Full wwPDB X-ray Structure Validation Report ⓘ

Oct 2, 2023 – 07:17 AM EDT

PDB ID	:	6MJQ
Title	:	Crystal structure of the mCD1d/xxp (JJ295) /iNKTCR ternary complex
Authors	:	Zajonc, D.M.; Bitra, A.; Janssens, J.
Deposited on	:	2018-09-21
Resolution	:	3.00 Å(reported)

This is a Full wwPDB X-ray Structure 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/XrayValidationReportHelp
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:

MolProbity	:	FAILED
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

There are no overall percentile quality scores available for this entry.

MolProbity and EDS failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition (i)

There are 12 unique types of molecules in this entry. The entry contains 13257 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 T cell receptor alpha variable 11,T cell receptor alpha variable 11,T cell receptor alpha joining 18,Human nkt tcr alpha chain, chimeric protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	201	Total	C	N	O	S	0	1	0
			1543	957	265	313	8			
1	G	201	Total	C	N	O	S	0	1	0
			1542	957	263	314	8			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	0	MET	-	initiating methionine	UNP A0A0B4J1J9
C	113	ILE	-	linker	UNP A0A0B4J1J9
G	0	MET	-	initiating methionine	UNP A0A0B4J1J9
G	113	ILE	-	linker	UNP A0A0B4J1J9

- Molecule 2 is a protein called Beta-chain,T cell receptor chain,T cell receptor beta constant 2, CHIMERIC PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	240	Total	C	N	O	S	0	0	0
			1885	1182	334	363	6			
2	H	239	Total	C	N	O	S	0	1	0
			1884	1181	335	362	6			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	95	ASP	-	linker	UNP A2NTY6
D	96	GLU	-	linker	UNP A2NTY6
D	97	GLY	-	linker	UNP A2NTY6
D	98	TYR	-	linker	UNP A2NTY6
D	130	ALA	ALA	linker	UNP A0N8J3
D	168	CYS	SER	variant	UNP A0A5B9

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Chain	Residue	Modelled	Actual	Comment	Reference
D	186	SER	CYS	variant	UNP A0A5B9
H	95	ASP	-	linker	UNP A2NTY6
H	96	GLU	-	linker	UNP A2NTY6
H	97	GLY	-	linker	UNP A2NTY6
H	98	TYR	-	linker	UNP A2NTY6
H	130	ALA	ALA	linker	UNP A0N8J3
H	168	CYS	SER	variant	UNP A0A5B9
H	186	SER	CYS	variant	UNP A0A5B9

- Molecule 3 is a protein called Antigen-presenting glycoprotein CD1d1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	274	Total	C	N	O	S	0	0	0
			2187	1394	376	404	13			
3	E	274	Total	C	N	O	S	0	0	0
			2193	1397	379	404	13			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	280	HIS	-	expression tag	UNP A0A0R4J090
A	281	HIS	-	expression tag	UNP A0A0R4J090
A	282	HIS	-	expression tag	UNP A0A0R4J090
A	283	HIS	-	expression tag	UNP A0A0R4J090
A	284	HIS	-	expression tag	UNP A0A0R4J090
A	285	HIS	-	expression tag	UNP A0A0R4J090
E	280	HIS	-	expression tag	UNP A0A0R4J090
E	281	HIS	-	expression tag	UNP A0A0R4J090
E	282	HIS	-	expression tag	UNP A0A0R4J090
E	283	HIS	-	expression tag	UNP A0A0R4J090
E	284	HIS	-	expression tag	UNP A0A0R4J090
E	285	HIS	-	expression tag	UNP A0A0R4J090

- Molecule 4 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	97	Total	C	N	O	S	0	0	0
			776	496	131	142	7			
4	F	97	Total	C	N	O	S	0	0	0
			776	496	131	142	7			

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-a

cetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	I	2	Total	C	N	O	0	0	0
			28	16	2	10			
5	K	2	Total	C	N	O	0	0	0
			28	16	2	10			
5	L	2	Total	C	N	O	0	0	0
			28	16	2	10			

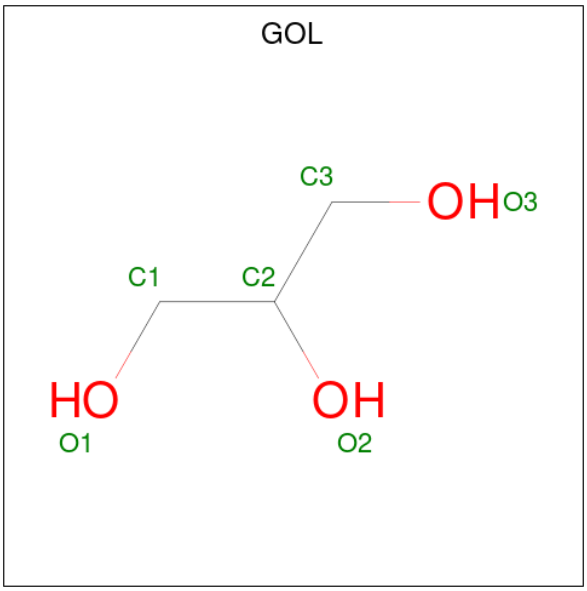
- Molecule 6 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	J	4	Total	C	N	O	0	0	0
			49	28	2	19			

- Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	M	5	Total	C	N	O	0	0	0
			60	34	2	24			

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

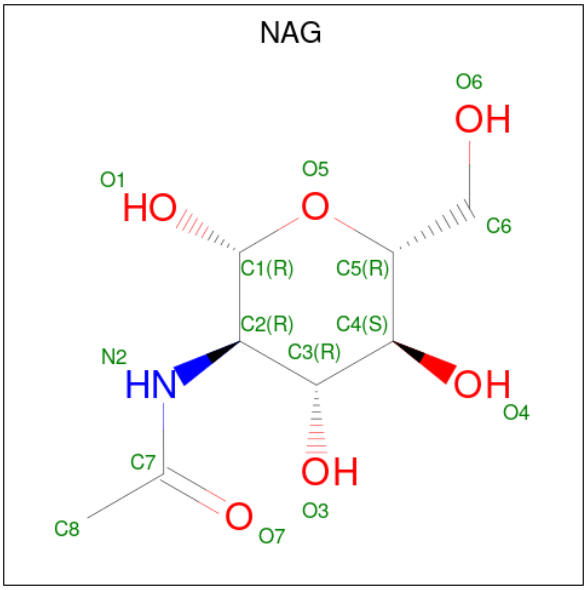


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	C	1	Total C O 6 3 3	0	0
8	E	1	Total C O 6 3 3	0	0
8	H	1	Total C O 6 3 3	0	0

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

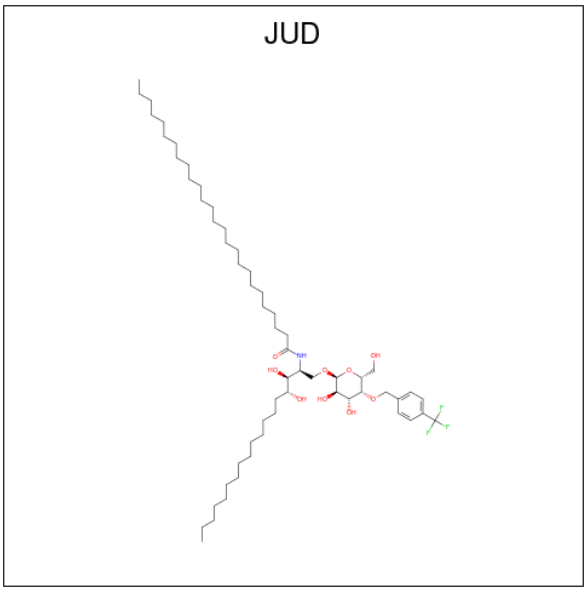
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	D	1	Total Na 1 1	0	0
9	H	2	Total Na 2 2	0	0

- Molecule 10 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 11 is N-{(2S,3S,4R)-3,4-dihydroxy-1-[(4-O-{[4-(trifluoromethyl)phenyl]methyl}-alpha-D-galactopyranosyl)oxy]octadecan-2-yl}hexacosanamide (three-letter code: JUD) (formula: $C_{58}H_{104}F_3NO_9$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	A	1	Total	C	F	N	O	0	0
			71	58	3	1	9		
11	E	1	Total	C	F	N	O	0	0
			71	58	3	1	9		

- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	C	14	Total	O	0	0
			14	14		
12	D	12	Total	O	0	0
			12	12		
12	A	15	Total	O	0	0
			15	15		
12	B	6	Total	O	0	0
			6	6		
12	E	15	Total	O	0	0
			15	15		
12	G	10	Total	O	0	0
			10	10		
12	H	17	Total	O	0	0
			17	17		
12	F	12	Total	O	0	0
			12	12		

MolProbity and EDS failed to run properly - this section is therefore empty.

3 Data and refinement statistics (i)

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	78.97Å 191.86Å 150.96Å 90.00° 90.02° 90.00°	Depositor
Resolution (Å)	49.75 – 3.00	Depositor
% Data completeness (in resolution range)	95.2 (49.75-3.00)	Depositor
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.73 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.8.0222	Depositor
R, R_{free}	0.215 , 0.258	Depositor
Wilson B-factor (Å^2)	51.6	Xtriage
Anisotropy	0.054	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.428 for h,-k,-l	Xtriage
Total number of atoms	13257	wwPDB-VP
Average B, all atoms (Å^2)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.97% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

4 Model quality

4.1 Standard geometry

MolProbity failed to run properly - this section is therefore empty.

4.2 Too-close contacts

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles

4.3.1 Protein backbone

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA

MolProbity failed to run properly - this section is therefore empty.

