



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 10, 2020 – 11:51 AM BST

PDB ID : 1RVZ
Title : 1934 H1 Hemagglutinin in complex with LSTC
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 : 2.25 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

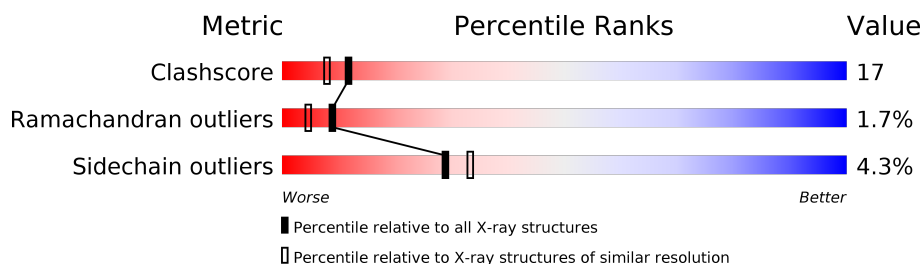
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)

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	
1	C	327	
1	E	327	
1	G	327	
1	I	327	
1	K	327	
2	B	160	
2	D	160	

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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	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 25452 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.

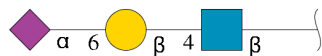
- Molecule 1 is a protein called hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	323	Total	C	N	O	S	0	0	0
			2556	1611	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.

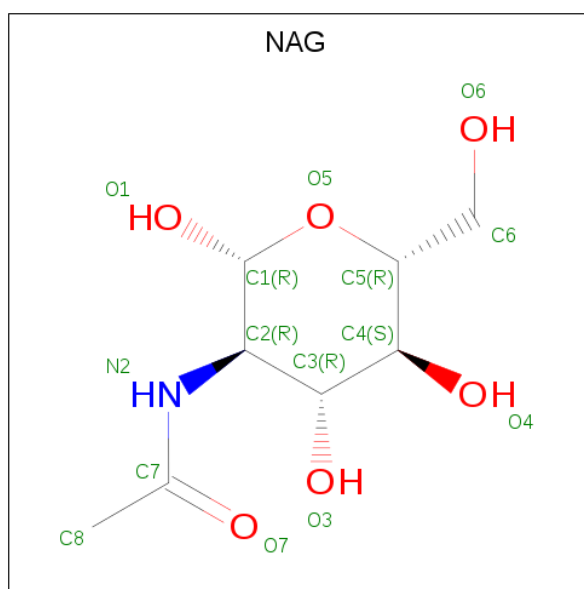
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	160	Total	C	N	O	S	0	0	0
			1283	805	218	253	7			
2	D	160	Total	C	N	O	S	0	0	0
			1283	805	218	253	7			
2	F	160	Total	C	N	O	S	0	0	0
			1283	805	218	253	7			
2	H	160	Total	C	N	O	S	0	0	0
			1283	805	218	253	7			
2	J	160	Total	C	N	O	S	0	0	0
			1283	805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

- Molecule 3 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-6)-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	E	1	Total	C	N	O	0	0
			15	8	1	6		
4	F	1	Total	C	N	O	0	0
			15	8	1	6		

- Molecule 5 is water.

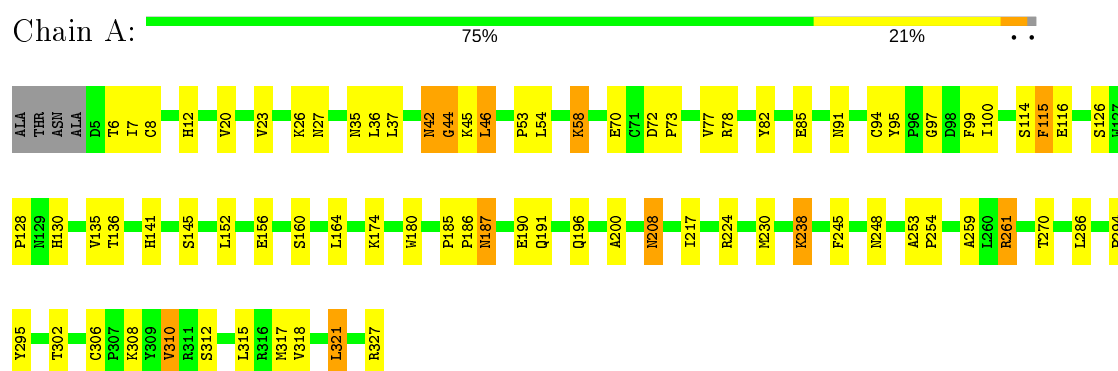
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	254	Total 254	O 254	0	0
5	B	69	Total 69	O 69	0	0
5	C	254	Total 254	O 254	0	0
5	D	97	Total 97	O 97	0	0
5	E	250	Total 250	O 250	0	0
5	F	81	Total 81	O 81	0	0
5	G	300	Total 300	O 300	0	0
5	H	76	Total 76	O 76	0	0
5	I	290	Total 290	O 290	0	0
5	J	76	Total 76	O 76	0	0
5	K	274	Total 274	O 274	0	0
5	L	77	Total 77	O 77	0	0

