WORLDWIDE wwPDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

Oct 5, 2024 – 07:32 AM EDT

PDB ID	:	1NCA
Title	:	REFINED CRYSTAL STRUCTURE OF THE INFLUENZA VIRUS N9 NEURAMINIDASE-NC41 FAB COMPLEX
Authors	:	Tulip, W.R.; Varghese, J.N.; Colman, P.M.
Deposited on	:	1992-01-21
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:

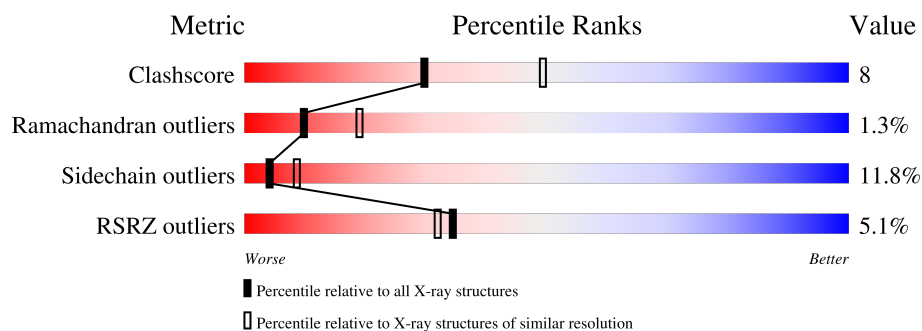|		
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 2.50 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	Percentile Ranks	Value
Clashscore		8
Ramachandran outliers		1.3%
Sidechain outliers		11.8%
RSRZ outliers		5.1%

Worse ... *Better*

▮ Percentile relative to all X-ray structures
〖 Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	180529	6282 (2.50-2.50)
Ramachandran outliers	177936	6191 (2.50-2.50)
Sidechain outliers	177891	6193 (2.50-2.50)
RSRZ outliers	164620	5504 (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% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	N	389	2% / 67% / 26% / 6% ·
2	L	214	7% / 64% / 28% / 7% ·
3	H	221	9% / 65% / 29% / 5% ·
4	A	6	100%

2 Entry composition ⓘ

There are 7 unique types of molecules in this entry. The entry contains 6577 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 INFLUENZA A SUBTYPE N9 NEURAMINIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	N	389	Total 3075	C 1920	N 539	O 593	S 23	0	0	0

- Molecule 2 is a protein called IGG2A-KAPPA NC41 FAB (LIGHT CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	214	Total 1667	C 1043	N 280	O 336	S 8	0	0	0

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	20	THR	SER	conflict	EMBL Y11589
L	21	ILE	VAL	conflict	EMBL Y11589
L	28	ASP	ILE	conflict	EMBL Y11589
L	30	SER	GLY	conflict	EMBL Y11589
L	32	ALA	ASN	conflict	EMBL Y11589
L	34	VAL	ALA	conflict	EMBL Y11589
L	46	LEU	ALA	conflict	EMBL Y11589
L	50	TRP	SER	conflict	EMBL Y11589
L	53	THR	TYR	conflict	EMBL Y11589
L	55	HIS	TYR	conflict	EMBL Y11589
L	56	ILE	SER	conflict	EMBL Y11589
L	63	ALA	THR	conflict	EMBL Y11589
L	71	TYR	PHE	conflict	EMBL Y11589
L	77	SER	ASN	conflict	EMBL Y11589
L	80	ALA	SER	conflict	EMBL Y11589
L	85	LEU	GLU	conflict	EMBL Y11589
L	87	TYR	PHE	conflict	EMBL Y11589
L	91	HIS	TYR	conflict	EMBL Y11589
L	92	TYR	ASN	conflict	EMBL Y11589
L	93	SER	ARG	conflict	EMBL Y11589

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
L	94	PRO	TYR	conflict	EMBL Y11589

- Molecule 3 is a protein called IGG2A-KAPPA NC41 FAB (HEAVY CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	221	Total 1662	C 1048	N 273	O 334	S 7	0	0	0

- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyran ose-(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.
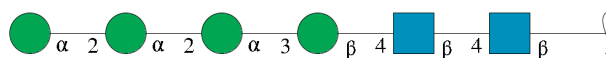
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	A	6	Total 72	C 40	N 2	O 30	0	0	0

