wwPDB EM Validation Summary Report

Jun 11, 2024 – 08:12 PM JST

PDB ID	:	8X53
EMDB ID	:	EMD-38060
Title	:	Cryo-EM structure of human gamma-secretase in complex with Abeta46
Authors	:	Guo, X.; Yan, C.; Lei, J.; Zhou, R.; Shi, Y.
Deposited on	:	2023-11-16
Resolution	:	3.00 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 ⓘ 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:

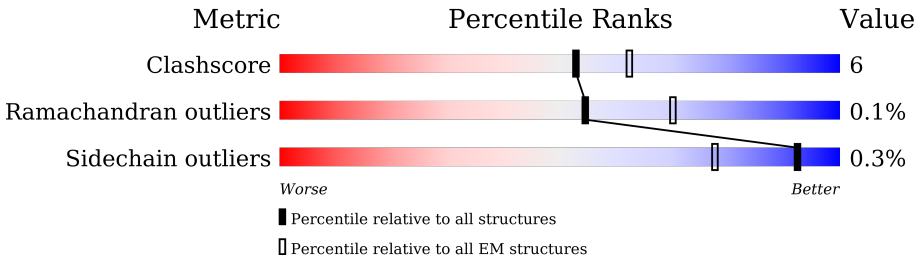
EMDB validation analysis	:	FAILED
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance

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

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
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%

Mol	Chain	Length	Quality of chain
1	A	709	84% 10% 6%
2	B	467	53% 10% • 34%
3	C	265	86% 5% 8%
4	D	143	59% 8% 33%
5	E	46	17% 28% • 52%
6	F	2	100%
6	H	2	50% 50%
6	I	2	100%
6	J	2	50% 50%

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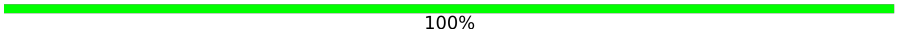
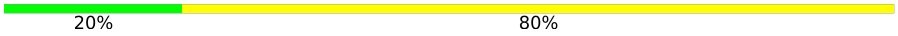
Mol	Chain	Length	Quality of chain
6	K	2	
7	G	5	

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 10947 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 Nicastrin.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	667	5235	3321	890	1003	21	0	0

- Molecule 2 is a protein called Presenilin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	306	2424	1640	369	401	14	0	0

- Molecule 3 is a protein called Gamma-secretase subunit APH-1A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	243	1872	1254	299	315	4	0	0

- Molecule 4 is a protein called Gamma-secretase subunit PEN-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	96	814	559	126	128	1	0	0

There are 43 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-41	MET	-	initiating methionine	UNP Q9NZ42
D	-40	ALA	-	expression tag	UNP Q9NZ42
D	-39	SER	-	expression tag	UNP Q9NZ42
D	-38	TRP	-	expression tag	UNP Q9NZ42
D	-37	SER	-	expression tag	UNP Q9NZ42
D	-36	HIS	-	expression tag	UNP Q9NZ42
D	-35	PRO	-	expression tag	UNP Q9NZ42
D	-34	GLN	-	expression tag	UNP Q9NZ42
D	-33	PHE	-	expression tag	UNP Q9NZ42

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-32	GLU	-	expression tag	UNP Q9NZ42
D	-31	LYS	-	expression tag	UNP Q9NZ42
D	-30	GLY	-	expression tag	UNP Q9NZ42
D	-29	GLY	-	expression tag	UNP Q9NZ42
D	-28	GLY	-	expression tag	UNP Q9NZ42
D	-27	ALA	-	expression tag	UNP Q9NZ42
D	-26	ARG	-	expression tag	UNP Q9NZ42
D	-25	GLY	-	expression tag	UNP Q9NZ42
D	-24	GLY	-	expression tag	UNP Q9NZ42
D	-23	SER	-	expression tag	UNP Q9NZ42
D	-22	GLY	-	expression tag	UNP Q9NZ42
D	-21	GLY	-	expression tag	UNP Q9NZ42
D	-20	GLY	-	expression tag	UNP Q9NZ42
D	-19	SER	-	expression tag	UNP Q9NZ42
D	-18	TRP	-	expression tag	UNP Q9NZ42
D	-17	SER	-	expression tag	UNP Q9NZ42
D	-16	HIS	-	expression tag	UNP Q9NZ42
D	-15	PRO	-	expression tag	UNP Q9NZ42
D	-14	GLN	-	expression tag	UNP Q9NZ42
D	-13	PHE	-	expression tag	UNP Q9NZ42
D	-12	GLU	-	expression tag	UNP Q9NZ42
D	-11	LYS	-	expression tag	UNP Q9NZ42
D	-10	GLY	-	expression tag	UNP Q9NZ42
D	-9	PHE	-	expression tag	UNP Q9NZ42
D	-8	ASP	-	expression tag	UNP Q9NZ42
D	-7	TYR	-	expression tag	UNP Q9NZ42
D	-6	LYS	-	expression tag	UNP Q9NZ42
D	-5	ASP	-	expression tag	UNP Q9NZ42
D	-4	ASP	-	expression tag	UNP Q9NZ42
D	-3	ASP	-	expression tag	UNP Q9NZ42
D	-2	ASP	-	expression tag	UNP Q9NZ42
D	-1	LYS	-	expression tag	UNP Q9NZ42
D	0	GLY	-	expression tag	UNP Q9NZ42
D	1	THR	-	expression tag	UNP Q9NZ42

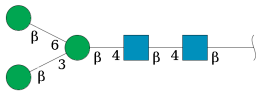
- Molecule 5 is a protein called Amyloid-beta precursor protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	22	142	93	24	24	1	0	0

- Molecule 6 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

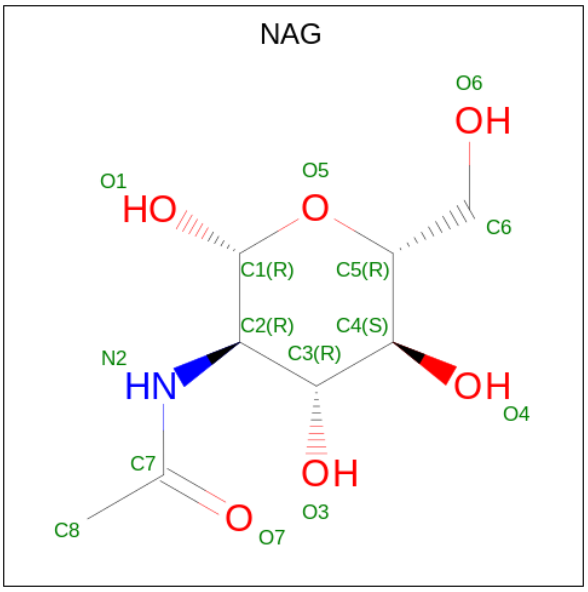
Mol	Chain	Residues	Atoms				AltConf	Trace
6	F	2	Total	C	N	O	0	0
			28	16	2	10		
6	H	2	Total	C	N	O	0	0
			28	16	2	10		
6	I	2	Total	C	N	O	0	0
			28	16	2	10		
6	J	2	Total	C	N	O	0	0
			28	16	2	10		
6	K	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 7 is an oligosaccharide called beta-D-mannopyranose-(1-3)-[beta-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.