3 Residue-property plots

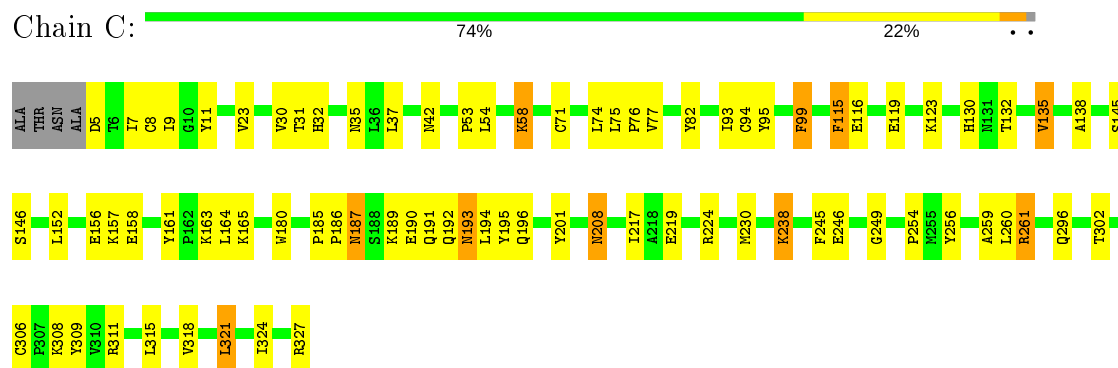
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

