



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 21, 2026 – 04:09 pm BST

PDB ID : 9T26 / pdb_00009t26
Title : Plant HSL3/NUT receptor in complex with disulfide-stabilized CT-NIP4/SCREW2 peptide
Authors : Jimenez Sandoval, P.; Santiago, J.
Deposited on : 2025-10-22
Resolution : 2.12 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

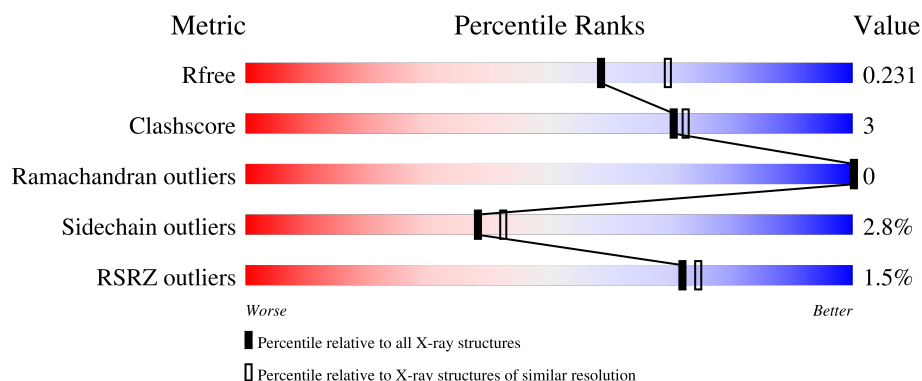
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.12 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))
R_{free}	180053	8290 (2.14-2.10)
Clashscore	190562	8817 (2.14-2.10)
Ramachandran outliers	187476	8738 (2.14-2.10)
Sidechain outliers	187428	8739 (2.14-2.10)
RSRZ outliers	180081	8294 (2.14-2.10)

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 $\leq 5\%$. 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	A	594	2% 88% 11%
2	B	25	84% 16%
3	C	2	100%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10044 atoms, of which 4873 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 Kinase family with leucine-rich repeat domain-containing protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	594	Total	C	H	N	O	S	148	0	0
			9018	2896	4476	736	897	13			

- Molecule 2 is a protein called Transmembrane protein.

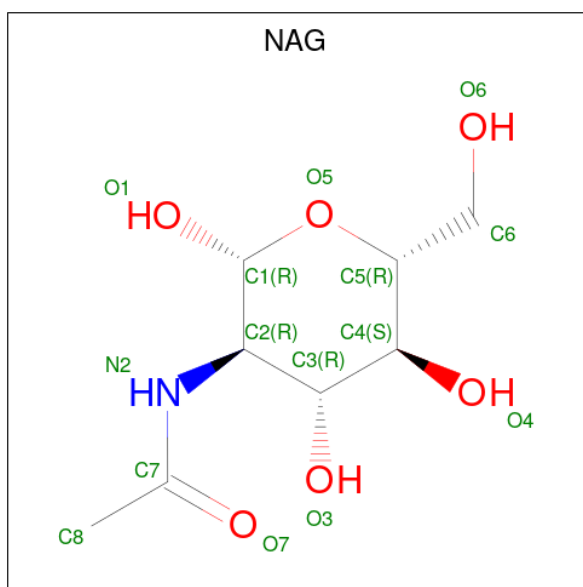
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	25	Total	C	H	N	O	S	7	0	0
			353	100	174	45	32	2			

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



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	C	2	Total	C	H	N	O		0	0	0
			55	16	27	2	10				

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
4	A	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
4	A	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
4	A	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
4	A	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
4	A	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
4	A	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
4	A	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
4	A	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
4	A	1	Total	C	H	N	O	0	0
			28	8	14	1	5		

