



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 9, 2020 – 04:18 AM BST

PDB ID : 3R05
Title : Structure of neurexin 1 alpha (domains LNS1-LNS6), with splice insert SS3
Authors : Venugopal, V.; Rudenko, G.
Deposited on : 2011-03-07
Resolution : 2.95 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) : 1.13
EDS : 2.13.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

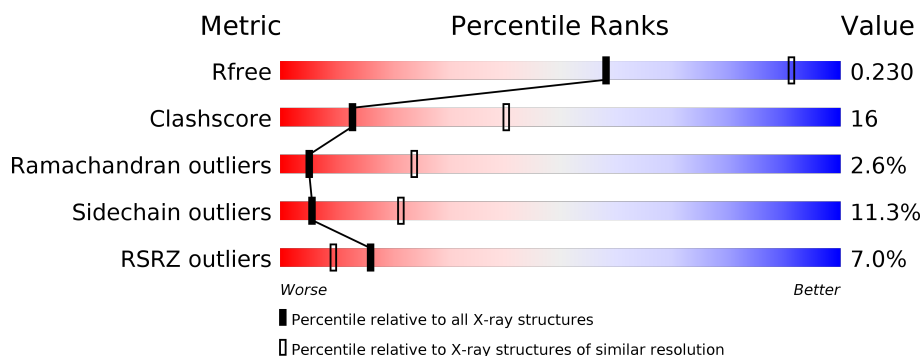
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 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}	130704	3104 (3.00-2.92)
Clashscore	141614	3462 (3.00-2.92)
Ramachandran outliers	138981	3340 (3.00-2.92)
Sidechain outliers	138945	3343 (3.00-2.92)
RSRZ outliers	127900	2986 (3.00-2.92)

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 $\leq 5\%$. 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	1254	<div> <div>6%</div> <div> <div></div> <div>50%</div> <div>24%</div> <div>5%</div> <div>20%</div> </div> </div>
1	B	1254	<div> <div>5%</div> <div> <div></div> <div>50%</div> <div>24%</div> <div>6%</div> <div>20%</div> </div> </div>
2	C	2	<div> <div></div> <div>100%</div> </div>
2	D	2	<div> <div></div> <div> <div>50%</div> <div>50%</div> </div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 15522 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 Neurexin-1-alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1008	Total	C	N	O	S	0	0	0
			7733	4857	1334	1499	43			
1	B	1008	Total	C	N	O	S	0	0	0
			7733	4857	1334	1499	43			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1340	ALA	-	expression tag	UNP Q28146
A	1341	SER	-	expression tag	UNP Q28146
A	1342	THR	-	expression tag	UNP Q28146
A	1343	SER	-	expression tag	UNP Q28146
A	1344	HIS	-	expression tag	UNP Q28146
A	1345	HIS	-	expression tag	UNP Q28146
A	1346	HIS	-	expression tag	UNP Q28146
A	1347	HIS	-	expression tag	UNP Q28146
A	1348	HIS	-	expression tag	UNP Q28146
A	1349	HIS	-	expression tag	UNP Q28146
B	1340	ALA	-	expression tag	UNP Q28146
B	1341	SER	-	expression tag	UNP Q28146
B	1342	THR	-	expression tag	UNP Q28146
B	1343	SER	-	expression tag	UNP Q28146
B	1344	HIS	-	expression tag	UNP Q28146
B	1345	HIS	-	expression tag	UNP Q28146
B	1346	HIS	-	expression tag	UNP Q28146
B	1347	HIS	-	expression tag	UNP Q28146
B	1348	HIS	-	expression tag	UNP Q28146
B	1349	HIS	-	expression tag	UNP Q28146

