



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 9, 2020 – 11:22 AM BST

PDB ID : 1RVX
Title : 1934 H1 Hemagglutinin in complex with LSTA
Authors : Gamblin, S.J.; Haire, L.F.; Russell, R.J.; Stevens, D.J.; Xiao, B.; Ha, Y.; Vasisht, N.; Steinhauer, D.A.; Daniels, R.S.; Elliot, A.; Wiley, D.C.; Skehel, J.J.
Deposited on : 2003-12-15
Resolution : 2.20 Å(reported)

This is a wwPDB X-ray Structure 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/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
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) : 2.13.1

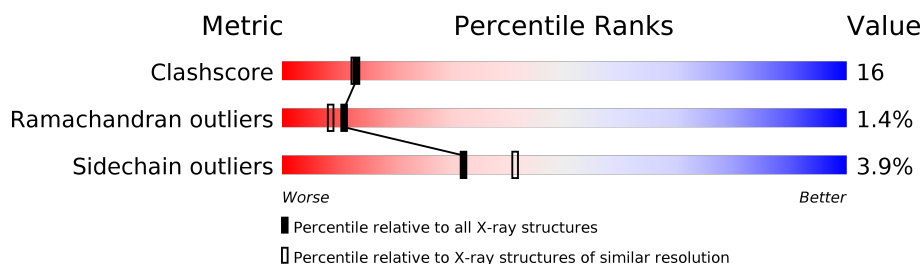
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	327	76% 20% ..
1	C	327	76% 20% ..
1	E	327	74% 22% ..
1	G	327	71% 26% ..
1	I	327	72% 24% ..
1	K	327	79% 17% ..
2	B	160	68% 24% 7% .
2	D	160	71% 25% ..

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Mol	Chain	Length	Quality of chain
2	F	160	
2	H	160	
2	J	160	
2	L	160	
3	M	3	
3	N	3	
3	O	3	
3	P	3	
3	Q	3	
3	R	3	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	NAG	L	3016	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 25966 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.

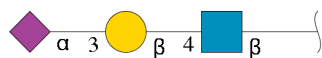
- Molecule 1 is a protein called hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	323	Total	C	N	O	S	0	0	0
			2557	1612	450	482	13			
1	C	323	Total	C	N	O	S	0	0	0
			2557	1612	450	482	13			
1	E	323	Total	C	N	O	S	0	0	0
			2557	1612	450	482	13			
1	G	323	Total	C	N	O	S	0	0	0
			2557	1612	450	482	13			
1	I	323	Total	C	N	O	S	0	0	0
			2557	1612	450	482	13			
1	K	323	Total	C	N	O	S	0	0	0
			2557	1612	450	482	13			

- Molecule 2 is a protein called Hemagglutinin.

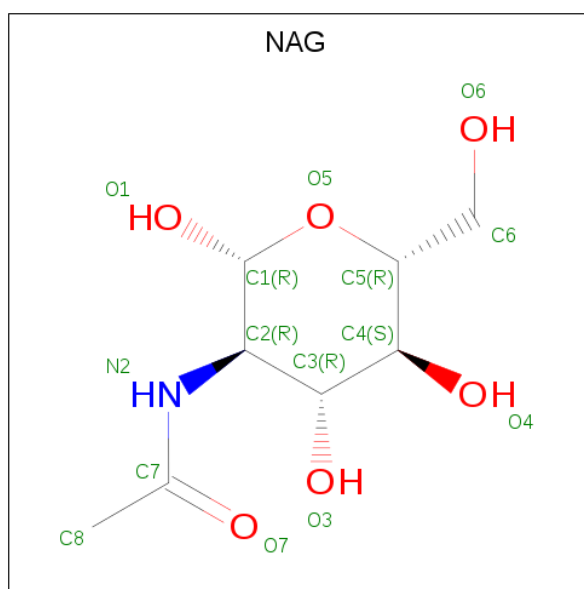
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	160	Total	C	N	O	S	0	0	0
			1283	805	218	253	7			
2	D	160	Total	C	N	O	S	0	0	0
			1283	805	218	253	7			
2	F	159	Total	C	N	O	S	0	0	0
			1275	800	217	251	7			
2	H	160	Total	C	N	O	S	0	0	0
			1283	805	218	253	7			
2	J	160	Total	C	N	O	S	0	0	0
			1283	805	218	253	7			
2	L	159	Total	C	N	O	S	0	0	0
			1275	800	217	251	7			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	M	3	Total	C	N	O	0	0	0
			45	25	2	18			
3	N	3	Total	C	N	O	0	0	0
			45	25	2	18			
3	O	3	Total	C	N	O	0	0	0
			45	25	2	18			
3	P	3	Total	C	N	O	0	0	0
			45	25	2	18			
3	Q	3	Total	C	N	O	0	0	0
			45	25	2	18			
3	R	3	Total	C	N	O	0	0	0
			45	25	2	18			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			15	8	1	6		
4	A	1	Total	C	N	O	0	0
			15	8	1	6		
4	B	1	Total	C	N	O	0	0
			15	8	1	6		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	C	1	Total	C	N	O	0	0
			15	8	1	6		
4	G	1	Total	C	N	O	0	0
			15	8	1	6		
4	G	1	Total	C	N	O	0	0
			15	8	1	6		
4	I	1	Total	C	N	O	0	0
			15	8	1	6		
4	J	1	Total	C	N	O	0	0
			15	8	1	6		
4	K	1	Total	C	N	O	0	0
			15	8	1	6		
4	L	1	Total	C	N	O	0	0
			15	8	1	6		

- Molecule 5 is water.

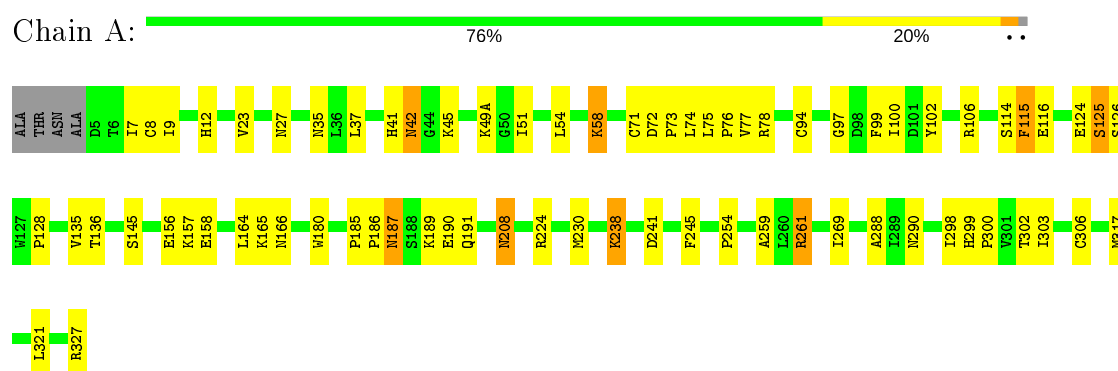
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	295	Total	O	0	0
			295	295		
5	B	107	Total	O	0	0
			107	107		
5	C	296	Total	O	0	0
			296	296		
5	D	122	Total	O	0	0
			122	122		
5	E	340	Total	O	0	0
			340	340		
5	F	122	Total	O	0	0
			122	122		
5	G	307	Total	O	0	0
			307	307		
5	H	101	Total	O	0	0
			101	101		
5	I	303	Total	O	0	0
			303	303		
5	J	105	Total	O	0	0
			105	105		
5	K	315	Total	O	0	0
			315	315		
5	L	109	Total	O	0	0
			109	109		