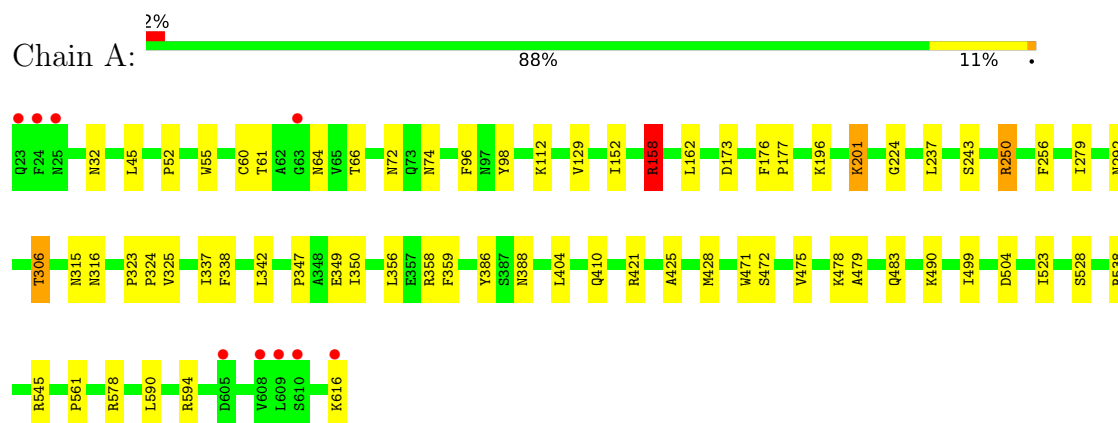
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	204	Total 204	O 204	0	0
5	B	22	Total 22	O 22	0	0

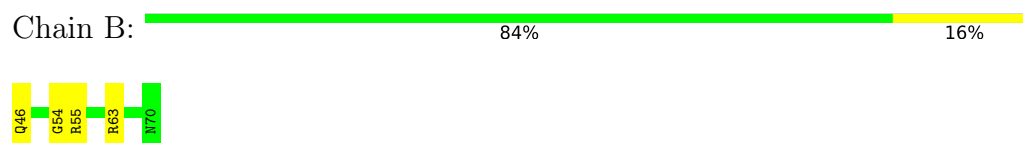
3 Residue-property plots

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: Kinase family with leucine-rich repeat domain-containing protein



- Molecule 2: Transmembrane protein



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



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	56.70Å 131.10Å 220.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	110.50 – 2.12 110.50 – 2.12	Depositor EDS
% Data completeness (in resolution range)	97.6 (110.50-2.12) 95.9 (110.50-2.12)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.40 (at 2.12Å)	Xtriage
Refinement program	REFMAC 5.8.0430 (refmacat 0.4.100)	Depositor
R, R_{free}	0.188 , 0.232 0.184 , 0.231	Depositor DCC
R_{free} test set	2312 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	41.7	Xtriage
Anisotropy	0.692	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 45.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	10044	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.39% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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

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	0.99	2/4631 (0.0%)	1.23	8/6307 (0.1%)
2	B	1.37	1/181 (0.6%)	1.72	4/239 (1.7%)
All	All	1.00	3/4812 (0.1%)	1.25	12/6546 (0.2%)

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	A	0	6

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	472	SER	CA-CB	5.20	1.62	1.53
1	A	243	SER	CA-CB	5.17	1.61	1.53
2	B	54	GLY	C-O	5.02	1.28	1.23

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	306	THR	CA-CB-OG1	-7.16	98.86	109.60
2	B	46	GLN	N-CA-CB	-6.98	98.63	110.50
1	A	479	ALA	CA-C-N	6.48	126.25	120.10
1	A	479	ALA	C-N-CA	6.48	126.25	120.10
1	A	590	LEU	N-CA-CB	-6.20	100.67	110.22
1	A	338	PHE	CA-CB-CG	6.05	119.85	113.80
2	B	63	ARG	NE-CZ-NH1	-5.66	115.84	121.50
1	A	162	LEU	N-CA-CB	5.14	117.62	109.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	55	ARG	NE-CZ-NH1	-5.13	116.37	121.50
1	A	616	LYS	CA-C-O	-5.11	112.11	120.80
2	B	55	ARG	CG-CD-NE	-5.09	100.79	112.00
1	A	176	PHE	CB-CA-C	5.06	116.49	108.84

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	158	ARG	Sidechain
1	A	250	ARG	Sidechain
1	A	358	ARG	Sidechain
1	A	545	ARG	Sidechain
1	A	578	ARG	Sidechain
1	A	594	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	A	4542	4476	4426	26	0
2	B	179	174	168	0	0
3	C	28	27	25	0	0
4	A	196	196	181	7	0
5	A	204	0	0	11	0
5	B	22	0	0	0	0
All	All	5171	4873	4800	33	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 3.

