wwPDB EM Validation Summary Report

Nov 20, 2022 – 08:04 AM EST

PDB ID	:	7M8K
EMDB ID	:	EMD-23718
Title	:	Cryo-EM structure of Brazil (P.1) SARS-CoV-2 spike glycoprotein variant in the prefusion state (1 RBD up)
Authors	:	Casner, R.G.; Cerutti, G.; Shapiro, L.; Ho, D.D.
Deposited on	:	2021-03-29
Resolution	:	Not provided

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:

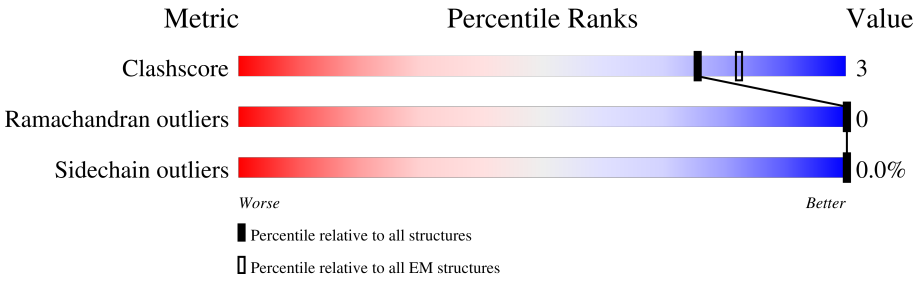
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al.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

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 unknown.

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	1257	78% · 18%
1	B	1257	74% 8% 18%
1	C	1257	75% 6% 18%
2	D	2	100%
2	E	2	50% 50%
2	F	2	100%
2	G	2	100%
2	H	2	100%
2	I	2	100%

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Mol	Chain	Length	Quality of chain
2	J	2	100%
2	K	2	50% 50%
2	L	2	100%
2	M	2	50% 50%
2	N	2	100%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 24826 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 Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1025	Total	C	N	O	S	1	0
			8020	5130	1328	1527	35		
1	B	1033	Total	C	N	O	S	0	0
			8072	5167	1335	1535	35		
1	C	1026	Total	C	N	O	S	0	0
			8020	5131	1329	1525	35		

There are 195 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	18	PHE	LEU	conflict	UNP P0DTC2
A	20	ASN	THR	conflict	UNP P0DTC2
A	26	SER	PRO	conflict	UNP P0DTC2
A	138	TYR	ASP	conflict	UNP P0DTC2
A	190	SER	ARG	conflict	UNP P0DTC2
A	417	THR	LYS	conflict	UNP P0DTC2
A	484	LYS	GLU	conflict	UNP P0DTC2
A	501	TYR	ASN	conflict	UNP P0DTC2
A	614	GLY	ASP	conflict	UNP P0DTC2
A	655	TYR	HIS	conflict	UNP P0DTC2
A	682	GLY	ARG	conflict	UNP P0DTC2
A	683	SER	ARG	conflict	UNP P0DTC2
A	685	SER	ARG	conflict	UNP P0DTC2
A	986	PRO	LYS	conflict	UNP P0DTC2
A	987	PRO	VAL	conflict	UNP P0DTC2
A	1027	ILE	THR	conflict	UNP P0DTC2
A	1209	GLY	-	expression tag	UNP P0DTC2
A	1210	SER	-	expression tag	UNP P0DTC2
A	1211	GLY	-	expression tag	UNP P0DTC2
A	1212	TYR	-	expression tag	UNP P0DTC2
A	1213	ILE	-	expression tag	UNP P0DTC2
A	1214	PRO	-	expression tag	UNP P0DTC2
A	1215	GLU	-	expression tag	UNP P0DTC2
A	1216	ALA	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1217	PRO	-	expression tag	UNP P0DTC2
A	1218	ARG	-	expression tag	UNP P0DTC2
A	1219	ASP	-	expression tag	UNP P0DTC2
A	1220	GLY	-	expression tag	UNP P0DTC2
A	1221	GLN	-	expression tag	UNP P0DTC2
A	1222	ALA	-	expression tag	UNP P0DTC2
A	1223	TYR	-	expression tag	UNP P0DTC2
A	1224	VAL	-	expression tag	UNP P0DTC2
A	1225	ARG	-	expression tag	UNP P0DTC2
A	1226	LYS	-	expression tag	UNP P0DTC2
A	1227	ASP	-	expression tag	UNP P0DTC2
A	1228	GLY	-	expression tag	UNP P0DTC2
A	1229	GLU	-	expression tag	UNP P0DTC2
A	1230	TRP	-	expression tag	UNP P0DTC2
A	1231	VAL	-	expression tag	UNP P0DTC2
A	1232	LEU	-	expression tag	UNP P0DTC2
A	1233	LEU	-	expression tag	UNP P0DTC2
A	1234	SER	-	expression tag	UNP P0DTC2
A	1235	THR	-	expression tag	UNP P0DTC2
A	1236	PHE	-	expression tag	UNP P0DTC2
A	1237	LEU	-	expression tag	UNP P0DTC2
A	1238	GLY	-	expression tag	UNP P0DTC2
A	1239	ARG	-	expression tag	UNP P0DTC2
A	1240	SER	-	expression tag	UNP P0DTC2
A	1241	LEU	-	expression tag	UNP P0DTC2
A	1242	GLU	-	expression tag	UNP P0DTC2
A	1243	VAL	-	expression tag	UNP P0DTC2
A	1244	LEU	-	expression tag	UNP P0DTC2
A	1245	PHE	-	expression tag	UNP P0DTC2
A	1246	GLN	-	expression tag	UNP P0DTC2
A	1247	GLY	-	expression tag	UNP P0DTC2
A	1248	PRO	-	expression tag	UNP P0DTC2
A	1249	GLY	-	expression tag	UNP P0DTC2
A	1250	HIS	-	expression tag	UNP P0DTC2
A	1251	HIS	-	expression tag	UNP P0DTC2
A	1252	HIS	-	expression tag	UNP P0DTC2
A	1253	HIS	-	expression tag	UNP P0DTC2
A	1254	HIS	-	expression tag	UNP P0DTC2
A	1255	HIS	-	expression tag	UNP P0DTC2
A	1256	HIS	-	expression tag	UNP P0DTC2
A	1257	HIS	-	expression tag	UNP P0DTC2
B	18	PHE	LEU	conflict	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	20	ASN	THR	conflict	UNP P0DTC2
B	26	SER	PRO	conflict	UNP P0DTC2
B	138	TYR	ASP	conflict	UNP P0DTC2
B	190	SER	ARG	conflict	UNP P0DTC2
B	417	THR	LYS	conflict	UNP P0DTC2
B	484	LYS	GLU	conflict	UNP P0DTC2
B	501	TYR	ASN	conflict	UNP P0DTC2
B	614	GLY	ASP	conflict	UNP P0DTC2
B	655	TYR	HIS	conflict	UNP P0DTC2
B	682	GLY	ARG	conflict	UNP P0DTC2
B	683	SER	ARG	conflict	UNP P0DTC2
B	685	SER	ARG	conflict	UNP P0DTC2
B	986	PRO	LYS	conflict	UNP P0DTC2
B	987	PRO	VAL	conflict	UNP P0DTC2
B	1027	ILE	THR	conflict	UNP P0DTC2
B	1209	GLY	-	expression tag	UNP P0DTC2
B	1210	SER	-	expression tag	UNP P0DTC2
B	1211	GLY	-	expression tag	UNP P0DTC2
B	1212	TYR	-	expression tag	UNP P0DTC2
B	1213	ILE	-	expression tag	UNP P0DTC2
B	1214	PRO	-	expression tag	UNP P0DTC2
B	1215	GLU	-	expression tag	UNP P0DTC2
B	1216	ALA	-	expression tag	UNP P0DTC2
B	1217	PRO	-	expression tag	UNP P0DTC2
B	1218	ARG	-	expression tag	UNP P0DTC2
B	1219	ASP	-	expression tag	UNP P0DTC2
B	1220	GLY	-	expression tag	UNP P0DTC2
B	1221	GLN	-	expression tag	UNP P0DTC2
B	1222	ALA	-	expression tag	UNP P0DTC2
B	1223	TYR	-	expression tag	UNP P0DTC2
B	1224	VAL	-	expression tag	UNP P0DTC2
B	1225	ARG	-	expression tag	UNP P0DTC2
B	1226	LYS	-	expression tag	UNP P0DTC2
B	1227	ASP	-	expression tag	UNP P0DTC2
B	1228	GLY	-	expression tag	UNP P0DTC2
B	1229	GLU	-	expression tag	UNP P0DTC2
B	1230	TRP	-	expression tag	UNP P0DTC2
B	1231	VAL	-	expression tag	UNP P0DTC2
B	1232	LEU	-	expression tag	UNP P0DTC2
B	1233	LEU	-	expression tag	UNP P0DTC2
B	1234	SER	-	expression tag	UNP P0DTC2
B	1235	THR	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1236	PHE	-	expression tag	UNP P0DTC2
B	1237	LEU	-	expression tag	UNP P0DTC2
B	1238	GLY	-	expression tag	UNP P0DTC2
B	1239	ARG	-	expression tag	UNP P0DTC2
B	1240	SER	-	expression tag	UNP P0DTC2
B	1241	LEU	-	expression tag	UNP P0DTC2
B	1242	GLU	-	expression tag	UNP P0DTC2
B	1243	VAL	-	expression tag	UNP P0DTC2
B	1244	LEU	-	expression tag	UNP P0DTC2
B	1245	PHE	-	expression tag	UNP P0DTC2
B	1246	GLN	-	expression tag	UNP P0DTC2
B	1247	GLY	-	expression tag	UNP P0DTC2
B	1248	PRO	-	expression tag	UNP P0DTC2
B	1249	GLY	-	expression tag	UNP P0DTC2
B	1250	HIS	-	expression tag	UNP P0DTC2
B	1251	HIS	-	expression tag	UNP P0DTC2
B	1252	HIS	-	expression tag	UNP P0DTC2
B	1253	HIS	-	expression tag	UNP P0DTC2
B	1254	HIS	-	expression tag	UNP P0DTC2
B	1255	HIS	-	expression tag	UNP P0DTC2
B	1256	HIS	-	expression tag	UNP P0DTC2
B	1257	HIS	-	expression tag	UNP P0DTC2
C	18	PHE	LEU	conflict	UNP P0DTC2
C	20	ASN	THR	conflict	UNP P0DTC2
C	26	SER	PRO	conflict	UNP P0DTC2
C	138	TYR	ASP	conflict	UNP P0DTC2
C	190	SER	ARG	conflict	UNP P0DTC2
C	417	THR	LYS	conflict	UNP P0DTC2
C	484	LYS	GLU	conflict	UNP P0DTC2
C	501	TYR	ASN	conflict	UNP P0DTC2
C	614	GLY	ASP	conflict	UNP P0DTC2
C	655	TYR	HIS	conflict	UNP P0DTC2
C	682	GLY	ARG	conflict	UNP P0DTC2
C	683	SER	ARG	conflict	UNP P0DTC2
C	685	SER	ARG	conflict	UNP P0DTC2
C	986	PRO	LYS	conflict	UNP P0DTC2
C	987	PRO	VAL	conflict	UNP P0DTC2
C	1027	ILE	THR	conflict	UNP P0DTC2
C	1209	GLY	-	expression tag	UNP P0DTC2
C	1210	SER	-	expression tag	UNP P0DTC2
C	1211	GLY	-	expression tag	UNP P0DTC2
C	1212	TYR	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1213	ILE	-	expression tag	UNP P0DTC2
C	1214	PRO	-	expression tag	UNP P0DTC2
C	1215	GLU	-	expression tag	UNP P0DTC2
C	1216	ALA	-	expression tag	UNP P0DTC2
C	1217	PRO	-	expression tag	UNP P0DTC2
C	1218	ARG	-	expression tag	UNP P0DTC2
C	1219	ASP	-	expression tag	UNP P0DTC2
C	1220	GLY	-	expression tag	UNP P0DTC2
C	1221	GLN	-	expression tag	UNP P0DTC2
C	1222	ALA	-	expression tag	UNP P0DTC2
C	1223	TYR	-	expression tag	UNP P0DTC2
C	1224	VAL	-	expression tag	UNP P0DTC2
C	1225	ARG	-	expression tag	UNP P0DTC2
C	1226	LYS	-	expression tag	UNP P0DTC2
C	1227	ASP	-	expression tag	UNP P0DTC2
C	1228	GLY	-	expression tag	UNP P0DTC2
C	1229	GLU	-	expression tag	UNP P0DTC2
C	1230	TRP	-	expression tag	UNP P0DTC2
C	1231	VAL	-	expression tag	UNP P0DTC2
C	1232	LEU	-	expression tag	UNP P0DTC2
C	1233	LEU	-	expression tag	UNP P0DTC2
C	1234	SER	-	expression tag	UNP P0DTC2
C	1235	THR	-	expression tag	UNP P0DTC2
C	1236	PHE	-	expression tag	UNP P0DTC2
C	1237	LEU	-	expression tag	UNP P0DTC2
C	1238	GLY	-	expression tag	UNP P0DTC2
C	1239	ARG	-	expression tag	UNP P0DTC2
C	1240	SER	-	expression tag	UNP P0DTC2
C	1241	LEU	-	expression tag	UNP P0DTC2
C	1242	GLU	-	expression tag	UNP P0DTC2
C	1243	VAL	-	expression tag	UNP P0DTC2
C	1244	LEU	-	expression tag	UNP P0DTC2
C	1245	PHE	-	expression tag	UNP P0DTC2
C	1246	GLN	-	expression tag	UNP P0DTC2
C	1247	GLY	-	expression tag	UNP P0DTC2
C	1248	PRO	-	expression tag	UNP P0DTC2
C	1249	GLY	-	expression tag	UNP P0DTC2
C	1250	HIS	-	expression tag	UNP P0DTC2
C	1251	HIS	-	expression tag	UNP P0DTC2
C	1252	HIS	-	expression tag	UNP P0DTC2
C	1253	HIS	-	expression tag	UNP P0DTC2
C	1254	HIS	-	expression tag	UNP P0DTC2

