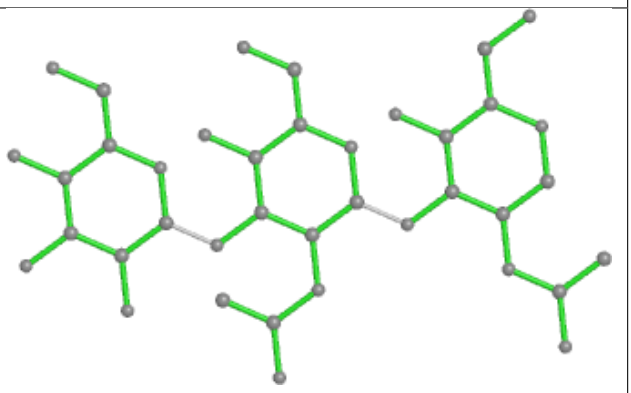


Rings

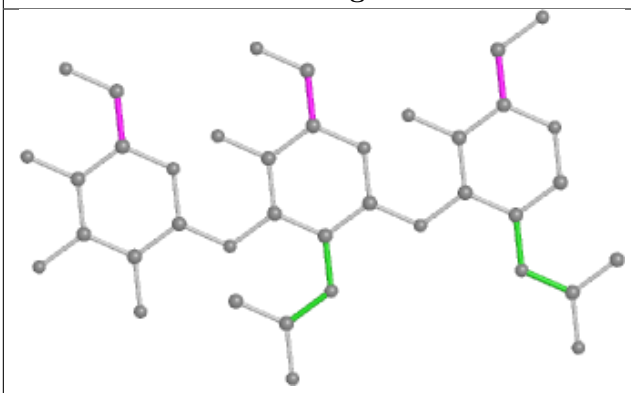
Oligosaccharide Chain H



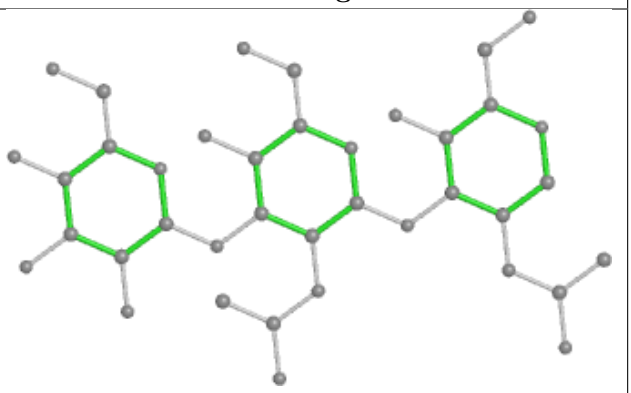
Bond lengths



Bond angles

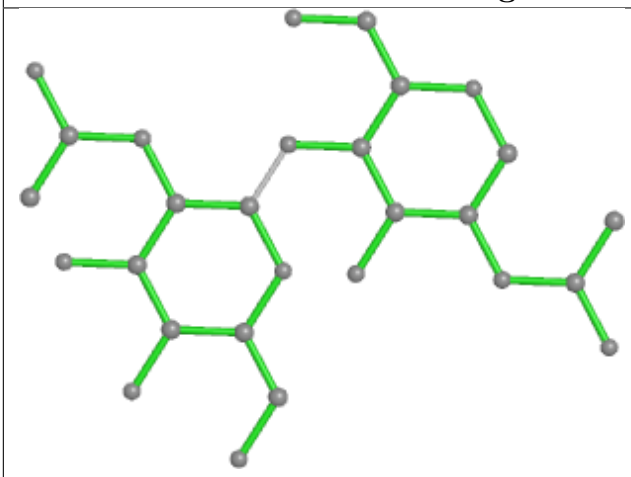


Torsions

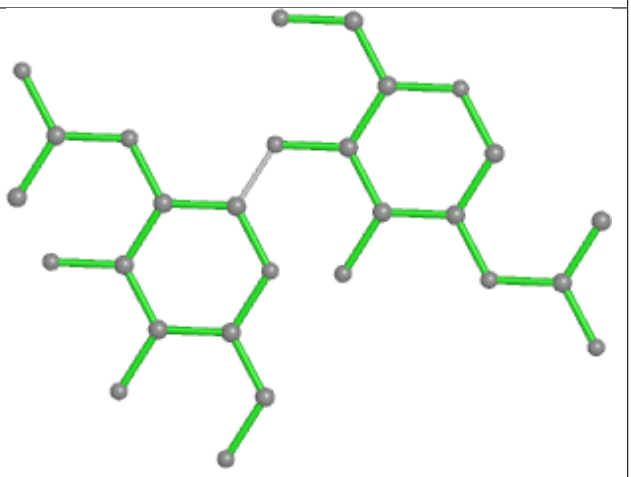


Rings

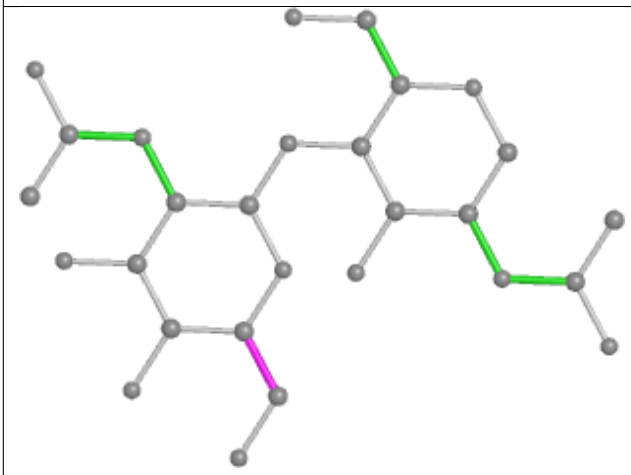
Oligosaccharide Chain J



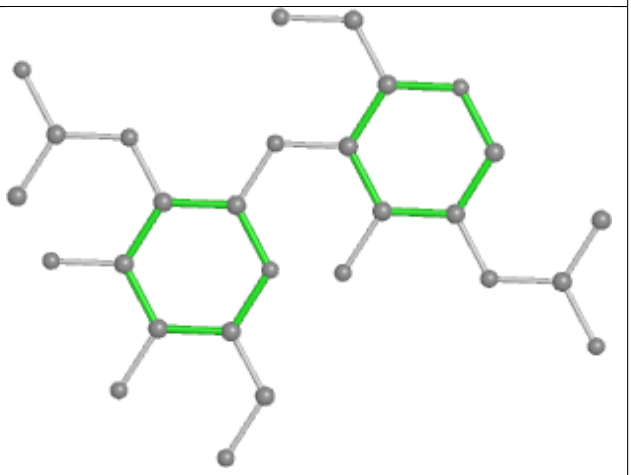
Bond lengths



Bond angles