All (33) 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:A:499:ILE:HG23	1:A:523:ILE:HD12	1.68	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:705:NAG:O6	5:A:801:HOH:O	2.07	0.72
1:A:425:ALA:HB3	1:A:428:MET:HG2	1.76	0.67
1:A:347:PRO:HB2	1:A:350:ILE:HG13	1.83	0.59
4:A:714:NAG:H5	5:A:946:HOH:O	2.04	0.57
1:A:292:ASN:HB2	1:A:316:ASN:HD21	1.70	0.57
4:A:714:NAG:O5	5:A:802:HOH:O	2.18	0.55
1:A:388:ASN:O	5:A:802:HOH:O	2.18	0.55
1:A:337:ILE:HD12	1:A:342:LEU:HD12	1.89	0.55
1:A:386:TYR:HB2	1:A:410:GLN:HG2	1.90	0.54
4:A:714:NAG:C5	5:A:946:HOH:O	2.56	0.54
1:A:52:PRO:HA	1:A:55:TRP:CD2	2.43	0.52
1:A:201:LYS:HG3	1:A:224:GLY:HA3	1.92	0.52
1:A:158:ARG:HD3	5:A:871:HOH:O	2.10	0.50
1:A:315:ASN:HB2	5:A:963:HOH:O	2.12	0.50
4:A:714:NAG:C6	5:A:946:HOH:O	2.62	0.46
1:A:152:ILE:HB	1:A:177:PRO:HD3	1.98	0.46
4:A:714:NAG:H62	5:A:946:HOH:O	2.17	0.45
1:A:356:LEU:HD21	1:A:359:PHE:HB2	1.99	0.45
1:A:475:VAL:HG13	1:A:499:ILE:HG13	1.98	0.45
1:A:504:ASP:HA	1:A:528:SER:O	2.16	0.43
1:A:538:ARG:HB3	1:A:561:PRO:HB3	2.00	0.43
1:A:471:TRP:CD1	1:A:471:TRP:N	2.84	0.43
1:A:425:ALA:HB3	1:A:428:MET:CG	2.47	0.43
4:A:709:NAG:H61	5:A:829:HOH:O	2.19	0.42
1:A:129:VAL:HG23	5:A:837:HOH:O	2.20	0.42
1:A:74:ASN:OD1	1:A:98:TYR:HE2	2.02	0.42
1:A:323:PRO:HA	1:A:324:PRO:HD3	1.93	0.42
1:A:173:ASP:HA	1:A:196:LYS:O	2.20	0.41
1:A:256:PHE:CD1	1:A:279:ILE:HG12	2.56	0.41
1:A:60:CYS:HA	1:A:64:ASN:O	2.20	0.41
1:A:72:ASN:HA	1:A:96:PHE:O	2.21	0.41
1:A:61:THR:HB	1:A:66:THR:HG21	2.03	0.40

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	A	592/594 (100%)	560 (95%)	32 (5%)	0	100	100
2	B	23/25 (92%)	23 (100%)	0	0	100	100
All	All	615/619 (99%)	583 (95%)	32 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	510/533 (96%)	495 (97%)	15 (3%)	37	41
2	B	18/19 (95%)	18 (100%)	0	100	100
All	All	528/552 (96%)	513 (97%)	15 (3%)	38	42

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	ASN
1	A	45	LEU
1	A	112	LYS
1	A	158	ARG
1	A	201	LYS
1	A	237	LEU
1	A	250	ARG
1	A	306	THR
1	A	325	VAL
1	A	349	GLU
1	A	404	LEU
1	A	421	ARG
1	A	478	LYS
1	A	483	GLN

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Mol	Chain	Res	Type
1	A	490	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	GLN
1	A	221	ASN
1	A	316	ASN
1	A	408	GLN
1	A	411	ASN
1	A	555	GLN
1	A	589	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 ⓘ

2 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	C	1	1,3	14,14,15	0.50	0	17,19,21	1.27	1 (5%)
3	NAG	C	2	3	14,14,15	0.70	0	17,19,21	1.27	2 (11%)

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	C	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	C	2	3	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1	NAG	O7-C7-C8	-3.53	115.51	122.06
3	C	2	NAG	C4-C3-C2	-2.63	107.17	111.02
3	C	2	NAG	C1-C2-N2	2.28	114.38	110.49

There are no chirality outliers.