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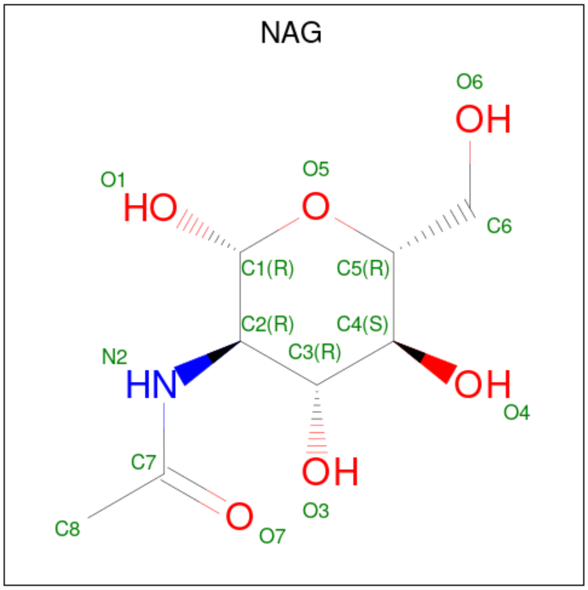
Chain	Residue	Modelled	Actual	Comment	Reference
C	1255	HIS	-	expression tag	UNP P0DTC2
C	1256	HIS	-	expression tag	UNP P0DTC2
C	1257	HIS	-	expression tag	UNP P0DTC2

- Molecule 2 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
2	D	2	Total	C	N	O	0	0
			28	16	2	10		
2	E	2	Total	C	N	O	0	0
			28	16	2	10		
2	F	2	Total	C	N	O	0	0
			28	16	2	10		
2	G	2	Total	C	N	O	0	0
			28	16	2	10		
2	H	2	Total	C	N	O	0	0
			28	16	2	10		
2	I	2	Total	C	N	O	0	0
			28	16	2	10		
2	J	2	Total	C	N	O	0	0
			28	16	2	10		
2	K	2	Total	C	N	O	0	0
			28	16	2	10		
2	L	2	Total	C	N	O	0	0
			28	16	2	10		
2	M	2	Total	C	N	O	0	0
			28	16	2	10		
2	N	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total 140	C 80	N 10	O 50	0
3	A	1	Total 140	C 80	N 10	O 50	0
3	A	1	Total 140	C 80	N 10	O 50	0
3	A	1	Total 140	C 80	N 10	O 50	0
3	A	1	Total 140	C 80	N 10	O 50	0
3	A	1	Total 140	C 80	N 10	O 50	0
3	A	1	Total 140	C 80	N 10	O 50	0
3	A	1	Total 140	C 80	N 10	O 50	0
3	A	1	Total 140	C 80	N 10	O 50	0
3	A	1	Total 140	C 80	N 10	O 50	0
3	B	1	Total 140	C 80	N 10	O 50	0
3	B	1	Total 140	C 80	N 10	O 50	0
3	B	1	Total 140	C 80	N 10	O 50	0
3	B	1	Total 140	C 80	N 10	O 50	0

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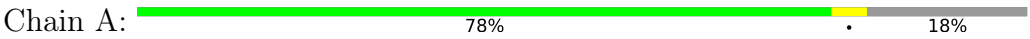
Mol	Chain	Residues	Atoms				AltConf
3	B	1	Total 140	C 80	N 10	O 50	0
3	B	1	Total 140	C 80	N 10	O 50	0
3	B	1	Total 140	C 80	N 10	O 50	0
3	B	1	Total 140	C 80	N 10	O 50	0
3	B	1	Total 140	C 80	N 10	O 50	0
3	B	1	Total 140	C 80	N 10	O 50	0
3	C	1	Total 126	C 72	N 9	O 45	0
3	C	1	Total 126	C 72	N 9	O 45	0
3	C	1	Total 126	C 72	N 9	O 45	0
3	C	1	Total 126	C 72	N 9	O 45	0
3	C	1	Total 126	C 72	N 9	O 45	0
3	C	1	Total 126	C 72	N 9	O 45	0
3	C	1	Total 126	C 72	N 9	O 45	0
3	C	1	Total 126	C 72	N 9	O 45	0
3	C	1	Total 126	C 72	N 9	O 45	0

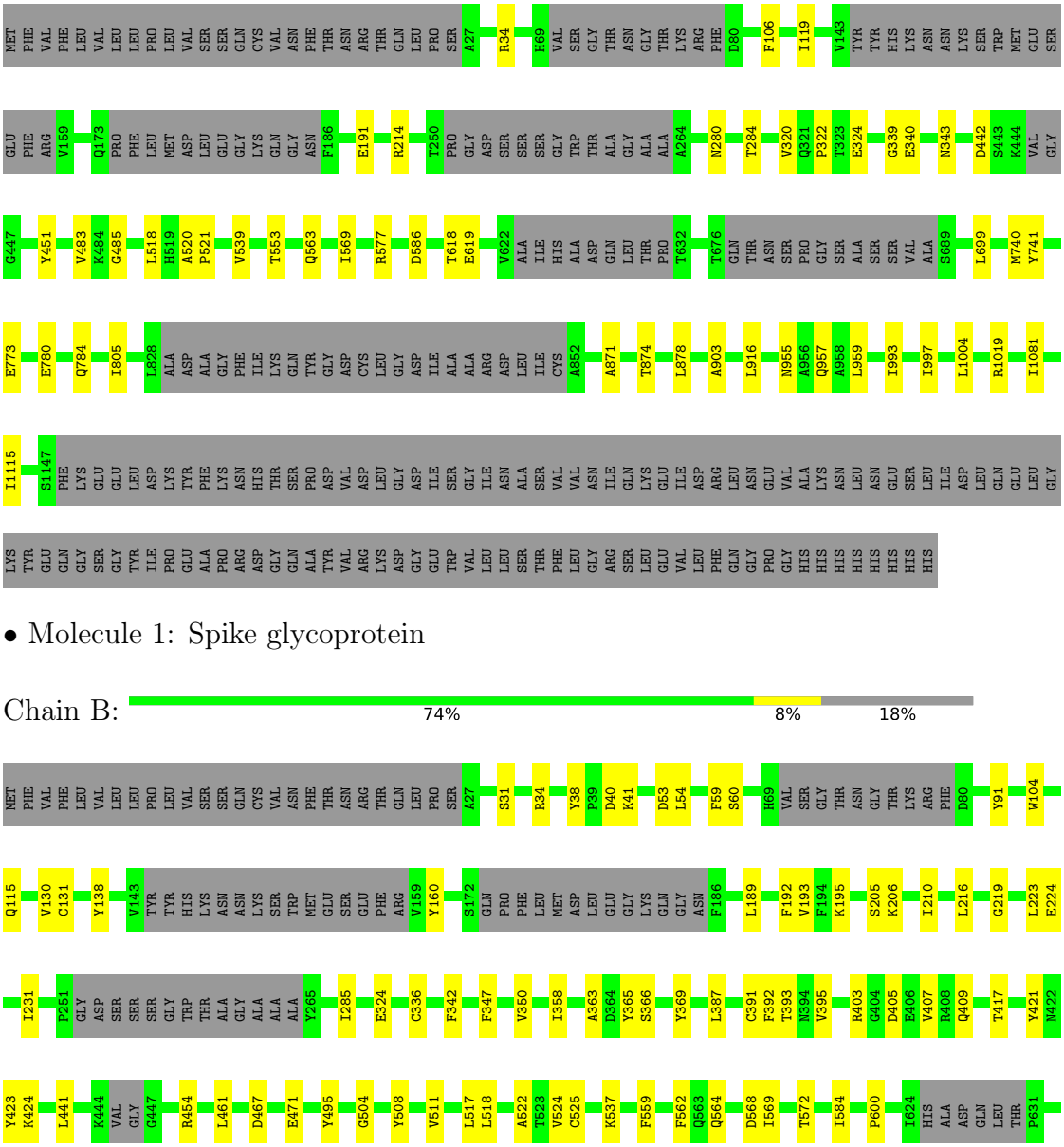
3 Residue-property plots (i)