3 Residue-property plots [i](#)

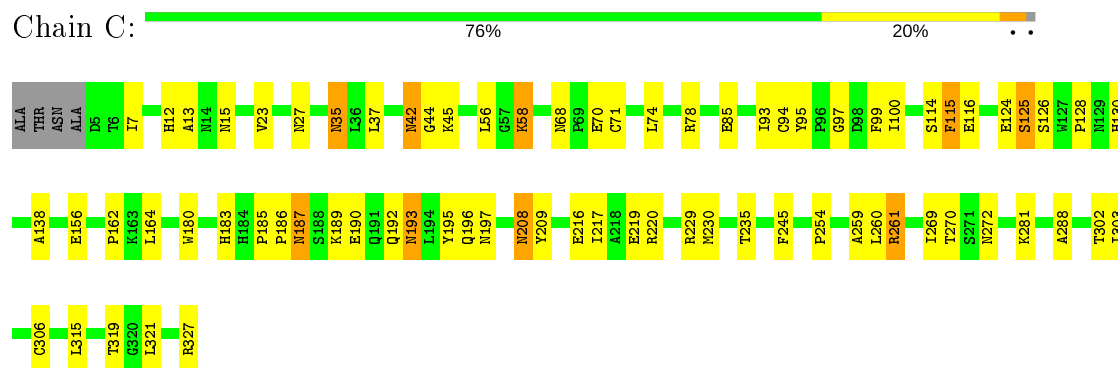
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

Note EDS was not executed.

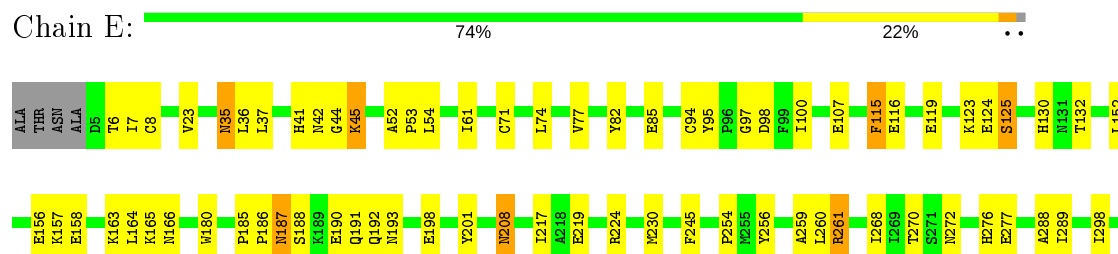
- Molecule 1: hemagglutinin



- Molecule 1: hemagglutinin



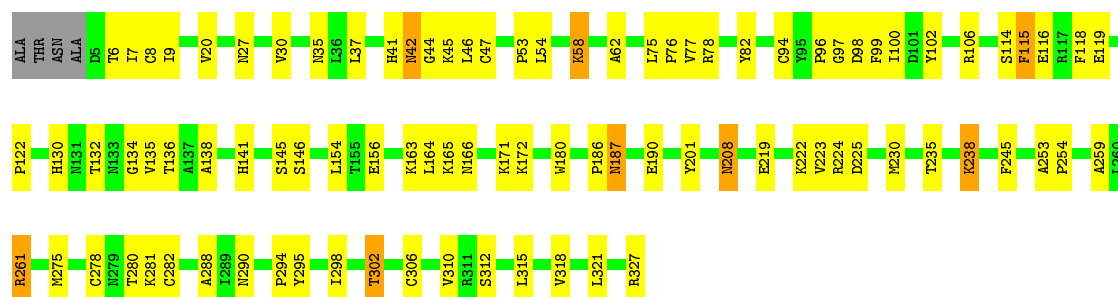
- Molecule 1: hemagglutinin





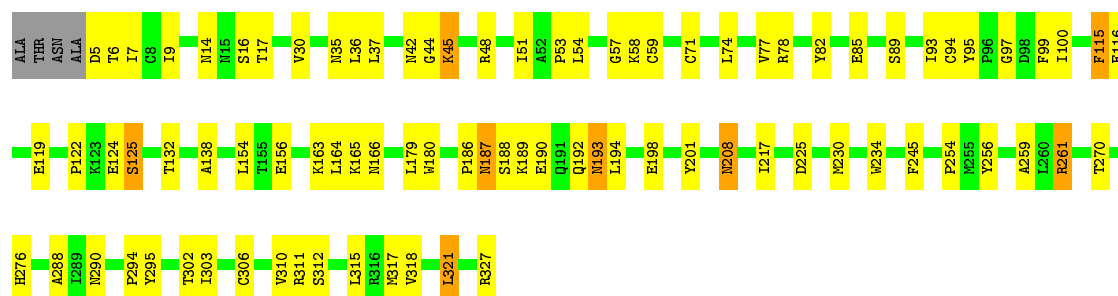
- Molecule 1: hemagglutinin

Chain G: 71% 26% ..



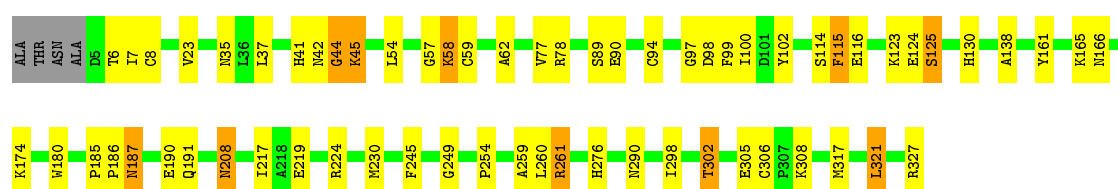
- Molecule 1: hemagglutinin

Chain I: 72% 24% ..



