



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 25, 2026 – 06:49 PM UTC

PDB ID : 4LSA / pdb_00004lsa
Title : Crystal structure of BRI1 sud1 (Gly643Glu) bound to brassinolide
Authors : Santiago, J.; Henzler, C.; Hothorn, M.
Deposited on : 2013-07-22
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 ⓘ 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	:	FAILED
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

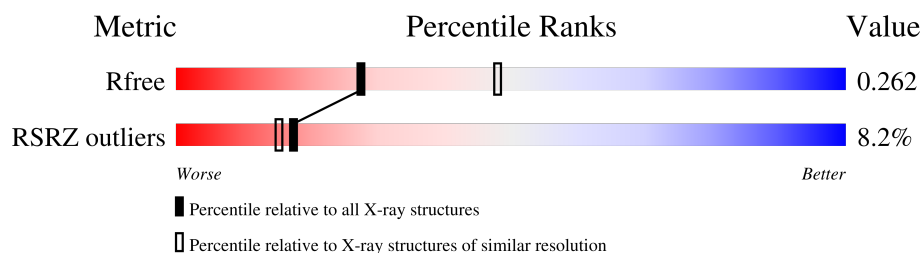
1 Overall quality at a glance

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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5829 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11337 atoms, of which 5478 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 BRASSINOSTEROID INSENSITIVE 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	743	11048	3518	5478	915	1106	31	0	5	0

There are 15 discrepancies between the modelled and reference sequences:

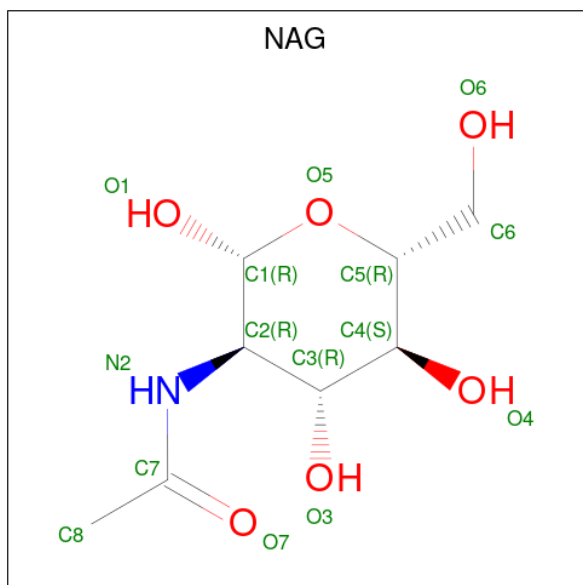
Chain	Residue	Modelled	Actual	Comment	Reference
A	24	GLY	-	expression tag	UNP O22476
A	25	SER	-	expression tag	UNP O22476
A	26	SER	-	expression tag	UNP O22476
A	27	MET	-	expression tag	UNP O22476
A	28	GLY	-	expression tag	UNP O22476
A	643	GLU	GLY	engineered mutation	UNP O22476
A	789	LEU	-	expression tag	UNP O22476
A	790	GLU	-	expression tag	UNP O22476
A	791	ASN	-	expression tag	UNP O22476
A	792	LEU	-	expression tag	UNP O22476
A	793	TYR	-	expression tag	UNP O22476
A	794	PHE	-	expression tag	UNP O22476
A	795	GLN	-	expression tag	UNP O22476
A	796	GLY	-	expression tag	UNP O22476
A	797	ALA	-	expression tag	UNP O22476

- Molecule 2 is an oligosaccharide called 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.