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: Spike glycoprotein

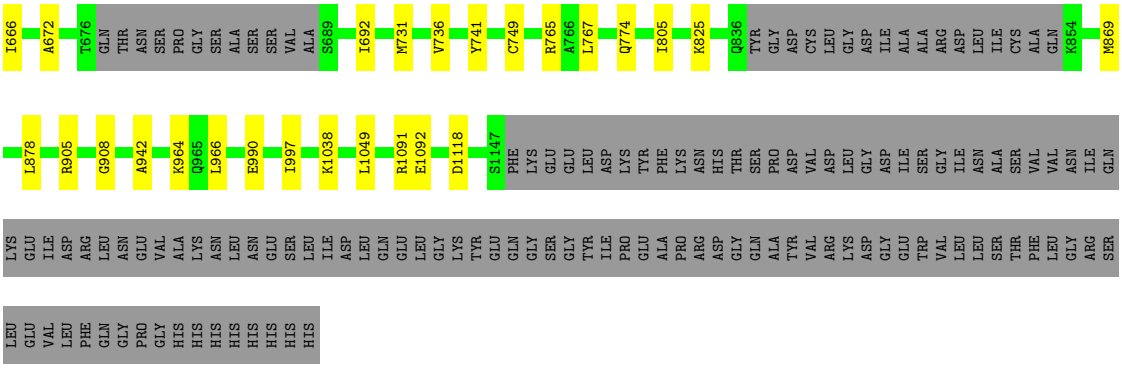
Chain A:





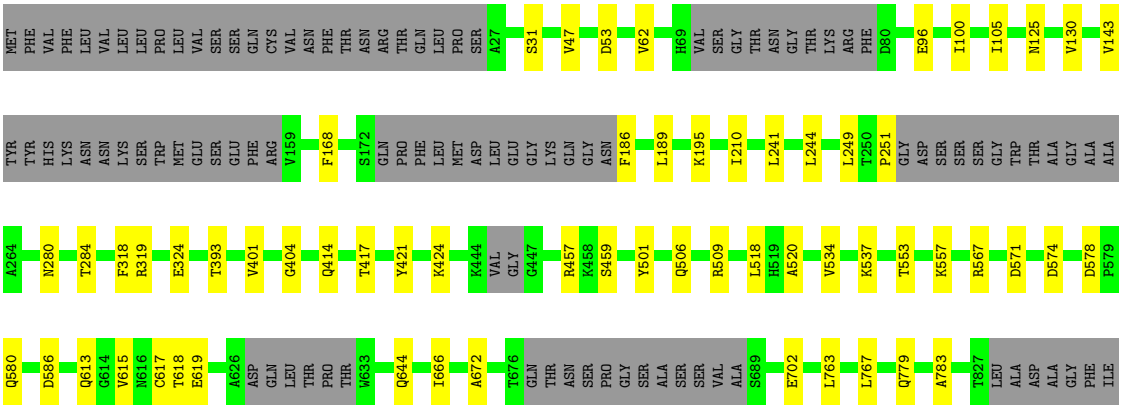
- Molecule 1: Spike glycoprotein

Chain B:



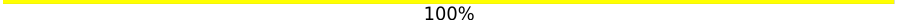
• Molecule 1: Spike glycoprotein

Chain C:



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

Chain D:



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

Chain E:

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

Chain F:

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

Chain G:

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

Chain H:

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

Chain I:

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

Chain J:

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

Chain K:

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

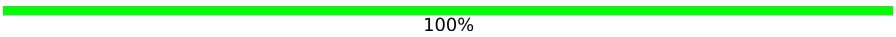
Chain L:

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

Chain M:

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

Chain N:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	120543	Depositor
Resolution determination method	Not provided	
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	42	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
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: NAG

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	0.44	0/8206	0.74	1/11169 (0.0%)
1	B	0.45	0/8258	0.75	0/11240
1	C	0.44	0/8205	0.73	0/11169
All	All	0.44	0/24669	0.74	1/33578 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	214	ARG	NE-CZ-NH1	5.96	123.28	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8020	0	7822	34	0
1	B	8072	0	7879	59	0
1	C	8020	0	7820	54	0
2	D	28	0	25	0	0
2	E	28	0	25	2	0
2	F	28	0	25	2	0
2	G	28	0	25	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	28	0	25	2	0
2	I	28	0	25	1	0
2	J	28	0	25	1	0
2	K	28	0	25	3	0
2	L	28	0	25	3	0
2	M	28	0	25	2	0
2	N	28	0	25	0	0
3	A	140	0	130	0	0
3	B	140	0	130	0	0
3	C	126	0	117	0	0
All	All	24826	0	24173	153	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 3.

The worst 5 of 153 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:205:SER:O	1:B:223:LEU:HD22	1.75	0.86
1:A:740:MET:CE	1:C:319:ARG:HE	1.92	0.81
1:A:740:MET:HE2	1:C:319:ARG:HE	1.44	0.81
1:A:740:MET:HB2	1:C:319:ARG:HH21	1.47	0.79
1:C:1101:HIS:ND1	2:M:1:NAG:H5	2.04	0.72

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	1008/1257 (80%)	980 (97%)	28 (3%)	0	100	100
1	B	1015/1257 (81%)	971 (96%)	44 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	1008/1257 (80%)	982 (97%)	26 (3%)	0	100	100
All	All	3031/3771 (80%)	2933 (97%)	98 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	898/1092 (82%)	898 (100%)	0	100	100
1	B	903/1092 (83%)	902 (100%)	1 (0%)	93	93
1	C	897/1092 (82%)	897 (100%)	0	100	100
All	All	2698/3276 (82%)	2697 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	216	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	121	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)

22 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	$\#\|Z\| > 2$
2	NAG	D	1	1,2	14,14,15	0.33	0	17,19,21	0.99	1 (5%)
2	NAG	D	2	2	14,14,15	0.37	0	17,19,21	1.12	1 (5%)
2	NAG	E	1	1,2	14,14,15	0.35	0	17,19,21	0.86	0
2	NAG	E	2	2	14,14,15	0.40	0	17,19,21	1.01	2 (11%)
2	NAG	F	1	1,2	14,14,15	0.30	0	17,19,21	1.04	2 (11%)
2	NAG	F	2	2	14,14,15	0.37	0	17,19,21	1.07	1 (5%)
2	NAG	G	1	1,2	14,14,15	0.34	0	17,19,21	1.26	2 (11%)
2	NAG	G	2	2	14,14,15	0.35	0	17,19,21	1.19	1 (5%)
2	NAG	H	1	1,2	14,14,15	0.32	0	17,19,21	1.14	2 (11%)
2	NAG	H	2	2	14,14,15	0.43	0	17,19,21	1.20	2 (11%)
2	NAG	I	1	1,2	14,14,15	0.36	0	17,19,21	1.14	3 (17%)
2	NAG	I	2	2	14,14,15	0.43	0	17,19,21	1.32	1 (5%)
2	NAG	J	1	1,2	14,14,15	0.33	0	17,19,21	1.12	2 (11%)
2	NAG	J	2	2	14,14,15	0.37	0	17,19,21	1.12	1 (5%)
2	NAG	K	1	1,2	14,14,15	0.35	0	17,19,21	1.10	2 (11%)
2	NAG	K	2	2	14,14,15	0.41	0	17,19,21	0.78	0
2	NAG	L	1	1,2	14,14,15	0.25	0	17,19,21	1.25	3 (17%)
2	NAG	L	2	2	14,14,15	0.45	0	17,19,21	0.85	1 (5%)
2	NAG	M	1	1,2	14,14,15	0.40	0	17,19,21	0.99	0
2	NAG	M	2	2	14,14,15	0.24	0	17,19,21	1.28	2 (11%)
2	NAG	N	1	1,2	14,14,15	0.28	0	17,19,21	0.63	0
2	NAG	N	2	2	14,14,15	0.31	0	17,19,21	0.77	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
2	NAG	D	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	D	2	2	-	0/6/23/26	0/1/1/1
2	NAG	E	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	E	2	2	-	0/6/23/26	0/1/1/1
2	NAG	F	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	F	2	2	-	0/6/23/26	0/1/1/1
2	NAG	G	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	G	2	2	-	1/6/23/26	0/1/1/1
2	NAG	H	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	H	2	2	-	0/6/23/26	0/1/1/1
2	NAG	I	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	I	2	2	-	0/6/23/26	0/1/1/1
2	NAG	J	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	J	2	2	-	0/6/23/26	0/1/1/1
2	NAG	K	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	K	2	2	-	2/6/23/26	0/1/1/1
2	NAG	L	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	L	2	2	-	4/6/23/26	0/1/1/1
2	NAG	M	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	M	2	2	-	4/6/23/26	0/1/1/1
2	NAG	N	1	1,2	-	3/6/23/26	0/1/1/1
2	NAG	N	2	2	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 29 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	I	2	NAG	C1-O5-C5	4.37	118.11	112.19
2	G	2	NAG	C1-O5-C5	4.11	117.75	112.19
2	F	2	NAG	C1-O5-C5	3.65	117.13	112.19
2	D	2	NAG	C1-O5-C5	3.56	117.02	112.19
2	J	2	NAG	C1-O5-C5	3.49	116.92	112.19

There are no chirality outliers.