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

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

4.5 Carbohydrates

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	$\#\|Z\|>2$
5	NAG	I	1	5,3	14,14,15	0.33	0	17,19,21	0.77	1 (5%)
5	NAG	I	2	5	14,14,15	0.34	0	17,19,21	0.76	1 (5%)
6	NAG	J	1	6,3	14,14,15	0.31	0	17,19,21	0.70	0
6	NAG	J	2	6	14,14,15	0.36	0	17,19,21	0.75	0
6	BMA	J	3	6	11,11,12	0.31	0	15,15,17	0.65	0
6	FUC	J	4	6	10,10,11	0.32	0	14,14,16	0.59	0
5	NAG	K	1	5,3	14,14,15	0.33	0	17,19,21	0.63	0
5	NAG	K	2	5	14,14,15	0.26	0	17,19,21	0.74	0
5	NAG	L	1	5,3	14,14,15	0.31	0	17,19,21	0.72	0
5	NAG	L	2	5	14,14,15	0.30	0	17,19,21	0.63	0
7	NAG	M	1	7,3	14,14,15	0.32	0	17,19,21	0.70	0
7	NAG	M	2	7	14,14,15	0.32	0	17,19,21	0.83	1 (5%)
7	BMA	M	3	7	11,11,12	0.37	0	15,15,17	0.79	0
7	MAN	M	4	7	11,11,12	0.41	0	15,15,17	1.29	2 (13%)
7	FUC	M	5	7	10,10,11	0.32	0	14,14,16	0.61	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
5	NAG	I	1	5,3	-	0/6/23/26	0/1/1/1
5	NAG	I	2	5	-	2/6/23/26	0/1/1/1
6	NAG	J	1	6,3	-	0/6/23/26	0/1/1/1
6	NAG	J	2	6	-	0/6/23/26	0/1/1/1
6	BMA	J	3	6	-	0/2/19/22	0/1/1/1
6	FUC	J	4	6	-	-	0/1/1/1
5	NAG	K	1	5,3	-	0/6/23/26	0/1/1/1
5	NAG	K	2	5	-	0/6/23/26	0/1/1/1
5	NAG	L	1	5,3	-	0/6/23/26	0/1/1/1
5	NAG	L	2	5	-	0/6/23/26	0/1/1/1
7	NAG	M	1	7,3	-	0/6/23/26	0/1/1/1
7	NAG	M	2	7	-	2/6/23/26	0/1/1/1
7	BMA	M	3	7	-	0/2/19/22	0/1/1/1
7	MAN	M	4	7	-	0/2/19/22	0/1/1/1
7	FUC	M	5	7	-	-	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	M	4	MAN	C1-C2-C3	3.69	114.20	109.67
5	I	1	NAG	C1-O5-C5	2.24	115.22	112.19
7	M	4	MAN	O5-C5-C6	2.21	110.67	107.20
5	I	2	NAG	O5-C5-C6	2.17	110.61	107.20
7	M	2	NAG	O5-C5-C6	2.07	110.44	107.20

There are no chirality outliers.

All (4) torsion outliers are listed below:

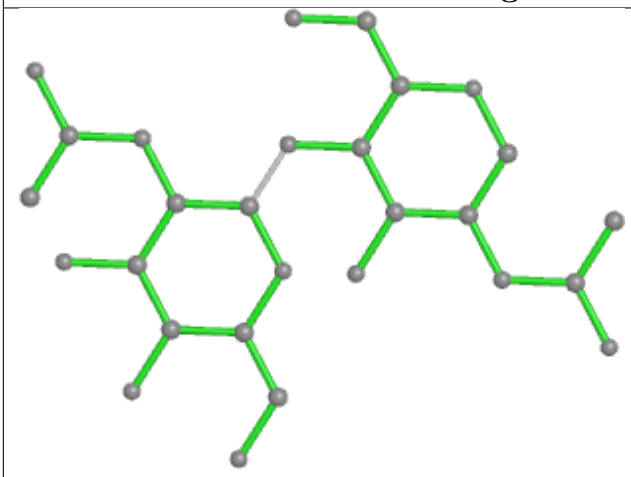
Mol	Chain	Res	Type	Atoms
7	M	2	NAG	O5-C5-C6-O6
5	I	2	NAG	O5-C5-C6-O6
7	M	2	NAG	C4-C5-C6-O6
5	I	2	NAG	C4-C5-C6-O6

There are no ring outliers.

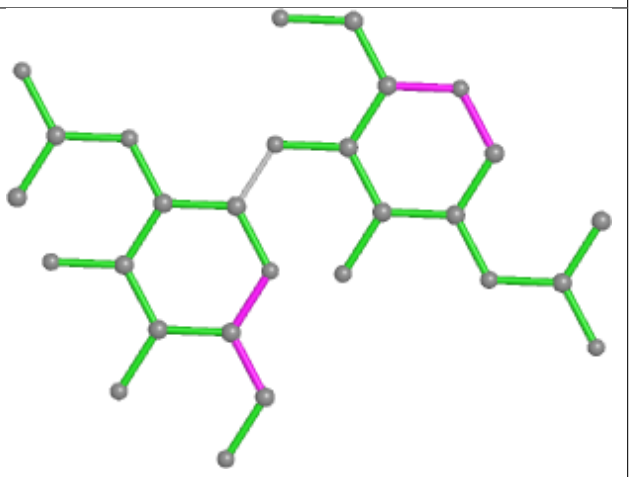
No monomer is involved in short contacts.