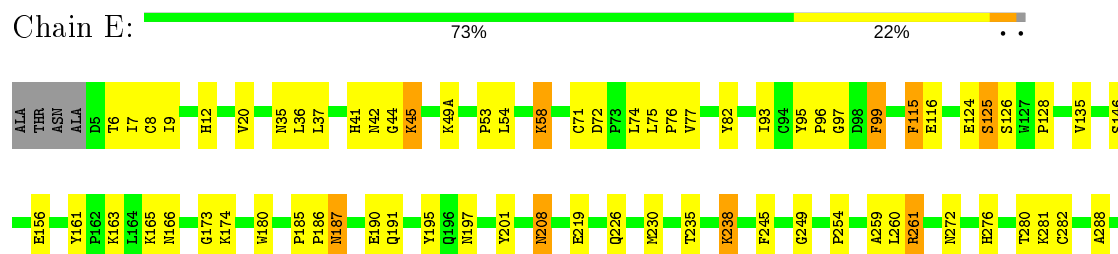
- Molecule 1: hemagglutinin



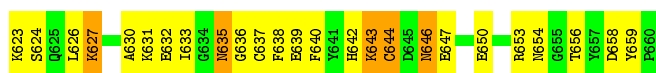
- Molecule 1: hemagglutinin



- Molecule 1: hemagglutinin

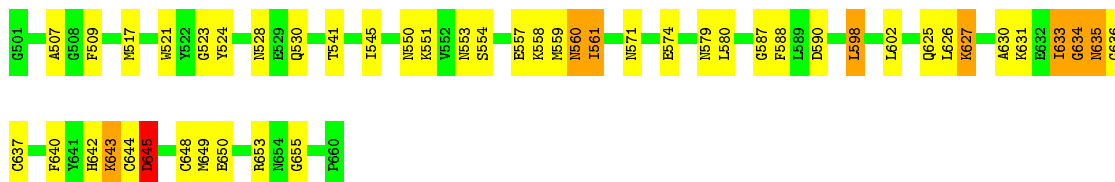






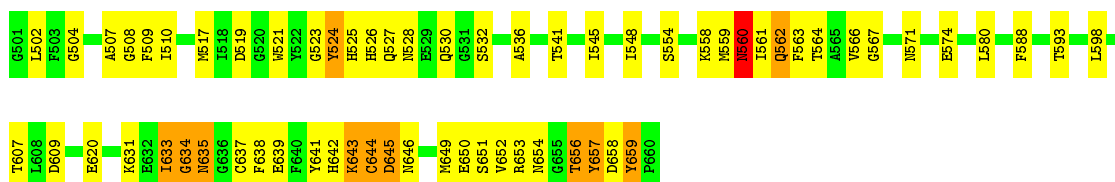
- Molecule 2: hemagglutinin

Chain D: 70% 24% 5%



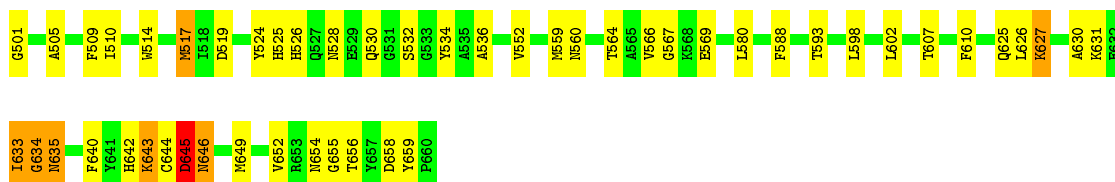
- Molecule 2: hemagglutinin

Chain F: 61% 32% 7%



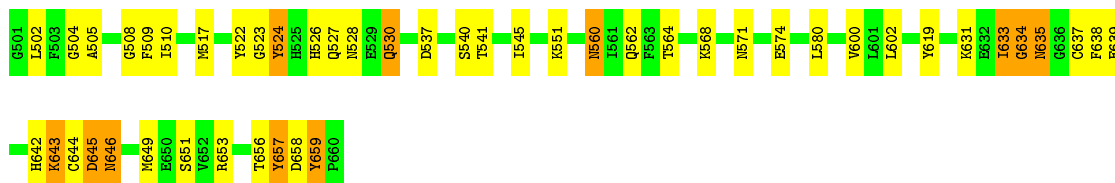
- Molecule 2: hemagglutinin

Chain H: 69% 26% 5%



- Molecule 2: hemagglutinin

Chain J: 70% 23% 7%



- Molecule 2: hemagglutinin

Chain L: 68% 29% 3%





- Molecule 3: N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M: 100%



- Molecule 3: N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N: 67% 33%



- Molecule 3: N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O: 100%



- Molecule 3: N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P: 33% 67%



- Molecule 3: N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q: 100%



- Molecule 3: N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R: 100%



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	227.58Å 131.52Å 175.02Å 90.00° 110.07° 90.00°	Depositor
Resolution (Å)	20.00 – 2.25	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-2.25)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.225 , 0.257	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	25452	wwPDB-VP
Average B, all atoms (Å ²)	44.0	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	0.34	0/2620	0.62	0/3561
1	C	0.34	0/2621	0.63	0/3563
1	E	0.35	0/2620	0.63	0/3560
1	G	0.36	0/2621	0.64	0/3563
1	I	0.34	0/2621	0.61	0/3563
1	K	0.34	0/2621	0.62	0/3563
2	B	0.32	0/1309	0.52	0/1761
2	D	0.34	0/1309	0.56	0/1761
2	F	0.34	0/1309	0.57	0/1761
2	H	0.33	0/1309	0.56	0/1761
2	J	0.34	0/1309	0.56	0/1761
2	L	0.32	0/1309	0.52	0/1761
All	All	0.34	0/23578	0.60	0/31939

There are no bond length outliers.

There are no bond angle outliers.