5 of 36 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	1	NAG	C8-C7-N2-C2
2	F	1	NAG	O7-C7-N2-C2
2	K	1	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
2	K	1	NAG	O7-C7-N2-C2
2	L	1	NAG	C8-C7-N2-C2

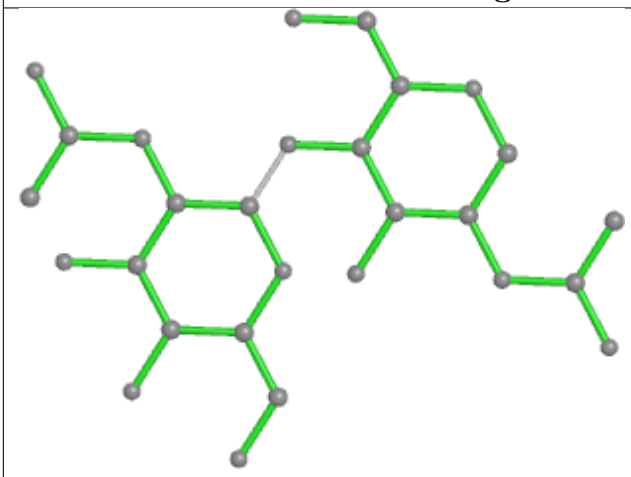
There are no ring outliers.

18 monomers are involved in 18 short contacts:

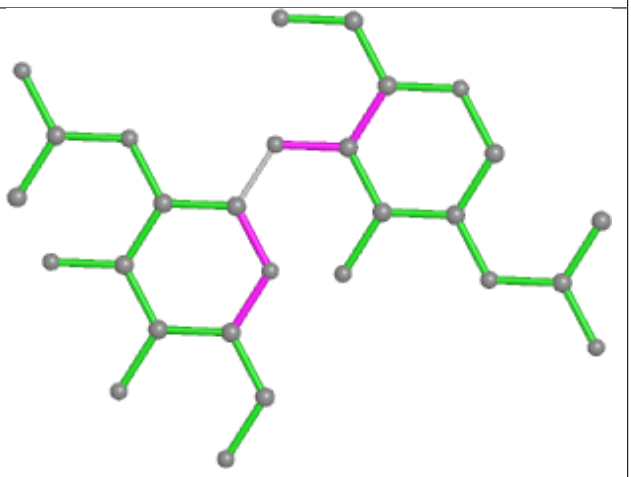
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	I	1	NAG	1	0
2	H	2	NAG	2	0
2	F	2	NAG	1	0
2	L	2	NAG	2	0
2	F	1	NAG	2	0
2	M	1	NAG	2	0
2	K	1	NAG	3	0
2	K	2	NAG	2	0
2	E	1	NAG	2	0
2	E	2	NAG	2	0
2	H	1	NAG	2	0
2	G	1	NAG	2	0
2	G	2	NAG	2	0
2	M	2	NAG	1	0
2	J	1	NAG	1	0
2	I	2	NAG	1	0
2	J	2	NAG	1	0
2	L	1	NAG	3	0