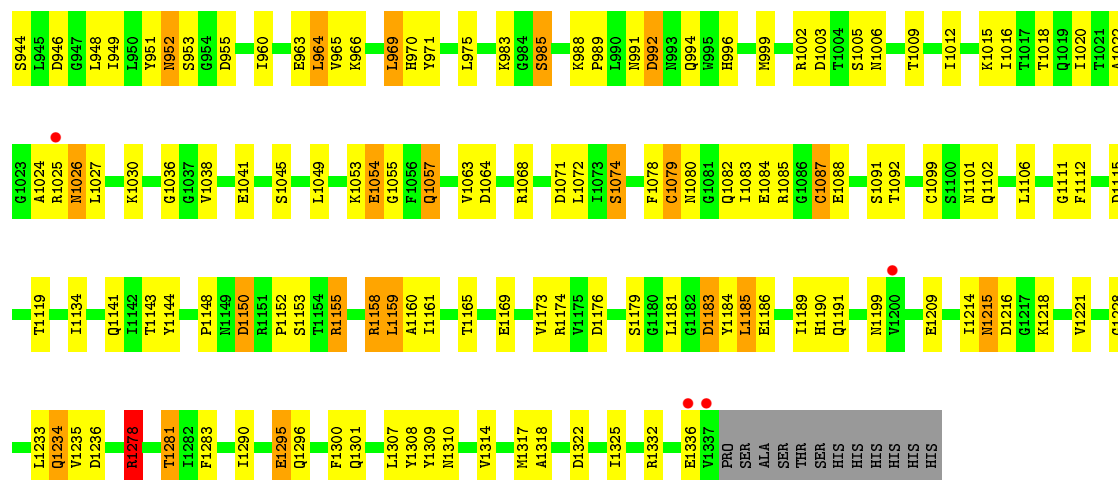
- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



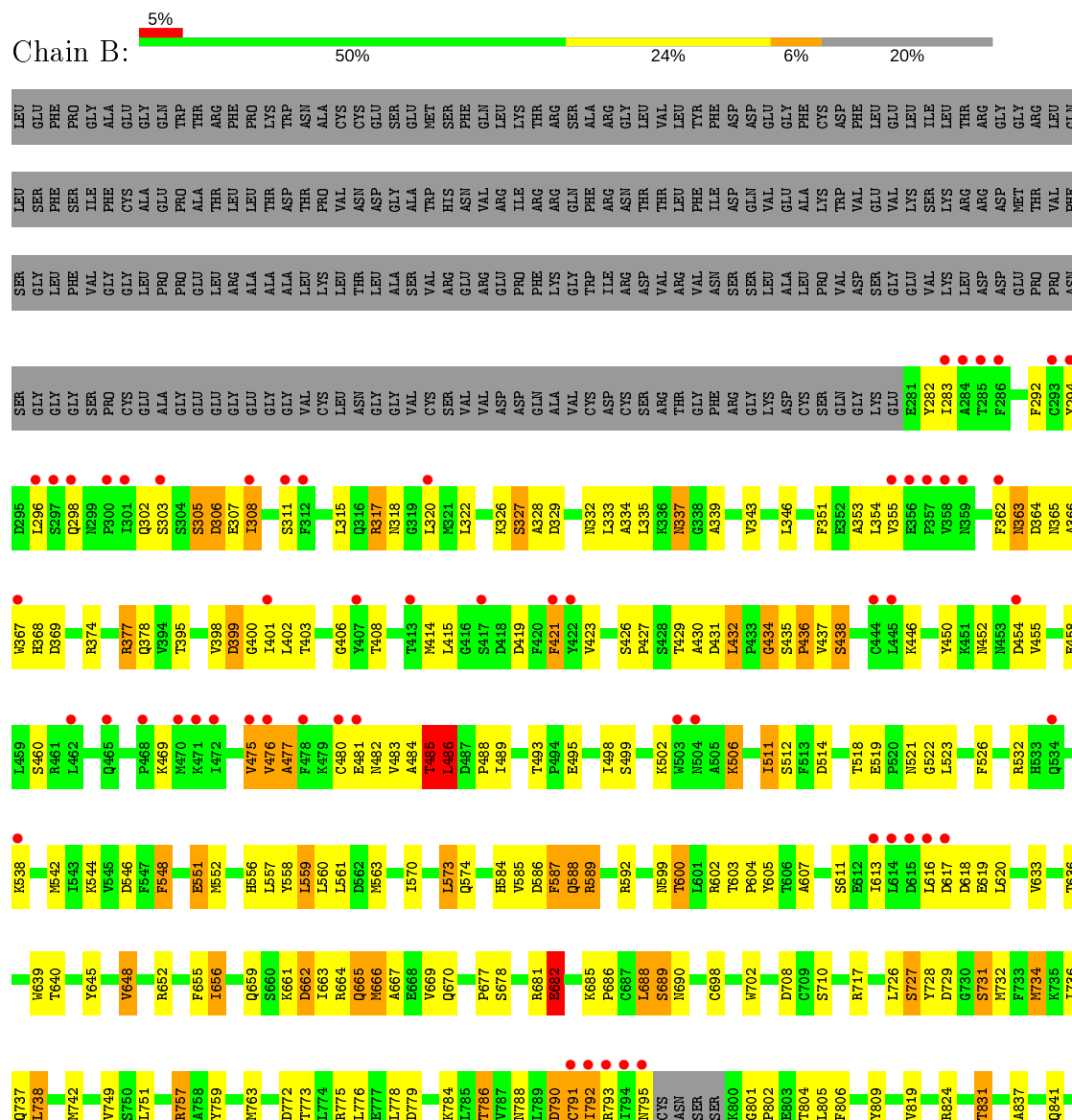
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	D	2	Total	C	N	O	0	0	0
			28	16	2	10			