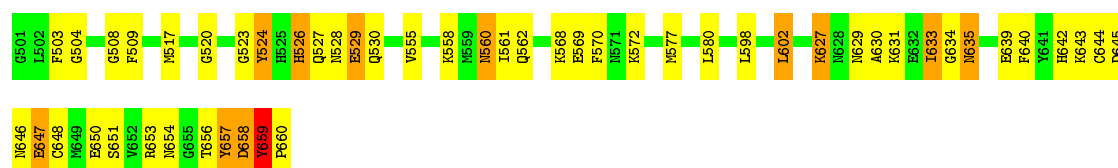
- Molecule 1: hemagglutinin

Chain K: 79% 17% ..



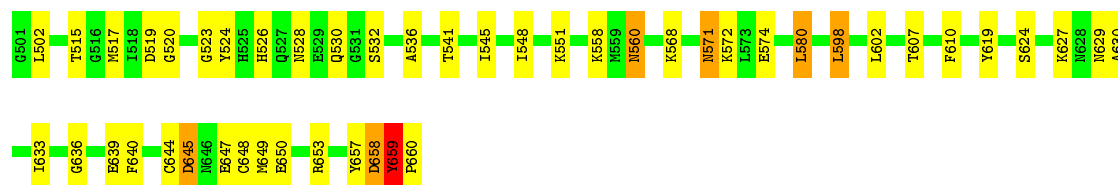
- Molecule 2: Hemagglutinin

Chain B: 68% 24% 7% .



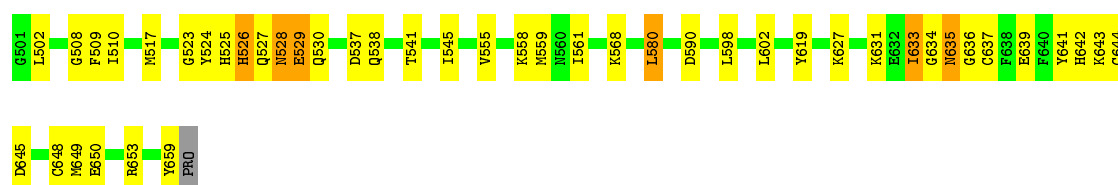
- Molecule 2: Hemagglutinin

Chain D:  71% 25% . .



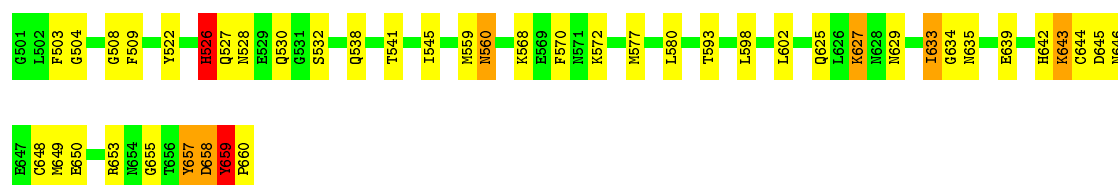
- Molecule 2: Hemagglutinin

Chain F:  71% 24% . .



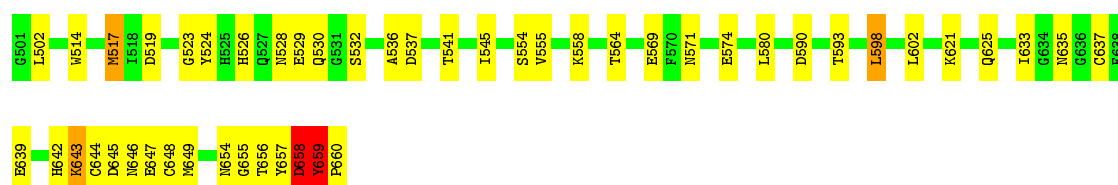
- Molecule 2: Hemagglutinin

Chain H:  73% 23% . .



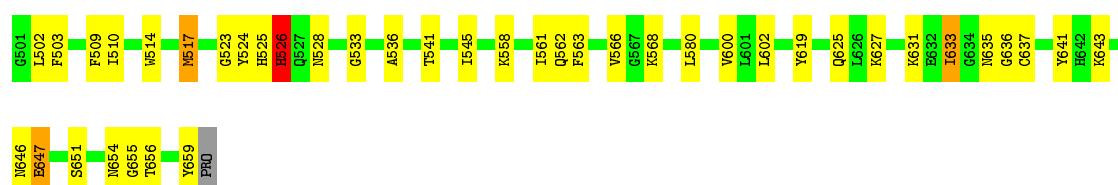
- Molecule 2: Hemagglutinin

Chain J:  70% 27% . .



- Molecule 2: Hemagglutinin

Chain L:  74% 23% . .



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

Chain M:  100%

MAG1
GAL2
SIA3

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

Chain N:  33% 67%

MAG1
GAL2
SIA3

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

Chain O:  100%

MAG1
GAL2
SIA3

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

Chain P:  33% 33% 33%

MAG1
GAL2
SIA3

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

Chain Q:  100%

MAG1
GAL2
SIA3

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

Chain R:  33% 67%

MAG1
GAL2
SIA3

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	227.88Å 131.34Å 174.71Å 90.00° 110.09° 90.00°	Depositor
Resolution (Å)	20.00 – 2.20	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-2.20)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.227 , 0.260	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	25966	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

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: SIA, GAL, 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	0.33	0/2621	0.61	0/3563
1	C	0.34	0/2621	0.62	0/3563
1	E	0.33	0/2620	0.62	0/3560
1	G	0.34	0/2621	0.63	0/3563
1	I	0.34	0/2620	0.62	0/3560
1	K	0.33	0/2621	0.64	1/3563 (0.0%)
2	B	0.32	0/1309	0.53	0/1761
2	D	0.33	0/1309	0.53	0/1761
2	F	0.33	0/1300	0.51	0/1749
2	H	0.32	0/1309	0.52	0/1761
2	J	0.32	0/1309	0.53	0/1761
2	L	0.32	0/1300	0.52	0/1749
All	All	0.33	0/23560	0.59	1/31914 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	44	GLY	N-CA-C	-8.24	92.50	113.10

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	2557	0	2495	84	0
1	C	2557	0	2495	81	0
1	E	2557	0	2494	72	0
1	G	2557	0	2497	102	0
1	I	2557	0	2494	88	0
1	K	2557	0	2495	67	0
2	B	1283	0	1207	69	0
2	D	1283	0	1207	41	0
2	F	1275	0	1200	39	0
2	H	1283	0	1207	54	0
2	J	1283	0	1207	58	0
2	L	1275	0	1200	50	0
3	M	45	0	38	0	0
3	N	45	0	38	0	0
3	O	45	0	38	0	0
3	P	45	0	38	1	0
3	Q	45	0	38	0	0
3	R	45	0	38	0	0
4	A	30	0	30	8	0
4	B	15	0	15	2	0
4	C	15	0	15	5	0
4	G	30	0	30	7	0
4	I	15	0	15	3	0
4	J	15	0	15	5	0
4	K	15	0	15	3	0
4	L	15	0	15	7	0
5	A	295	0	0	6	0
5	B	107	0	0	5	0
5	C	296	0	0	8	0
5	D	122	0	0	5	0
5	E	340	0	0	6	0
5	F	122	0	0	0	0
5	G	307	0	0	11	0
5	H	101	0	0	2	0
5	I	303	0	0	6	0
5	J	105	0	0	1	0
5	K	315	0	0	5	0
5	L	109	0	0	5	0
All	All	25966	0	22576	751	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 16.