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

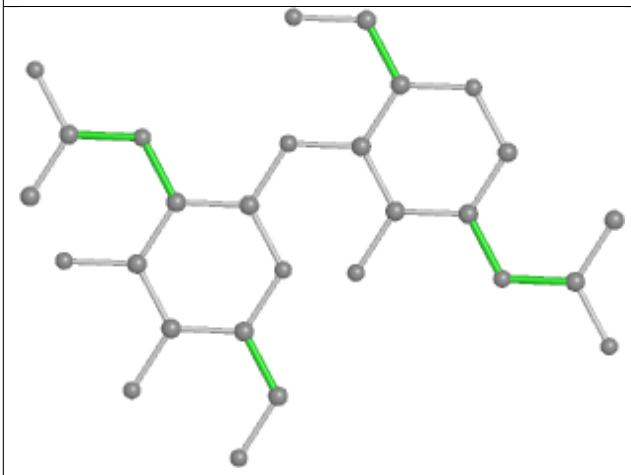
Oligosaccharide Chain D



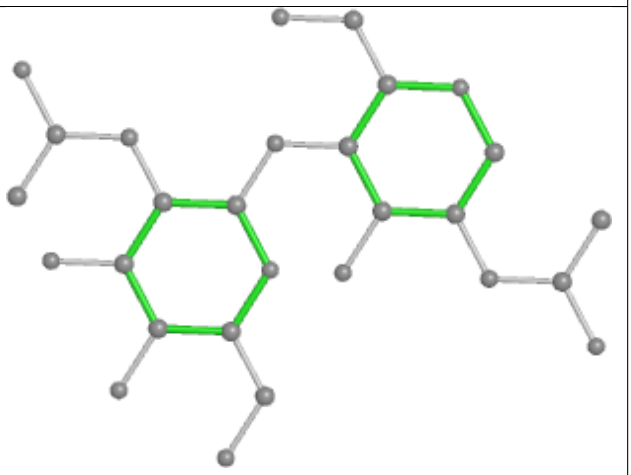
Bond lengths



Bond angles

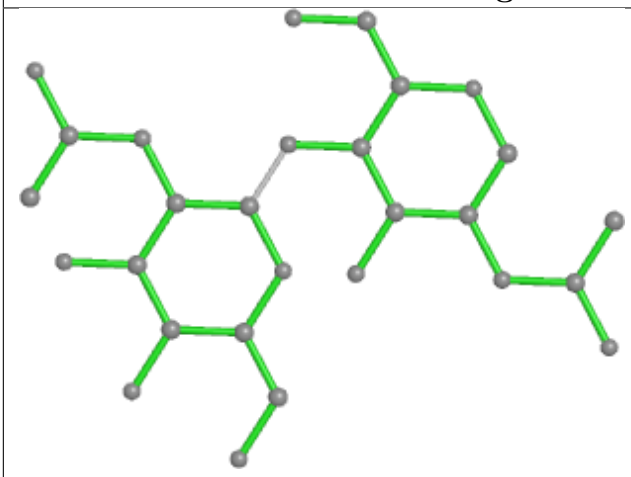


Torsions

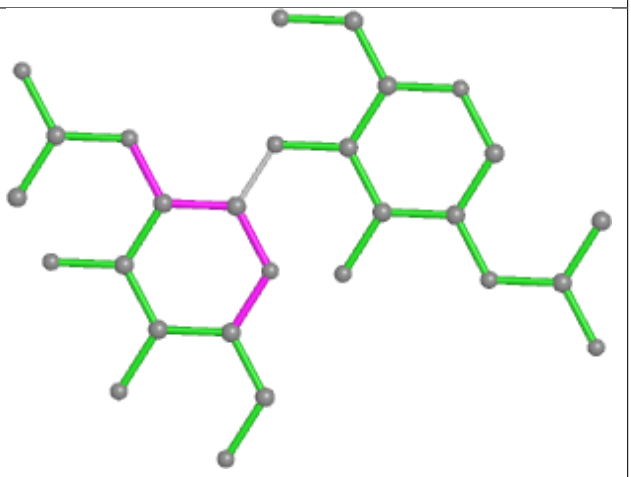


Rings

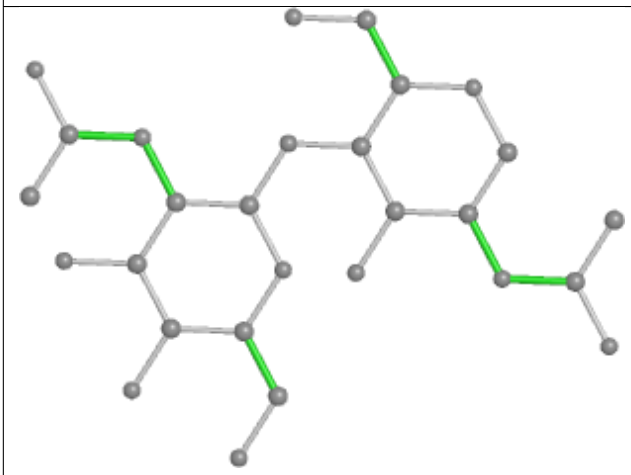
Oligosaccharide Chain E



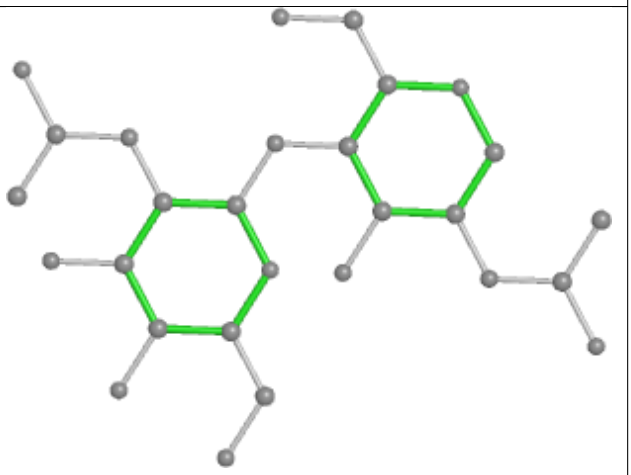
Bond lengths



Bond angles

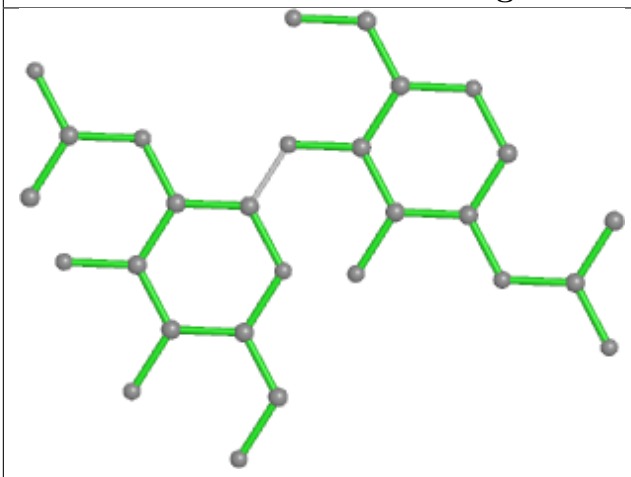


Torsions

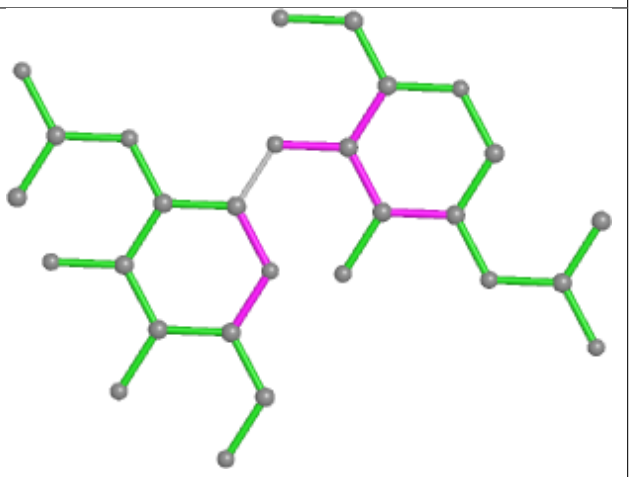


Rings

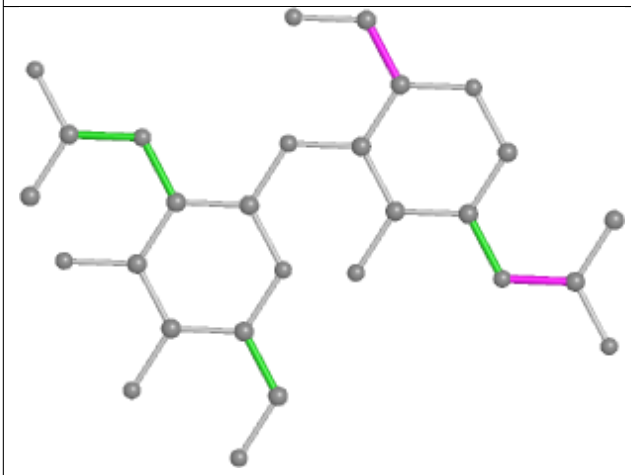
Oligosaccharide Chain F



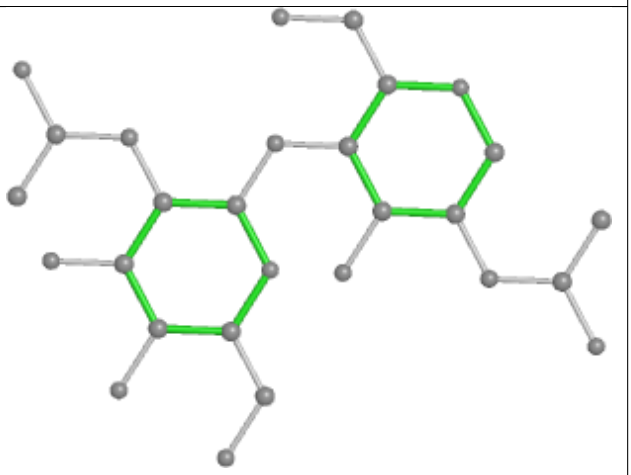
Bond lengths



Bond angles

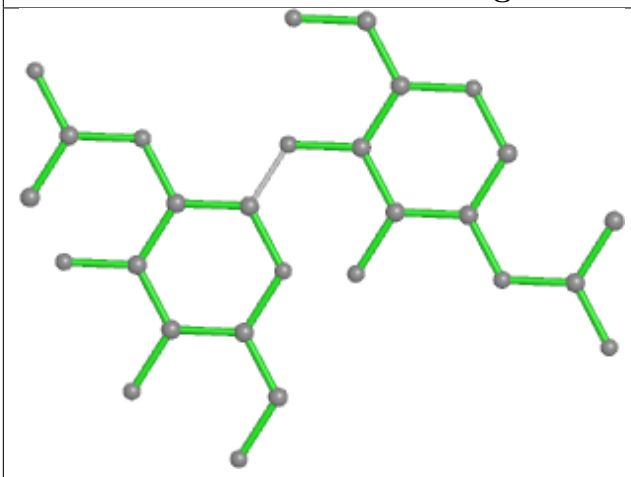


Torsions

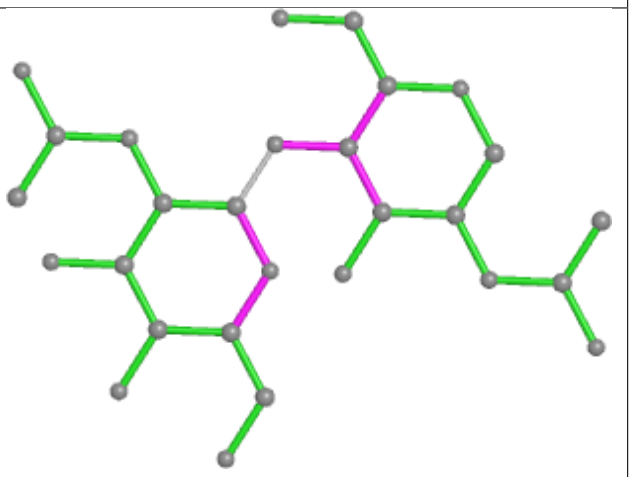


Rings

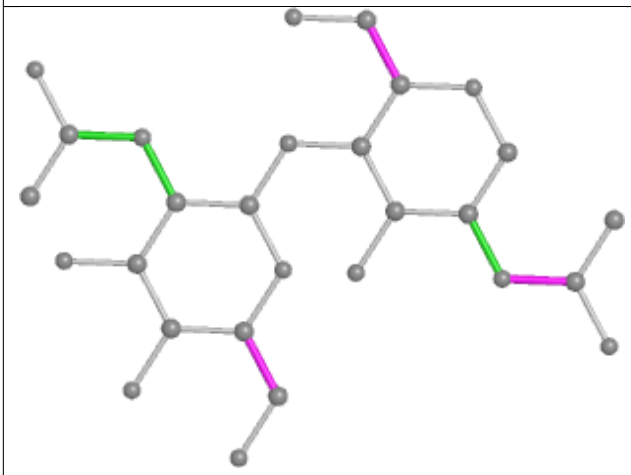
Oligosaccharide Chain G



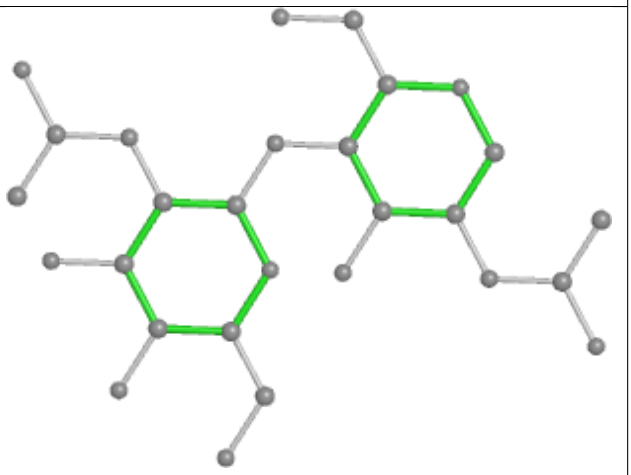
Bond lengths



Bond angles

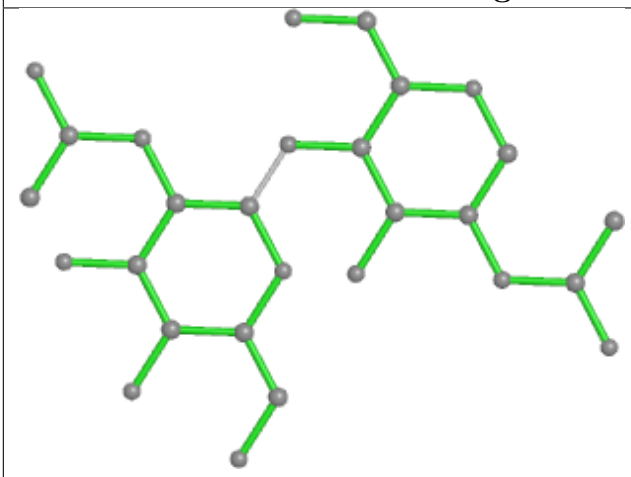


Torsions

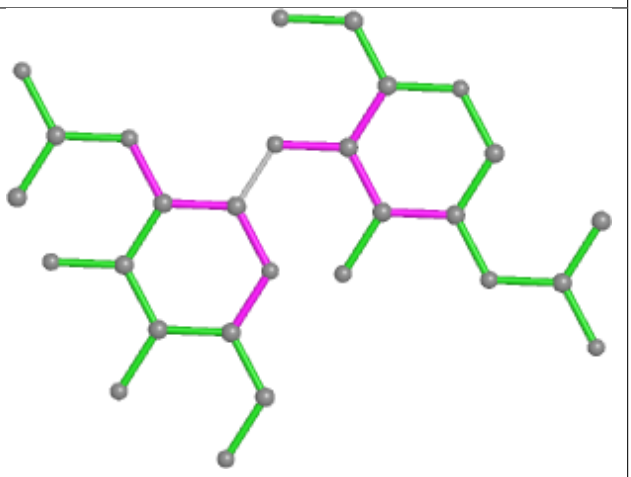


Rings

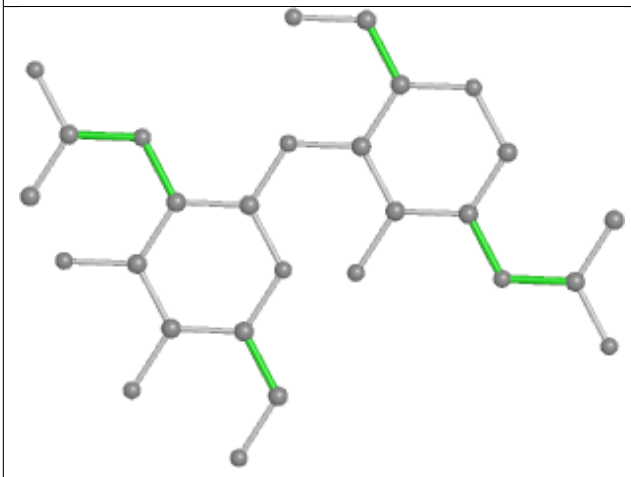
Oligosaccharide Chain H



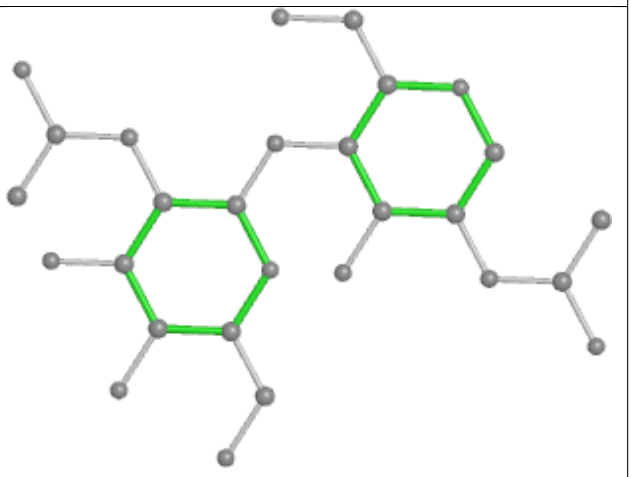
Bond lengths



Bond angles

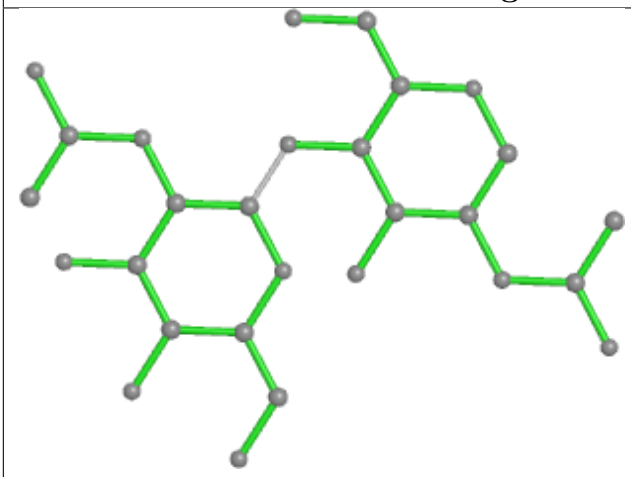


Torsions

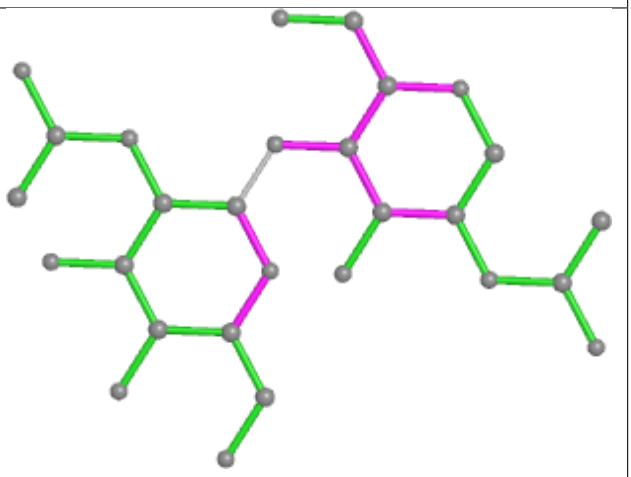


Rings

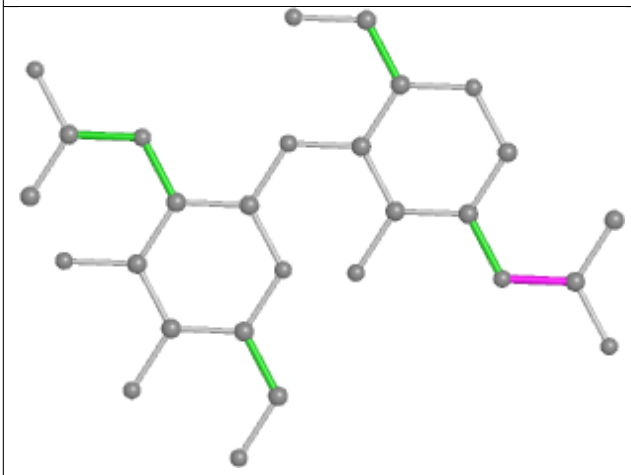
Oligosaccharide Chain I



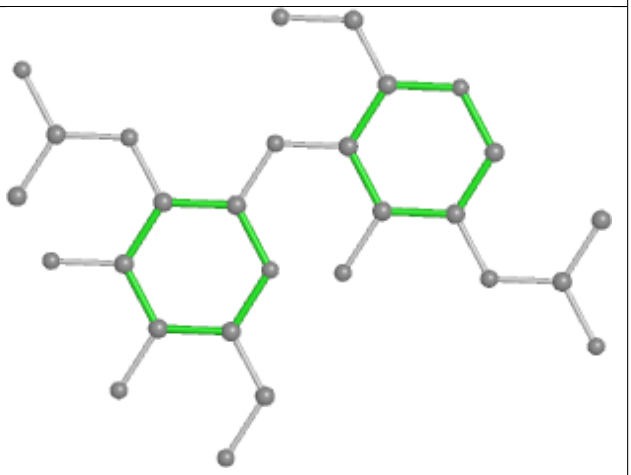
Bond lengths



Bond angles

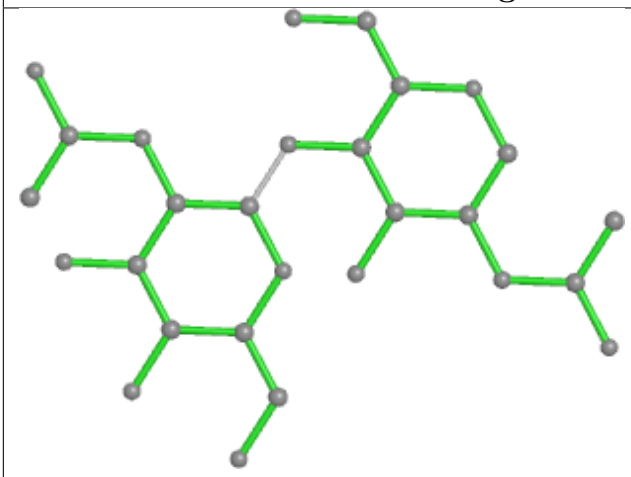


Torsions

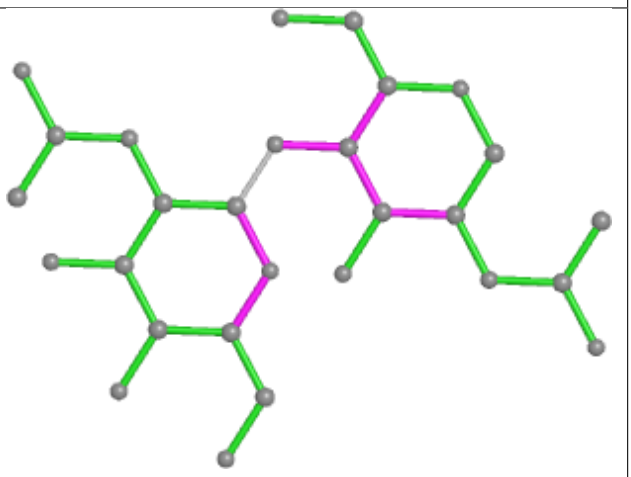


Rings

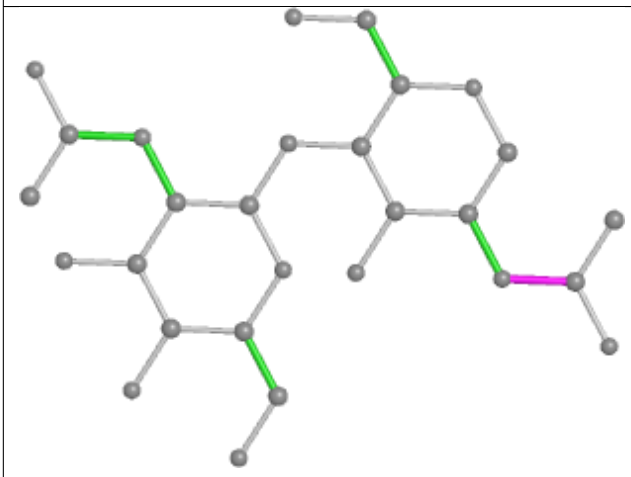
Oligosaccharide Chain J



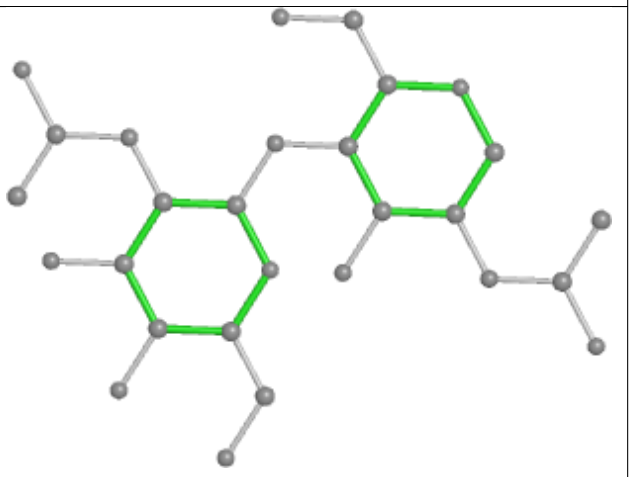
Bond lengths