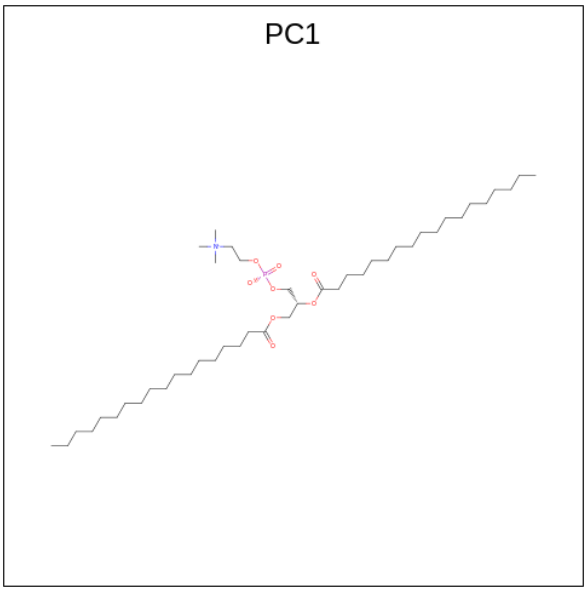
Mol	Chain	Residues	Atoms				AltConf	Trace
7	G	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



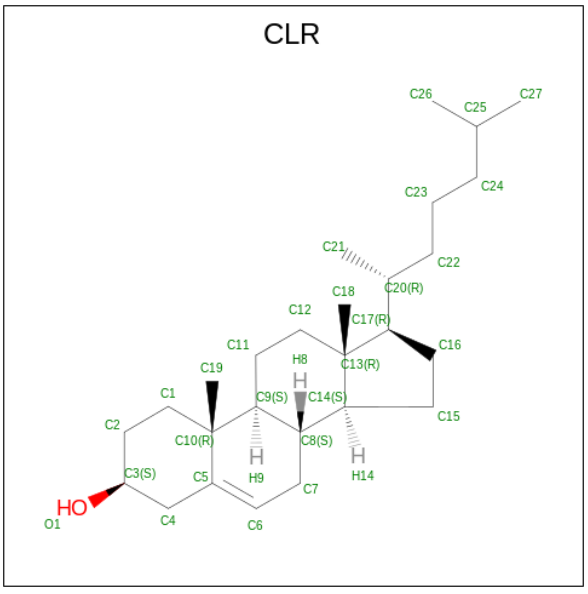
Mol	Chain	Residues	Atoms				AltConf
8	A	1	Total	C	N	O	0
			14	8	1	5	
8	A	1	Total	C	N	O	0
			14	8	1	5	
8	A	1	Total	C	N	O	0
			14	8	1	5	
8	A	1	Total	C	N	O	0
			14	8	1	5	
8	A	1	Total	C	N	O	0
			14	8	1	5	
8	A	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 9 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PC1) (formula: $C_{44}H_{88}NO_8P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
9	B	1	Total	C	N	O	P	0
			37	27	1	8	1	
9	B	1	Total	C	N	O	P	0
			41	31	1	8	1	
9	C	1	Total	C	N	O	P	0
			41	31	1	8	1	

- Molecule 10 is CHOLESTEROL (three-letter code: CLR) (formula: $C_{27}H_{46}O$) (labeled as "Ligand of Interest" by depositor).



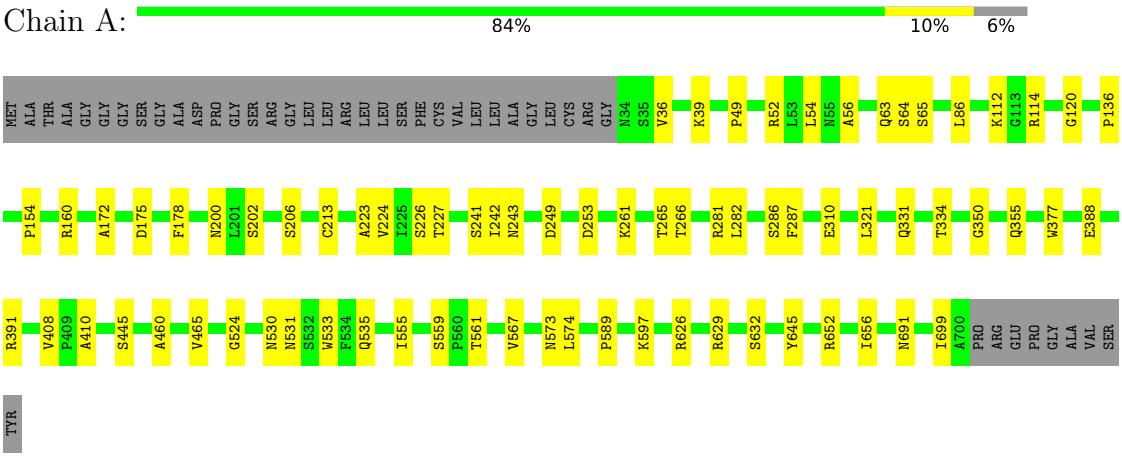
Mol	Chain	Residues	Atoms			AltConf
10	C	1	Total	C	O	0
			28	27	1	
10	C	1	Total	C	O	0
			28	27	1	

3 Residue-property plots (i)

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

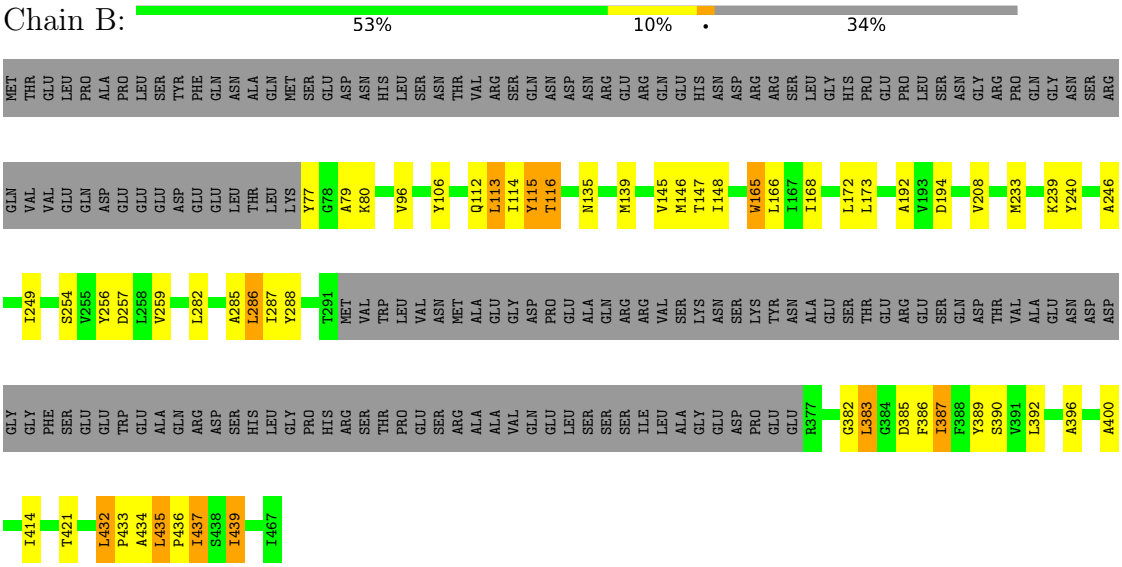
• Molecule 1: Nicastrin

Chain A:



• Molecule 2: Presenilin-1

Chain B:

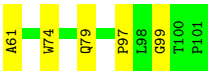


• Molecule 3: Gamma-secretase subunit APH-1A

Chain C:

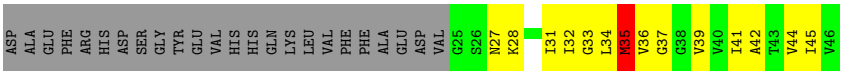
• Molecule 4: Gamma-secretase subunit PEN-2

Chain D:



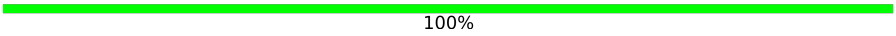
• Molecule 5: Amyloid-beta precursor protein

