wwPDB X-ray Structure Validation Summary Report (i)

Jul 26, 2023 – 04:32 AM EDT

PDB ID	:	1A14
Title	:	COMPLEX BETWEEN NC10 ANTI-INFLUENZA VIRUS NEURAMINIDASE SINGLE CHAIN ANTIBODY WITH A 5 RESIDUE LINKER AND INFLUENZA VIRUS NEURAMINIDASE
Authors	:	Malby, R.L.; Mccoy, A.J.; Kortt, A.A.; Hudson, P.J.; Colman, P.M.
Deposited on	:	1997-12-21
Resolution	:	2.50 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 (i) 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 (i)) were used in the production of this report:

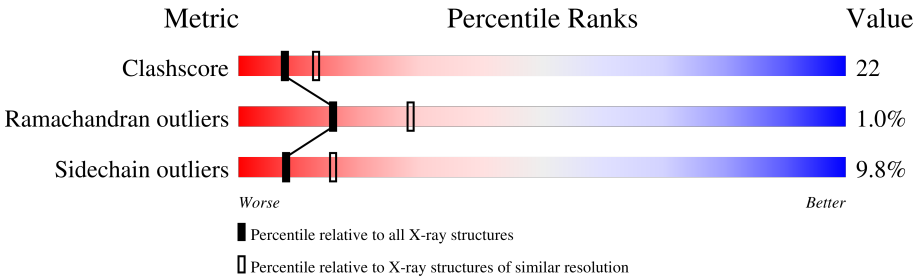
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.34

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.50 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	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)

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 of 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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	N	388	53% 43% .
2	H	120	50% 46% .
3	L	104	59% 37% 5%
4	A	6	83% 17%

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
6	NAG	N	477(A)	X	-	-	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 5124 atoms, of which 212 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 NEURAMINIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	N	388	3067	1914	538	592	23	8	0	0

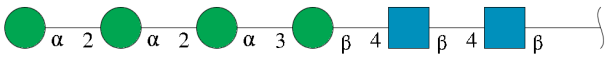
- Molecule 2 is a protein called NC10 FV (HEAVY CHAIN).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
2	H	120	1143	585	212	153	188	5	22	0	0

- Molecule 3 is a protein called NC10 FV (LIGHT CHAIN).

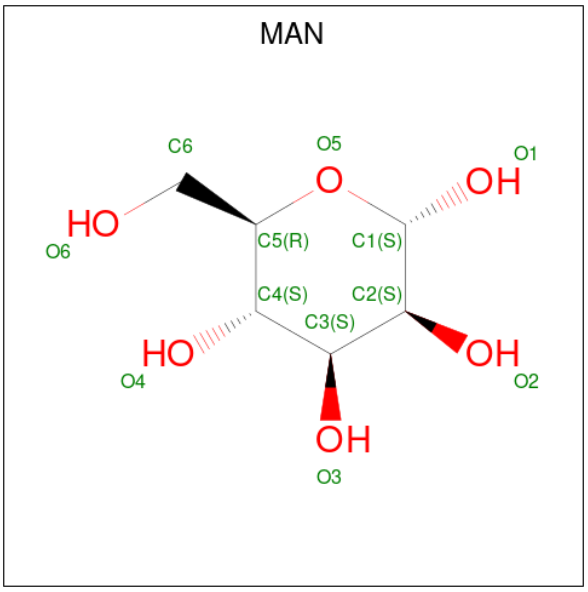
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	L	104	802	499	129	172	2	0	0	0

- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



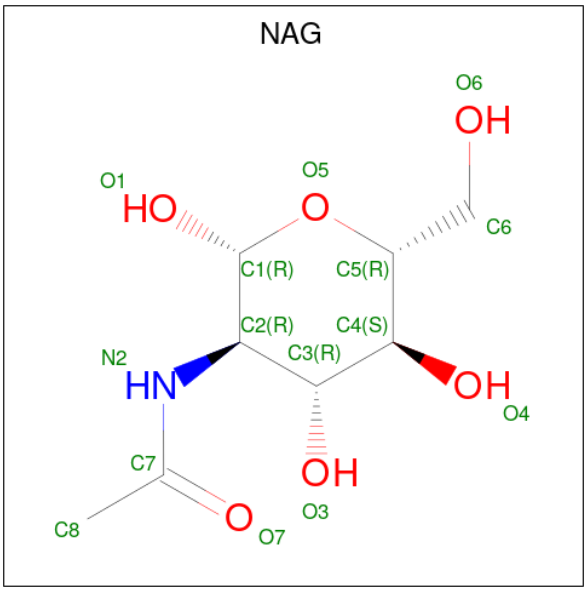
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	A	6	72	40	2	30	0	0	0