The worst 5 of 751 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:C:15:ASN:HD21	4:C:3020:NAG:H61	1.08	1.19
1:A:27:ASN:HD21	4:A:3017:NAG:H4	1.04	1.14
1:A:238:LYS:H	1:A:238:LYS:CE	1.63	1.11
1:A:58:LYS:H	1:A:58:LYS:HD3	0.98	1.10
1:K:290:ASN:HD21	4:K:3015:NAG:H3	1.00	1.10

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 X-ray entries followed by that with respect to entries of similar resolution.

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	321/327 (98%)	309 (96%)	11 (3%)	1 (0%)	41	46
1	C	321/327 (98%)	311 (97%)	8 (2%)	2 (1%)	25	26
1	E	319/327 (98%)	309 (97%)	8 (2%)	2 (1%)	25	26
1	G	321/327 (98%)	308 (96%)	13 (4%)	0	100	100
1	I	319/327 (98%)	307 (96%)	10 (3%)	2 (1%)	25	26
1	K	321/327 (98%)	307 (96%)	12 (4%)	2 (1%)	25	26
2	B	158/160 (99%)	139 (88%)	11 (7%)	8 (5%)	2	0
2	D	158/160 (99%)	138 (87%)	16 (10%)	4 (2%)	5	3
2	F	157/160 (98%)	140 (89%)	11 (7%)	6 (4%)	3	1
2	H	158/160 (99%)	140 (89%)	11 (7%)	7 (4%)	2	1
2	J	158/160 (99%)	145 (92%)	9 (6%)	4 (2%)	5	3
2	L	157/160 (98%)	150 (96%)	6 (4%)	1 (1%)	25	26
All	All	2868/2922 (98%)	2703 (94%)	126 (4%)	39 (1%)	11	8

5 of 39 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	657	TYR
2	B	659	TYR
1	C	44	GLY
2	D	645	ASP
2	D	658	ASP

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	285/287 (99%)	274 (96%)	11 (4%)	32	41
1	C	285/287 (99%)	274 (96%)	11 (4%)	32	41
1	E	285/287 (99%)	277 (97%)	8 (3%)	43	56
1	G	285/287 (99%)	273 (96%)	12 (4%)	30	38
1	I	285/287 (99%)	275 (96%)	10 (4%)	36	46
1	K	285/287 (99%)	276 (97%)	9 (3%)	39	50
2	B	136/136 (100%)	127 (93%)	9 (7%)	16	19
2	D	136/136 (100%)	127 (93%)	9 (7%)	16	19
2	F	135/136 (99%)	132 (98%)	3 (2%)	52	65
2	H	136/136 (100%)	129 (95%)	7 (5%)	24	29
2	J	136/136 (100%)	131 (96%)	5 (4%)	34	43
2	L	135/136 (99%)	130 (96%)	5 (4%)	34	43
All	All	2524/2538 (99%)	2425 (96%)	99 (4%)	32	41

5 of 99 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	187	ASN
1	G	156	GLU
1	K	261	ARG
1	E	261	ARG
2	F	580	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 98 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	276	HIS
1	G	130	HIS
1	K	208	ASN
2	F	528	ASN
2	F	646	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

18 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	$\# Z > 2$
3	NAG	M	1	3	14,14,15	1.10	1 (7%)	17,19,21	0.59	0
3	GAL	M	2	3	11,11,12	1.77	4 (36%)	15,15,17	0.74	0
3	SIA	M	3	3	17,20,21	1.87	5 (29%)	21,28,31	1.03	2 (9%)
3	NAG	N	1	3	14,14,15	1.14	0	17,19,21	0.67	0
3	GAL	N	2	3	11,11,12	1.72	3 (27%)	15,15,17	0.76	0
3	SIA	N	3	3	17,20,21	1.90	6 (35%)	21,28,31	1.04	2 (9%)
3	NAG	O	1	3	14,14,15	1.17	1 (7%)	17,19,21	0.61	0
3	GAL	O	2	3	11,11,12	1.68	4 (36%)	15,15,17	0.79	0
3	SIA	O	3	3	17,20,21	1.93	5 (29%)	21,28,31	1.06	2 (9%)
3	NAG	P	1	3	14,14,15	1.03	0	17,19,21	0.65	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GAL	P	2	3	11,11,12	1.72	4 (36%)	15,15,17	0.71	0
3	SIA	P	3	3	17,20,21	1.95	5 (29%)	21,28,31	1.00	2 (9%)
3	NAG	Q	1	3	14,14,15	1.57	3 (21%)	17,19,21	0.86	0
3	GAL	Q	2	3	11,11,12	1.86	4 (36%)	15,15,17	0.73	0
3	SIA	Q	3	3	17,20,21	1.95	6 (35%)	21,28,31	0.98	2 (9%)
3	NAG	R	1	3	14,14,15	1.07	0	17,19,21	0.63	0
3	GAL	R	2	3	11,11,12	1.76	4 (36%)	15,15,17	0.74	0
3	SIA	R	3	3	17,20,21	1.86	5 (29%)	21,28,31	1.05	2 (9%)

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	M	1	3	-	2/6/23/26	0/1/1/1
3	GAL	M	2	3	-	0/2/19/22	0/1/1/1
3	SIA	M	3	3	-	0/14/34/38	0/1/1/1
3	NAG	N	1	3	-	0/6/23/26	0/1/1/1
3	GAL	N	2	3	-	0/2/19/22	0/1/1/1
3	SIA	N	3	3	-	0/14/34/38	0/1/1/1
3	NAG	O	1	3	-	0/6/23/26	0/1/1/1
3	GAL	O	2	3	-	0/2/19/22	0/1/1/1
3	SIA	O	3	3	-	0/14/34/38	0/1/1/1
3	NAG	P	1	3	-	0/6/23/26	0/1/1/1
3	GAL	P	2	3	-	0/2/19/22	0/1/1/1
3	SIA	P	3	3	-	0/14/34/38	0/1/1/1
3	NAG	Q	1	3	-	1/6/23/26	0/1/1/1
3	GAL	Q	2	3	-	0/2/19/22	0/1/1/1
3	SIA	Q	3	3	-	0/14/34/38	0/1/1/1
3	NAG	R	1	3	-	0/6/23/26	0/1/1/1
3	GAL	R	2	3	-	0/2/19/22	0/1/1/1
3	SIA	R	3	3	-	0/14/34/38	0/1/1/1