Chain E:



• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:

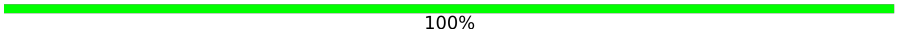


• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:

• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:

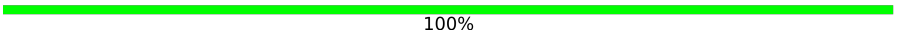


• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:

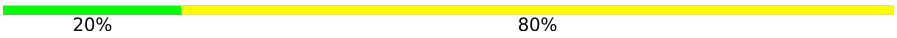
• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:



• Molecule 7: beta-D-mannopyranose-(1-3)-[beta-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 G:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	1447171	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: CLR, PC1, NAG, 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	0.40	2/5358 (0.0%)	0.55	3/7302 (0.0%)
2	B	0.79	14/2486 (0.6%)	0.78	9/3392 (0.3%)
3	C	0.39	0/1924	0.61	1/2624 (0.0%)
4	D	0.35	0/847	0.48	0/1157
5	E	0.99	1/141 (0.7%)	1.42	1/190 (0.5%)
All	All	0.52	17/10756 (0.2%)	0.63	14/14665 (0.1%)

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	437	ILE	C-O	-11.16	1.02	1.23
2	B	433	PRO	N-CA	11.08	1.66	1.47
1	A	243	ASN	C-N	9.60	1.52	1.34
2	B	116	THR	C-N	8.94	1.51	1.34
2	B	436	PRO	C-O	-8.75	1.05	1.23

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	233	GLY	N-CA-C	12.38	144.06	113.10
2	B	386	PHE	CB-CA-C	-9.38	91.65	110.40
2	B	433	PRO	CA-N-CD	-7.05	101.63	111.50
2	B	286	LEU	CA-CB-CG	6.90	131.16	115.30
2	B	112	GLN	CB-CA-C	-6.86	96.67	110.40

There are no chirality outliers.

There are no planarity outliers.

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	5235	0	5127	40	0
2	B	2424	0	2549	53	0
3	C	1872	0	1911	12	0
4	D	814	0	804	9	0
5	E	142	0	161	31	0
6	F	28	0	25	0	0
6	H	28	0	25	0	0
6	I	28	0	25	0	0
6	J	28	0	25	0	0
6	K	28	0	25	0	0
7	G	61	0	52	0	0
8	A	84	0	78	1	0
9	B	78	0	104	4	0
9	C	41	0	56	3	0
10	C	56	0	92	3	0
All	All	10947	0	11059	123	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 6.

The worst 5 of 123 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)
2:B:432:LEU:O	5:E:45:ILE:HG22	1.68	0.93
2:B:257:ASP:OD2	2:B:435:LEU:HB2	1.73	0.88
2:B:286:LEU:HD12	2:B:287:ILE:HG13	1.59	0.84
2:B:233:MET:SD	5:E:35:MET:CE	2.66	0.83
5:E:32:ILE:O	5:E:35:MET:HB2	1.79	0.82

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	665/709 (94%)	626 (94%)	39 (6%)	0	100 100
2	B	302/467 (65%)	292 (97%)	10 (3%)	0	100 100
3	C	241/265 (91%)	234 (97%)	7 (3%)	0	100 100
4	D	94/143 (66%)	90 (96%)	4 (4%)	0	100 100
5	E	20/46 (44%)	15 (75%)	4 (20%)	1 (5%)	2 12
All	All	1322/1630 (81%)	1257 (95%)	64 (5%)	1 (0%)	54 85

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	E	35	MET

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	584/612 (95%)	584 (100%)	0	100 100
2	B	264/408 (65%)	261 (99%)	3 (1%)	73 90
3	C	193/214 (90%)	193 (100%)	0	100 100
4	D	84/119 (71%)	84 (100%)	0	100 100
5	E	14/36 (39%)	14 (100%)	0	100 100
All	All	1139/1389 (82%)	1136 (100%)	3 (0%)	92 97

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	139	MET
2	B	383	LEU
2	B	439	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	531	ASN
1	A	691	ASN
2	B	464	GLN
2	B	405	ASN
1	A	355	GLN

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)

15 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	$\#\|Z\| > 2$
6	NAG	F	1	1,6	14,14,15	0.28	0	17,19,21	0.43	0
6	NAG	F	2	6	14,14,15	0.23	0	17,19,21	0.58	0
7	NAG	G	1	1,7	14,14,15	0.25	0	17,19,21	0.53	0
7	NAG	G	2	7	14,14,15	0.21	0	17,19,21	0.64	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	BMA	G	3	7	11,11,12	0.67	0	15,15,17	0.90	1 (6%)
7	BMA	G	4	7	11,11,12	0.68	0	15,15,17	0.92	1 (6%)
7	BMA	G	5	7	11,11,12	1.58	3 (27%)	15,15,17	1.89	4 (26%)
6	NAG	H	1	1,6	14,14,15	0.33	0	17,19,21	1.06	1 (5%)
6	NAG	H	2	6	14,14,15	0.39	0	17,19,21	0.49	0
6	NAG	I	1	6	14,14,15	0.23	0	17,19,21	0.47	0
6	NAG	I	2	6	14,14,15	0.23	0	17,19,21	0.56	0
6	NAG	J	1	1,6	14,14,15	0.24	0	17,19,21	0.51	0
6	NAG	J	2	6	14,14,15	0.72	1 (7%)	17,19,21	2.23	3 (17%)
6	NAG	K	1	1,6	14,14,15	0.32	0	17,19,21	0.54	0
6	NAG	K	2	6	14,14,15	0.26	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
6	NAG	F	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	F	2	6	-	2/6/23/26	0/1/1/1
7	NAG	G	1	1,7	-	4/6/23/26	0/1/1/1
7	NAG	G	2	7	-	1/6/23/26	0/1/1/1
7	BMA	G	3	7	-	2/2/19/22	0/1/1/1
7	BMA	G	4	7	-	1/2/19/22	0/1/1/1
7	BMA	G	5	7	-	0/2/19/22	0/1/1/1
6	NAG	H	1	1,6	-	1/6/23/26	0/1/1/1
6	NAG	H	2	6	-	4/6/23/26	0/1/1/1
6	NAG	I	1	6	-	2/6/23/26	0/1/1/1
6	NAG	I	2	6	-	2/6/23/26	0/1/1/1
6	NAG	J	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	J	2	6	-	3/6/23/26	0/1/1/1
6	NAG	K	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	K	2	6	-	2/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	5	BMA	C2-C3	3.09	1.57	1.52
7	G	5	BMA	C1-C2	2.92	1.58	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	5	BMA	O5-C1	2.07	1.47	1.43
6	J	2	NAG	C1-C2	2.04	1.55	1.52

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	J	2	NAG	C2-N2-C7	7.77	133.97	122.90
7	G	5	BMA	C1-O5-C5	4.96	118.91	112.19
6	J	2	NAG	C1-C2-N2	3.63	116.69	110.49
6	H	1	NAG	C2-N2-C7	3.17	127.42	122.90
7	G	5	BMA	C1-C2-C3	2.99	113.35	109.67

There are no chirality outliers.