- Molecule 5 is alpha-D-mannopyranose (three-letter code: MAN) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	N	1	Total C O 11 6 5	0	0

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	N	1	Total Ca 1 1	0	0

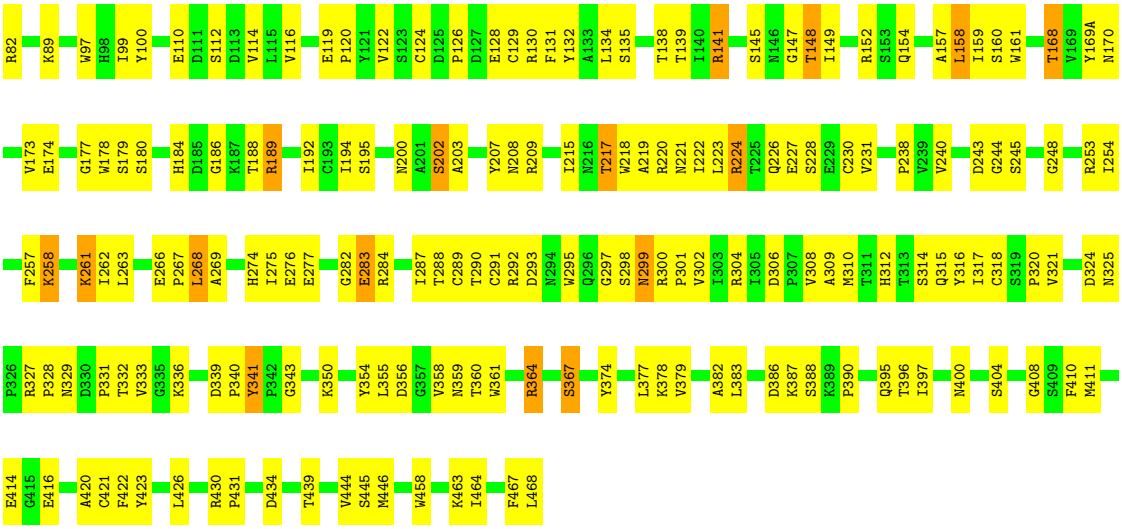
3 Residue-property plots (i)

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.

Note EDS was not executed.

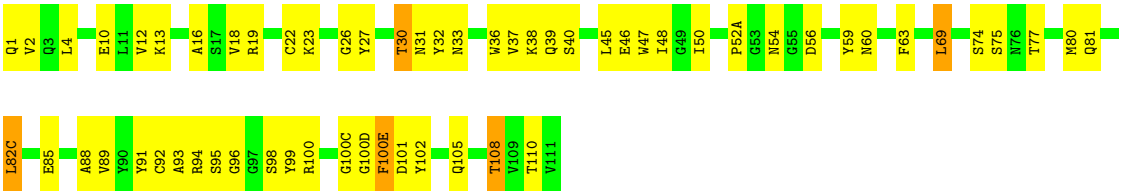
• Molecule 1: NEURAMINIDASE

Chain N:



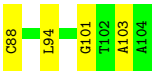
• Molecule 2: NC10 FV (HEAVY CHAIN)

Chain H:



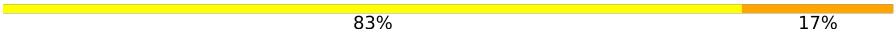
• Molecule 3: NC10 FV (LIGHT CHAIN)

Chain L:



• Molecule 4: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain A:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, α, β, γ	165.30Å 165.30Å 182.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	7.00 – 2.50	Depositor
% Data completeness (in resolution range)	80.0 (7.00-2.50)	Depositor
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.200 , 0.270	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5124	wwPDB-VP
Average B, all atoms (Å^2)	18.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MAN, CA, NAG, BMA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	N	0.73	0/3150	0.93	5/4290 (0.1%)
2	H	0.51	0/954	0.74	0/1290
3	L	0.58	0/818	0.70	0/1113
All	All	0.67	0/4922	0.86	5/6693 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	N	0	2

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	N	189	ARG	NE-CZ-NH1	6.11	123.35	120.30
1	N	189	ARG	NE-CZ-NH2	-6.10	117.25	120.30
1	N	299	ASN	N-CA-C	-5.95	94.94	111.00
1	N	226	GLN	N-CA-C	5.34	125.43	111.00
1	N	439	THR	N-CA-C	-5.20	96.97	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	N	341	TYR	Sidechain
1	N	374	TYR	Sidechain

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	N	3067	0	2892	133	0
2	H	931	212	870	42	0
3	L	802	0	748	34	0
4	A	72	0	60	2	0
5	N	11	0	9	3	0
6	N	28	0	26	0	0
7	N	1	0	0	0	0
All	All	4912	212	4605	208	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 22.