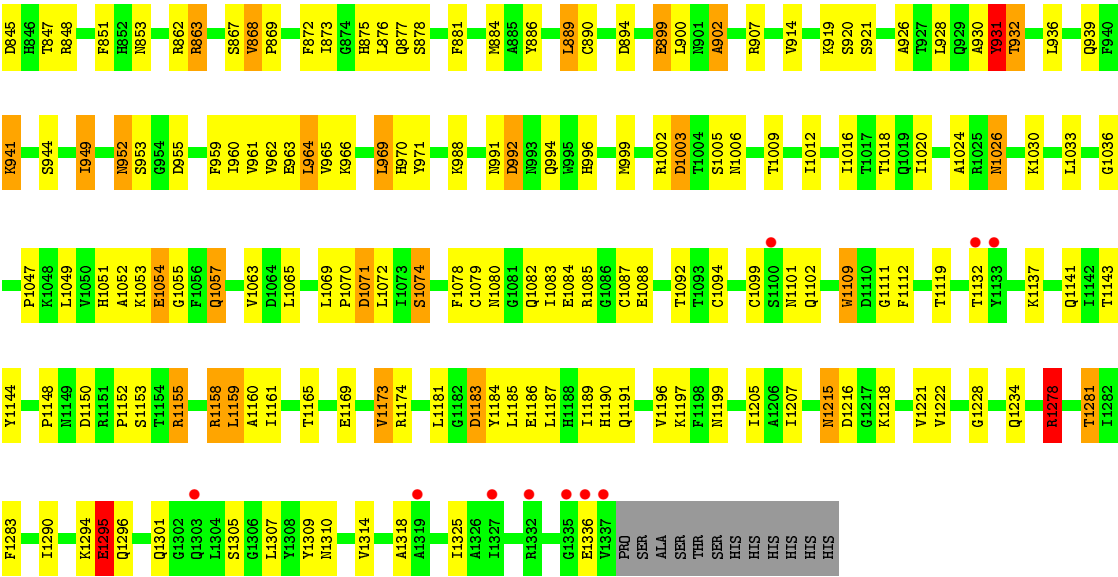
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

[illegible]