5 of 28 torsion outliers are listed below:

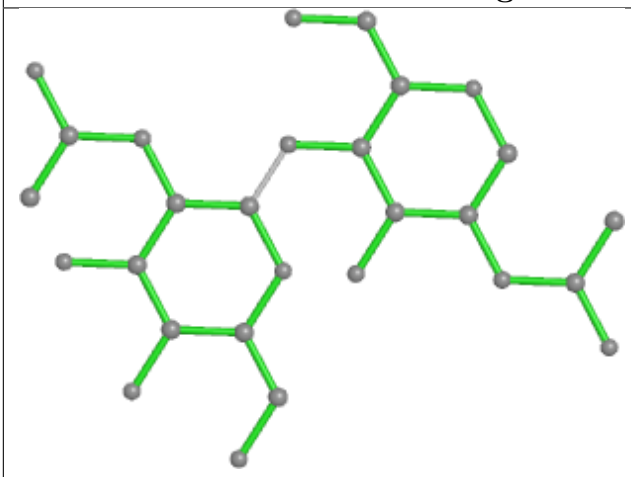
Mol	Chain	Res	Type	Atoms
6	J	1	NAG	O5-C5-C6-O6
7	G	3	BMA	C4-C5-C6-O6
6	K	1	NAG	O5-C5-C6-O6
6	J	1	NAG	C4-C5-C6-O6
7	G	3	BMA	O5-C5-C6-O6

There are no ring outliers.

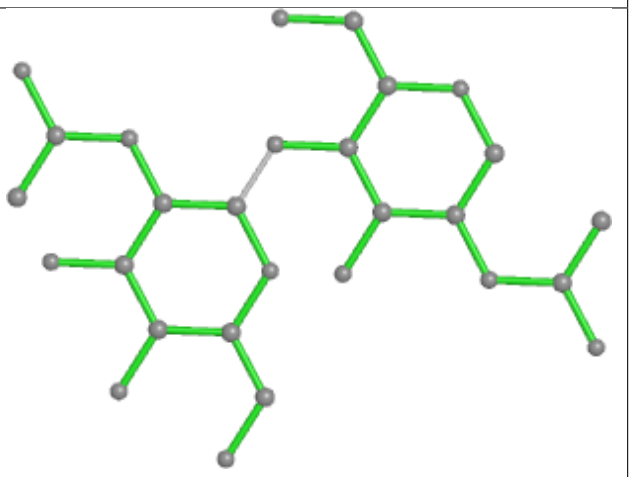
No monomer is involved in short contacts.

