



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 6, 2020 – 10:05 AM BST

PDB ID : 1QFU
Title : INFLUENZA VIRUS HEMAGGLUTININ COMPLEXED WITH A NEUTRALIZING ANTIBODY
Authors : Fleury, D.; Gigant, B.; Bizebard, T.; Daniels, R.S.; Skehel, J.J.; Knossow, M.
Deposited on : 1999-04-14
Resolution : 2.80 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

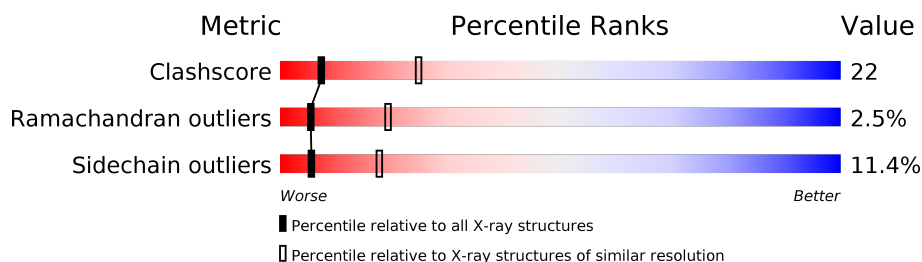
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)

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	328	
2	B	175	
3	L	217	
4	H	223	
5	C	2	
6	D	3	

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 7439 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 PROTEIN (HEMAGGLUTININ (HA1 CHAIN)).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	318	Total	C	N	O	S	0	0	1
			2447	1532	430	472	13			

- Molecule 2 is a protein called PROTEIN (HEMAGGLUTININ (HA2 CHAIN)).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	174	Total	C	N	O	S	0	0	1
			1408	874	248	280	6			

- Molecule 3 is a protein called PROTEIN (IMMUNOGLOBULIN IGG1-KAPPA ANTIBODY (LIGHT CHAIN)).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	217	Total	C	N	O	S	0	0	0
			1687	1056	289	336	6			

- Molecule 4 is a protein called PROTEIN (IMMUNOGLOBULIN IGG1-KAPPA ANTIBODY (HEAVY CHAIN)).

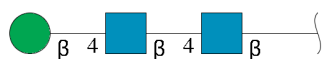
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	223	Total	C	N	O	S	0	0	0
			1718	1089	281	340	8			

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-alpha-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



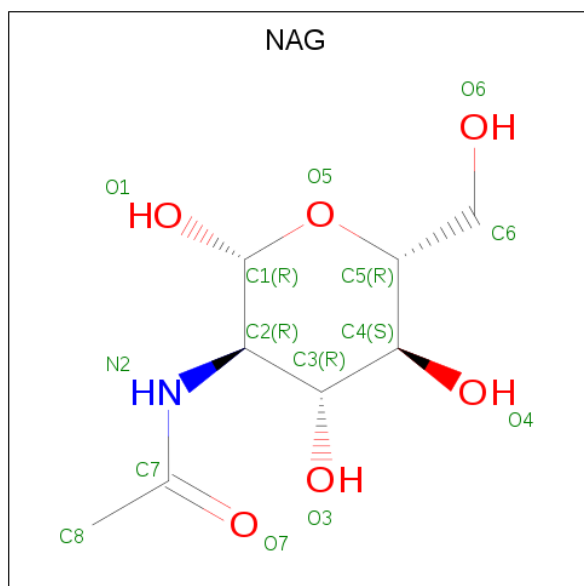
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	C	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 6 is an oligosaccharide called 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
6	D	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 8 is water.