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).
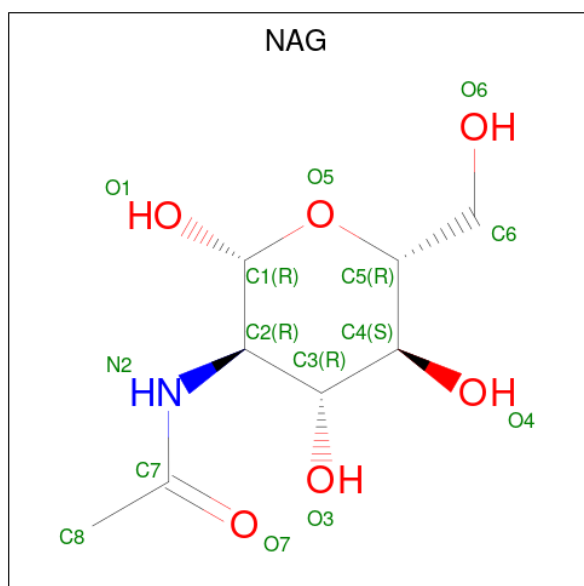
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	N	1	Total 14	C 8	N 1	O 5	0	0

Continued on next page...

Continued from previous page...

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

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 7 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	N	66	Total 66	O 66	0	0
7	L	2	Total 2	O 2	0	0
7	H	4	Total 4	O 4	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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). 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: INFLUENZA A SUBTYPE N9 NEURAMINIDASE
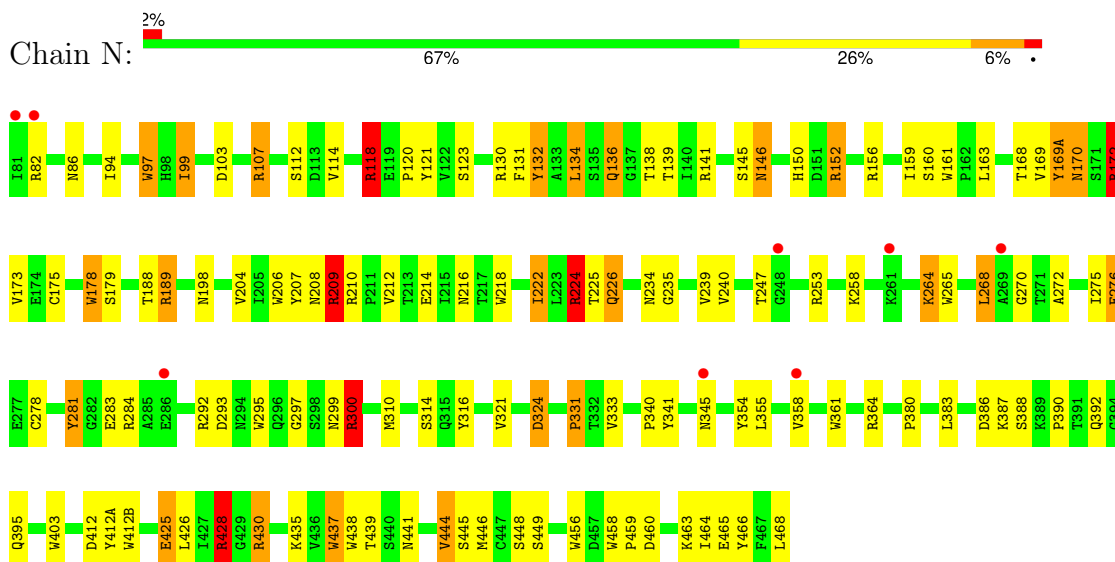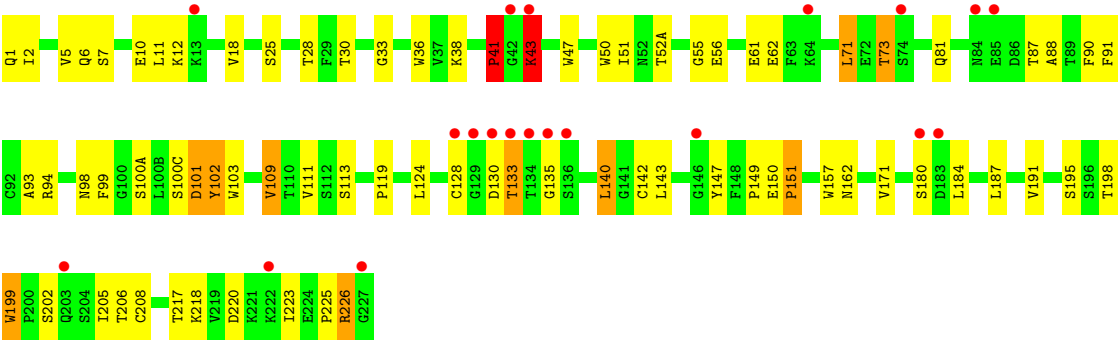
Chain N:

• Molecule 2: IGG2A-KAPPA NC41 FAB (LIGHT CHAIN)
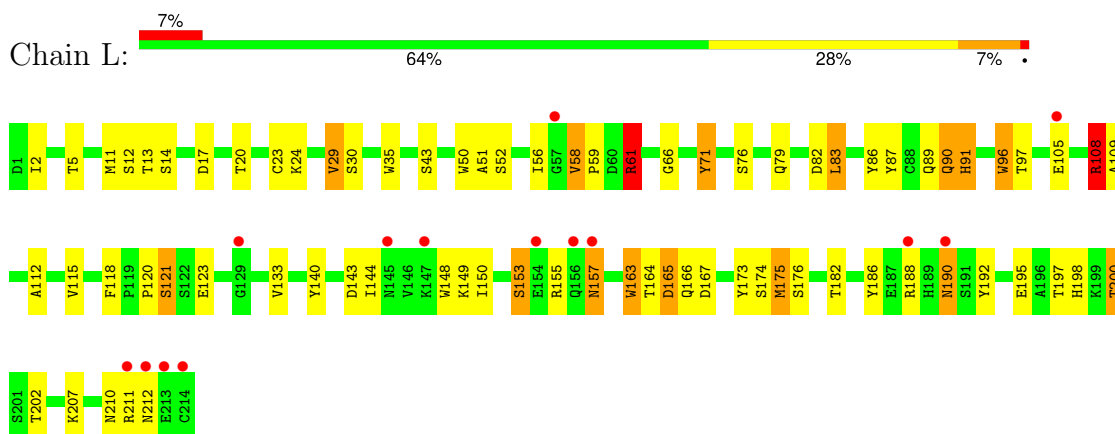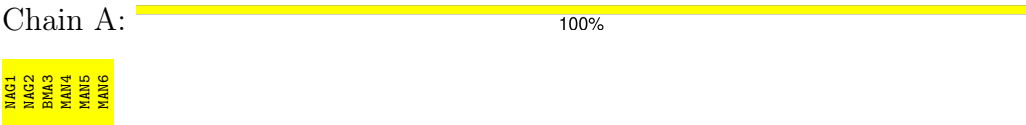
Chain L:

• Molecule 3: IGG2A-KAPPA NC41 FAB (HEAVY CHAIN)

Chain H:

● Molecule 4: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyran ose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetam ido-2-deoxy-beta-D-glucopyranose

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 4 21 2	Depositor
Cell constants a, b, c, α, β, γ	167.00Å 167.00Å 124.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.50 8.00 – 2.90	Depositor EDS
% Data completeness (in resolution range)	(Not available) (8.00-2.50) 47.5 (8.00-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$	-	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.191 , (Not available) 0.199 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	26.5	Xtriage
Anisotropy	0.118	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.17 , 30.3	EDS
L-test for twinning[1]	$<|L|> = 0.34, <L^2> = 0.17$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.84	EDS
Total number of atoms	6577	wwPDB-VP
Average B, all atoms (Å^2)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.63% of the height of the origin peak. No significant pseudotranslation is detected.*

---

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	1.04	1/3158 (0.0%)	1.93	106/4301 (2.5%)
2	L	0.88	0/1708	1.81	36/2323 (1.5%)
3	H	0.89	0/1704	1.69	28/2323 (1.2%)
All	All	0.96	1/6570 (0.0%)	1.84	170/8947 (1.9%)

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	7
2	L	0	3
All	All	0	10

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	425	GLU	CD-OE2	-5.47	1.19	1.25

The worst 5 of 170 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	N	300	ARG	NE-CZ-NH2	-15.62	112.49	120.30
1	N	107	ARG	CD-NE-CZ	-14.89	102.75	123.60
1	N	118	ARG	NE-CZ-NH2	-13.96	113.32	120.30
1	N	300	ARG	NE-CZ-NH1	12.80	126.70	120.30
1	N	430	ARG	NE-CZ-NH2	-12.63	113.99	120.30

There are no chirality outliers.

5 of 10 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	N	107	ARG	Sidechain
1	N	118	ARG	Sidechain
1	N	172	ARG	Sidechain
1	N	209	ARG	Sidechain
1	N	224	ARG	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	3075	0	2903	51	0
2	L	1667	0	1598	23	0
3	H	1662	0	1611	28	0
4	A	72	0	61	0	0
5	N	28	0	26	0	0
6	N	1	0	0	0	0
7	H	4	0	0	0	0
7	L	2	0	0	0	0
7	N	66	0	0	2	0
All	All	6577	0	6199	100	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 8.