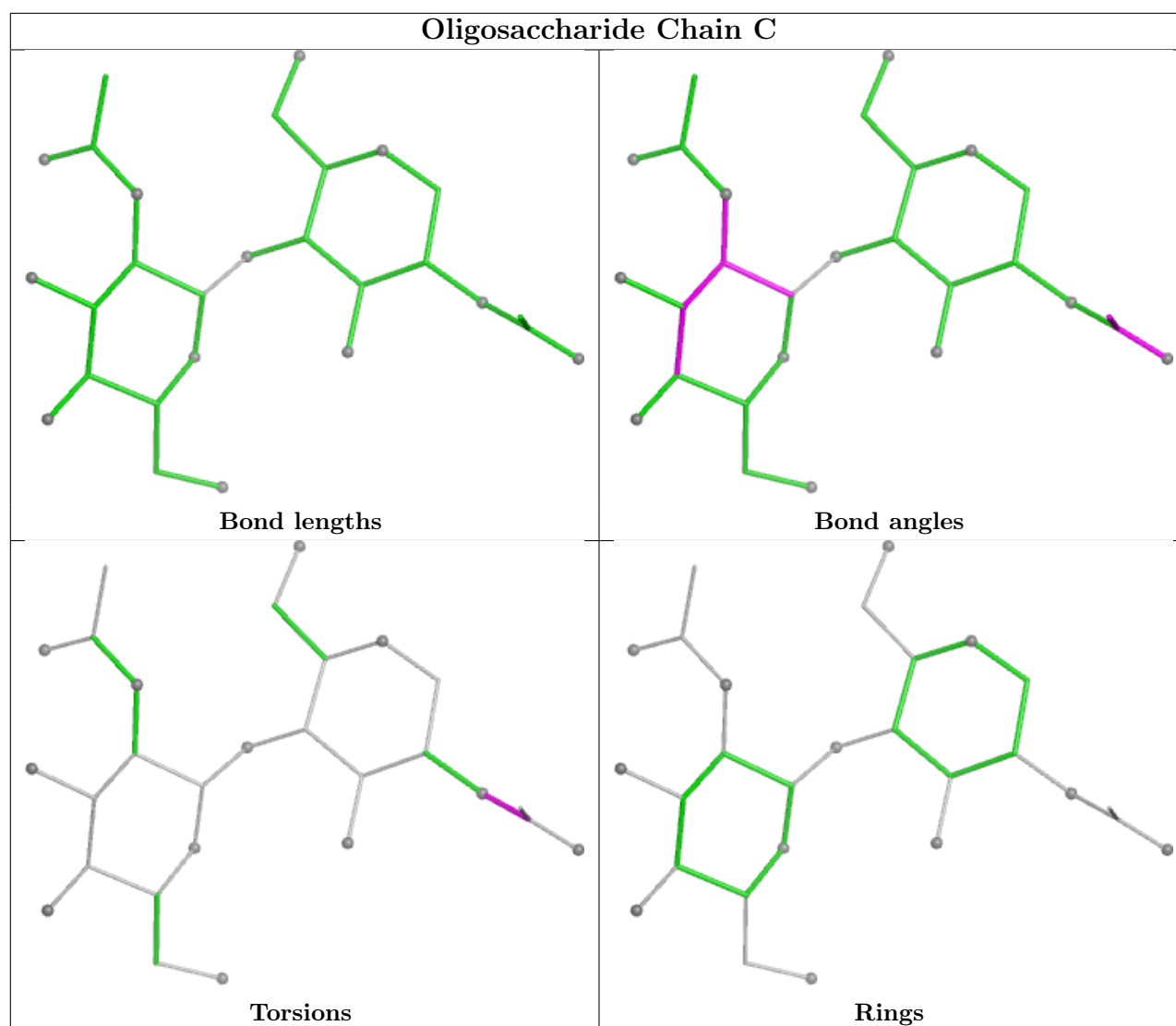
All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	1	NAG	C8-C7-N2-C2
3	C	1	NAG	O7-C7-N2-C2