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

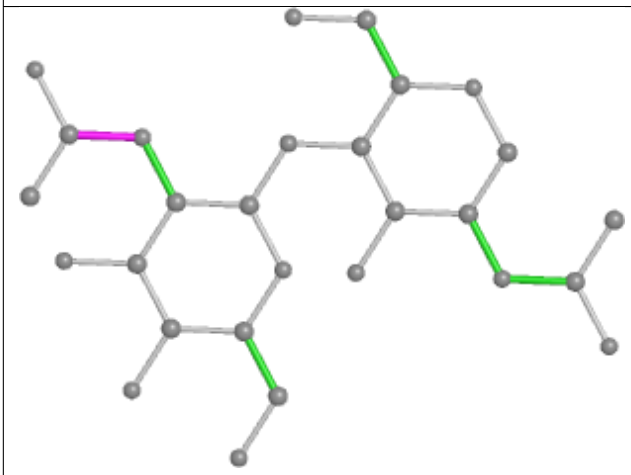
Oligosaccharide Chain F



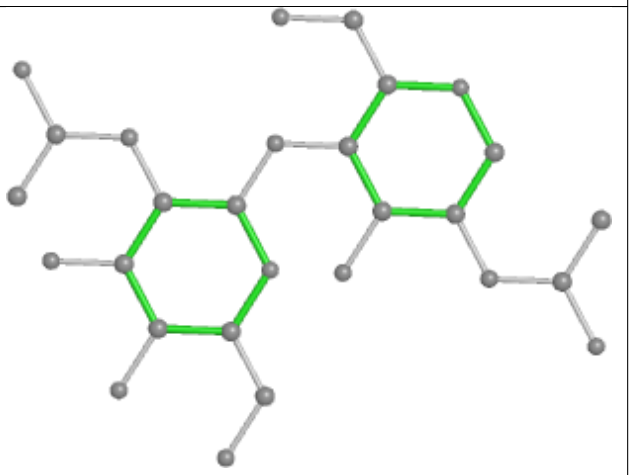
Bond lengths



Bond angles

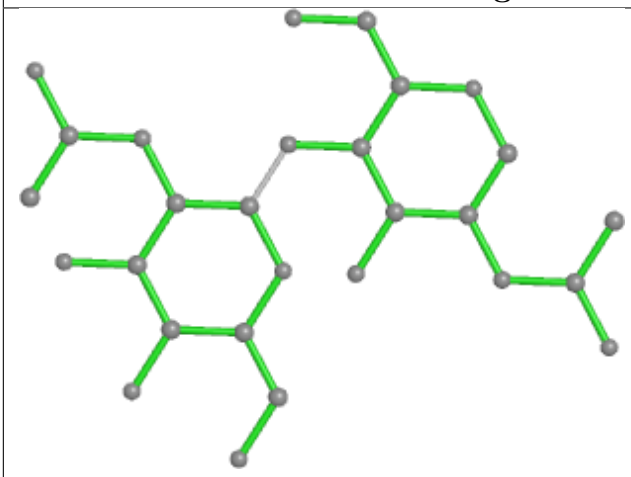


Torsions

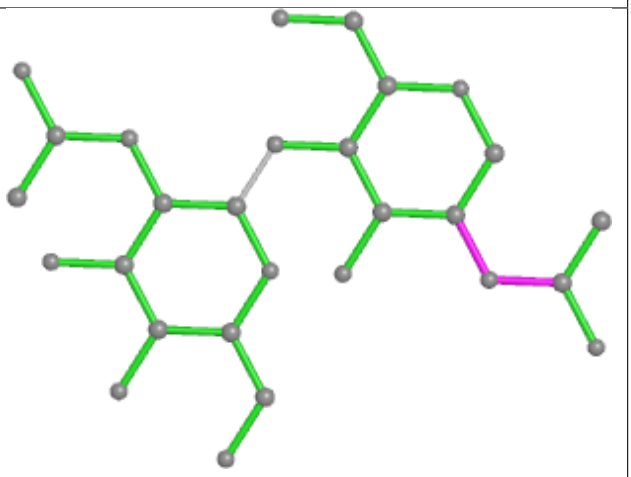


Rings

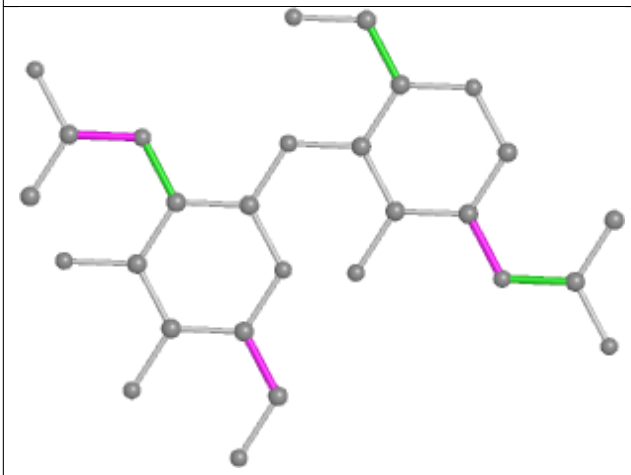
Oligosaccharide Chain H



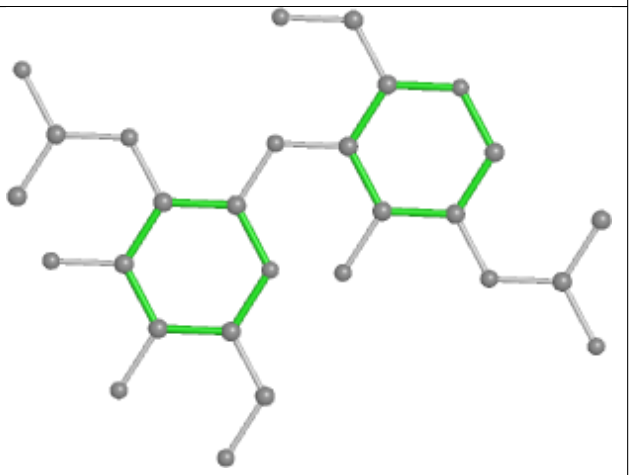
Bond lengths



Bond angles

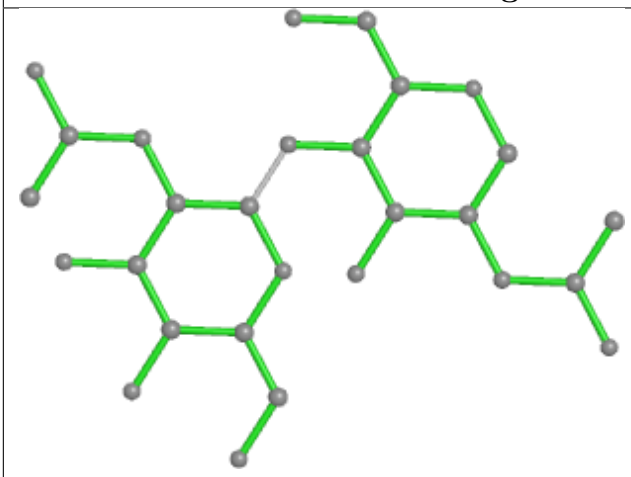


Torsions

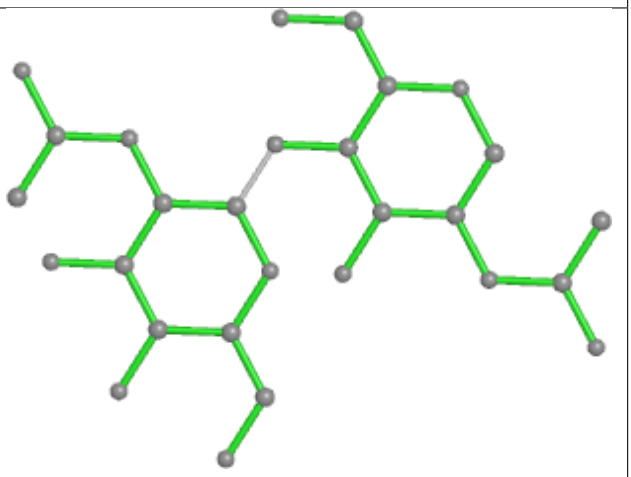


Rings

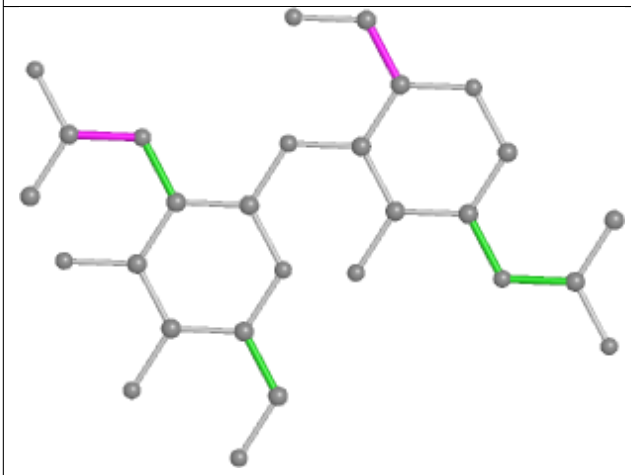
Oligosaccharide Chain I



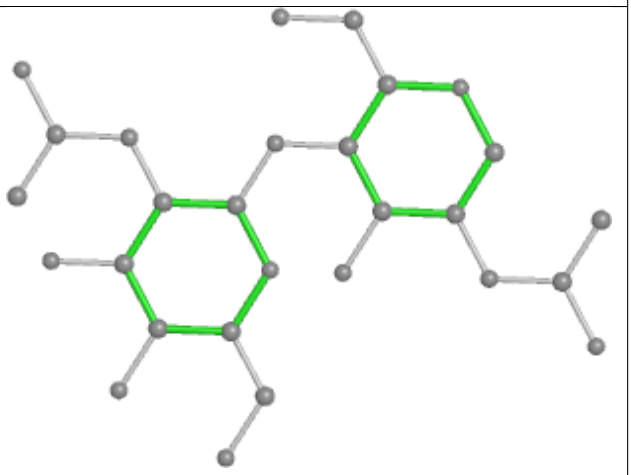
Bond lengths



Bond angles

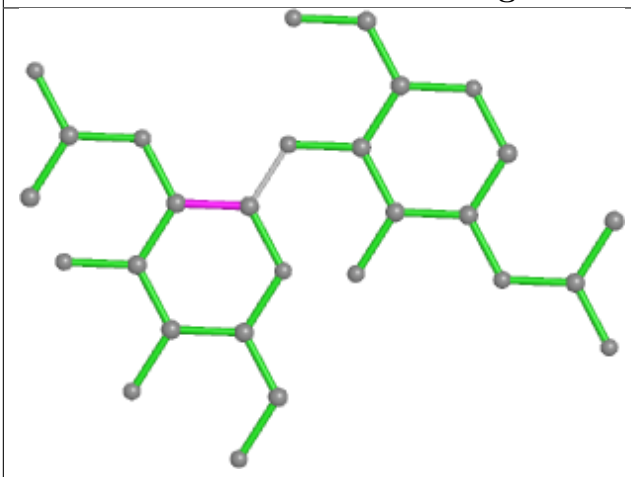


Torsions

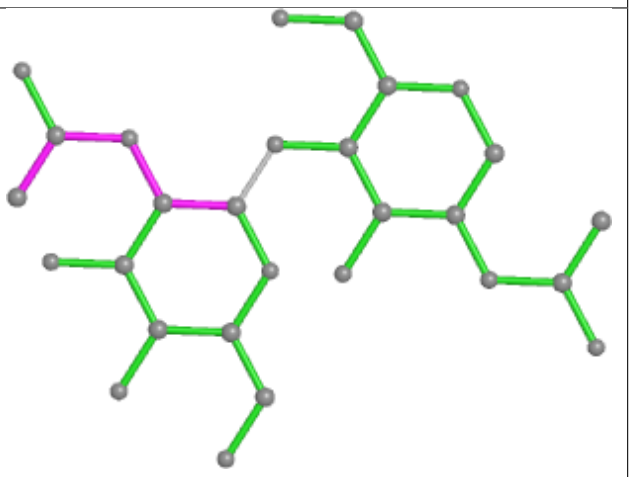


Rings

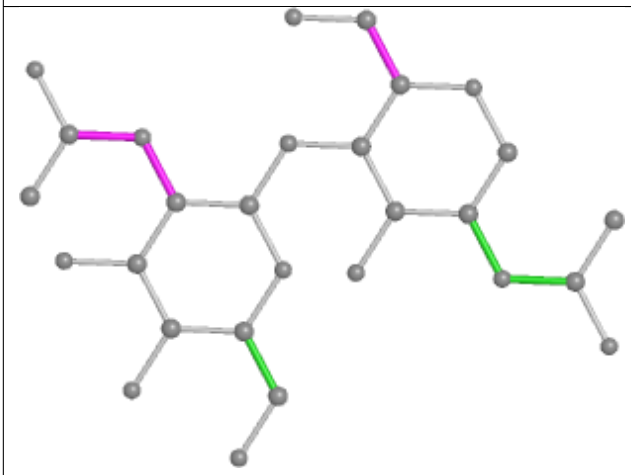
Oligosaccharide Chain J



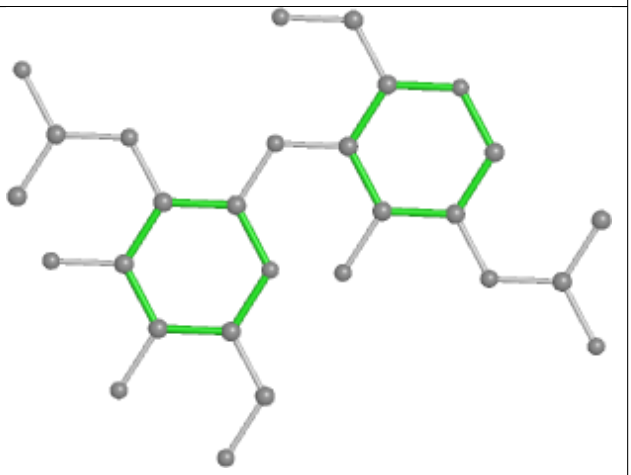
Bond lengths



Bond angles

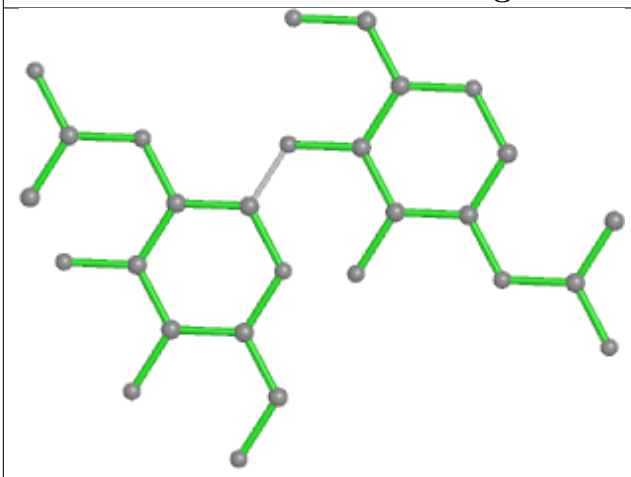


Torsions

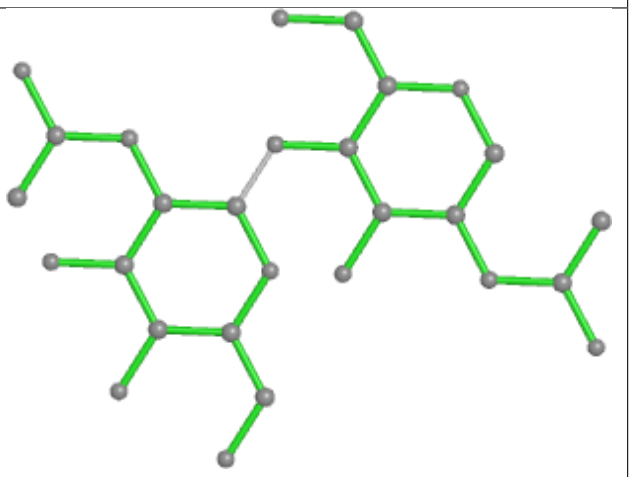


Rings

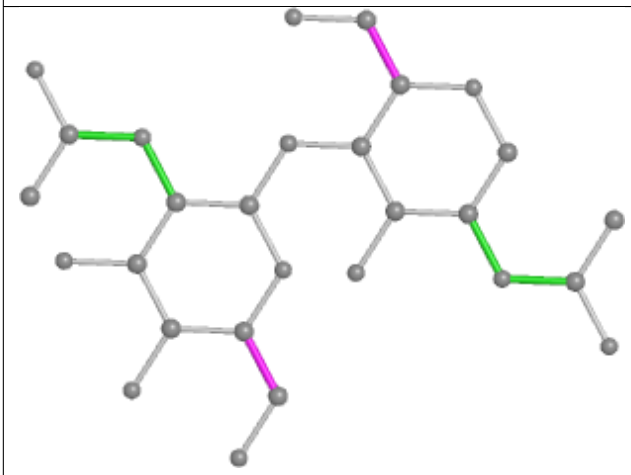