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

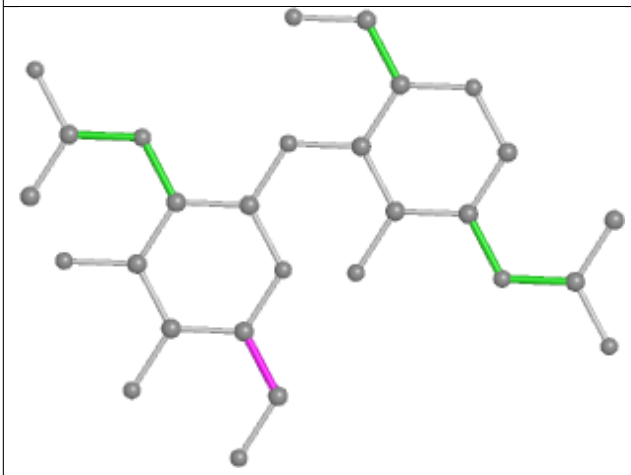
Oligosaccharide Chain I



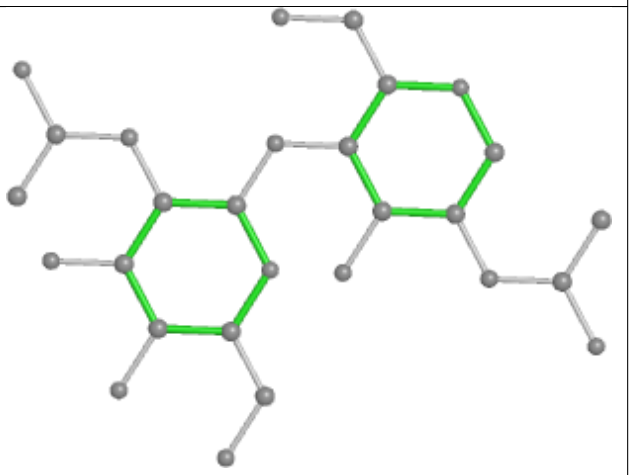
Bond lengths



Bond angles

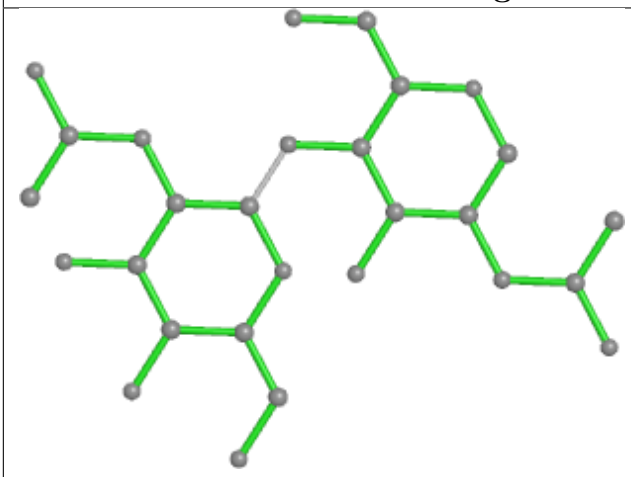


Torsions

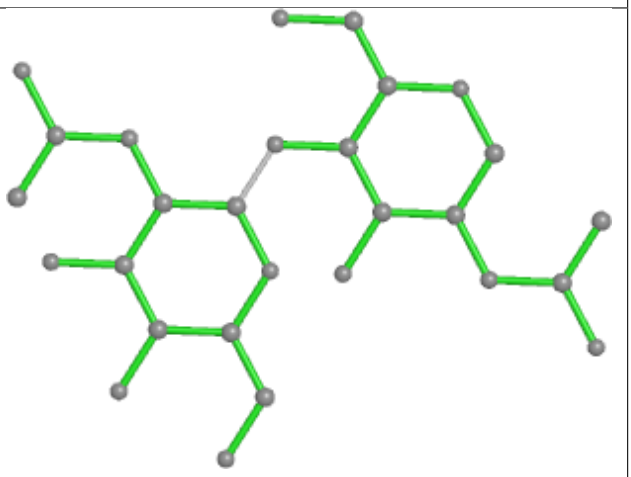


Rings

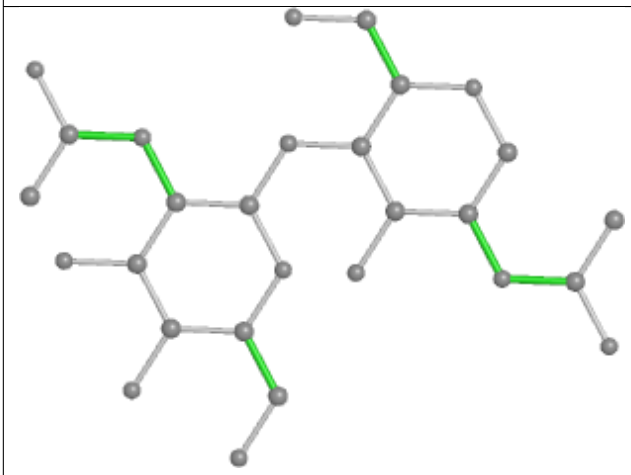
Oligosaccharide Chain K



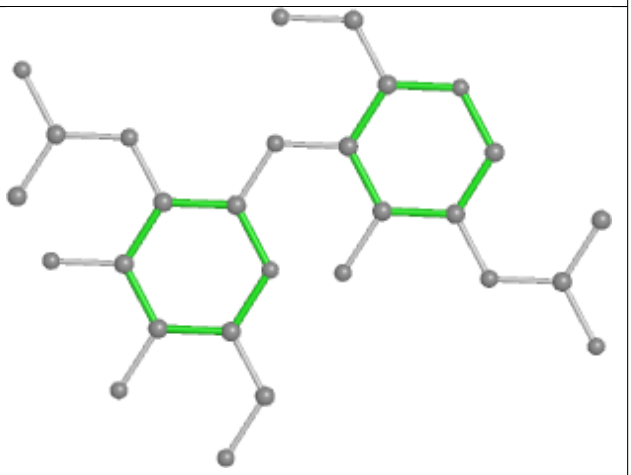
Bond lengths



Bond angles

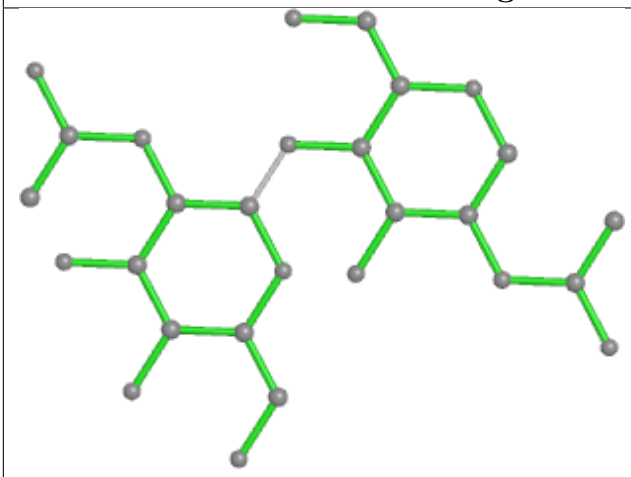


Torsions

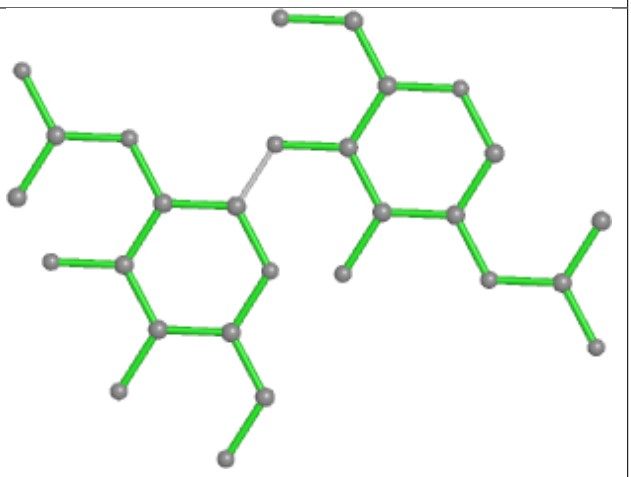


Rings

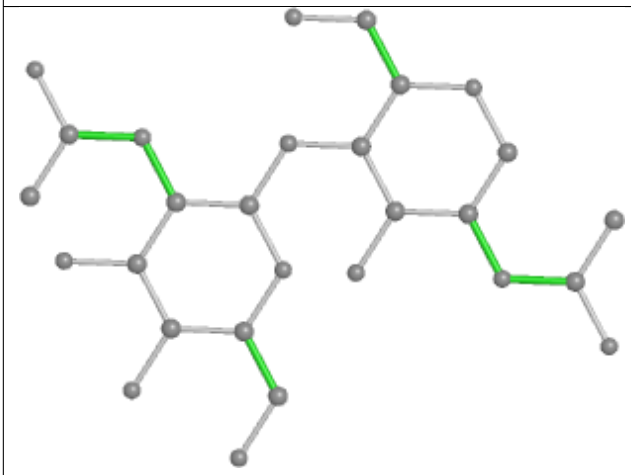
Oligosaccharide Chain L



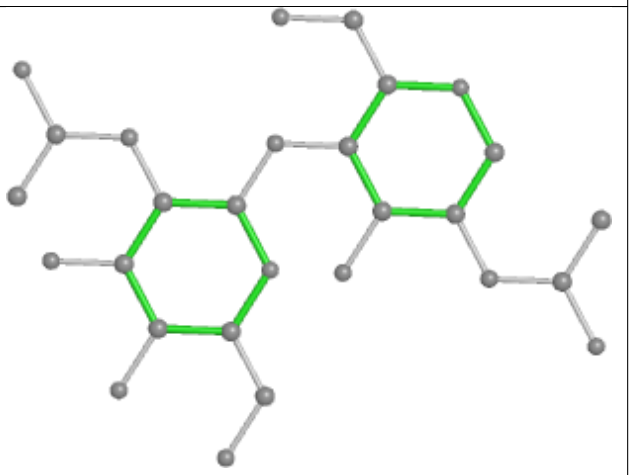
Bond lengths



Bond angles

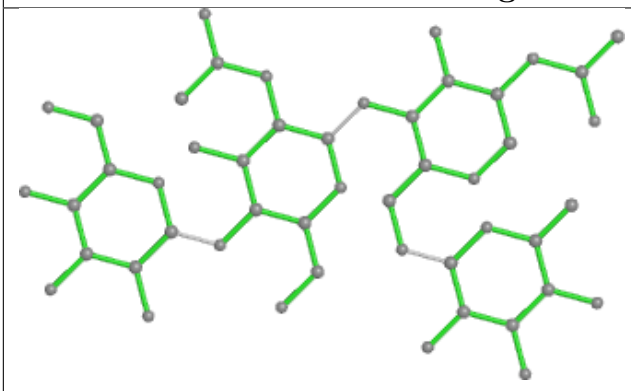


Torsions

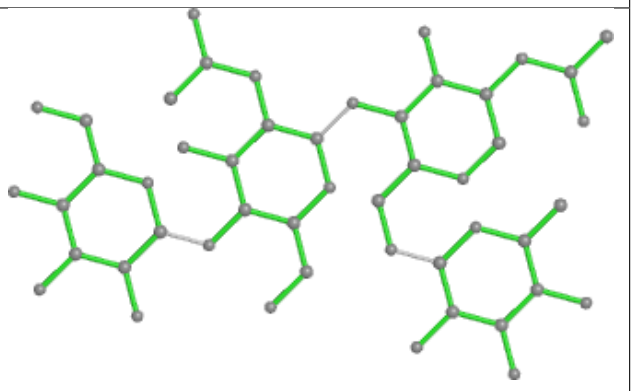


Rings