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	2556	0	2491	93	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2557	0	2495	85	0
1	E	2557	0	2494	98	0
1	G	2557	0	2495	89	1
1	I	2557	0	2495	66	0
1	K	2557	0	2495	93	0
2	B	1283	0	1205	64	0
2	D	1283	0	1205	45	0
2	F	1283	0	1205	82	0
2	H	1283	0	1205	57	0
2	J	1283	0	1205	51	0
2	L	1283	0	1205	53	0
3	M	45	0	37	0	0
3	N	45	0	37	1	0
3	O	45	0	37	0	0
3	P	45	0	37	1	0
3	Q	45	0	37	0	0
3	R	45	0	37	0	0
4	A	15	0	15	4	0
4	E	15	0	15	4	0
4	F	15	0	15	4	0
5	A	254	0	0	5	1
5	B	69	0	0	2	0
5	C	254	0	0	3	0
5	D	97	0	0	3	0
5	E	250	0	0	4	0
5	F	81	0	0	4	0
5	G	300	0	0	9	0
5	H	76	0	0	2	0
5	I	290	0	0	2	0
5	J	76	0	0	4	0
5	K	274	0	0	5	1
5	L	77	0	0	1	0
All	All	25452	0	22462	795	2

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 17.

The worst 5 of 795 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:G:238:LYS:H	1:G:238:LYS:CE	1.65	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:58:LYS:H	1:G:58:LYS:HD3	1.14	1.07
1:G:238:LYS:H	1:G:238:LYS:HE3	0.94	1.06
1:G:280:THR:HG22	1:G:282:CYS:H	1.19	1.03
1:E:280:THR:HG22	1:E:282:CYS:H	1.23	1.02

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:K:3421:HOH:O	5:K:3421:HOH:O[2_555]	2.14	0.06
1:G:276:HIS:ND1	5:A:3354:HOH:O[2_555]	2.15	0.05

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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%)	310 (97%)	9 (3%)	2 (1%)	25	25
1	C	321/327 (98%)	311 (97%)	10 (3%)	0	100	100
1	E	319/327 (98%)	308 (97%)	9 (3%)	2 (1%)	25	25
1	G	321/327 (98%)	309 (96%)	10 (3%)	2 (1%)	25	25
1	I	321/327 (98%)	312 (97%)	7 (2%)	2 (1%)	25	25
1	K	321/327 (98%)	307 (96%)	13 (4%)	1 (0%)	41	46
2	B	158/160 (99%)	137 (87%)	17 (11%)	4 (2%)	5	3
2	D	158/160 (99%)	138 (87%)	13 (8%)	7 (4%)	2	0
2	F	158/160 (99%)	139 (88%)	10 (6%)	9 (6%)	1	0
2	H	158/160 (99%)	136 (86%)	16 (10%)	6 (4%)	3	1
2	J	158/160 (99%)	139 (88%)	10 (6%)	9 (6%)	1	0
2	L	158/160 (99%)	141 (89%)	11 (7%)	6 (4%)	3	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	2872/2922 (98%)	2687 (94%)	135 (5%)	50 (2%)	9 4