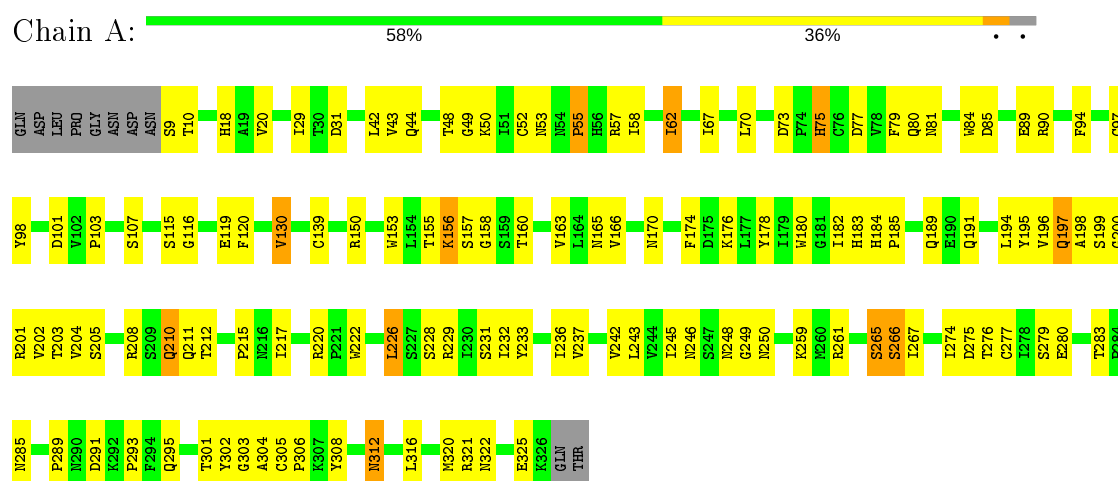
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	28	Total 28	O 28	0	0
8	B	30	Total 30	O 30	0	0
8	L	3	Total 3	O 3	0	0
8	H	9	Total 9	O 9	0	0

3 Residue-property plots

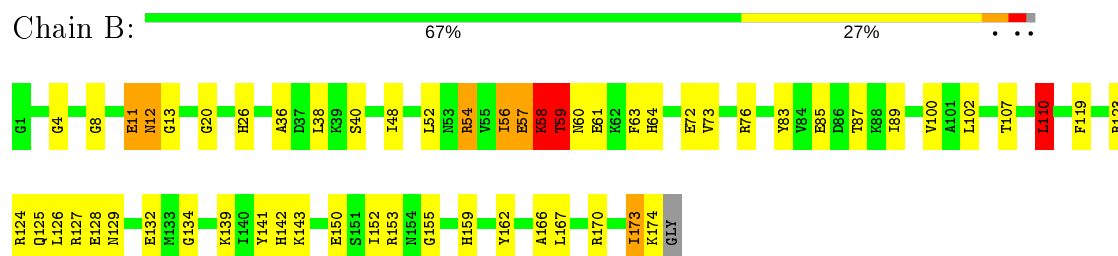
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

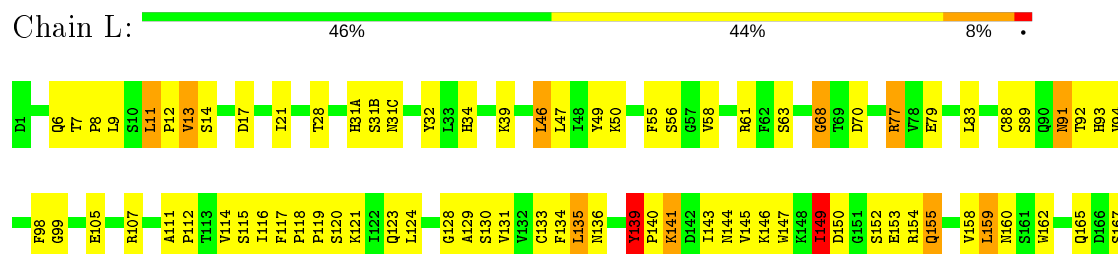
- Molecule 1: PROTEIN (HEMAGGLUTININ (HA1 CHAIN))