Bond angles

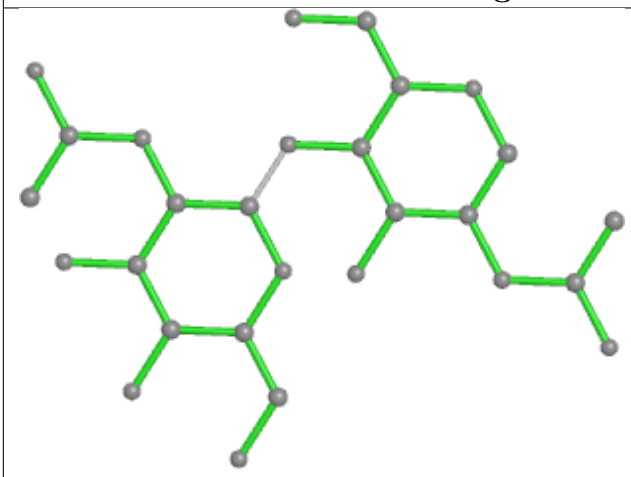


Torsions

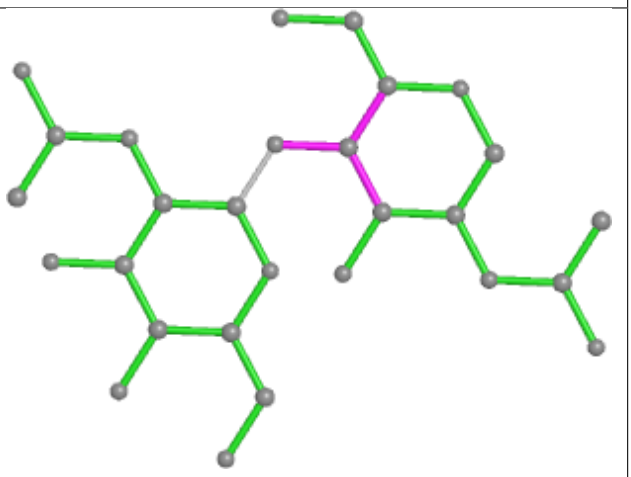


Rings

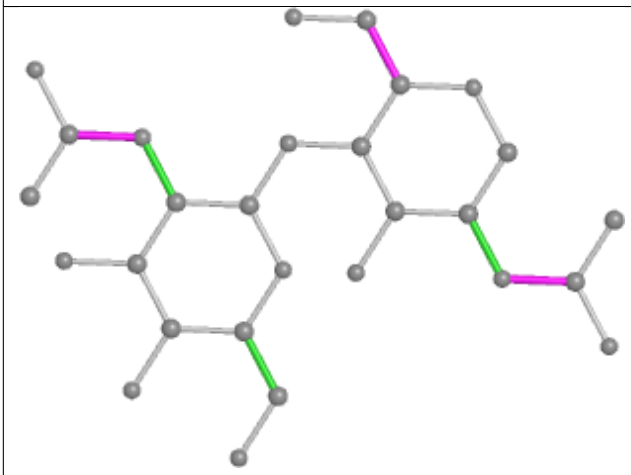
Oligosaccharide Chain K



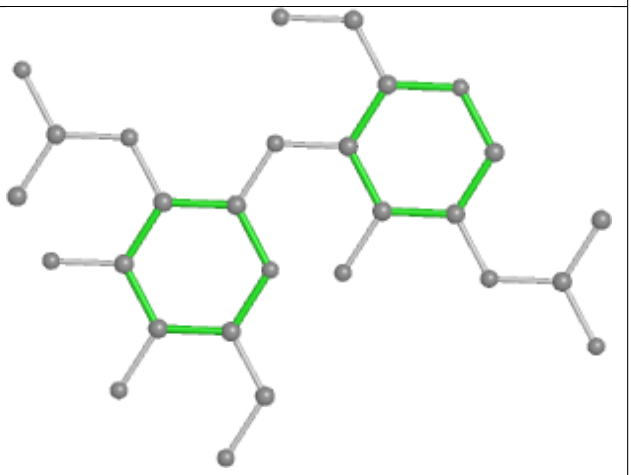
Bond lengths



Bond angles

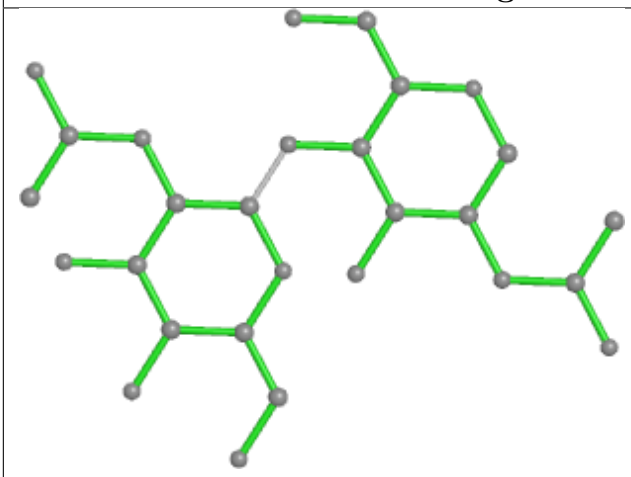


Torsions

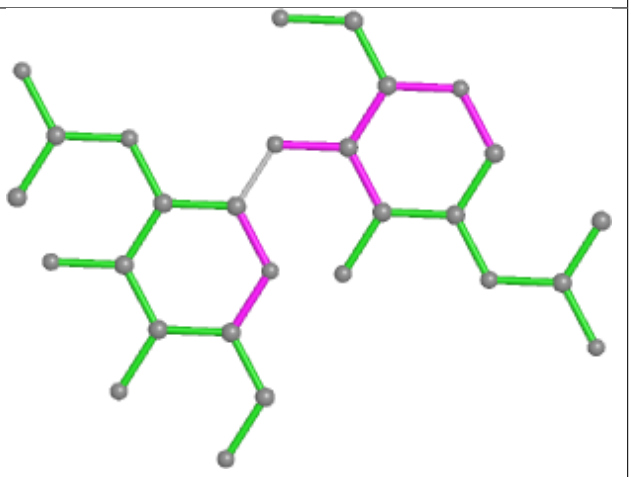


Rings

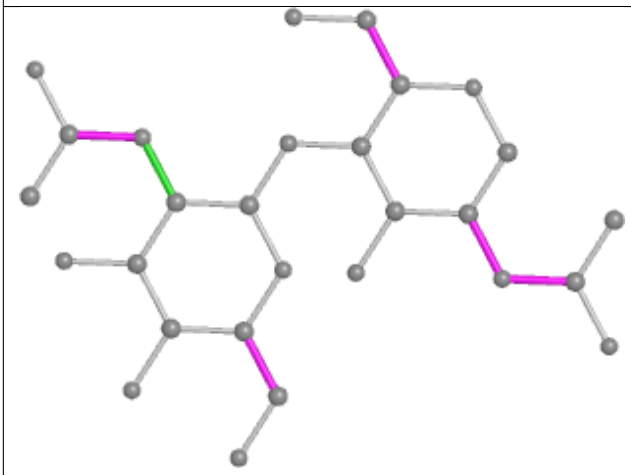
Oligosaccharide Chain L



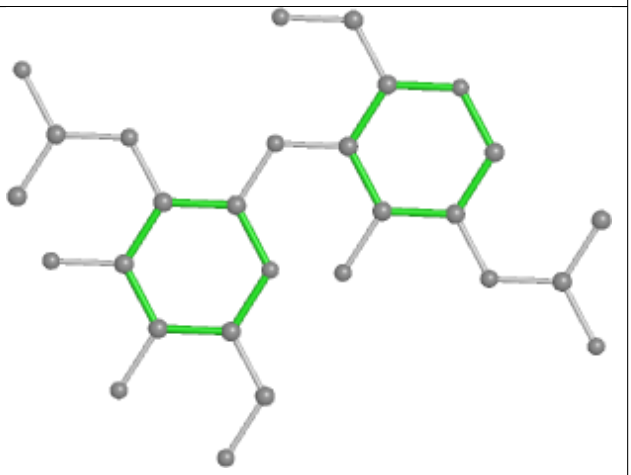
Bond lengths



Bond angles

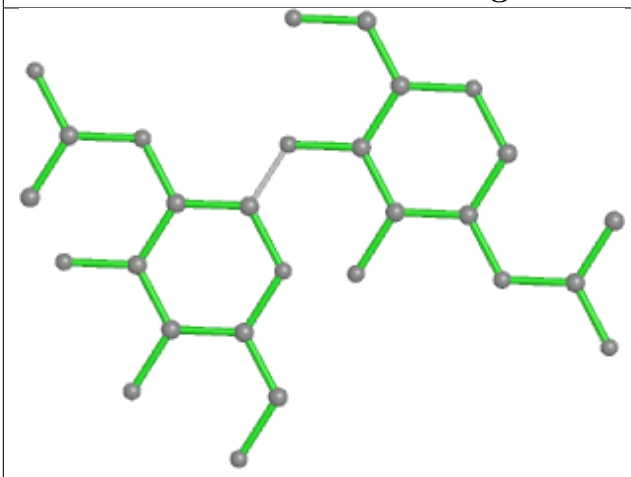


Torsions

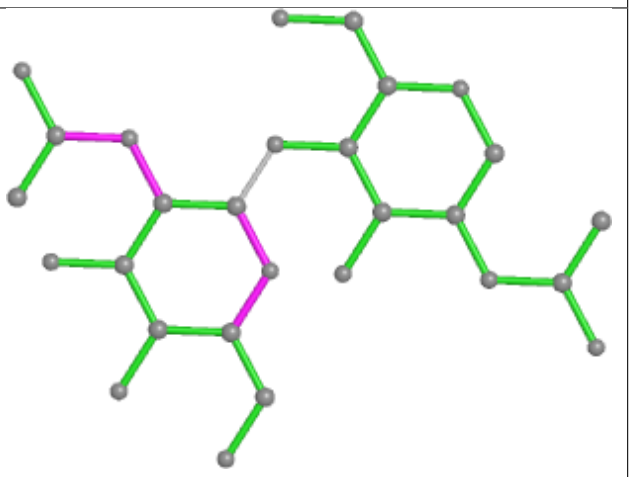


Rings

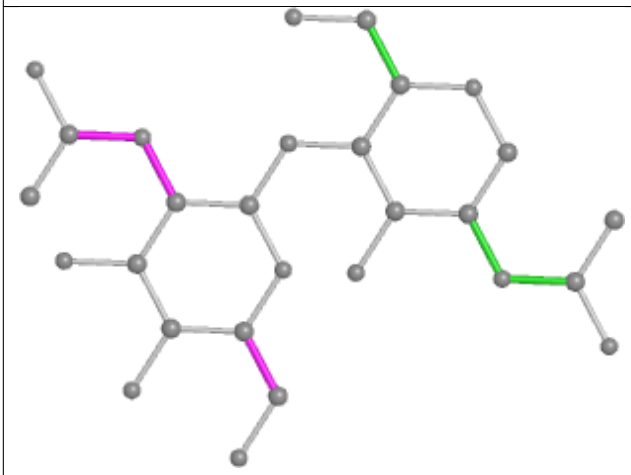
Oligosaccharide Chain M



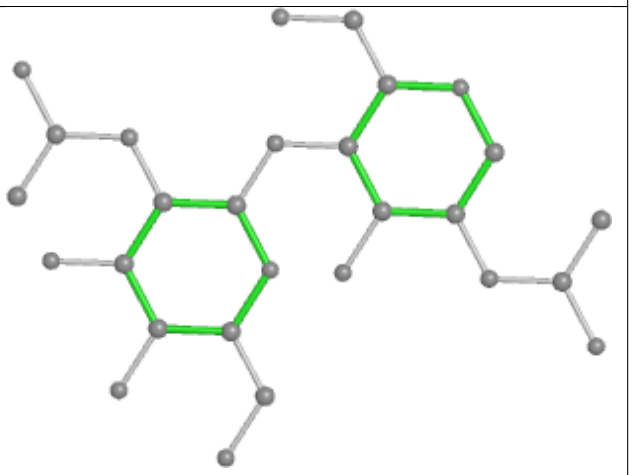
Bond lengths



Bond angles

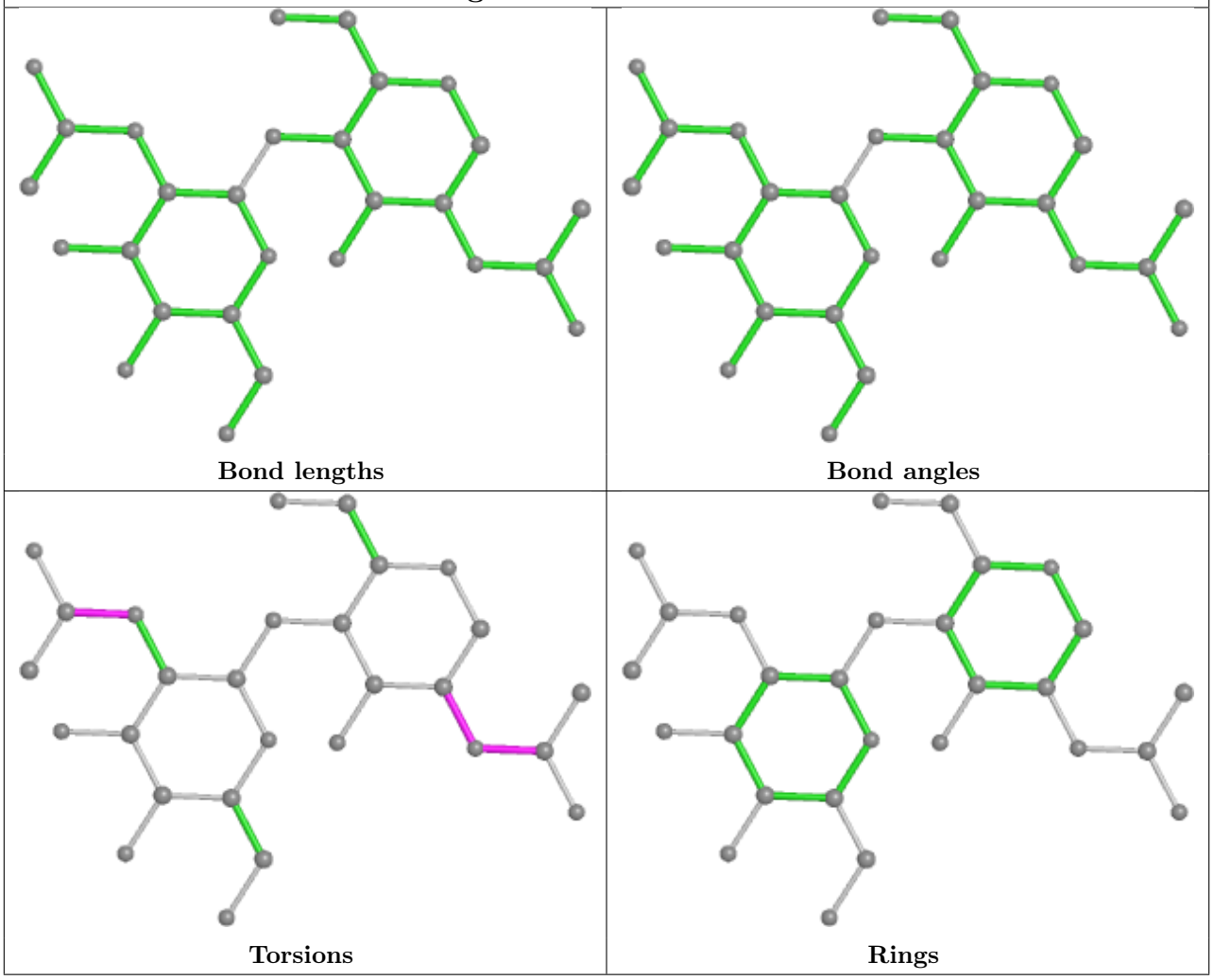


Torsions



Rings

Oligosaccharide Chain N



5.6 Ligand geometry (i)

29 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	$\#\|Z\| > 2$
3	NAG	A	1309	-	14,14,15	0.26	0	17,19,21	1.18	1 (5%)
3	NAG	C	1308	-	14,14,15	0.52	0	17,19,21	1.25	2 (11%)
3	NAG	C	1305	1	14,14,15	0.19	0	17,19,21	0.60	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	NAG	B	1306	1	14,14,15	0.22	0	17,19,21	0.48	0
3	NAG	A	1304	-	14,14,15	0.33	0	17,19,21	1.44	3 (17%)
3	NAG	B	1302	1	14,14,15	0.31	0	17,19,21	1.47	3 (17%)
3	NAG	A	1310	1	14,14,15	0.30	0	17,19,21	0.71	0
3	NAG	B	1301	1	14,14,15	0.26	0	17,19,21	0.65	0
3	NAG	B	1303	-	14,14,15	0.27	0	17,19,21	1.29	2 (11%)
3	NAG	A	1308	-	14,14,15	0.29	0	17,19,21	0.56	0
3	NAG	B	1304	1	14,14,15	0.26	0	17,19,21	0.63	0
3	NAG	B	1310	1	14,14,15	0.28	0	17,19,21	0.70	0
3	NAG	C	1303	1	14,14,15	0.26	0	17,19,21	0.61	0