5 of 50 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	627	LYS
2	D	635	ASN
2	D	645	ASP
2	F	635	ASN
2	F	645	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%)	273 (96%)	12 (4%)	30 34
1	C	285/287 (99%)	273 (96%)	12 (4%)	30 34
1	E	285/287 (99%)	274 (96%)	11 (4%)	32 38
1	G	285/287 (99%)	271 (95%)	14 (5%)	25 27
1	I	285/287 (99%)	276 (97%)	9 (3%)	39 47
1	K	285/287 (99%)	273 (96%)	12 (4%)	30 34
2	B	136/136 (100%)	129 (95%)	7 (5%)	24 25
2	D	136/136 (100%)	128 (94%)	8 (6%)	19 19
2	F	136/136 (100%)	131 (96%)	5 (4%)	34 40
2	H	136/136 (100%)	129 (95%)	7 (5%)	24 25
2	J	136/136 (100%)	131 (96%)	5 (4%)	34 40
2	L	136/136 (100%)	130 (96%)	6 (4%)	28 32
All	All	2526/2538 (100%)	2418 (96%)	108 (4%)	29 33

5 of 108 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	261	ARG
1	G	115	PHE
1	K	238	LYS
2	F	524	TYR
2	F	644	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 100 such sidechains are listed below:

Mol	Chain	Res	Type
2	F	614	ASN
1	G	187	ASN
1	K	276	HIS
2	F	629	ASN
1	G	35	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	2.05	5 (35%)	17,19,21	0.72	0
3	GAL	M	2	3	11,11,12	2.33	4 (36%)	15,15,17	1.20	1 (6%)
3	SIA	M	3	3	17,20,21	3.10	6 (35%)	21,28,31	3.06	7 (33%)
3	NAG	N	1	3	14,14,15	2.10	5 (35%)	17,19,21	0.85	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GAL	N	2	3	11,11,12	2.27	5 (45%)	15,15,17	1.01	1 (6%)
3	SIA	N	3	3	17,20,21	3.19	6 (35%)	21,28,31	3.08	4 (19%)
3	NAG	O	1	3	14,14,15	1.87	4 (28%)	17,19,21	1.09	1 (5%)
3	GAL	O	2	3	11,11,12	2.79	4 (36%)	15,15,17	1.62	3 (20%)
3	SIA	O	3	3	17,20,21	3.17	6 (35%)	21,28,31	3.04	4 (19%)
3	NAG	P	1	3	14,14,15	2.31	7 (50%)	17,19,21	1.14	1 (5%)
3	GAL	P	2	3	11,11,12	2.45	4 (36%)	15,15,17	1.62	3 (20%)
3	SIA	P	3	3	17,20,21	3.20	6 (35%)	21,28,31	3.07	4 (19%)
3	NAG	Q	1	3	14,14,15	2.09	5 (35%)	17,19,21	0.82	0
3	GAL	Q	2	3	11,11,12	2.19	4 (36%)	15,15,17	0.96	0
3	SIA	Q	3	3	17,20,21	3.21	6 (35%)	21,28,31	3.11	6 (28%)
3	NAG	R	1	3	14,14,15	2.13	6 (42%)	17,19,21	0.86	0
3	GAL	R	2	3	11,11,12	2.26	5 (45%)	15,15,17	1.00	1 (6%)
3	SIA	R	3	3	17,20,21	3.20	6 (35%)	21,28,31	3.05	4 (19%)

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SIA	R	3	3	-	2/14/34/38	0/1/1/1

The worst 5 of 94 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	M	3	SIA	O4-C4	-8.11	1.26	1.43
3	Q	3	SIA	O4-C4	-8.09	1.26	1.43
3	R	3	SIA	O4-C4	-8.05	1.26	1.43
3	N	3	SIA	O4-C4	-7.94	1.26	1.43
3	O	3	SIA	O4-C4	-7.87	1.26	1.43

The worst 5 of 40 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Q	3	SIA	C6-O6-C2	12.59	138.26	111.34
3	N	3	SIA	C6-O6-C2	12.47	138.00	111.34
3	P	3	SIA	C6-O6-C2	12.37	137.81	111.34
3	R	3	SIA	C6-O6-C2	12.37	137.81	111.34
3	O	3	SIA	C6-O6-C2	12.31	137.68	111.34

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	M	3	SIA	C11-C10-N5-C5
3	O	3	SIA	C11-C10-N5-C5
3	Q	3	SIA	C11-C10-N5-C5
3	M	3	SIA	O10-C10-N5-C5
3	O	3	SIA	O10-C10-N5-C5