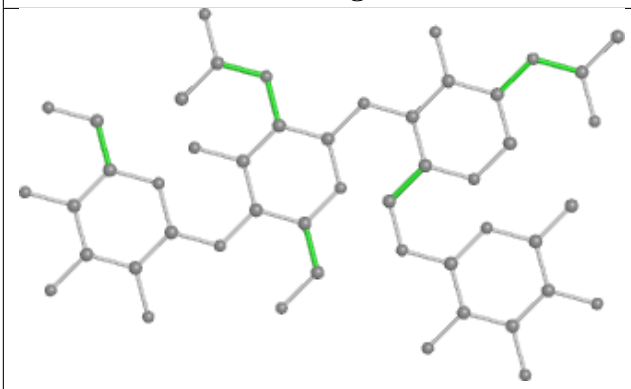
Oligosaccharide Chain J



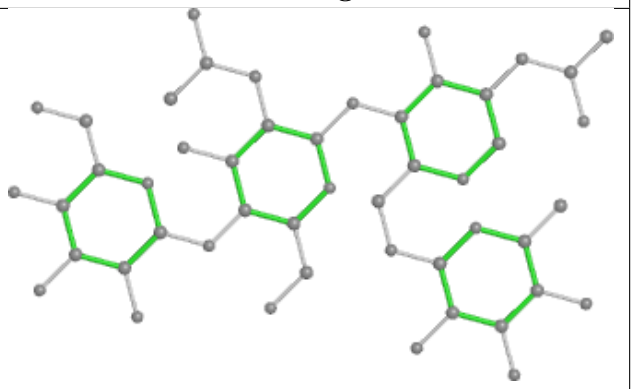
Bond lengths



Bond angles

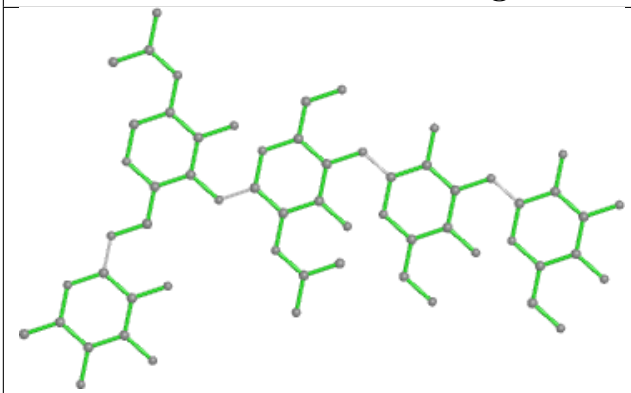


Torsions

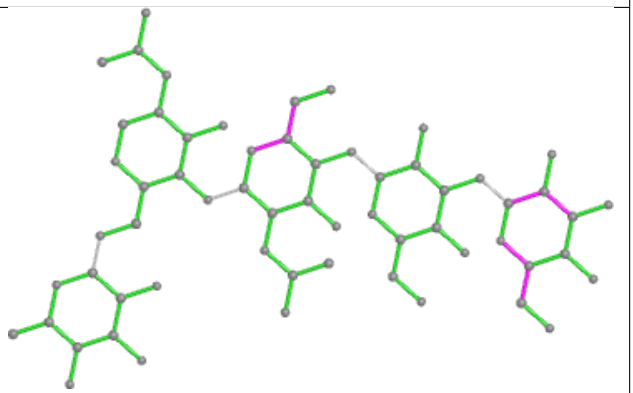


Rings

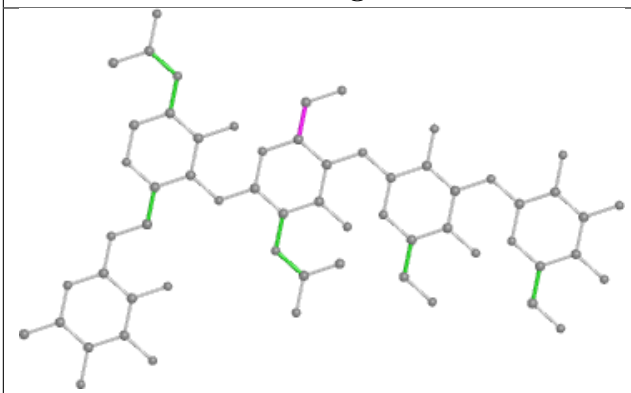
Oligosaccharide Chain M



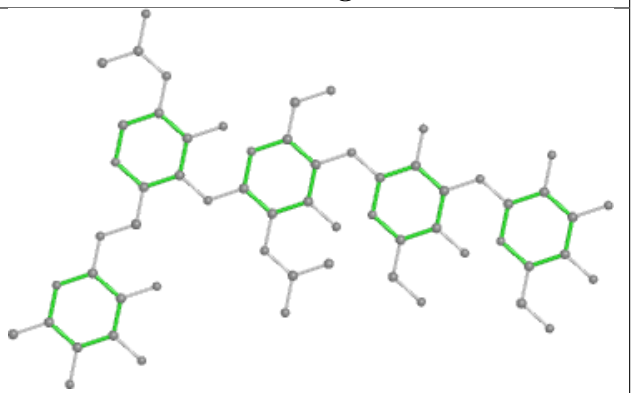
Bond lengths



Bond angles



Torsions



Rings

4.6 Ligand geometry (i)

Of 9 ligands modelled in this entry, 3 are monoatomic - leaving 6 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	$\#\|Z\| > 2$
11	JUD	A	308	-	72,72,72	0.95	3 (4%)	83,87,87	0.77	0
10	NAG	A	301	3	14,14,15	0.33	0	17,19,21	0.73	0
8	GOL	C	301	-	5,5,5	0.28	0	5,5,5	0.17	0
8	GOL	E	310	-	5,5,5	0.26	0	5,5,5	0.23	0
8	GOL	H	301	-	5,5,5	0.30	0	5,5,5	0.21	0