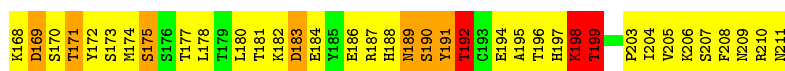


- Molecule 2: PROTEIN (HEMAGGLUTININ (HA2 CHAIN))

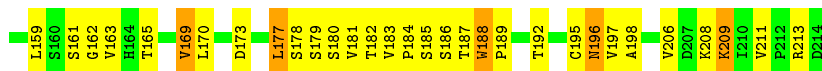
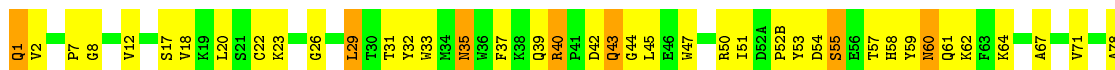


- Molecule 3: PROTEIN (IMMUNOGLOBULIN IGG1-KAPPA ANTIBODY (LIGHT CHAIN))





● Molecule 4: PROTEIN (IMMUNOGLOBULIN IGG1-KAPPA ANTIBODY (HEAVY CHAIN))



● Molecule 5: 2-acetamido-2-deoxy-alpha-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



● Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants a, b, c, α , β , γ	138.00Å 138.00Å 135.00Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	7.00 – 2.80	Depositor
% Data completeness (in resolution range)	98.0 (7.00-2.80)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.84	Depositor
R, R_{free}	0.198 , 0.284	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7439	wwPDB-VP
Average B, all atoms (Å ²)	44.0	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: BMA, NAG, NDG

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	0.52	0/2503	0.80	1/3412 (0.0%)
2	B	0.63	0/1432	0.83	2/1925 (0.1%)
3	L	0.49	0/1726	0.83	2/2342 (0.1%)
4	H	0.54	1/1764 (0.1%)	0.84	2/2413 (0.1%)
All	All	0.54	1/7425 (0.0%)	0.82	7/10092 (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
3	L	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	92	CYS	CB-SG	-6.64	1.71	1.82

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	177	LEU	CA-CB-CG	6.82	130.98	115.30
1	A	197	GLN	N-CA-C	5.64	126.22	111.00
2	B	58	LYS	N-CA-C	5.55	126.00	111.00
3	L	152	SER	N-CA-C	5.53	125.93	111.00
4	H	161	SER	N-CA-C	5.12	124.83	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	L	139	TYR	Sidechain
3	L	191	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	A	2447	0	2393	95	0
2	B	1408	0	1329	49	0
3	L	1687	0	1640	112	0
4	H	1718	0	1680	104	0
5	C	28	0	24	0	0
6	D	39	0	34	0	0
7	A	28	0	26	0	0
7	B	14	0	13	1	0
8	A	28	0	0	1	0
8	B	30	0	0	3	0
8	H	9	0	0	1	0
8	L	3	0	0	0	0
All	All	7439	0	7139	324	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 324 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:194:GLU:HG3	3:L:205:VAL:HG22	1.34	1.08
3:L:189:ASN:HD21	3:L:209:ASN:HA	1.21	1.04
1:A:53:ASN:OD1	1:A:276:THR:HA	1.72	0.87
3:L:8:PRO:HG3	3:L:11:LEU:HD23	1.56	0.87
3:L:189:ASN:ND2	3:L:209:ASN:HA	1.93	0.84

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	316/328 (96%)	285 (90%)	29 (9%)	2 (1%)	25	56
2	B	172/175 (98%)	150 (87%)	17 (10%)	5 (3%)	4	15
3	L	215/217 (99%)	184 (86%)	21 (10%)	10 (5%)	2	7
4	H	221/223 (99%)	188 (85%)	27 (12%)	6 (3%)	5	17
All	All	924/943 (98%)	807 (87%)	94 (10%)	23 (2%)	5	19

5 of 23 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	59	THR
2	B	173	ILE
3	L	190	SER
3	L	198	LYS
4	H	185	SER