Oligosaccharide Chain K



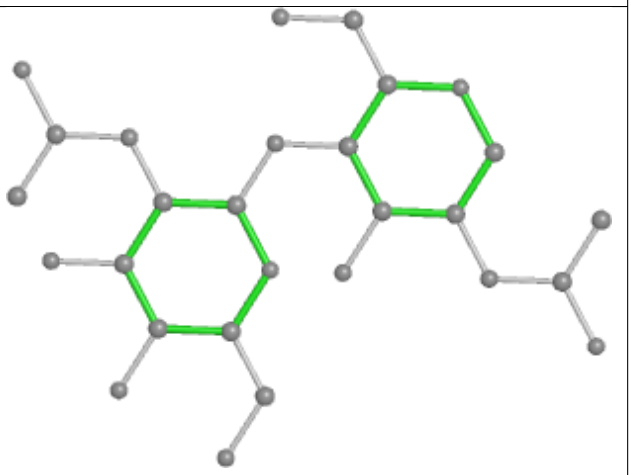
Bond lengths



Bond angles

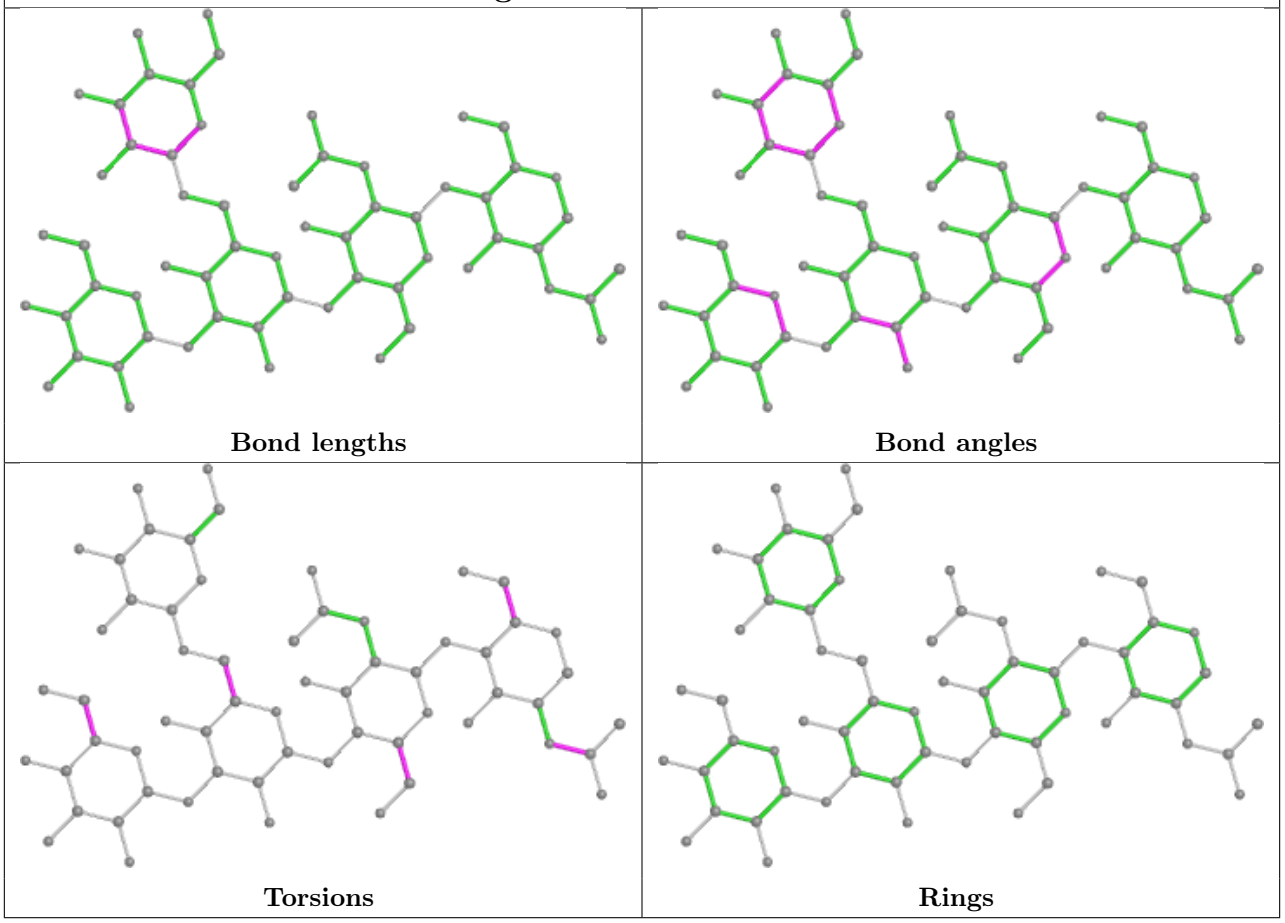


Torsions



Rings

Oligosaccharide Chain G



5.6 Ligand geometry (i)

11 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	$\#\|Z\| > 2$
8	NAG	A	804	1	14,14,15	0.91	1 (7%)	17,19,21	2.27	3 (17%)
8	NAG	A	801	1	14,14,15	0.36	0	17,19,21	0.58	1 (5%)
8	NAG	A	802	1	14,14,15	0.51	0	17,19,21	1.00	1 (5%)
10	CLR	C	301	-	31,31,31	0.29	0	48,48,48	0.33	0
8	NAG	A	803	1	14,14,15	0.45	0	17,19,21	0.46	0
9	PC1	B	801	-	36,36,53	0.31	0	42,44,61	0.34	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
8	NAG	A	806	1	14,14,15	0.23	0	17,19,21	0.61	1 (5%)
10	CLR	C	302	-	31,31,31	0.28	0	48,48,48	0.33	0
8	NAG	A	805	1	14,14,15	0.25	0	17,19,21	0.47	0
9	PC1	B	802	-	40,40,53	0.29	0	46,48,61	0.32	0
9	PC1	C	303	-	40,40,53	0.30	0	46,48,61	0.32	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
8	NAG	A	804	1	-	5/6/23/26	0/1/1/1
8	NAG	A	801	1	-	0/6/23/26	0/1/1/1
8	NAG	A	802	1	-	3/6/23/26	0/1/1/1
10	CLR	C	301	-	-	1/10/68/68	0/4/4/4
8	NAG	A	803	1	-	2/6/23/26	0/1/1/1