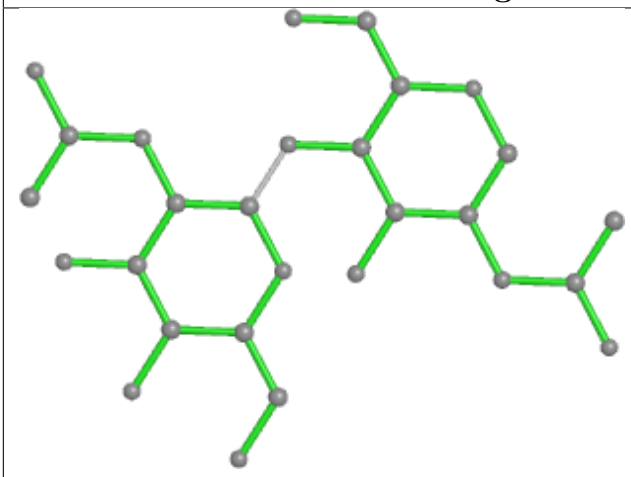


Torsions

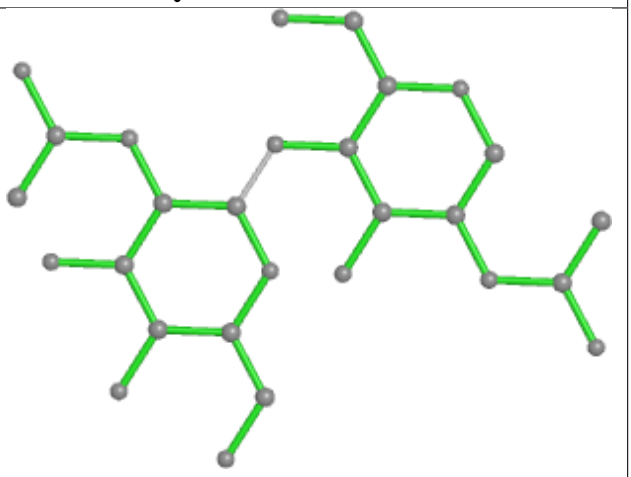


Rings

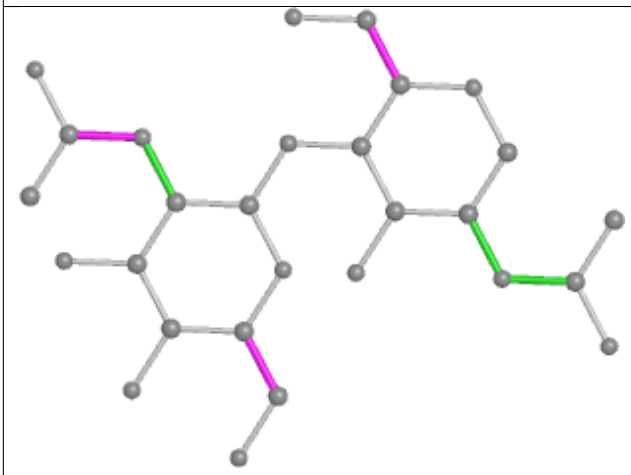
Oligosaccharide Chain Q



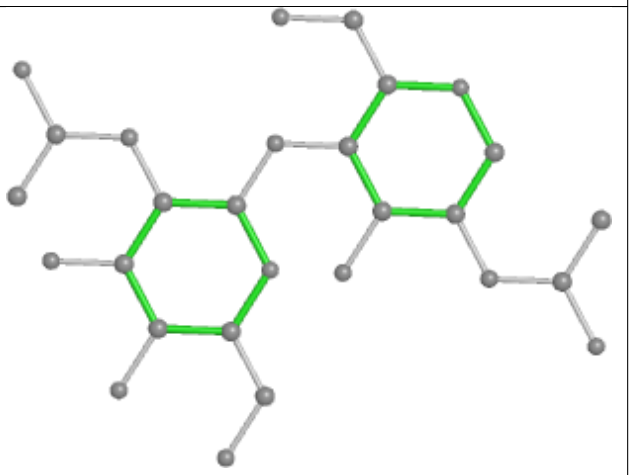
Bond lengths



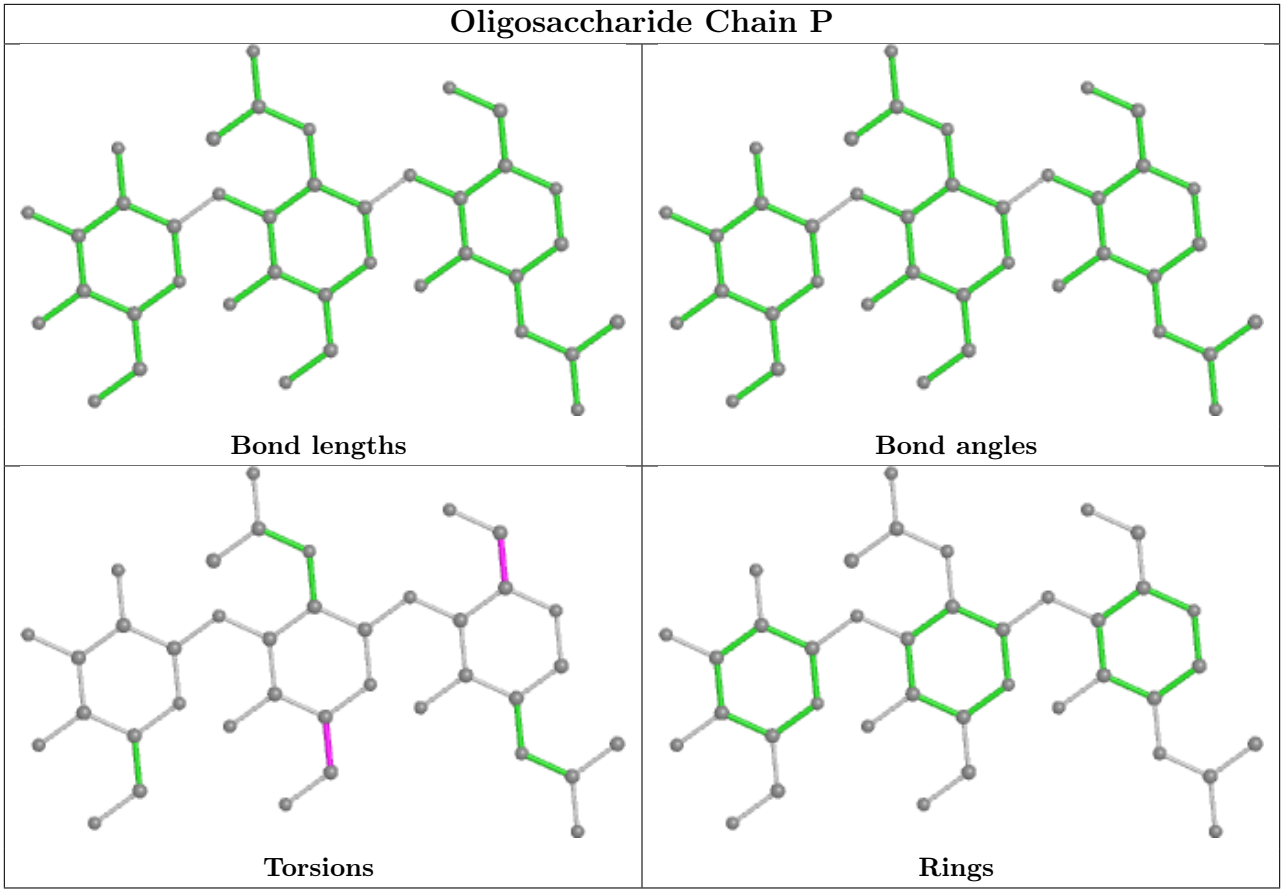
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

Of 9 ligands modelled in this entry, 2 are monoatomic - leaving 7 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