11	JUD	E	311	-	72,72,72	0.94	3 (4%)	83,87,87	0.78	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
11	JUD	A	308	-	-	16/69/89/89	0/2/2/2
10	NAG	A	301	3	-	0/6/23/26	0/1/1/1
8	GOL	C	301	-	-	0/4/4/4	-
8	GOL	E	310	-	-	0/4/4/4	-
8	GOL	H	301	-	-	0/4/4/4	-
11	JUD	E	311	-	-	16/69/89/89	0/2/2/2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	E	311	JUD	CAT-CAU	-4.22	1.40	1.50
11	A	308	JUD	CAT-CAU	-4.16	1.40	1.50
11	A	308	JUD	CBA-CAX	-3.93	1.41	1.49
11	E	311	JUD	CBA-CAX	-3.87	1.41	1.49
11	E	311	JUD	O1-C1	2.62	1.44	1.40
11	A	308	JUD	O1-C1	2.46	1.44	1.40

There are no bond angle outliers.

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	E	311	JUD	CBN-CBO-CBP-CBQ
11	A	308	JUD	O6-C2-C3-O2
11	E	311	JUD	O6-C2-C3-O2
11	A	308	JUD	CBN-CBO-CBP-CBQ
11	A	308	JUD	CCK-CCL-CCM-CCN