9	PC1	B	801	-	-	11/40/40/57	-
8	NAG	A	806	1	-	0/6/23/26	0/1/1/1
10	CLR	C	302	-	-	8/10/68/68	0/4/4/4
8	NAG	A	805	1	-	0/6/23/26	0/1/1/1
9	PC1	B	802	-	-	29/44/44/57	-
9	PC1	C	303	-	-	7/44/44/57	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	804	NAG	C1-C2	2.89	1.56	1.52

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	A	804	NAG	C2-N2-C7	7.90	134.16	122.90
8	A	804	NAG	C1-C2-N2	3.69	116.78	110.49
8	A	802	NAG	C2-N2-C7	3.08	127.28	122.90
8	A	806	NAG	C1-O5-C5	2.14	115.09	112.19
8	A	804	NAG	C8-C7-N2	2.14	119.72	116.10

There are no chirality outliers.

5 of 66 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	B	801	PC1	C11-O13-P-O14
9	B	802	PC1	C1-O11-P-O14
9	B	802	PC1	O13-C11-C12-N
9	C	303	PC1	C11-O13-P-O14
9	C	303	PC1	C12-C11-O13-P

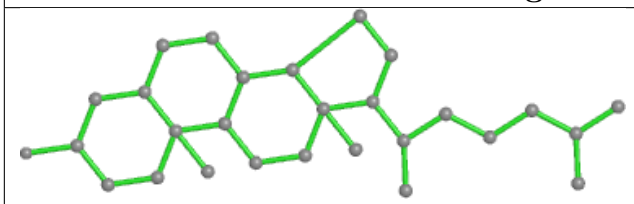
There are no ring outliers.

6 monomers are involved in 11 short contacts:

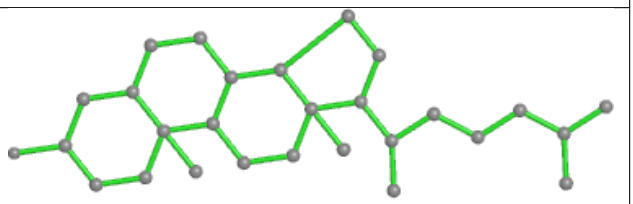
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	804	NAG	1	0
10	C	301	CLR	1	0
9	B	801	PC1	1	0
10	C	302	CLR	2	0
9	B	802	PC1	3	0
9	C	303	PC1	3	0