15	CLR	S	301	-	31,31,31	0.40	0	48,48,48	0.72	0
14	NAG	A	401	1	14,14,15	0.38	0	17,19,21	0.43	0
15	CLR	D	301	-	31,31,31	0.36	0	48,48,48	0.48	0
15	CLR	D	302	-	31,31,31	0.37	0	48,48,48	0.50	0
14	NAG	A	402	1	14,14,15	0.22	0	17,19,21	0.38	0
17	P5S	G	301	-	31,32,53	0.51	0	35,39,60	0.49	0
14	NAG	O	801	8	14,14,15	0.20	0	17,19,21	0.37	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
15	CLR	S	301	-	-	5/10/68/68	0/4/4/4
14	NAG	A	401	1	-	2/6/23/26	0/1/1/1
15	CLR	D	301	-	-	5/10/68/68	0/4/4/4
15	CLR	D	302	-	-	4/10/68/68	0/4/4/4
14	NAG	A	402	1	-	2/6/23/26	0/1/1/1
17	P5S	G	301	-	-	19/38/38/59	-
14	NAG	O	801	8	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 38 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	G	301	P5S	O-C-CA-N
17	G	301	P5S	C-CA-CB-OG
17	G	301	P5S	N-CA-CB-OG
17	G	301	P5S	CB-OG-P12-O16
17	G	301	P5S	C3-O16-P12-OG

There are no ring outliers.