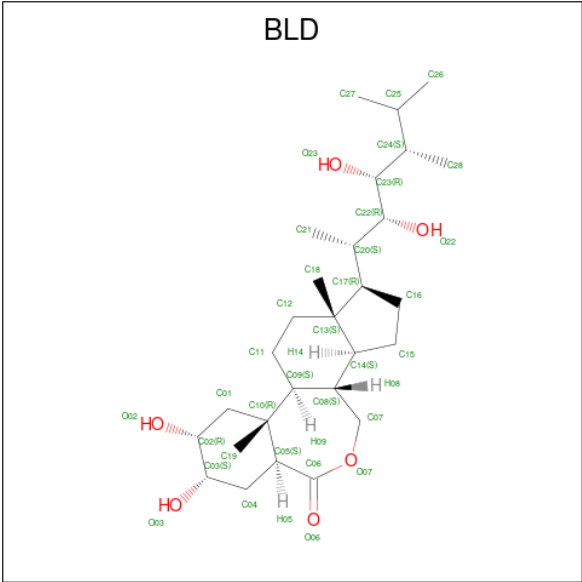
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	4	Total	C	N	O	0	0	0
			50	28	2	20			
2	C	4	Total	C	N	O	0	0	0
			50	28	2	20			
2	D	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 4 is Brassinolide (CCD ID: BLD) (formula: $C_{28}H_{48}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			34	28	6		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	49	Total	O	0	0
			49	49		

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3 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	174.03Å 67.30Å 120.90Å 90.00° 121.09° 90.00°	Depositor
Resolution (Å)	49.56 – 2.50 49.56 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.3 (49.56-2.50) 99.4 (49.56-2.50)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.03 (at 2.51Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1334)	Depositor
R, R_{free}	0.205 , 0.251 0.220 , 0.262	Depositor DCC
R_{free} test set	2086 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	58.6	Xtriage
Anisotropy	0.306	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 52.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11337	wwPDB-VP
Average B, all atoms (Å ²)	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.68% 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.

4 Model quality [i](#)

4.1 Standard geometry [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.2 Too-close contacts [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA [i](#)

MolProbity failed to run properly - this section is therefore empty.

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

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

4.5 Carbohydrates [i](#)

12 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	B	1	2,1	14,14,15	0.35	0	17,19,21	0.39	0
2	NAG	B	2	2	14,14,15	0.30	0	17,19,21	0.51	0
2	BMA	B	3	2	11,11,12	0.71	0	15,15,17	0.94	0
2	MAN	B	4	2	11,11,12	0.75	0	15,15,17	0.96	2 (13%)
2	NAG	C	1	2,1	14,14,15	0.31	0	17,19,21	0.46	0
2	NAG	C	2	2	14,14,15	0.44	0	17,19,21	0.38	0
2	BMA	C	3	2	11,11,12	0.63	0	15,15,17	0.74	0
2	MAN	C	4	2	11,11,12	0.65	0	15,15,17	1.01	2 (13%)
2	NAG	D	1	2,1	14,14,15	0.36	0	17,19,21	0.42	0
2	NAG	D	2	2	14,14,15	0.29	0	17,19,21	0.36	0
2	BMA	D	3	2	11,11,12	0.91	0	15,15,17	1.24	1 (6%)
2	MAN	D	4	2	11,11,12	0.82	1 (9%)	15,15,17	0.91	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
2	NAG	B	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	B	2	2	-	4/6/23/26	0/1/1/1
2	BMA	B	3	2	-	0/2/19/22	0/1/1/1
2	MAN	B	4	2	-	1/2/19/22	0/1/1/1
2	NAG	C	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	2/6/23/26	0/1/1/1
2	BMA	C	3	2	-	2/2/19/22	0/1/1/1
2	MAN	C	4	2	-	0/2/19/22	0/1/1/1
2	NAG	D	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1
2	BMA	D	3	2	-	2/2/19/22	0/1/1/1
2	MAN	D	4	2	-	2/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	4	MAN	O5-C1	-2.20	1.40	1.43

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	3	BMA	C1-C2-C3	2.88	113.84	109.64
2	C	4	MAN	C1-O5-C5	2.64	115.72	112.19
2	B	4	MAN	C1-O5-C5	2.32	115.29	112.19
2	D	4	MAN	O2-C2-C3	-2.24	105.50	110.15
2	B	4	MAN	O2-C2-C3	-2.14	105.72	110.15

There are no chirality outliers.