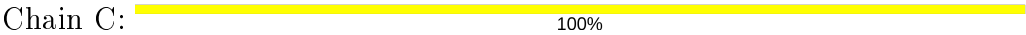


• Molecule 1: Neurexin-1-alpha

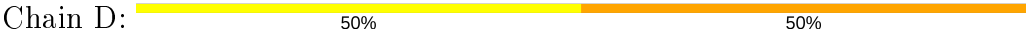




● Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



● Molecule 2: 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	P 1	Depositor
Cell constants a, b, c, α , β , γ	61.03Å 114.57Å 160.13Å 89.60° 89.98° 87.96°	Depositor
Resolution (Å)	44.29 – 2.95 44.29 – 2.94	Depositor EDS
% Data completeness (in resolution range)	98.2 (44.29-2.95) 97.7 (44.29-2.94)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.32 (at 2.96Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.208 , 0.235 0.202 , 0.230	Depositor DCC
R_{free} test set	4662 reflections (5.20%)	wwPDB-VP
Wilson B-factor (Å ²)	62.7	Xtriage
Anisotropy	0.812	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 47.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.125 for h,-k,-l 0.004 for -h,k,-l 0.010 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	15522	wwPDB-VP
Average B, all atoms (Å ²)	92.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.10% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² Theoretical 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	1.19	32/7886 (0.4%)	1.12	25/10691 (0.2%)
1	B	1.19	29/7886 (0.4%)	1.13	28/10691 (0.3%)
All	All	1.19	61/15772 (0.4%)	1.13	53/21382 (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	3
1	B	0	3
All	All	0	6

The worst 5 of 61 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1057	GLN	CG-CD	14.07	1.83	1.51
1	B	1057	GLN	CG-CD	13.73	1.82	1.51
1	A	898	CYS	CB-SG	10.65	2.00	1.82
1	B	868	VAL	CB-CG2	-9.30	1.33	1.52
1	B	963	GLU	CD-OE2	9.26	1.35	1.25

The worst 5 of 53 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1071	ASP	CB-CG-OD1	10.07	127.37	118.30
1	A	824	ARG	NE-CZ-NH1	9.87	125.23	120.30
1	B	1053	LYS	CD-CE-NZ	-9.41	90.05	111.70
1	A	941	LYS	CD-CE-NZ	-8.72	91.65	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	824	ARG	NE-CZ-NH2	-8.72	115.94	120.30

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1215	ASN	Peptide
1	A	484	ALA	Peptide
1	A	747	GLU	Peptide
1	B	484	ALA	Peptide
1	B	790	ASP	Peptide

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	7733	0	7482	253	0
1	B	7733	0	7482	260	0
2	C	28	0	25	0	0
2	D	28	0	25	4	0
All	All	15522	0	15014	503	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 16.

The worst 5 of 503 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:B:1057:GLN:CG	1:B:1057:GLN:CD	1.82	1.46
1:A:1057:GLN:CG	1:A:1057:GLN:CD	1.83	1.44
1:B:519:GLU:HG3	1:B:648:VAL:HG22	1.40	1.02
1:A:988:LYS:HG3	1:B:731:SER:HB3	1.41	1.02
1:A:727:SER:HB2	1:A:875:HIS:CD2	1.94	1.01

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	1004/1254 (80%)	881 (88%)	97 (10%)	26 (3%)	5	24
1	B	1004/1254 (80%)	881 (88%)	96 (10%)	27 (3%)	5	23
All	All	2008/2508 (80%)	1762 (88%)	193 (10%)	53 (3%)	5	24

5 of 53 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	327	SER
1	A	401	ILE
1	A	476	VAL
1	A	477	ALA
1	A	506	LYS

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	839/1068 (79%)	742 (88%)	97 (12%)	5	20
1	B	839/1068 (79%)	747 (89%)	92 (11%)	6	22
All	All	1678/2136 (79%)	1489 (89%)	189 (11%)	6	21

5 of 189 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1176	ASP

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Mol	Chain	Res	Type
1	B	377	ARG
1	B	1155	ARG
1	A	1185	LEU
1	A	1295	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	378	GLN
1	B	452	ASN
1	B	1008	HIS
1	B	365	ASN
1	B	1141	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 ⓘ