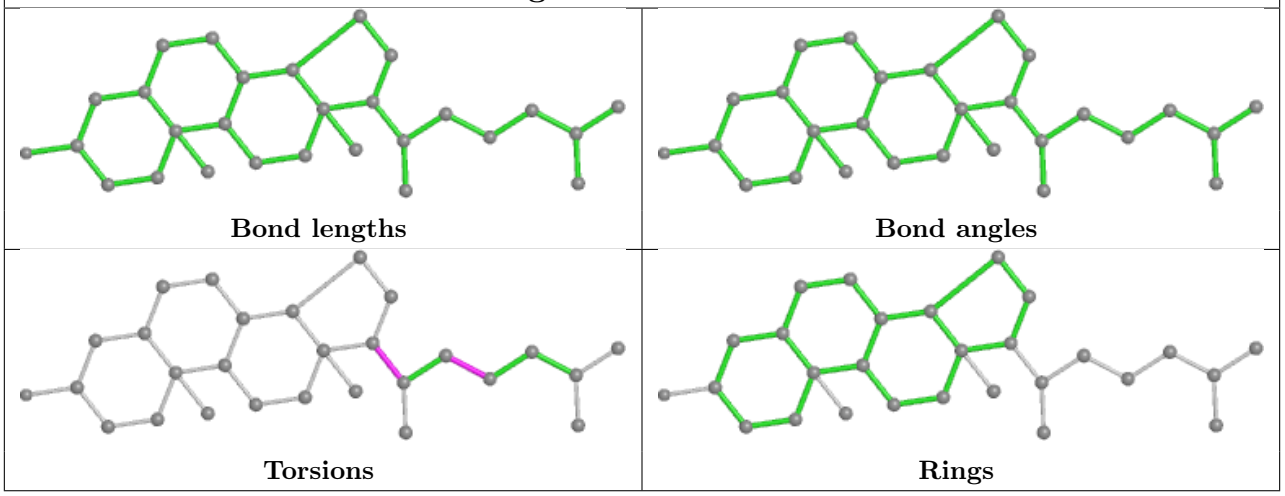
6 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	S	301	CLR	4	0
14	A	401	NAG	2	0
15	D	301	CLR	1	0
15	D	302	CLR	3	0
17	G	301	P5S	3	0
14	O	801	NAG	1	0

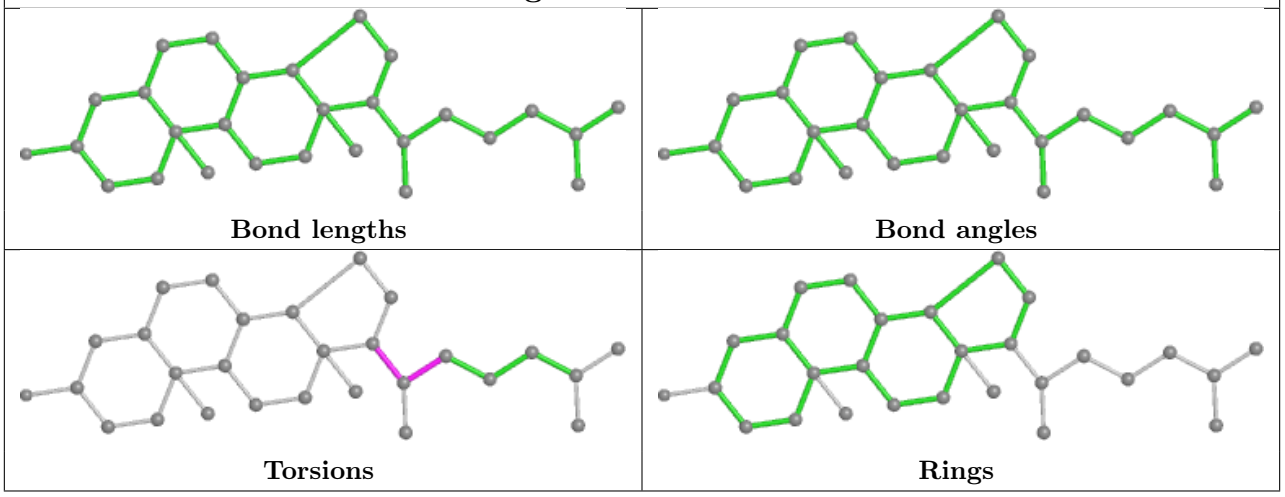
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