The worst 5 of 208 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)
3:L:39:ASN:HD21	3:L:45:LYS:HD3	1.40	0.86
1:N:283:GLU:HG2	1:N:284:ARG:HG3	1.56	0.85
1:N:168:THR:HG22	1:N:170:ASN:H	1.41	0.84
1:N:141:ARG:NH2	1:N:467:PHE:HA	1.91	0.83
1:N:159:ILE:HG22	1:N:173:VAL:HA	1.60	0.81

There are no symmetry-related clashes.

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	N	386/388 (100%)	354 (92%)	29 (8%)	3 (1%)	19 35
2	H	118/120 (98%)	104 (88%)	13 (11%)	1 (1%)	19 35
3	L	102/104 (98%)	92 (90%)	8 (8%)	2 (2%)	7 12
All	All	606/612 (99%)	550 (91%)	50 (8%)	6 (1%)	15 28

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	N	148	THR
3	L	28	ASP
1	N	295	TRP
1	N	222	ILE
2	H	16	ALA

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 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	N	341/341 (100%)	311 (91%)	30 (9%)	10 19
2	H	98/98 (100%)	86 (88%)	12 (12%)	5 9
3	L	91/91 (100%)	81 (89%)	10 (11%)	6 12
All	All	530/530 (100%)	478 (90%)	52 (10%)	8 15

5 of 52 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	N	464	ILE
2	H	80	MET
3	L	69	THR
1	N	468	LEU
2	H	50	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
2	H	39	GLN
2	H	76	ASN
3	L	38	GLN
1	N	345	ASN
1	N	338	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)

6 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	$\#\|Z\| > 2$
4	NAG	A	1	1,4	14,14,15	1.53	2 (14%)	17,19,21	2.52	5 (29%)
4	NAG	A	2	4	14,14,15	1.53	3 (21%)	17,19,21	1.65	4 (23%)
4	BMA	A	3	4	11,11,12	2.57	3 (27%)	15,15,17	1.93	3 (20%)
4	MAN	A	4	4	11,11,12	2.56	5 (45%)	15,15,17	1.39	2 (13%)
4	MAN	A	5	4	11,11,12	1.75	3 (27%)	15,15,17	2.31	6 (40%)
4	MAN	A	6	4	11,11,12	1.50	2 (18%)	15,15,17	1.92	2 (13%)

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	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	2	4	-	2/6/23/26	0/1/1/1
4	BMA	A	3	4	-	0/2/19/22	0/1/1/1
4	MAN	A	4	4	-	0/2/19/22	0/1/1/1
4	MAN	A	5	4	-	0/2/19/22	0/1/1/1
4	MAN	A	6	4	-	2/2/19/22	0/1/1/1

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	3	BMA	O3-C3	-5.75	1.29	1.43
4	A	4	MAN	C2-C3	-5.69	1.44	1.52
4	A	3	BMA	O5-C5	5.31	1.54	1.43
4	A	5	MAN	C4-C3	3.65	1.61	1.52
4	A	1	NAG	C4-C5	3.49	1.60	1.53

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1	NAG	C8-C7-N2	-6.70	104.75	116.10
4	A	6	MAN	C1-O5-C5	6.26	120.68	112.19
4	A	5	MAN	C1-O5-C5	6.14	120.51	112.19
4	A	1	NAG	O7-C7-C8	5.00	131.35	122.06
4	A	3	BMA	O5-C5-C6	4.70	114.57	107.20

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	2	NAG	O5-C5-C6-O6
4	A	2	NAG	C4-C5-C6-O6
4	A	6	MAN	O5-C5-C6-O6
4	A	6	MAN	C4-C5-C6-O6