4 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$
2	NAG	C	1	1,2	14,14,15	0.88	0	17,19,21	2.97	10 (58%)
2	NAG	C	2	2	14,14,15	0.61	0	17,19,21	1.72	3 (17%)
2	NAG	D	1	1,2	14,14,15	0.84	0	17,19,21	3.05	9 (52%)
2	NAG	D	2	2	14,14,15	0.81	1 (7%)	17,19,21	1.60	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
2	NAG	C	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	C	2	2	-	2/6/23/26	0/1/1/1
2	NAG	D	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	2	NAG	C1-C2	2.06	1.55	1.52

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1	NAG	C1-O5-C5	7.00	121.67	112.19
2	C	1	NAG	C1-O5-C5	6.05	120.39	112.19
2	C	1	NAG	O5-C5-C6	4.63	114.46	107.20
2	C	2	NAG	O5-C5-C6	4.53	114.30	107.20
2	D	1	NAG	O5-C5-C6	4.49	114.24	107.20

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

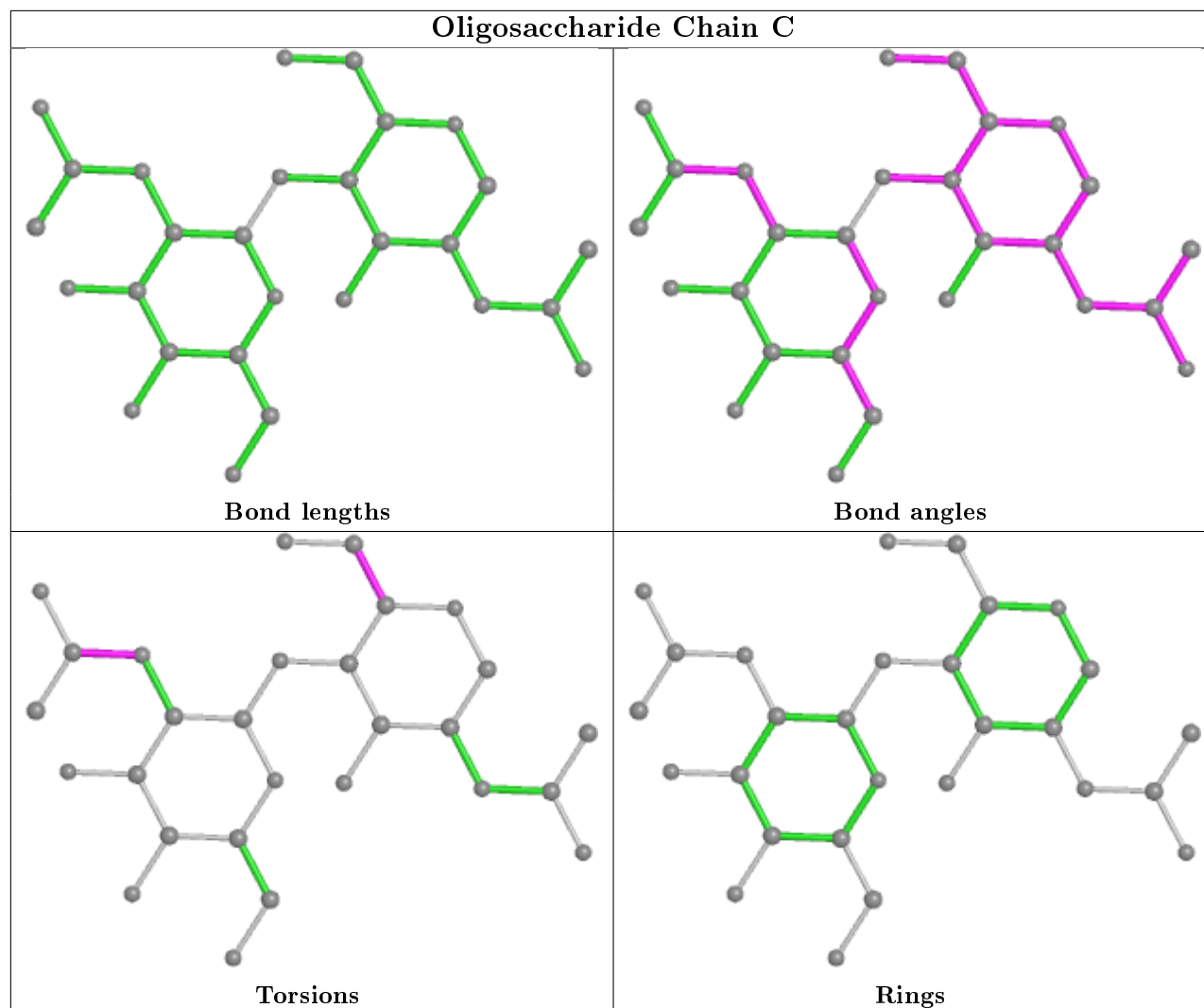
Mol	Chain	Res	Type	Atoms
2	D	2	NAG	C8-C7-N2-C2
2	C	2	NAG	C8-C7-N2-C2
2	D	2	NAG	O7-C7-N2-C2
2	C	2	NAG	O7-C7-N2-C2
2	C	1	NAG	O5-C5-C6-O6