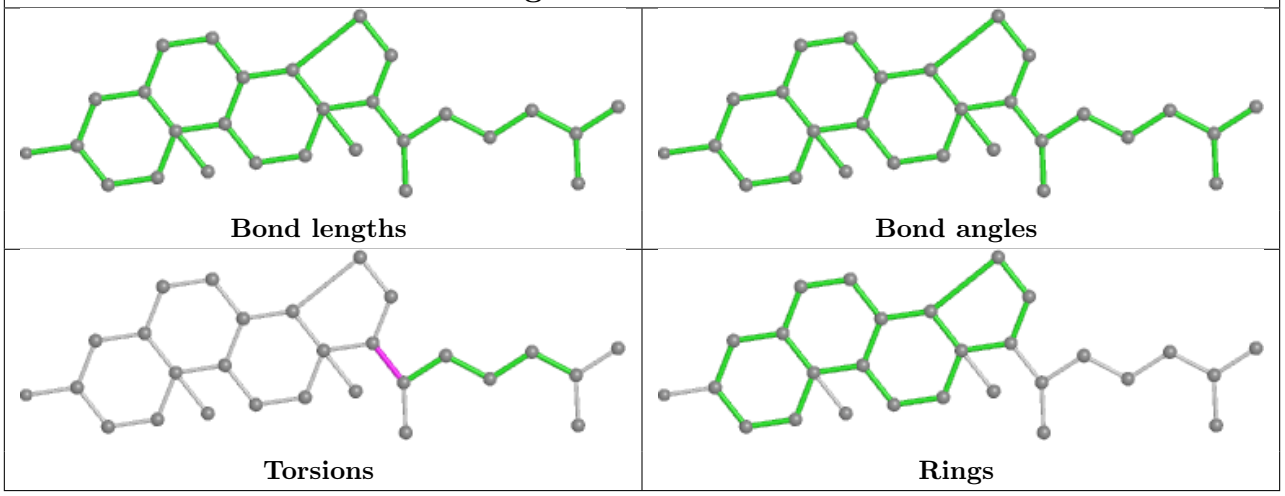
Ligand CLR S 301



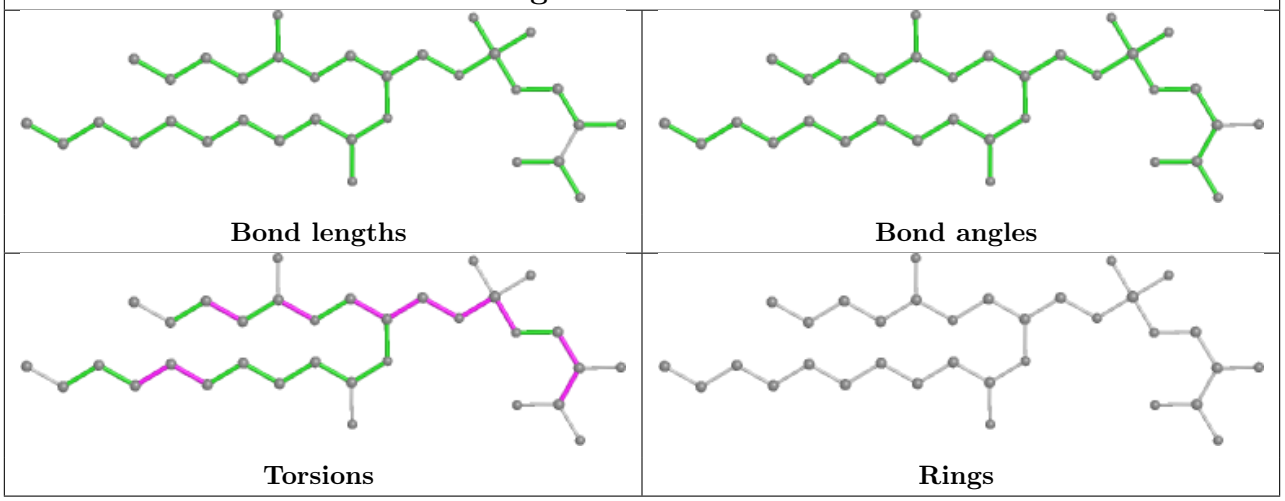
Ligand CLR D 301



Ligand CLR D 302



Ligand P5S G 301



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.