3	NAG	C	1307	1	14,14,15	0.22	0	17,19,21	0.54	0
3	NAG	B	1308	-	14,14,15	0.29	0	17,19,21	1.44	3 (17%)
3	NAG	A	1307	1	14,14,15	0.32	0	17,19,21	0.55	0
3	NAG	A	1305	-	14,14,15	0.24	0	17,19,21	1.12	2 (11%)
3	NAG	B	1305	1	14,14,15	0.22	0	17,19,21	0.49	0
3	NAG	B	1309	1	14,14,15	0.36	0	17,19,21	1.57	3 (17%)
3	NAG	C	1302	1	14,14,15	0.25	0	17,19,21	0.95	2 (11%)
3	NAG	A	1303	1	14,14,15	0.25	0	17,19,21	0.45	0
3	NAG	A	1302	1	14,14,15	0.22	0	17,19,21	0.47	0
3	NAG	C	1306	1	14,14,15	0.23	0	17,19,21	0.48	0
3	NAG	C	1304	1	14,14,15	0.19	0	17,19,21	0.58	0
3	NAG	C	1301	1	14,14,15	0.29	0	17,19,21	1.41	3 (17%)
3	NAG	A	1306	1	14,14,15	0.32	0	17,19,21	0.50	0
3	NAG	A	1301	-	14,14,15	0.31	0	17,19,21	1.62	3 (17%)
3	NAG	C	1309	1	14,14,15	0.31	0	17,19,21	0.74	1 (5%)
3	NAG	B	1307	1	14,14,15	0.26	0	17,19,21	0.59	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
3	NAG	A	1309	-	-	0/6/23/26	0/1/1/1
3	NAG	C	1308	-	-	0/6/23/26	0/1/1/1
3	NAG	C	1305	1	-	1/6/23/26	0/1/1/1
3	NAG	B	1306	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1304	-	-	2/6/23/26	0/1/1/1
3	NAG	B	1302	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1310	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	B	1301	1	-	1/6/23/26	0/1/1/1
3	NAG	B	1303	-	-	0/6/23/26	0/1/1/1
3	NAG	A	1308	-	-	0/6/23/26	0/1/1/1
3	NAG	B	1304	1	-	3/6/23/26	0/1/1/1
3	NAG	B	1310	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1303	1	-	1/6/23/26	0/1/1/1
3	NAG	C	1307	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1308	-	-	2/6/23/26	0/1/1/1
3	NAG	A	1307	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1305	-	-	1/6/23/26	0/1/1/1
3	NAG	B	1305	1	-	1/6/23/26	0/1/1/1