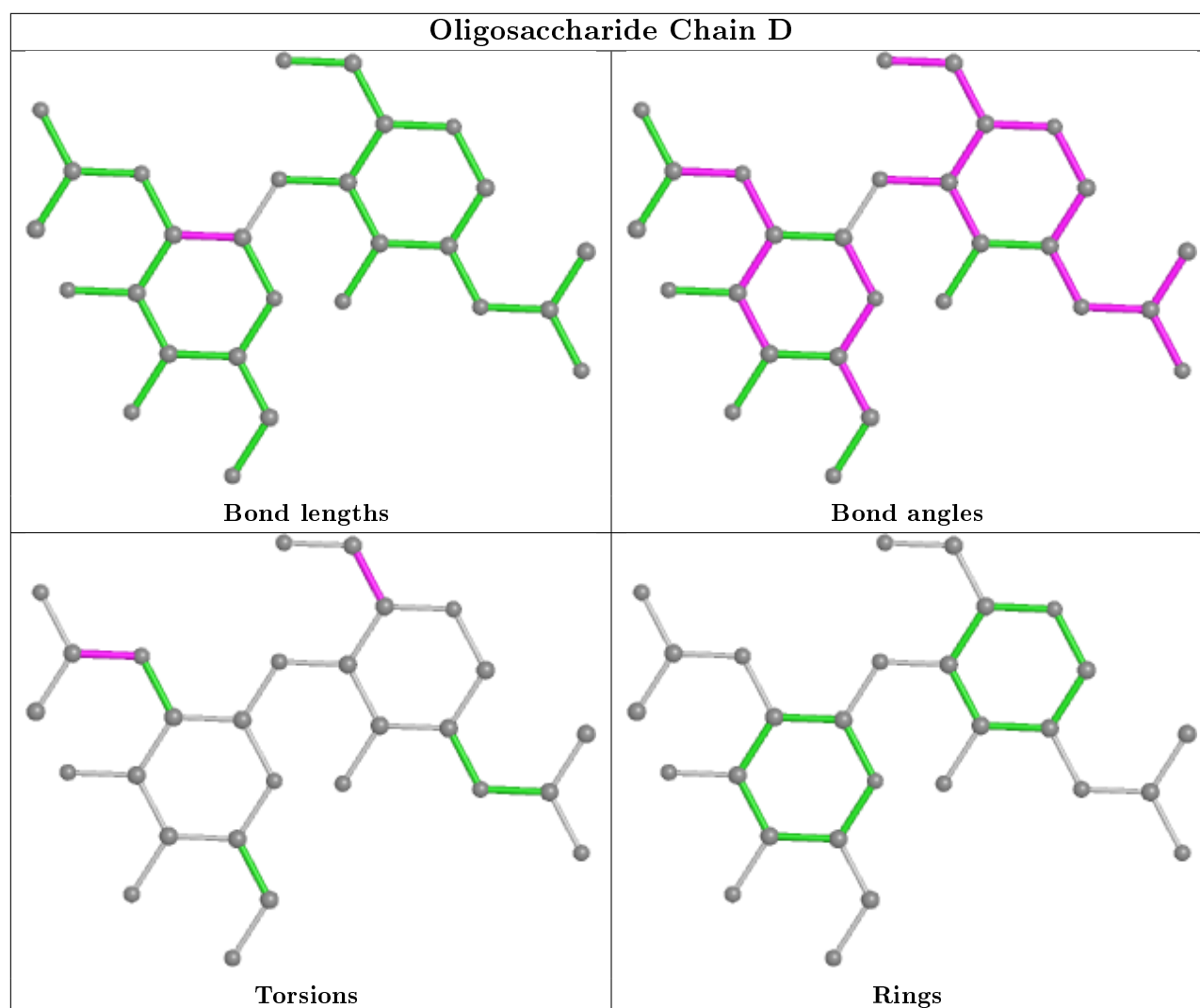
There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1	NAG	4	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](#)