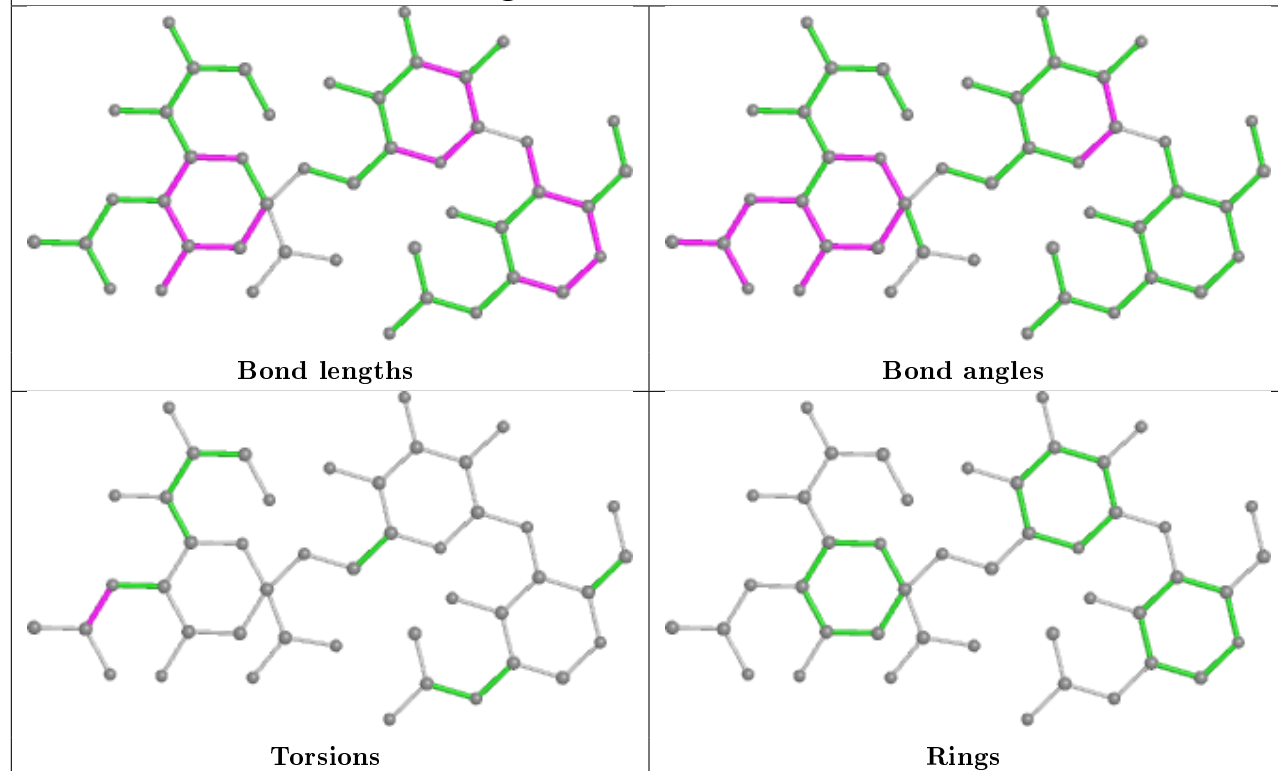
There are no ring outliers.

3 monomers are involved in 2 short contacts:

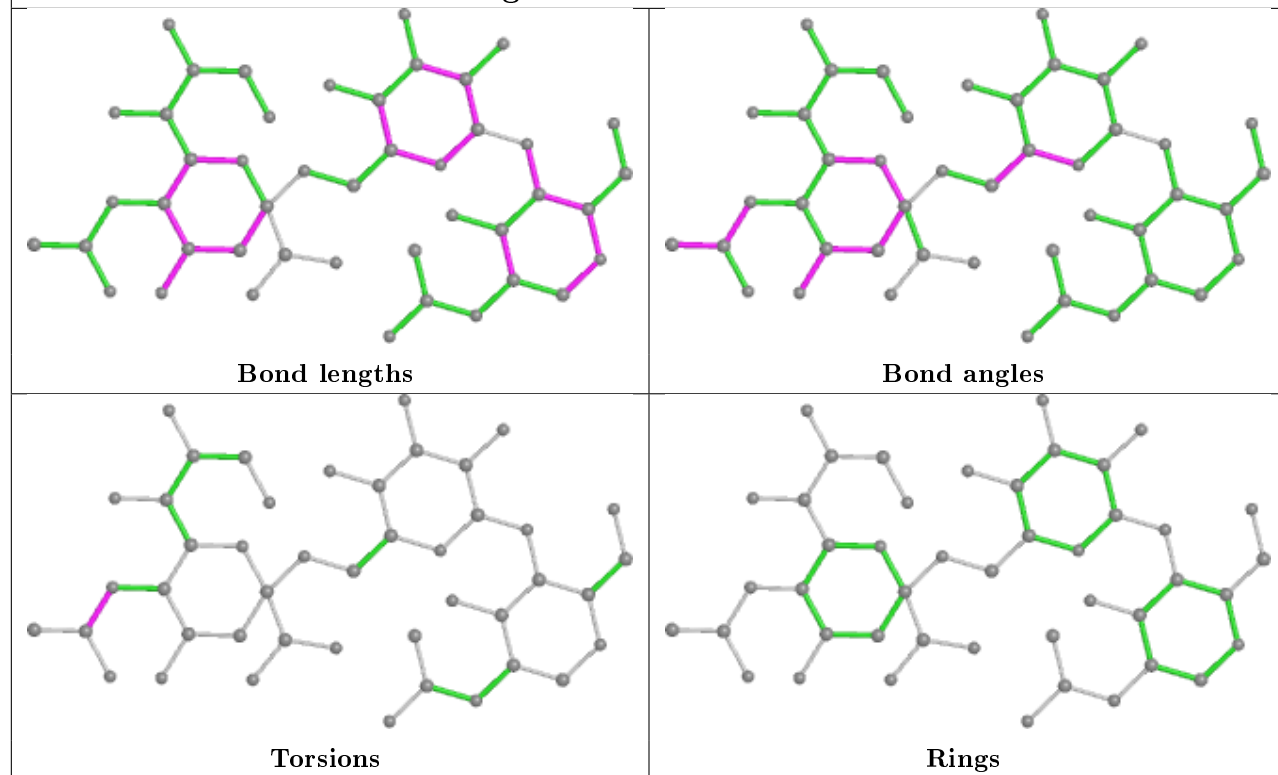
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	P	1	NAG	1	0
3	P	2	GAL	1	0
3	N	3	SIA	1	0