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 [i](#)

14 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	701	1	14,14,15	1.15	1 (7%)	17,19,21	3.16	12 (70%)
4	NAG	A	706	1	14,14,15	0.87	0	17,19,21	2.17	9 (52%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	A	711	1	14,14,15	0.73	0	17,19,21	1.62	4 (23%)
4	NAG	A	705	1	14,14,15	0.95	1 (7%)	17,19,21	2.26	7 (41%)
4	NAG	A	707	1	14,14,15	0.95	0	17,19,21	2.47	6 (35%)
4	NAG	A	703	1	14,14,15	0.80	0	17,19,21	3.01	7 (41%)
4	NAG	A	712	1	14,14,15	0.69	0	17,19,21	1.56	4 (23%)
4	NAG	A	709	1	14,14,15	0.80	1 (7%)	17,19,21	2.07	6 (35%)
4	NAG	A	710	1	14,14,15	0.69	0	17,19,21	1.80	3 (17%)
4	NAG	A	702	1	14,14,15	1.18	1 (7%)	17,19,21	2.29	6 (35%)
4	NAG	A	714	1	14,14,15	1.35	3 (21%)	17,19,21	2.87	8 (47%)
4	NAG	A	704	1	14,14,15	0.92	1 (7%)	17,19,21	2.34	7 (41%)
4	NAG	A	713	1	14,14,15	0.81	1 (7%)	17,19,21	2.34	4 (23%)
4	NAG	A	708	1	14,14,15	0.53	0	17,19,21	1.94	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
4	NAG	A	701	1	-	1/6/23/26	0/1/1/1
4	NAG	A	706	1	-	2/6/23/26	0/1/1/1
4	NAG	A	711	1	-	0/6/23/26	0/1/1/1
4	NAG	A	705	1	-	0/6/23/26	0/1/1/1
4	NAG	A	707	1	-	2/6/23/26	0/1/1/1
4	NAG	A	703	1	-	3/6/23/26	0/1/1/1
4	NAG	A	712	1	-	2/6/23/26	0/1/1/1
4	NAG	A	709	1	-	0/6/23/26	0/1/1/1
4	NAG	A	710	1	-	2/6/23/26	0/1/1/1
4	NAG	A	702	1	-	0/6/23/26	0/1/1/1
4	NAG	A	714	1	-	2/6/23/26	0/1/1/1
4	NAG	A	704	1	-	0/6/23/26	0/1/1/1
4	NAG	A	713	1	-	2/6/23/26	0/1/1/1
4	NAG	A	708	1	-	0/6/23/26	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	714	NAG	O5-C5	2.70	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	702	NAG	O4-C4	-2.56	1.36	1.43
4	A	714	NAG	C8-C7	2.36	1.55	1.50
4	A	704	NAG	C8-C7	-2.18	1.46	1.50
4	A	709	NAG	O7-C7	2.14	1.28	1.23
4	A	713	NAG	O5-C5	2.07	1.47	1.43
4	A	714	NAG	C6-C5	2.05	1.58	1.51
4	A	705	NAG	O7-C7	-2.03	1.18	1.23
4	A	701	NAG	C4-C5	2.01	1.57	1.53