There are no ligands in this entry.

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	1008/1254 (80%)	0.20	75 (7%) 14 8	35, 91, 151, 196	0
1	B	1008/1254 (80%)	0.20	67 (6%) 18 10	34, 92, 152, 201	0
All	All	2016/2508 (80%)	0.20	142 (7%) 16 9	34, 91, 152, 201	0

The worst 5 of 142 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	472	ILE	5.9
1	B	358	VAL	5.7
1	A	359	ASN	5.7
1	B	284	ALA	5.5
1	A	480	CYS	5.5

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](#)

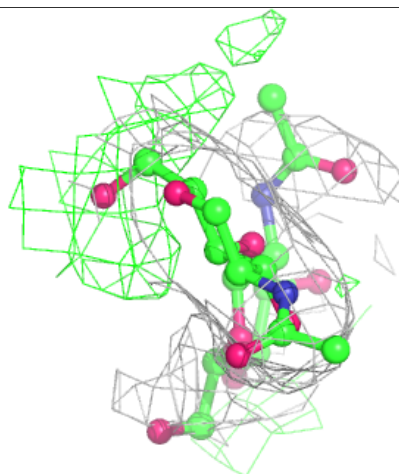
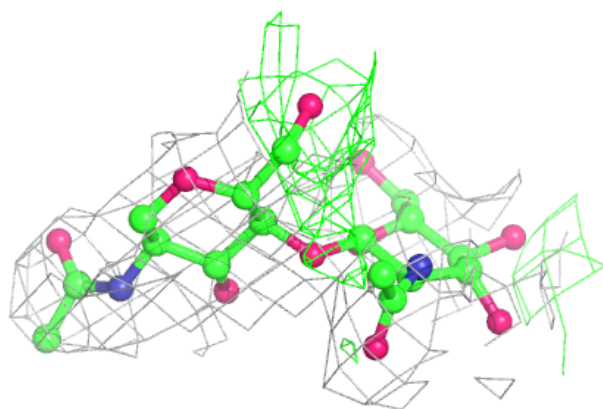
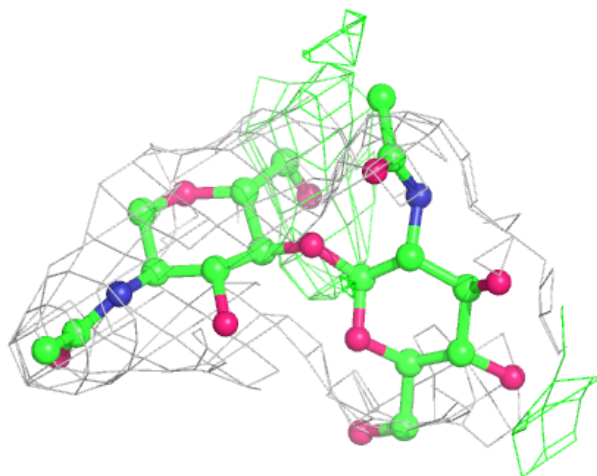
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