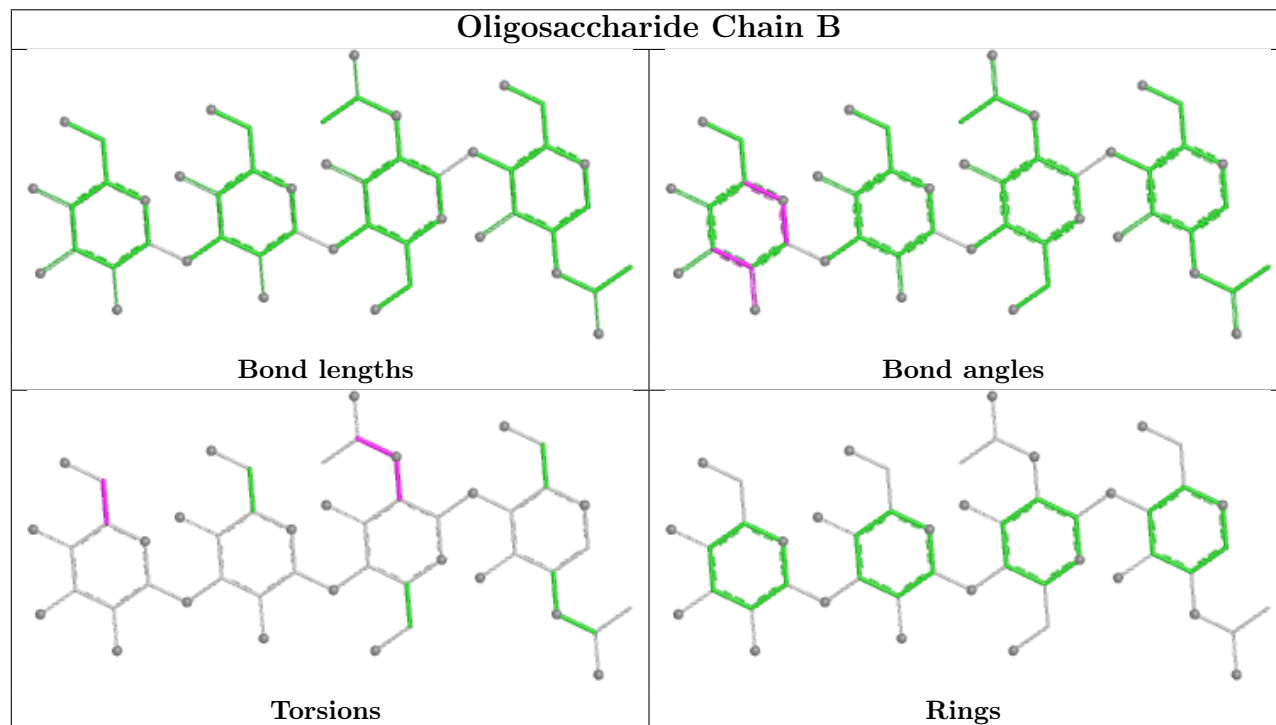
5 of 15 torsion outliers are listed below:

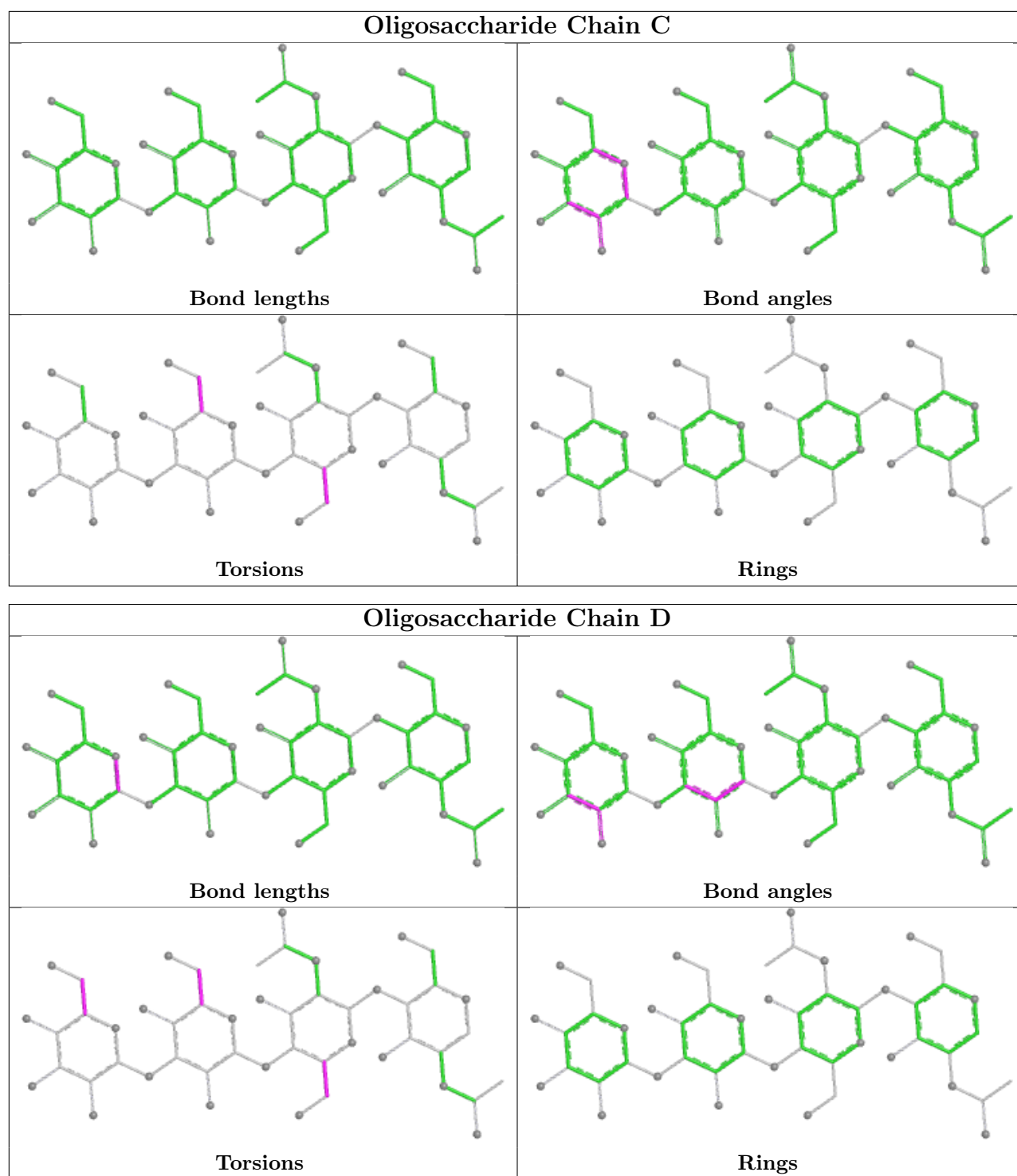
Mol	Chain	Res	Type	Atoms
2	D	2	NAG	C4-C5-C6-O6
2	D	2	NAG	O5-C5-C6-O6
2	C	2	NAG	C4-C5-C6-O6
2	C	3	BMA	C4-C5-C6-O6
2	C	2	NAG	O5-C5-C6-O6

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.





4.6 Ligand geometry [i](#)

5 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	$\# Z > 2$
3	NAG	A	801	1	14,14,15	0.19	0	17,19,21	0.42	0
3	NAG	A	811	1	14,14,15	0.27	0	17,19,21	0.40	0
3	NAG	A	806	1	14,14,15	0.22	0	17,19,21	0.43	0
3	NAG	A	816	1	14,14,15	0.19	0	17,19,21	0.44	0
4	BLD	A	817	-	36,37,37	3.22	12 (33%)	49,59,59	2.41	21 (42%)

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	A	801	1	-	2/6/23/26	0/1/1/1
3	NAG	A	811	1	-	2/6/23/26	0/1/1/1
3	NAG	A	806	1	-	0/6/23/26	0/1/1/1
3	NAG	A	816	1	-	0/6/23/26	0/1/1/1
4	BLD	A	817	-	-	1/20/85/85	0/4/4/4