The worst 5 of 60 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	P	3	SIA	C3-C2	4.69	1.59	1.52
3	R	3	SIA	C3-C2	4.58	1.59	1.52
3	O	3	SIA	C3-C2	4.26	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	M	3	SIA	C3-C2	4.23	1.59	1.52
3	Q	3	SIA	C3-C2	4.23	1.59	1.52

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	3	SIA	C3-C4-C5	-2.78	108.10	111.46
3	O	3	SIA	C3-C4-C5	-2.74	108.15	111.46
3	M	3	SIA	C3-C4-C5	-2.57	108.35	111.46
3	N	3	SIA	C3-C4-C5	-2.53	108.40	111.46
3	R	3	SIA	C3-C4-C5	-2.44	108.51	111.46

There are no chirality outliers.

All (3) torsion outliers are listed below:

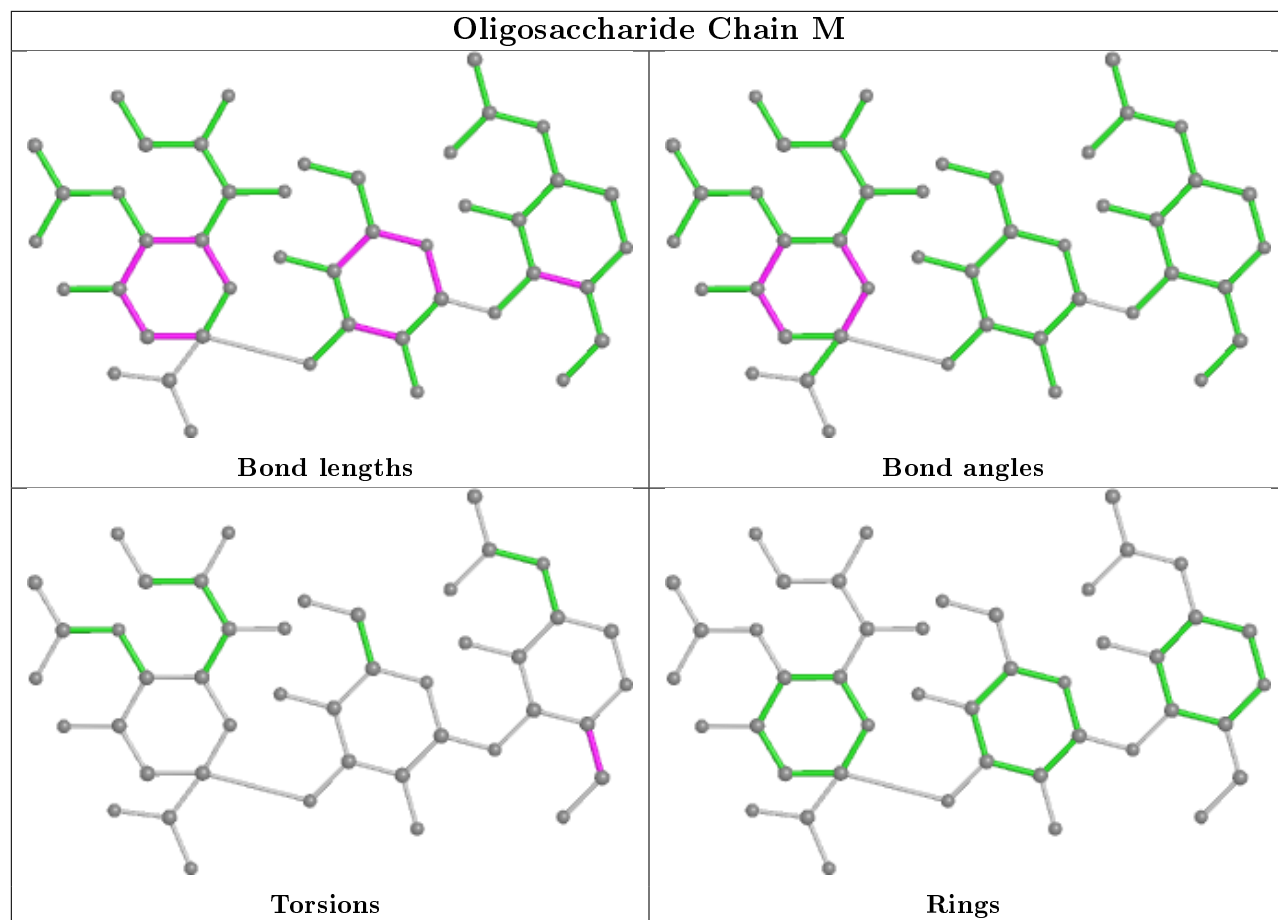
Mol	Chain	Res	Type	Atoms
3	M	1	NAG	C4-C5-C6-O6
3	Q	1	NAG	C3-C2-N2-C7
3	M	1	NAG	O5-C5-C6-O6