11	E	311	JUD	CBK-CBL-CBM-CBN
11	A	308	JUD	CBK-CBL-CBM-CBN
11	A	308	JUD	CCG-CCH-CCI-CCJ
11	E	311	JUD	CCG-CCH-CCI-CCJ
11	A	308	JUD	CBP-CBQ-CBR-CBS
11	E	311	JUD	CBW-CBX-CBY-CBZ
11	E	311	JUD	CCJ-CCK-CCL-CCM
11	E	311	JUD	CCK-CCL-CCM-CCN
11	E	311	JUD	CBP-CBQ-CBR-CBS
11	A	308	JUD	CCC-CCD-CCE-CCF
11	A	308	JUD	CCA-CCB-CCC-CCD
11	A	308	JUD	CAU-CAT-O4-C4
11	A	308	JUD	CBW-CBX-CBY-CBZ
11	A	308	JUD	CCJ-CCK-CCL-CCM
11	E	311	JUD	CCA-CCB-CCC-CCD
11	E	311	JUD	CCC-CCD-CCE-CCF
11	E	311	JUD	CCO-CCP-CCQ-CCR
11	A	308	JUD	CCH-CCI-CCJ-CCK
11	E	311	JUD	CCH-CCI-CCJ-CCK
11	A	308	JUD	CBE-CBU-CBV-CBW
11	E	311	JUD	CBE-CBU-CBV-CBW
11	A	308	JUD	CCL-CCM-CCN-CCO
11	E	311	JUD	CAU-CAT-O4-C4
11	A	308	JUD	CAP-CAN-NAO-CBE
11	E	311	JUD	CAP-CAN-NAO-CBE
11	E	311	JUD	CCL-CCM-CCN-CCO
11	A	308	JUD	CCM-CCN-CCO-CCP