The worst 5 of 100 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:H:150:GLU:HG2	3:H:151:PRO:HA	1.58	0.85
3:H:87:THR:HG22	3:H:111:VAL:H	1.44	0.83
3:H:11:LEU:HD22	3:H:149:PRO:HG3	1.61	0.80
1:N:146:ASN:OD1	1:N:437:TRP:HB3	1.83	0.77
2:L:112:ALA:HB2	2:L:200:THR:HG21	1.72	0.70

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	387/389 (100%)	362 (94%)	23 (6%)	2 (0%)	25	44
2	L	212/214 (99%)	197 (93%)	14 (7%)	1 (0%)	25	44
3	H	219/221 (99%)	195 (89%)	16 (7%)	8 (4%)	2	3
All	All	818/824 (99%)	754 (92%)	53 (6%)	11 (1%)	10	19

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	H	43	LYS
3	H	102	TYR
3	H	226	ARG
3	H	41	PRO
3	H	128	CYS

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	N	342/342 (100%)	313 (92%)	29 (8%)	8	18
2	L	190/190 (100%)	161 (85%)	29 (15%)	2	4
3	H	187/187 (100%)	160 (86%)	27 (14%)	2	5
All	All	719/719 (100%)	634 (88%)	85 (12%)	4	9

5 of 85 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	L	212	ASN
3	H	113	SER
3	H	5	VAL
3	H	61	GLU
3	H	151	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
3	H	98	ASN
3	H	79	ASN
1	N	441	ASN
3	H	53	ASN
1	N	395	GLN

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 ⓘ

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	0.57	0	17,19,21	1.18	1 (5%)
4	NAG	A	2	4	14,14,15	1.08	1 (7%)	17,19,21	1.34	1 (5%)
4	BMA	A	3	4	11,11,12	1.06	1 (9%)	15,15,17	1.25	2 (13%)
4	MAN	A	4	4	11,11,12	0.33	0	15,15,17	1.10	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
4	MAN	A	5	4	11,11,12	0.65	0	15,15,17	0.94	1 (6%)
4	MAN	A	6	4	11,11,12	0.83	0	15,15,17	1.66	1 (6%)

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	2	NAG	C4-C3	2.42	1.58	1.52
4	A	3	BMA	C6-C5	2.03	1.58	1.51

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	6	MAN	C1-O5-C5	6.00	120.23	112.19
4	A	2	NAG	C4-C3-C2	-3.17	106.37	111.02
4	A	3	BMA	C6-C5-C4	2.97	120.31	113.02
4	A	3	BMA	O5-C5-C4	-2.30	105.23	110.83
4	A	1	NAG	C1-C2-N2	-2.19	106.98	110.43