All (87) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	713	NAG	O5-C5-C6	7.92	119.62	107.20
4	A	707	NAG	C1-O5-C5	7.42	122.24	112.19
4	A	703	NAG	C8-C7-N2	6.15	126.50	116.10
4	A	714	NAG	C4-C3-C2	6.11	119.98	111.02
4	A	701	NAG	O5-C5-C6	5.76	116.24	107.20
4	A	708	NAG	C1-O5-C5	5.59	119.77	112.19
4	A	704	NAG	C1-O5-C5	-5.59	104.62	112.19
4	A	705	NAG	C2-N2-C7	5.35	130.53	122.90
4	A	703	NAG	O7-C7-N2	-5.32	112.17	121.95
4	A	701	NAG	C1-O5-C5	-5.32	104.99	112.19
4	A	714	NAG	O5-C5-C6	5.15	115.27	107.20
4	A	703	NAG	C1-O5-C5	5.00	118.97	112.19
4	A	703	NAG	C2-N2-C7	4.89	129.87	122.90
4	A	710	NAG	C1-O5-C5	-4.43	106.19	112.19
4	A	701	NAG	C6-C5-C4	4.40	123.32	113.00
4	A	714	NAG	C6-C5-C4	4.39	123.28	113.00
4	A	709	NAG	C8-C7-N2	-4.13	109.10	116.10
4	A	709	NAG	C1-O5-C5	4.12	117.77	112.19
4	A	704	NAG	O5-C5-C6	4.05	113.56	107.20
4	A	704	NAG	O5-C5-C4	-4.01	101.08	110.83
4	A	702	NAG	C6-C5-C4	3.97	122.29	113.00
4	A	702	NAG	O5-C5-C4	-3.85	101.46	110.83
4	A	702	NAG	C4-C3-C2	-3.77	105.49	111.02
4	A	705	NAG	C4-C3-C2	3.75	116.51	111.02
4	A	706	NAG	C6-C5-C4	3.74	121.76	113.00
4	A	714	NAG	O5-C5-C4	-3.72	101.77	110.83
4	A	703	NAG	C3-C4-C5	-3.67	103.68	110.24
4	A	706	NAG	C1-O5-C5	3.64	117.12	112.19
4	A	701	NAG	O5-C5-C4	-3.61	102.05	110.83
4	A	712	NAG	C2-N2-C7	3.61	128.04	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	702	NAG	C3-C4-C5	-3.60	103.82	110.24
4	A	701	NAG	C8-C7-N2	3.45	121.94	116.10
4	A	714	NAG	O3-C3-C2	-3.43	102.37	109.47
4	A	701	NAG	O6-C6-C5	-3.25	100.13	111.29
4	A	706	NAG	C4-C3-C2	-3.21	106.31	111.02
4	A	709	NAG	O4-C4-C3	-3.20	102.95	110.35
4	A	703	NAG	C4-C3-C2	-3.19	106.34	111.02
4	A	705	NAG	C3-C4-C5	-3.18	104.57	110.24
4	A	701	NAG	C1-C2-N2	-3.12	105.15	110.49
4	A	708	NAG	O7-C7-C8	3.08	127.78	122.06
4	A	701	NAG	C3-C4-C5	-3.04	104.82	110.24
4	A	709	NAG	O7-C7-C8	2.97	127.57	122.06
4	A	713	NAG	C6-C5-C4	-2.94	106.12	113.00
4	A	704	NAG	C8-C7-N2	-2.94	111.13	116.10
4	A	710	NAG	O4-C4-C5	2.89	116.46	109.30
4	A	702	NAG	O7-C7-N2	2.87	127.23	121.95
4	A	703	NAG	O4-C4-C5	2.84	116.36	109.30
4	A	711	NAG	O5-C5-C6	2.79	111.58	107.20
4	A	706	NAG	C8-C7-N2	2.77	120.78	116.10
4	A	707	NAG	C6-C5-C4	-2.74	106.59	113.00
4	A	711	NAG	C4-C3-C2	-2.73	107.02	111.02
4	A	706	NAG	C2-N2-C7	-2.73	119.02	122.90
4	A	707	NAG	O7-C7-C8	2.71	127.08	122.06
4	A	707	NAG	O5-C5-C6	-2.70	102.97	107.20
4	A	701	NAG	O4-C4-C5	2.67	115.93	109.30
4	A	709	NAG	O6-C6-C5	-2.66	102.16	111.29
4	A	705	NAG	O4-C4-C5	-2.63	102.76	109.30
4	A	706	NAG	O4-C4-C5	2.61	115.77	109.30
4	A	714	NAG	C1-C2-N2	-2.53	106.17	110.49
4	A	714	NAG	C2-N2-C7	2.52	126.50	122.90
4	A	707	NAG	C2-N2-C7	2.49	126.45	122.90
4	A	713	NAG	C2-N2-C7	2.44	126.38	122.90
4	A	714	NAG	C1-O5-C5	-2.37	108.98	112.19
4	A	704	NAG	C6-C5-C4	2.36	118.53	113.00
4	A	712	NAG	O4-C4-C3	2.35	115.79	110.35
4	A	708	NAG	C6-C5-C4	-2.35	107.50	113.00
4	A	702	NAG	O6-C6-C5	-2.34	103.28	111.29
4	A	707	NAG	C1-C2-N2	2.33	114.47	110.49
4	A	710	NAG	O7-C7-N2	-2.33	117.67	121.95
4	A	705	NAG	O5-C1-C2	-2.30	107.66	111.29
4	A	709	NAG	O3-C3-C4	-2.28	105.08	110.35
4	A	704	NAG	O6-C6-C5	-2.28	103.48	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	701	NAG	O3-C3-C4	2.26	115.58	110.35
4	A	712	NAG	O5-C5-C6	2.25	110.74	107.20
4	A	706	NAG	O7-C7-C8	-2.24	117.89	122.06
4	A	701	NAG	O5-C1-C2	2.22	114.79	111.29
4	A	708	NAG	C8-C7-N2	-2.22	112.34	116.10
4	A	705	NAG	O5-C5-C4	-2.21	105.44	110.83
4	A	713	NAG	C8-C7-N2	-2.17	112.43	116.10
4	A	706	NAG	C3-C4-C5	-2.15	106.40	110.24
4	A	701	NAG	C4-C3-C2	-2.10	107.94	111.02
4	A	712	NAG	C6-C5-C4	-2.09	108.10	113.00
4	A	711	NAG	C1-C2-N2	2.09	114.06	110.49
4	A	704	NAG	O7-C7-N2	2.08	125.78	121.95
4	A	706	NAG	O5-C5-C4	-2.07	105.78	110.83
4	A	711	NAG	O6-C6-C5	-2.04	104.29	111.29
4	A	705	NAG	O3-C3-C2	2.03	113.67	109.47