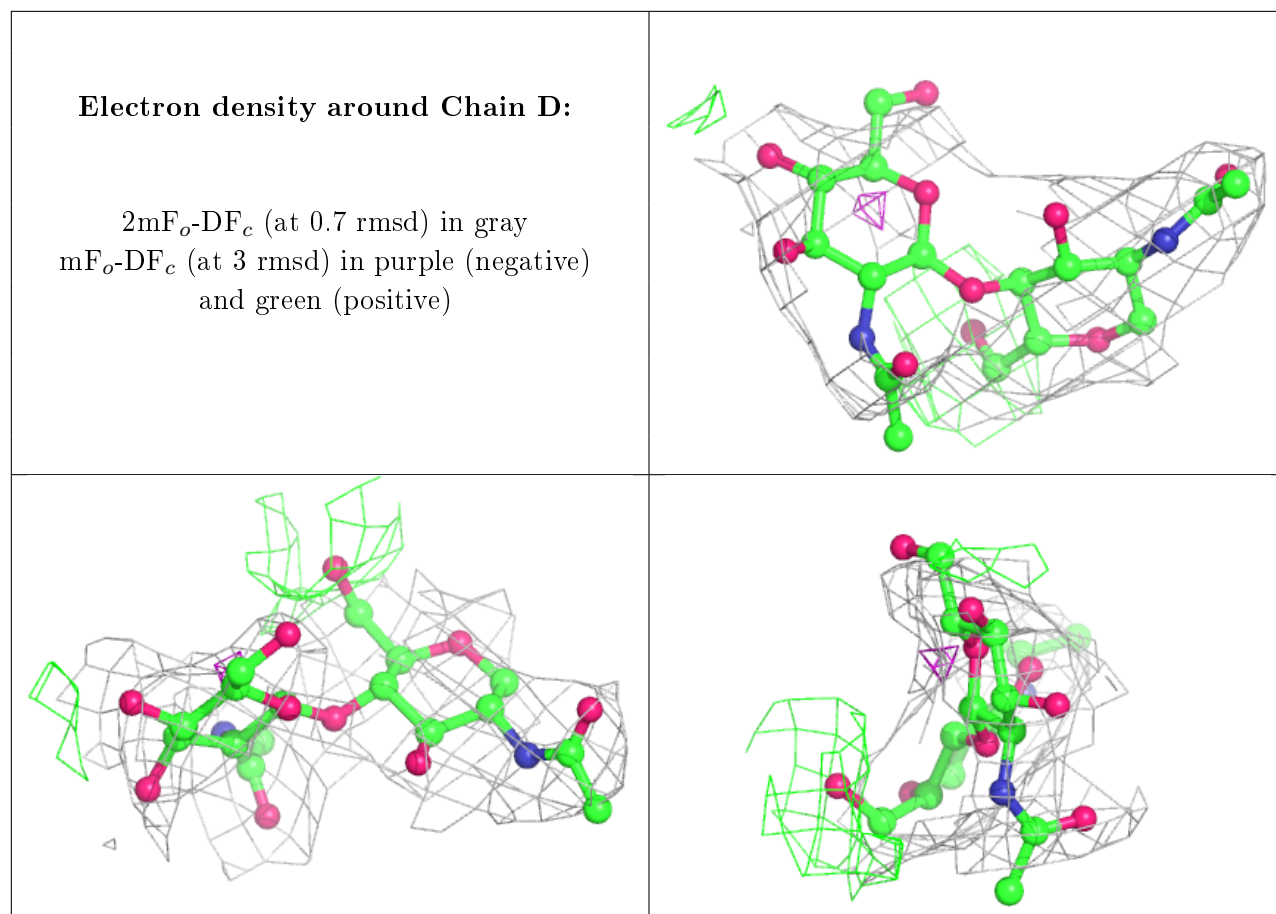
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAG	D	2	14/15	0.82	0.33	113,126,132,134	0
2	NAG	C	2	14/15	0.84	0.23	110,124,129,133	0
2	NAG	D	1	14/15	0.85	0.18	87,101,111,114	0
2	NAG	C	1	14/15	0.86	0.16	89,102,110,114	0

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.

Electron density around Chain C:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.