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	817	BLD	O07-C07	-10.83	1.29	1.45
4	A	817	BLD	O06-C06	9.68	1.45	1.21
4	A	817	BLD	C15-C14	-5.64	1.42	1.54
4	A	817	BLD	C11-C09	4.92	1.61	1.53
4	A	817	BLD	C20-C17	-3.53	1.48	1.54

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	817	BLD	C15-C14-C08	-7.01	107.91	119.10
4	A	817	BLD	C07-O07-C06	-6.02	112.63	120.98
4	A	817	BLD	C11-C09-C08	-4.18	105.95	111.78
4	A	817	BLD	C01-C10-C05	3.68	112.87	107.11
4	A	817	BLD	C12-C13-C17	3.54	121.81	116.60

There are no chirality outliers.

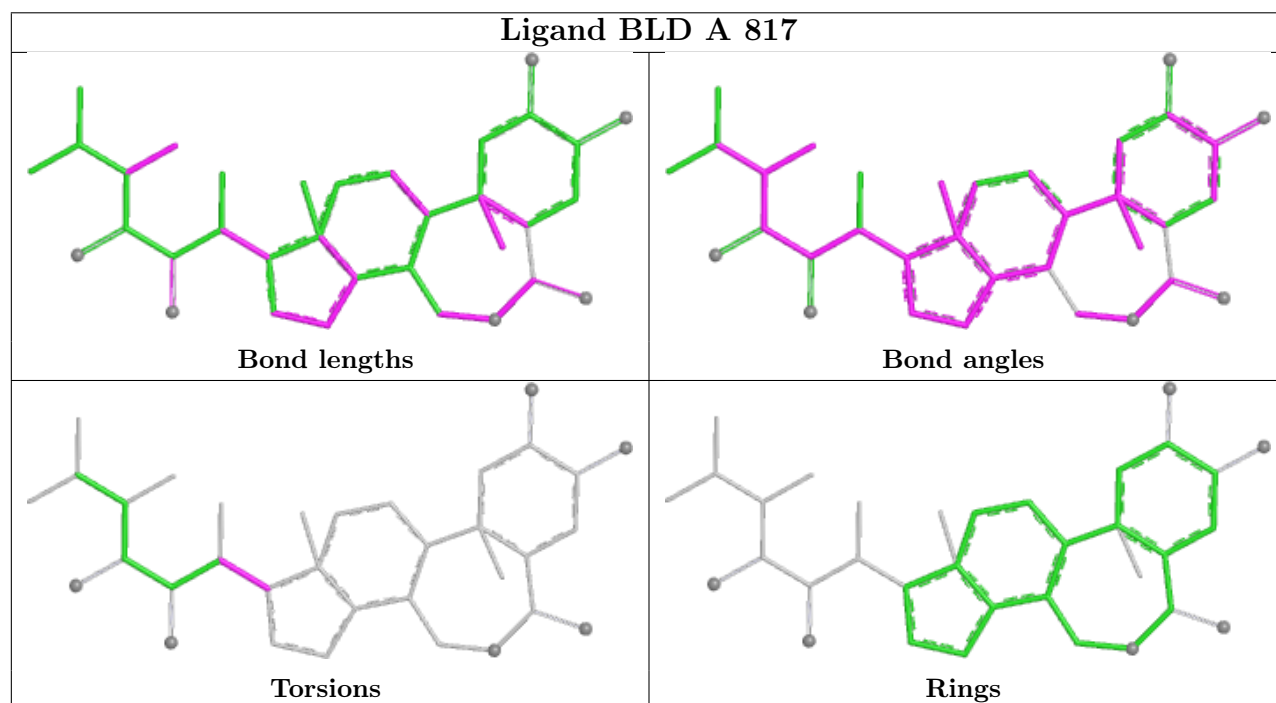
All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	811	NAG	O5-C5-C6-O6
3	A	811	NAG	C4-C5-C6-O6
4	A	817	BLD	C16-C17-C20-C22
3	A	801	NAG	C4-C5-C6-O6
3	A	801	NAG	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 all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

5 Fit of model and data [i](#)

5.1 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	743/774 (95%)	0.62	61 (8%) 17 15	37, 79, 124, 160	5 (0%)

The worst 5 of 61 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	771	ASP	8.3
1	A	29	SER	6.6
1	A	49	LYS	6.0
1	A	48	ASP	5.5
1	A	409	ASN	5.4

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

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

5.3 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.