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	714	NAG	C8-C7-N2-C2
4	A	714	NAG	O7-C7-N2-C2
4	A	713	NAG	O5-C5-C6-O6
4	A	712	NAG	O5-C5-C6-O6
4	A	712	NAG	C4-C5-C6-O6
4	A	713	NAG	C4-C5-C6-O6
4	A	703	NAG	C8-C7-N2-C2
4	A	703	NAG	O7-C7-N2-C2
4	A	706	NAG	C8-C7-N2-C2
4	A	706	NAG	O7-C7-N2-C2
4	A	710	NAG	C8-C7-N2-C2
4	A	710	NAG	O7-C7-N2-C2
4	A	707	NAG	C4-C5-C6-O6
4	A	707	NAG	O5-C5-C6-O6
4	A	703	NAG	C1-C2-N2-C7
4	A	701	NAG	C4-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	705	NAG	1	0
4	A	709	NAG	1	0
4	A	714	NAG	5	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	A	594/594 (100%)	-0.04	9 (1%) 72 74	34, 54, 80, 105	0
2	B	25/25 (100%)	-0.19	0 100 100	34, 45, 71, 76	0
All	All	619/619 (100%)	-0.05	9 (1%) 72 74	34, 54, 80, 105	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	608	VAL	5.0
1	A	24	PHE	4.4
1	A	25	ASN	3.2
1	A	609	LEU	2.9
1	A	23	GLN	2.9
1	A	610	SER	2.8
1	A	616	LYS	2.6
1	A	63	GLY	2.2
1	A	605	ASP	2.2

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

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.