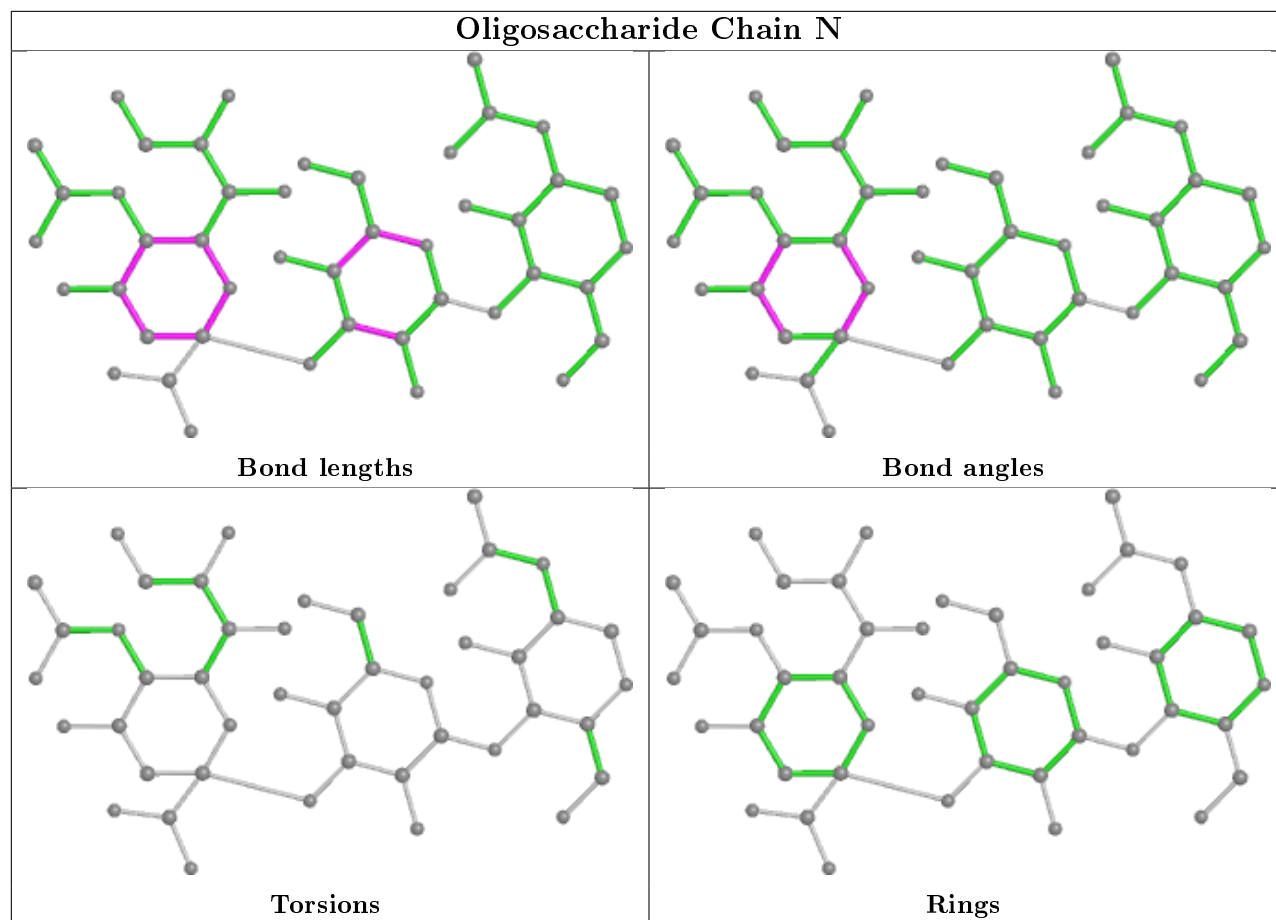
There are no ring outliers.

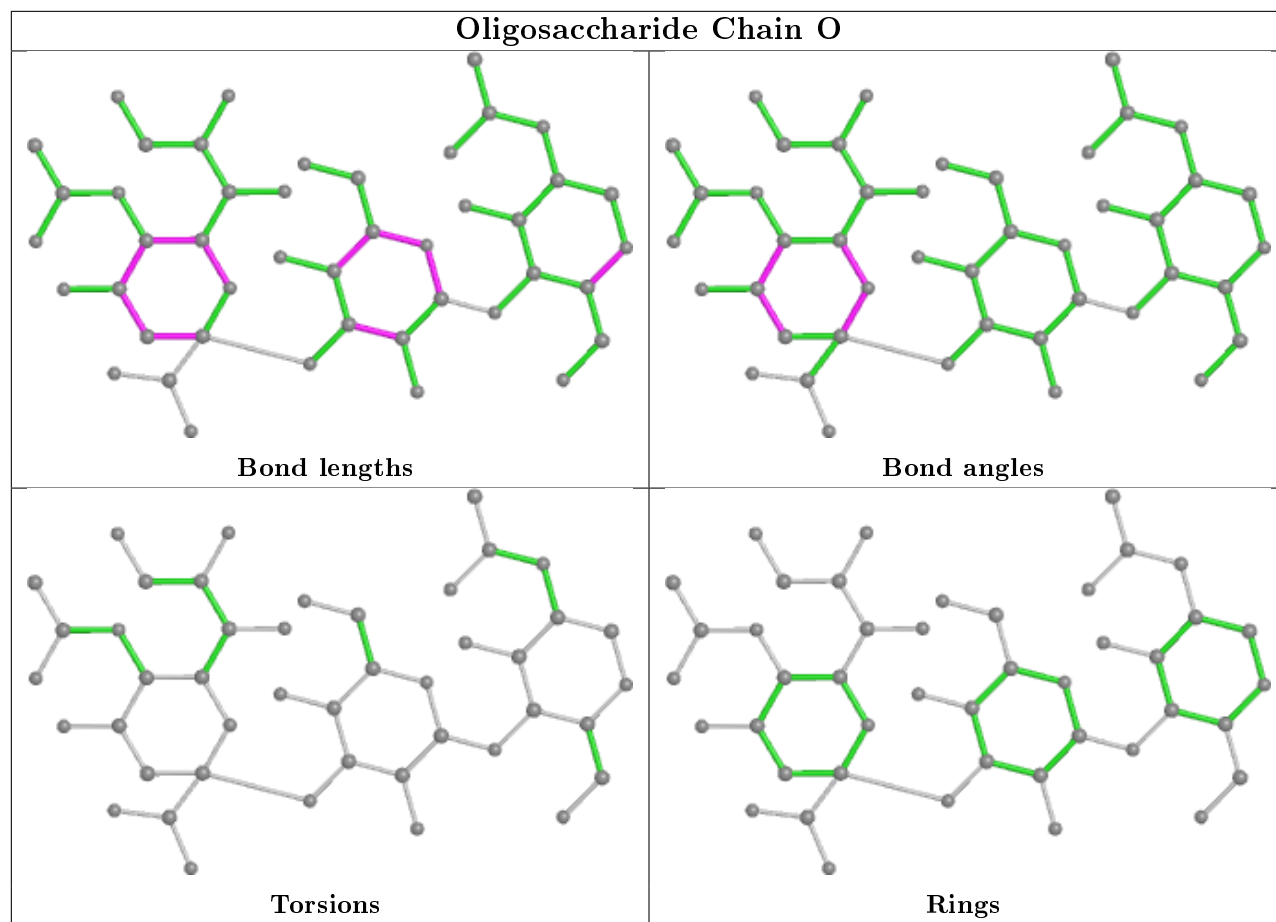
1 monomer is involved in 1 short contact:

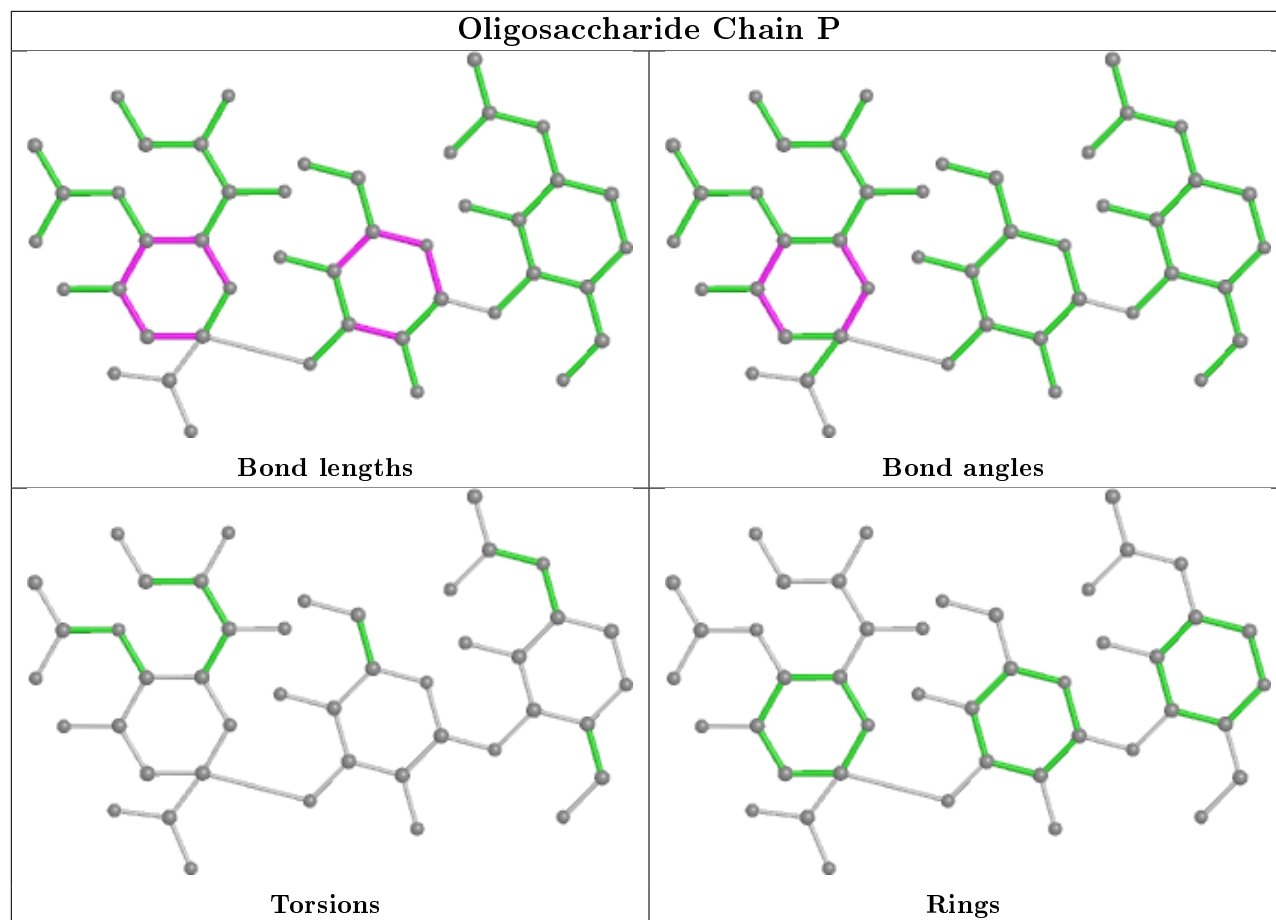
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	P	3	SIA	1	0

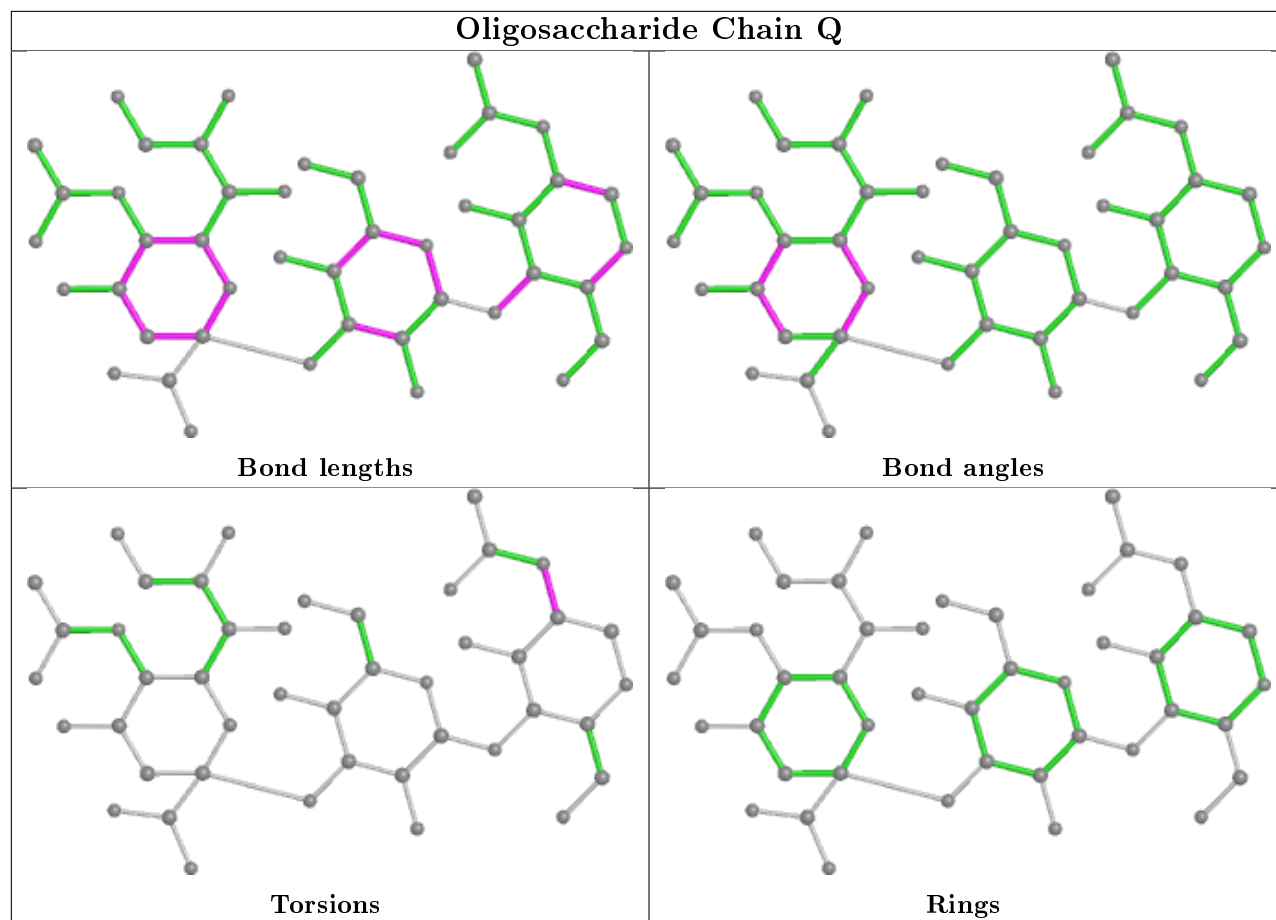
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