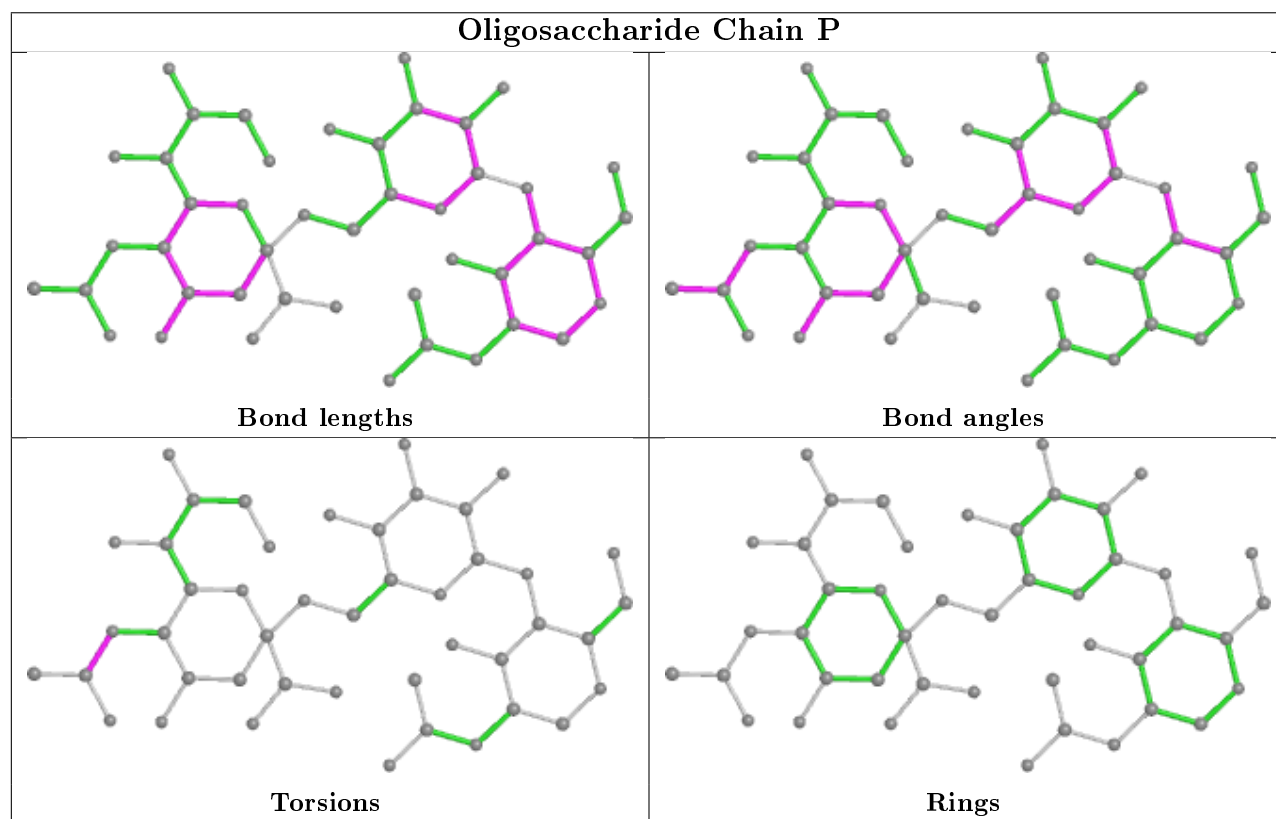
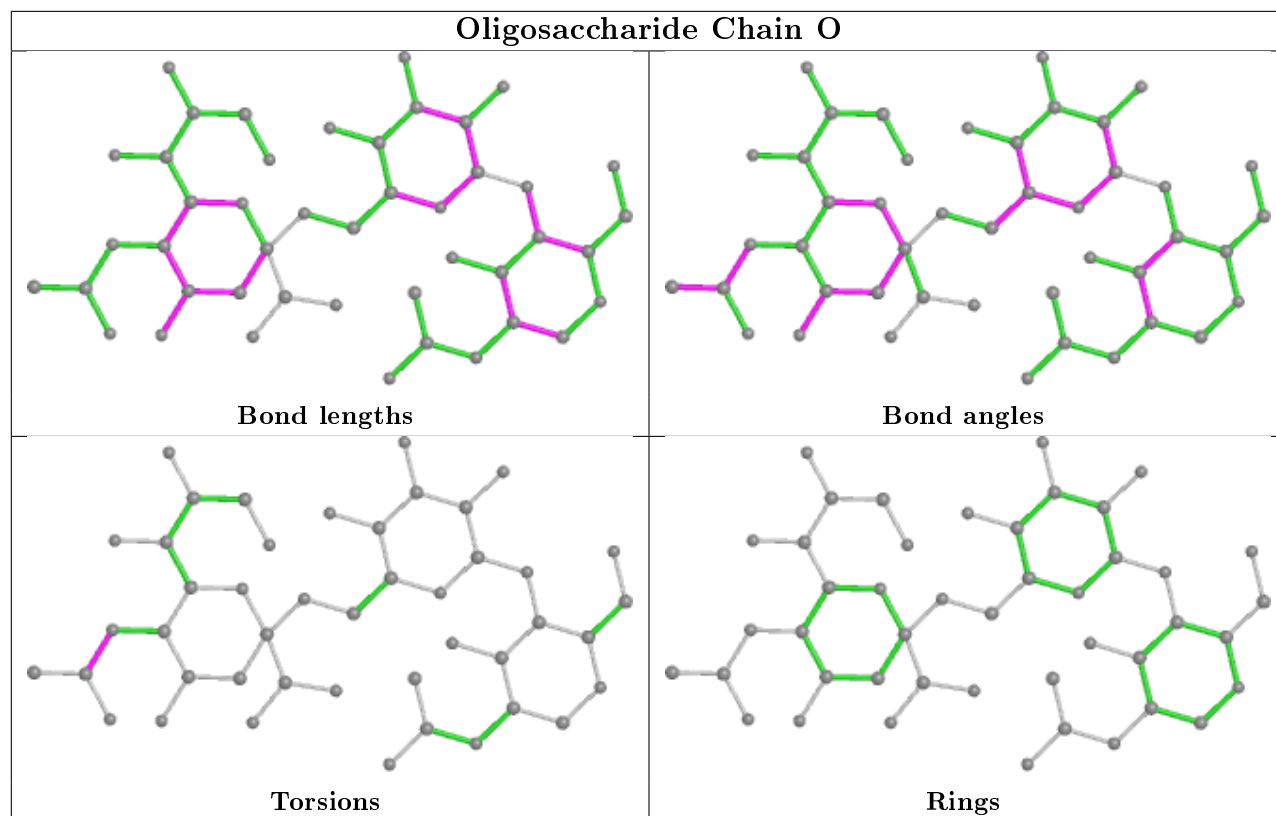
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