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

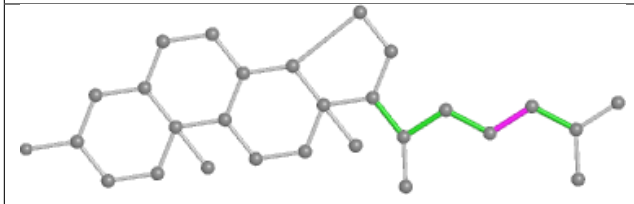
Ligand CLR C 301



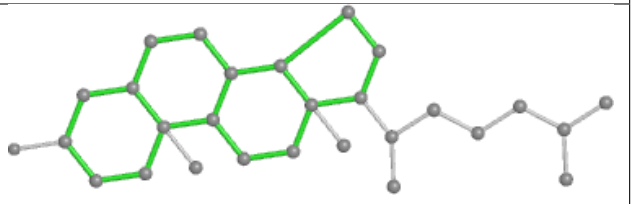
Bond lengths



Bond angles

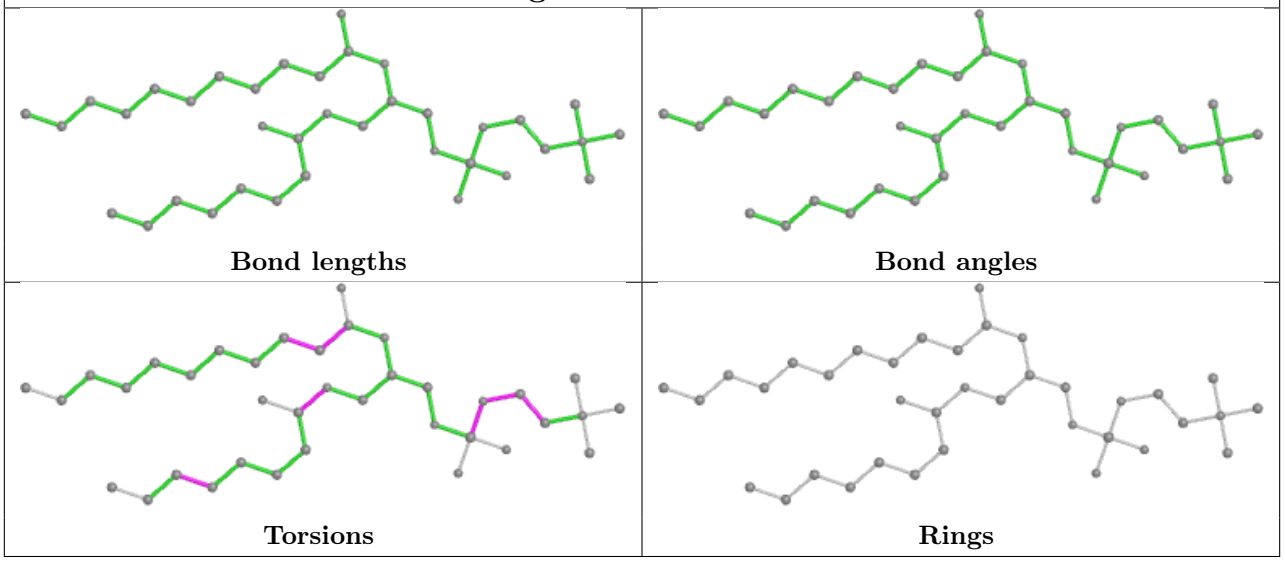


Torsions

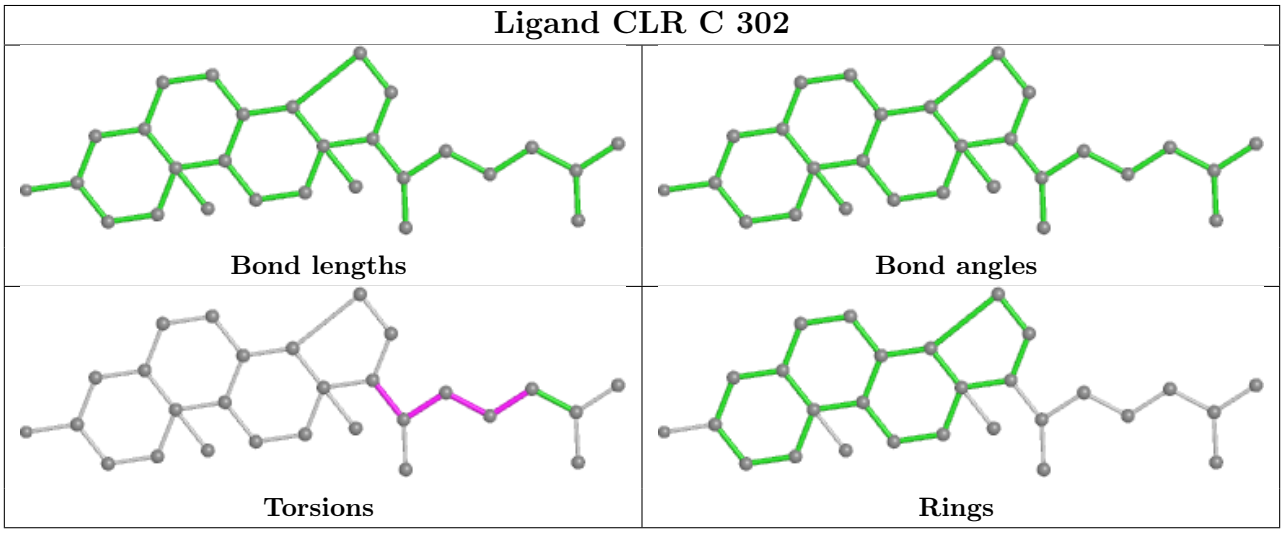


Rings

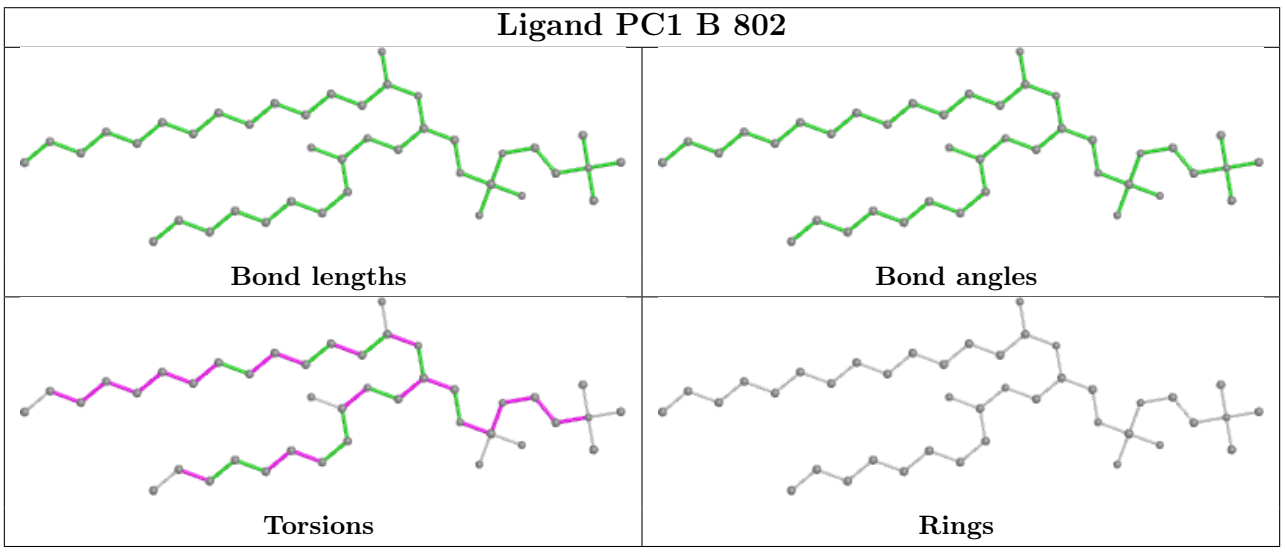
Ligand PC1 B 801



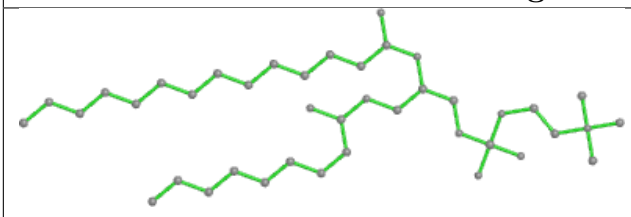
Ligand CLR C 302



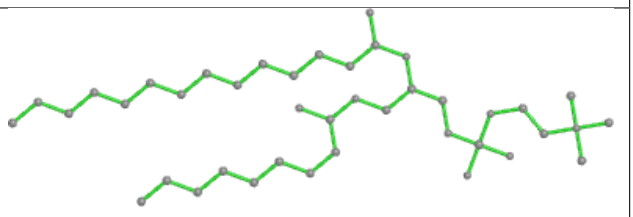
Ligand PC1 B 802



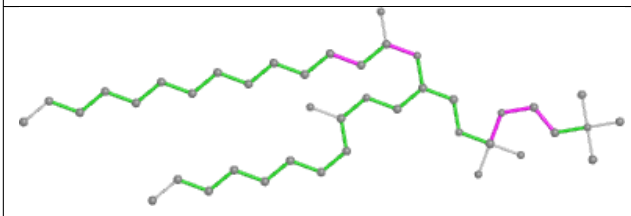
Ligand PC1 C 303



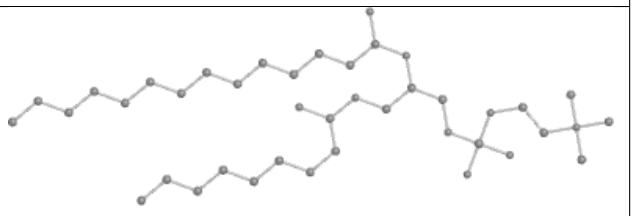
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.