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	3	BMA	C4-C5-C6-O6
4	A	3	BMA	O5-C5-C6-O6
4	A	6	MAN	O5-C5-C6-O6
4	A	6	MAN	C4-C5-C6-O6
4	A	4	MAN	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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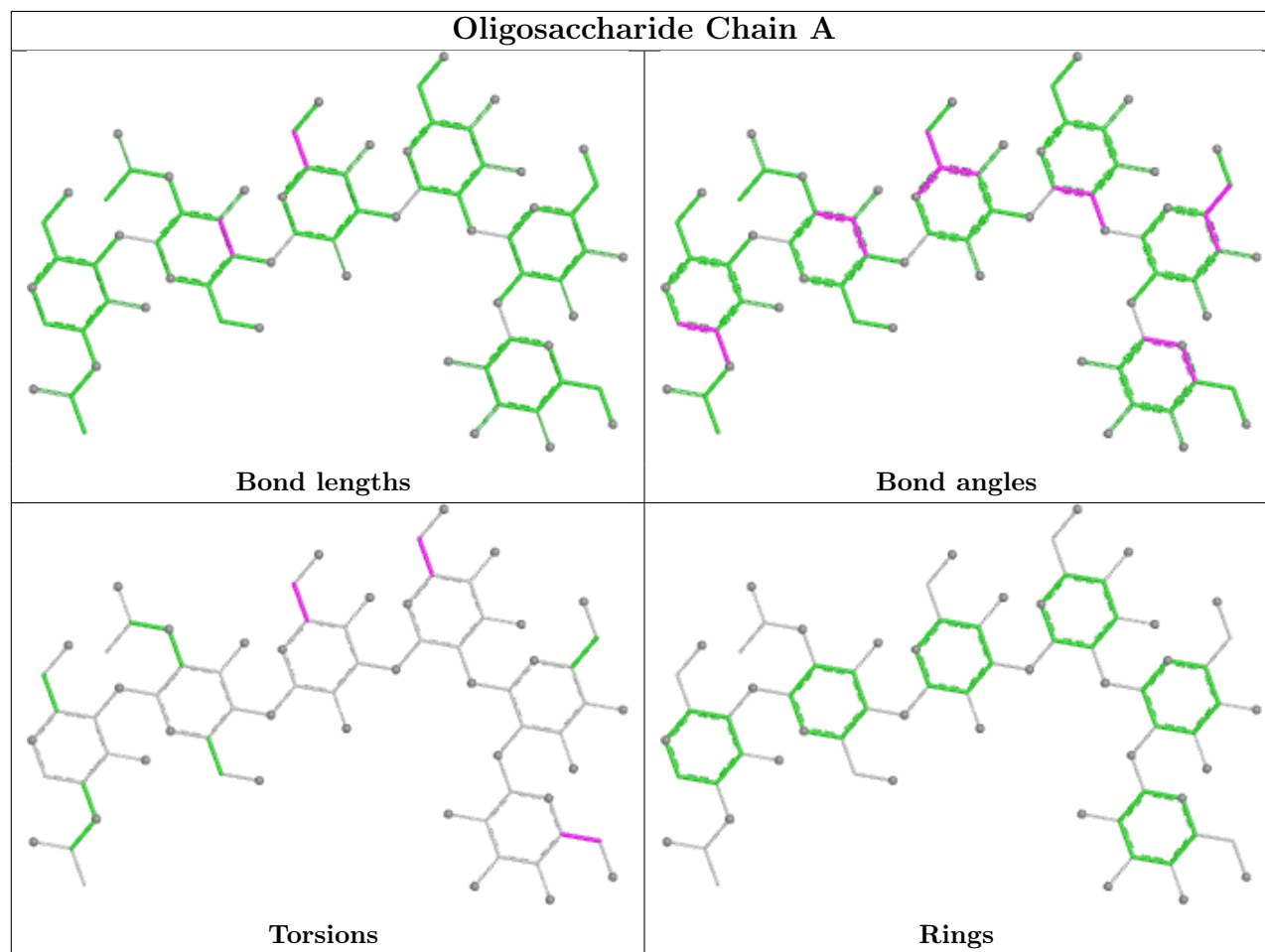
5.6 Ligand geometry ⓘ

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 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	NAG	N	475(A)	1	14,14,15	0.97	0	17,19,21	1.42	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
5	NAG	N	476(A)	1	14,14,15	1.21	1 (7%)	17,19,21	1.91	5 (29%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	N	475(A)	1	-	1/6/23/26	0/1/1/1
5	NAG	N	476(A)	1	-	3/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	N	476(A)	NAG	C1-C2	3.75	1.57	1.52

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	N	476(A)	NAG	C4-C3-C2	-5.35	103.18	111.02
5	N	475(A)	NAG	C1-O5-C5	3.85	117.35	112.19
5	N	476(A)	NAG	C8-C7-N2	3.15	121.34	116.12
5	N	475(A)	NAG	C1-C2-N2	2.64	114.59	110.43
5	N	476(A)	NAG	O3-C3-C4	2.61	116.52	110.38

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	N	476(A)	NAG	C1-C2-N2-C7
5	N	476(A)	NAG	O5-C5-C6-O6
5	N	475(A)	NAG	O5-C5-C6-O6
5	N	476(A)	NAG	C3-C2-N2-C7

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

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 ⓘ

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	N	389/389 (100%)	-0.27	8 (2%)	63	60	2, 7, 23, 48	5 (1%)
2	L	214/214 (100%)	0.42	14 (6%)	26	24	1, 26, 43, 48	11 (5%)
3	H	221/221 (100%)	0.72	20 (9%)	17	15	1, 25, 39, 45	22 (9%)
All	All	824/824 (100%)	0.18	42 (5%)	34	32	1, 16, 39, 48	38 (4%)

The worst 5 of 42 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	H	42	GLY	16.6
3	H	133	THR	13.5
3	H	180	SER	11.1
2	L	212	ASN	10.3
3	H	130	ASP	10.0

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

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

6.3 Carbohydrates ⓘ

SUGAR-RSR INFOmissingINFO

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
5	NAG	N	476(A)	14/15	0.77	0.16	40,44,54,57	0
5	NAG	N	475(A)	14/15	0.90	0.11	38,41,43,43	0
6	CA	N	1	1/1	0.93	0.11	85,85,85,85	0

6.5 Other polymers ⓘ

There are no such residues in this entry.