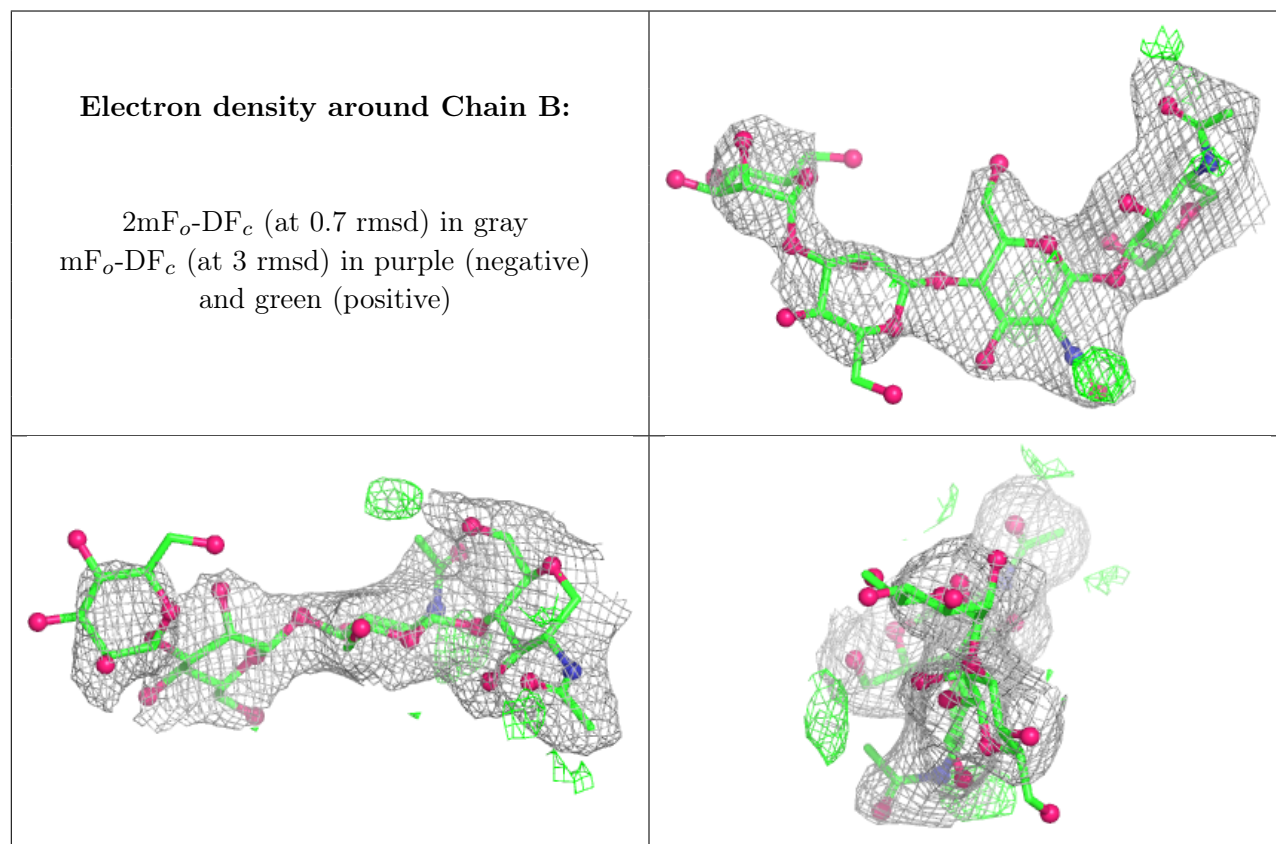
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	MAN	B	4	11/12	0.36	0.17	138,153,155,156	0
2	BMA	C	3	11/12	0.42	0.18	134,141,144,147	0
2	BMA	B	3	11/12	0.64	0.19	108,130,140,149	0
2	BMA	D	3	11/12	0.65	0.21	102,126,138,147	0
2	MAN	C	4	11/12	0.70	0.19	127,145,150,151	0
2	MAN	D	4	11/12	0.72	0.15	114,135,139,139	0
2	NAG	C	2	14/15	0.80	0.16	58,109,126,138	0