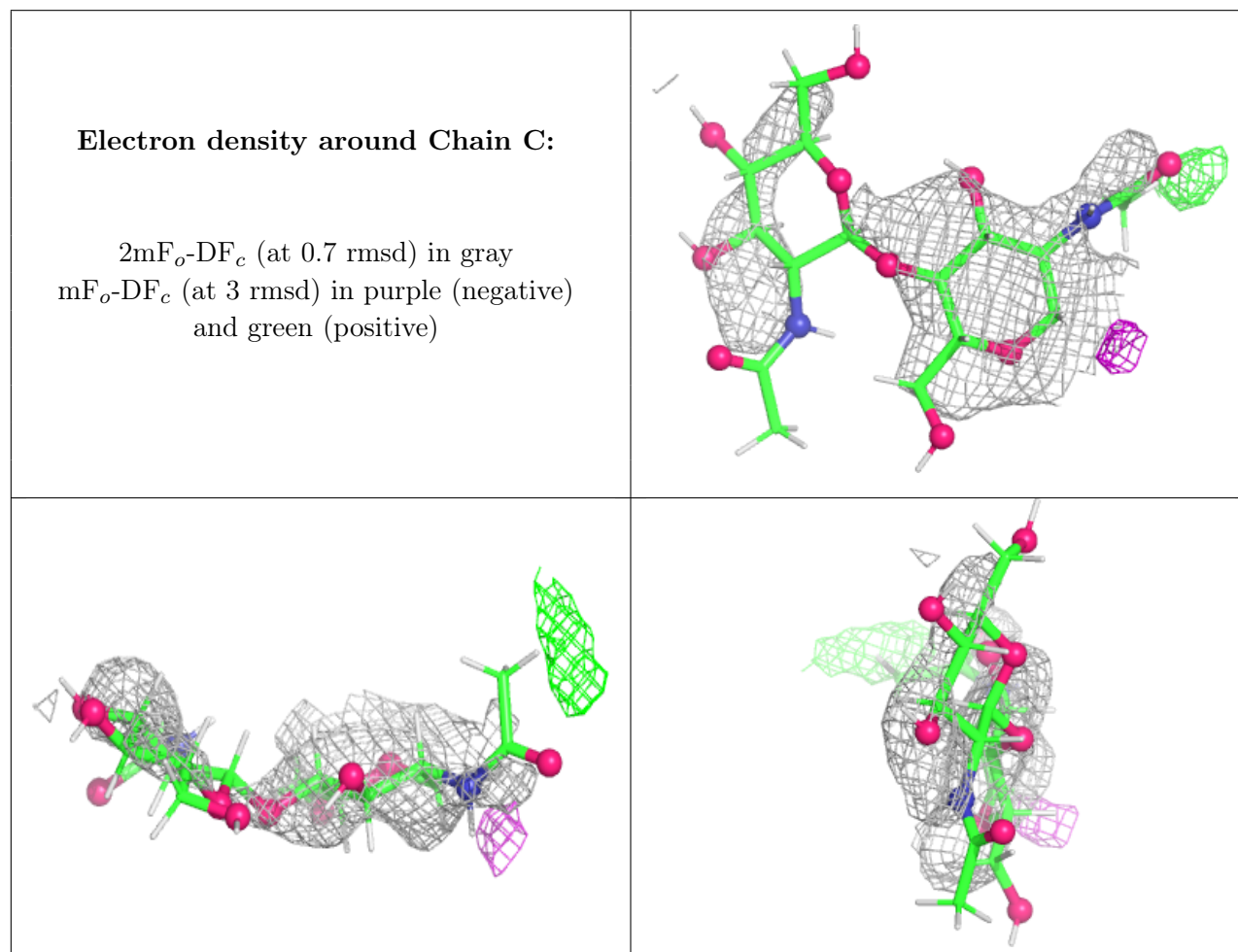
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAG	C	2	14/15	0.64	0.13	122,143,161,169	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NAG	C	1	14/15	0.77	0.12	113,126,143,151	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



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($\text{\AA}^2$)	Q<0.9
4	NAG	A	714	14/15	0.57	0.14	86,106,125,135	0
4	NAG	A	712	14/15	0.62	0.14	113,128,140,145	0
4	NAG	A	713	14/15	0.75	0.13	105,123,143,159	0
4	NAG	A	710	14/15	0.76	0.11	82,98,107,110	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NAG	A	708	14/15	0.76	0.10	98,113,122,123	0
4	NAG	A	707	14/15	0.77	0.12	61,85,92,94	0
4	NAG	A	711	14/15	0.81	0.09	66,91,107,115	0
4	NAG	A	706	14/15	0.81	0.09	68,91,116,129	0
4	NAG	A	709	14/15	0.86	0.11	90,99,107,108	0
4	NAG	A	704	14/15	0.88	0.09	66,81,95,103	0
4	NAG	A	703	14/15	0.88	0.10	74,86,94,105	0
4	NAG	A	705	14/15	0.91	0.09	63,69,75,85	0
4	NAG	A	702	14/15	0.91	0.09	57,73,78,88	0
4	NAG	A	701	14/15	0.94	0.08	51,65,76,76	0

6.5 Other polymers [i](#)

There are no such residues in this entry.