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	A	279/289 (96%)	257 (92%)	22 (8%)	12	34
2	B	148/149 (99%)	138 (93%)	10 (7%)	16	42
3	L	195/195 (100%)	166 (85%)	29 (15%)	3	9
4	H	197/197 (100%)	165 (84%)	32 (16%)	2	7
All	All	819/830 (99%)	726 (89%)	93 (11%)	5	18

5 of 93 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	L	91	ASN
3	L	180	LEU
4	H	163	VAL
3	L	107	ARG
3	L	155	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 25 such sidechains are listed below:

Mol	Chain	Res	Type
3	L	27	GLN
3	L	93	HIS
4	H	105	GLN
3	L	34	HIS
3	L	156	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 ⓘ

5 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	$\# Z > 2$
5	NAG	C	1	1,5	14,14,15	1.07	2 (14%)	17,19,21	2.36	4 (23%)
5	NDG	C	2	5	14,14,15	2.57	3 (21%)	17,19,21	3.02	5 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	D	1	1,6	14,14,15	0.98	1 (7%)	17,19,21	1.70	5 (29%)
6	NAG	D	2	6	14,14,15	0.81	1 (7%)	17,19,21	1.05	1 (5%)
6	BMA	D	3	6	11,11,12	1.27	1 (9%)	15,15,17	1.42	3 (20%)

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	C	1	1,5	-	2/6/23/26	0/1/1/1
5	NDG	C	2	5	-	2/6/23/26	0/1/1/1
6	NAG	D	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	D	2	6	-	0/6/23/26	0/1/1/1
6	BMA	D	3	6	-	0/2/19/22	0/1/1/1

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	2	NDG	C1-C2	7.71	1.63	1.52
5	C	2	NDG	O5-C1	3.66	1.49	1.43
6	D	3	BMA	C4-C5	2.55	1.58	1.53
5	C	2	NDG	C4-C5	2.50	1.58	1.53
6	D	2	NAG	C4-C5	-2.50	1.47	1.53

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	2	NDG	C1-O5-C5	9.18	124.64	112.19
5	C	1	NAG	C1-O5-C5	7.35	122.15	112.19
5	C	2	NDG	C6-C5-C4	5.37	125.57	113.00
5	C	2	NDG	C1-C2-N2	4.03	117.38	110.49
5	C	1	NAG	C6-C5-C4	3.95	122.25	113.00

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	1	NAG	C4-C5-C6-O6
5	C	2	NDG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	C	2	NDG	C4-C5-C6-O6
5	C	1	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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
7	NAG	A	430	1	14,14,15	1.74	4 (28%)	17,19,21	1.43	4 (23%)
7	NAG	A	460	1	14,14,15	1.79	4 (28%)	17,19,21	2.71	7 (41%)
7	NAG	B	410	2	14,14,15	1.49	2 (14%)	17,19,21	2.01	3 (17%)

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
7	NAG	A	430	1	-	0/6/23/26	0/1/1/1
7	NAG	A	460	1	-	2/6/23/26	0/1/1/1
7	NAG	B	410	2	-	0/6/23/26	0/1/1/1

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	430	NAG	C1-C2	-3.99	1.46	1.52
7	B	410	NAG	C1-C2	3.60	1.57	1.52
7	A	460	NAG	C1-C2	3.56	1.57	1.52
7	A	460	NAG	O5-C1	-3.40	1.38	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	430	NAG	O5-C1	-3.26	1.38	1.43

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	460	NAG	C1-O5-C5	7.18	121.92	112.19
7	B	410	NAG	C1-O5-C5	6.23	120.63	112.19
7	A	460	NAG	O5-C5-C6	-5.25	98.97	107.20
7	A	430	NAG	C3-C4-C5	3.51	116.50	110.24
7	A	460	NAG	O7-C7-C8	-3.29	115.95	122.06

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	460	NAG	O5-C5-C6-O6
7	A	460	NAG	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	410	NAG	1	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.