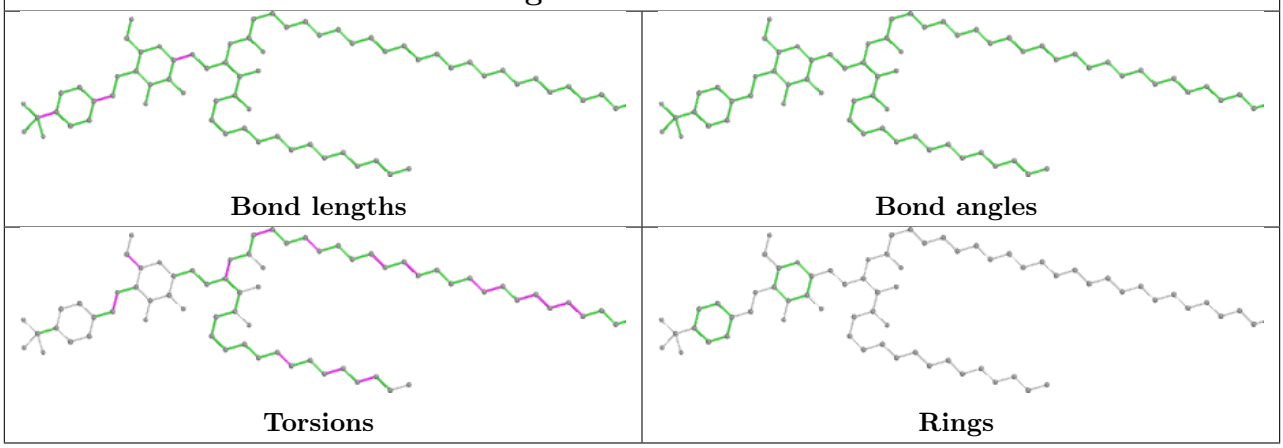
There are no ring outliers.

No monomer is involved in short contacts.

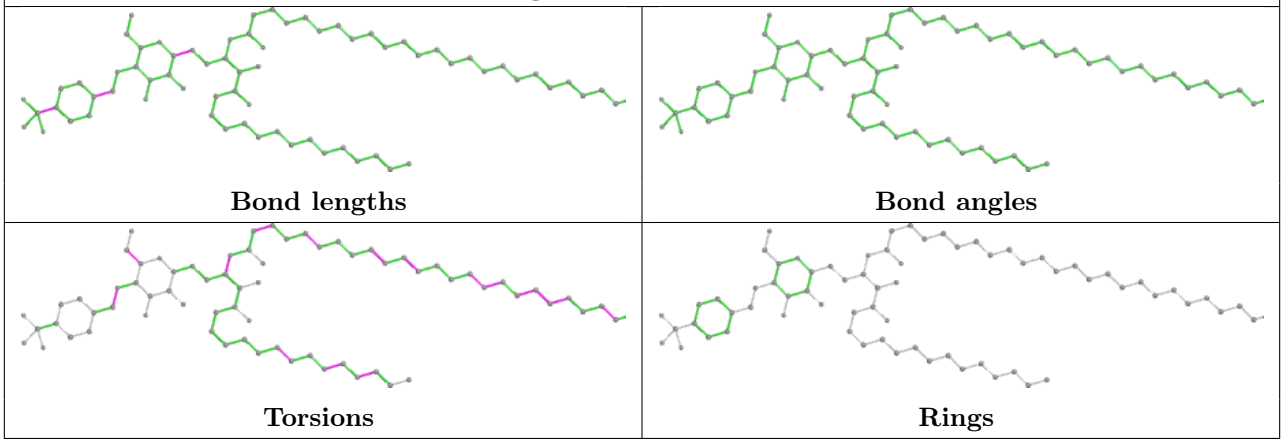
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

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 JUD A 308



Ligand JUD E 311



4.7 Other polymers (i)

There are no such residues in this entry.

4.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

5 Fit of model and data

5.1 Protein, DNA and RNA chains

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

5.3 Carbohydrates

EDS failed to run properly - this section is therefore empty.

5.4 Ligands

EDS failed to run properly - this section is therefore empty.

5.5 Other polymers

EDS failed to run properly - this section is therefore empty.