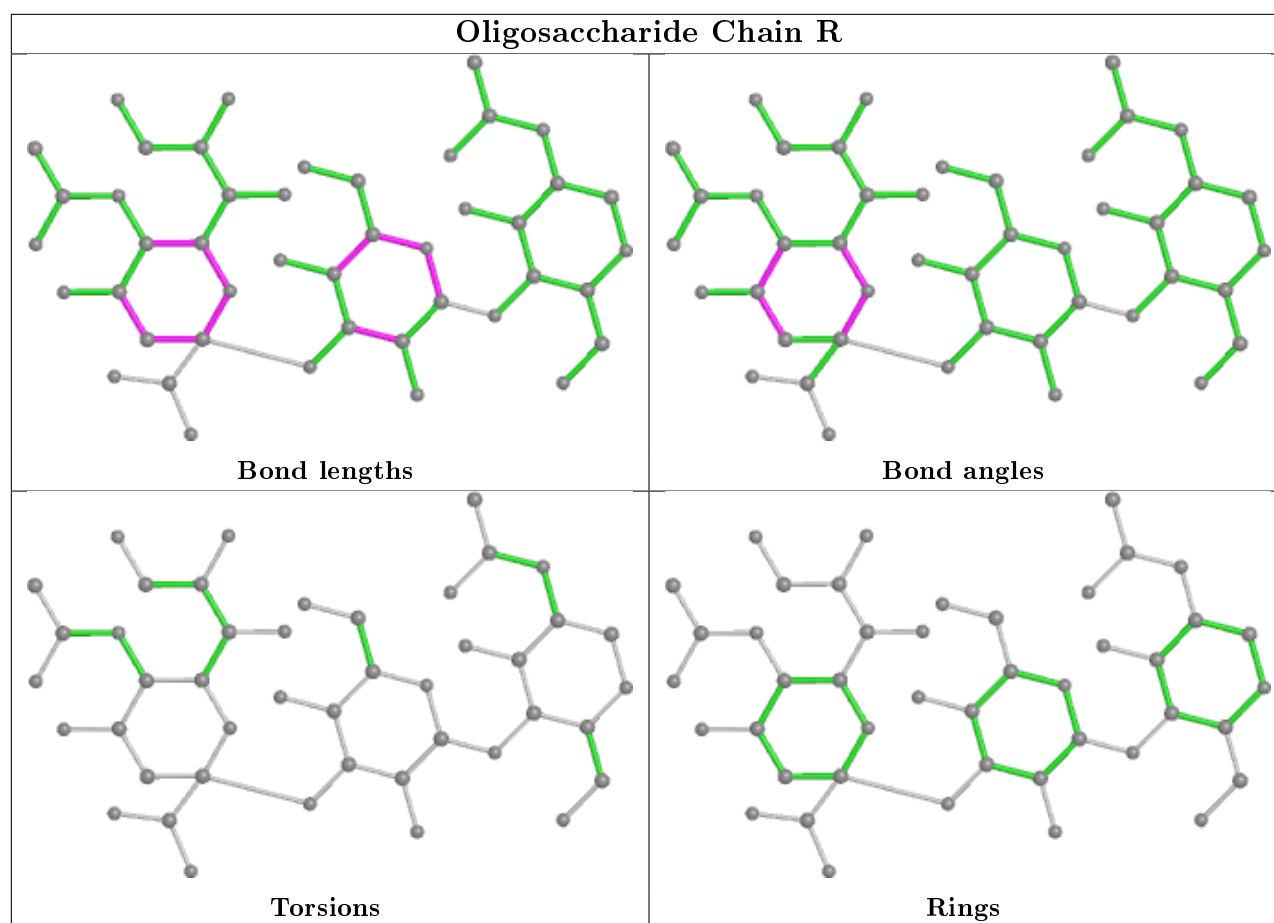












5.6 Ligand geometry [i](#)

10 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	$\# Z > 2$
4	NAG	B	3019	-	15,15,15	0.49	0	21,21,21	0.62	0
4	NAG	L	3016	-	15,15,15	0.55	0	21,21,21	0.60	0
4	NAG	A	3018	-	15,15,15	0.45	0	21,21,21	0.54	0
4	NAG	C	3020	-	15,15,15	0.50	0	21,21,21	0.57	0
4	NAG	G	3011	-	15,15,15	0.55	0	21,21,21	0.66	0
4	NAG	G	3012	-	15,15,15	0.42	0	21,21,21	0.55	0
4	NAG	A	3017	-	15,15,15	0.53	0	21,21,21	0.82	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	J	3014	-	15,15,15	0.49	0	21,21,21	0.60	0
4	NAG	I	3013	-	15,15,15	0.64	0	21,21,21	0.68	0
4	NAG	K	3015	-	15,15,15	0.50	0	21,21,21	0.67	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
4	NAG	B	3019	-	-	3/6/26/26	0/1/1/1
4	NAG	L	3016	-	-	6/6/26/26	0/1/1/1
4	NAG	A	3018	-	-	5/6/26/26	0/1/1/1
4	NAG	C	3020	-	-	4/6/26/26	0/1/1/1
4	NAG	G	3011	-	-	6/6/26/26	0/1/1/1
4	NAG	G	3012	-	-	4/6/26/26	0/1/1/1
4	NAG	A	3017	-	-	6/6/26/26	0/1/1/1
4	NAG	J	3014	-	-	5/6/26/26	0/1/1/1
4	NAG	I	3013	-	-	6/6/26/26	0/1/1/1
4	NAG	K	3015	-	-	2/6/26/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 47 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	3019	NAG	C8-C7-N2-C2
4	B	3019	NAG	O7-C7-N2-C2
4	L	3016	NAG	C8-C7-N2-C2
4	L	3016	NAG	O7-C7-N2-C2
4	A	3018	NAG	C8-C7-N2-C2

There are no ring outliers.

10 monomers are involved in 40 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	3019	NAG	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	L	3016	NAG	7	0
4	A	3018	NAG	4	0
4	C	3020	NAG	5	0
4	G	3011	NAG	4	0
4	G	3012	NAG	3	0
4	A	3017	NAG	4	0
4	J	3014	NAG	5	0
4	I	3013	NAG	3	0
4	K	3015	NAG	3	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	I	1
1	E	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	I	42:ASN	C	44:GLY	N	2.69
1	E	42:ASN	C	44:GLY	N	2.55

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.