3	NAG	B	1309	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1302	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1303	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1302	1	-	0/6/23/26	0/1/1/1
3	NAG	C	1306	1	-	0/6/23/26	0/1/1/1
3	NAG	C	1304	1	-	0/6/23/26	0/1/1/1
3	NAG	C	1301	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1306	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1301	-	-	1/6/23/26	0/1/1/1
3	NAG	C	1309	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1307	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	1309	NAG	C1-O5-C5	5.27	119.33	112.19
3	A	1301	NAG	C1-O5-C5	3.97	117.57	112.19
3	A	1304	NAG	C1-O5-C5	3.97	117.57	112.19
3	B	1308	NAG	C1-O5-C5	3.84	117.40	112.19
3	B	1303	NAG	C1-O5-C5	3.70	117.21	112.19

There are no chirality outliers.

5 of 27 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1310	NAG	C8-C7-N2-C2
3	A	1310	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
3	B	1310	NAG	O7-C7-N2-C2
3	C	1309	NAG	C8-C7-N2-C2
3	C	1309	NAG	O7-C7-N2-C2

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-23718. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal surface views

This section was not generated.

6.5 Mask visualisation

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

7 Map analysis

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

7.1 Map-value distribution

This section was not generated.

7.2 Volume estimate versus contour level

This section was not generated.

7.3 Rotationally averaged power spectrum

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation

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

9 Map-model fit

This section was not generated.