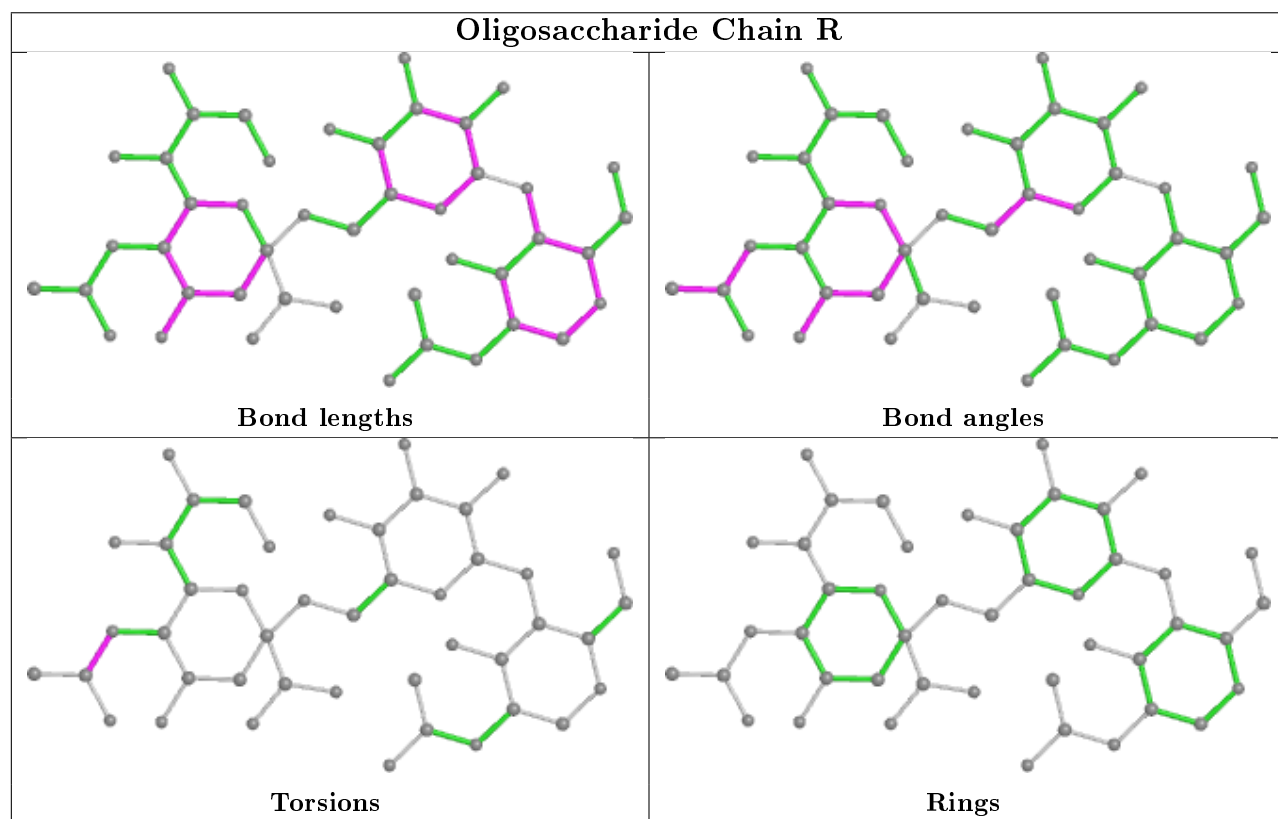
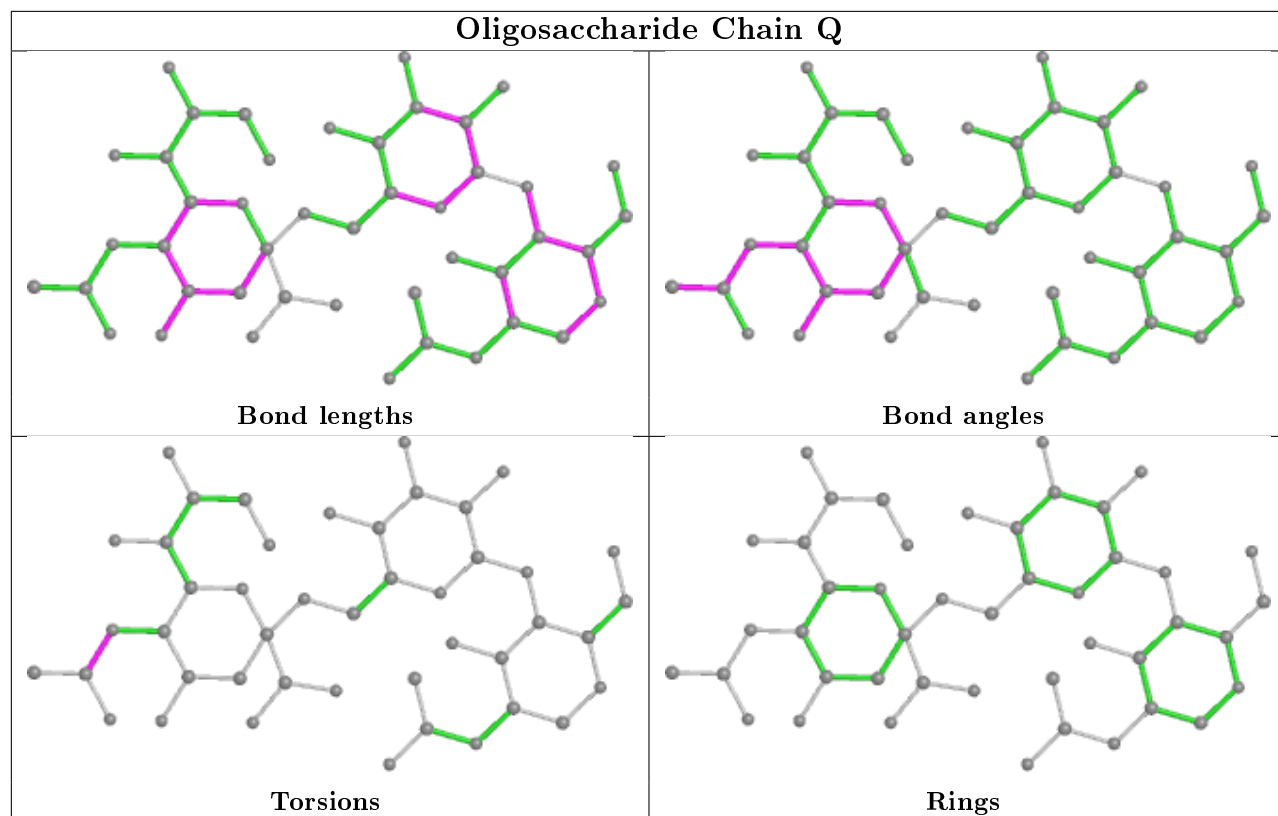
Oligosaccharide Chain M



Oligosaccharide Chain N







5.6 Ligand geometry

3 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	A	3321	-	15,15,15	0.47	0	21,21,21	0.68	0
4	NAG	E	3311	-	15,15,15	0.50	0	21,21,21	0.56	0
4	NAG	F	3331	-	15,15,15	0.48	0	21,21,21	0.60	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	A	3321	-	-	2/6/26/26	0/1/1/1
4	NAG	E	3311	-	-	4/6/26/26	0/1/1/1
4	NAG	F	3331	-	-	4/6/26/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	3321	NAG	C8-C7-N2-C2
4	A	3321	NAG	O7-C7-N2-C2
4	E	3311	NAG	C8-C7-N2-C2
4	E	3311	NAG	O7-C7-N2-C2
4	F	3331	NAG	C8-C7-N2-C2

There are no ring outliers.

3 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	3321	NAG	4	0
4	E	3311	NAG	4	0
4	F	3331	NAG	4	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	E	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	42:ASN	C	44:GLY	N	2.61

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.