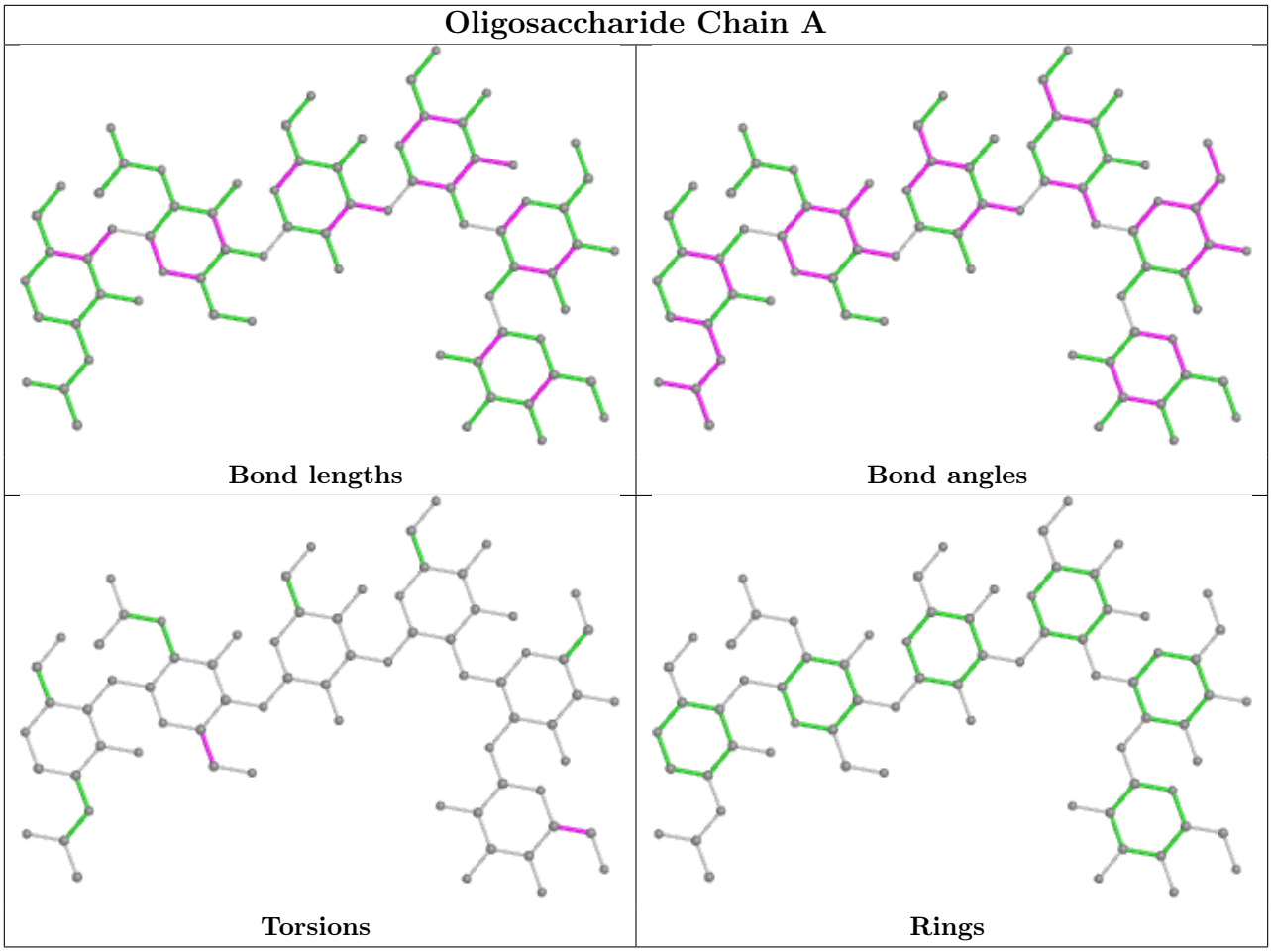
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	3	BMA	2	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)

Of 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	MAN	N	475(G)	-	11,11,12	2.57	5 (45%)	15,15,17	2.96	8 (53%)
6	NAG	N	477(A)	1	14,14,15	2.93	6 (42%)	17,19,21	2.88	5 (29%)
6	NAG	N	476(A)	1	14,14,15	1.71	4 (28%)	17,19,21	1.63	4 (23%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	MAN	N	475(G)	-	-	2/2/19/22	0/1/1/1
6	NAG	N	477(A)	1	1/1/5/7	1/6/23/26	0/1/1/1
6	NAG	N	476(A)	1	-	1/6/23/26	0/1/1/1

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	N	477(A)	NAG	C1-C2	6.56	1.62	1.52
6	N	477(A)	NAG	O5-C1	5.51	1.52	1.43
5	N	475(G)	MAN	O5-C1	4.90	1.51	1.43
6	N	477(A)	NAG	C8-C7	4.39	1.59	1.50
5	N	475(G)	MAN	C1-C2	4.25	1.61	1.52

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	N	477(A)	NAG	C1-C2-N2	8.10	124.32	110.49
5	N	475(G)	MAN	C3-C4-C5	5.74	120.48	110.24
6	N	477(A)	NAG	C1-O5-C5	5.21	119.26	112.19
5	N	475(G)	MAN	O2-C2-C1	4.98	119.33	109.15
5	N	475(G)	MAN	O4-C4-C3	-4.55	99.83	110.35

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	N	477(A)	NAG	C1

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	N	475(G)	MAN	O5-C5-C6-O6
5	N	475(G)	MAN	C4-C5-C6-O6
6	N	477(A)	NAG	O5-C5-C6-O6
6	N	476(A)	NAG	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	N	475(G)	MAN	3	0

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 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.