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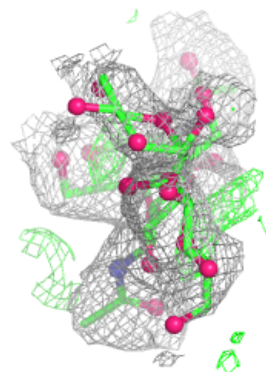
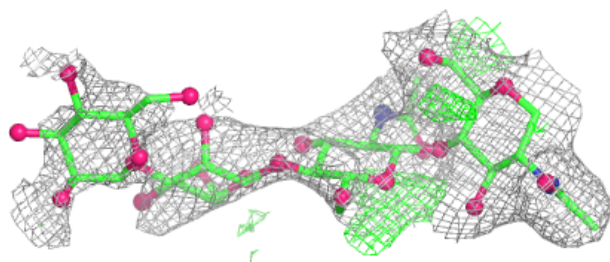
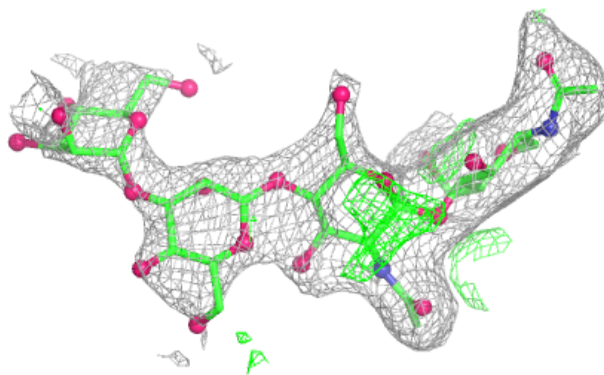
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	NAG	B	2	14/15	0.82	0.16	54,77,93,98	0
2	NAG	D	2	14/15	0.89	0.13	61,79,92,92	0
2	NAG	C	1	14/15	0.91	0.12	44,62,69,85	0
2	NAG	D	1	14/15	0.92	0.10	51,62,71,73	0
2	NAG	B	1	14/15	0.96	0.09	35,42,61,63	0

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.

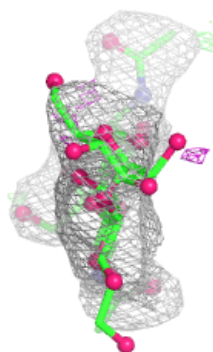
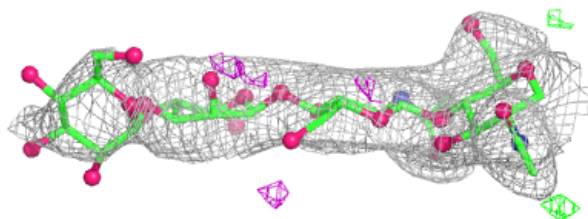
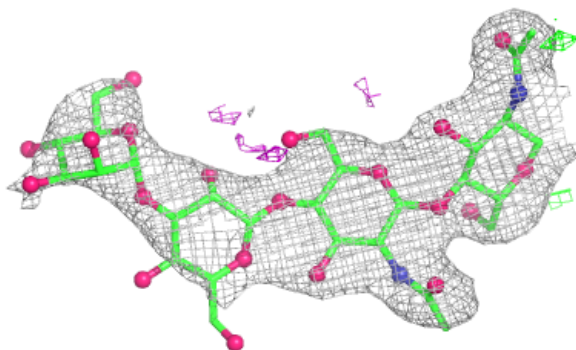


Electron density around Chain C:

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

**Electron density around Chain D:**

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

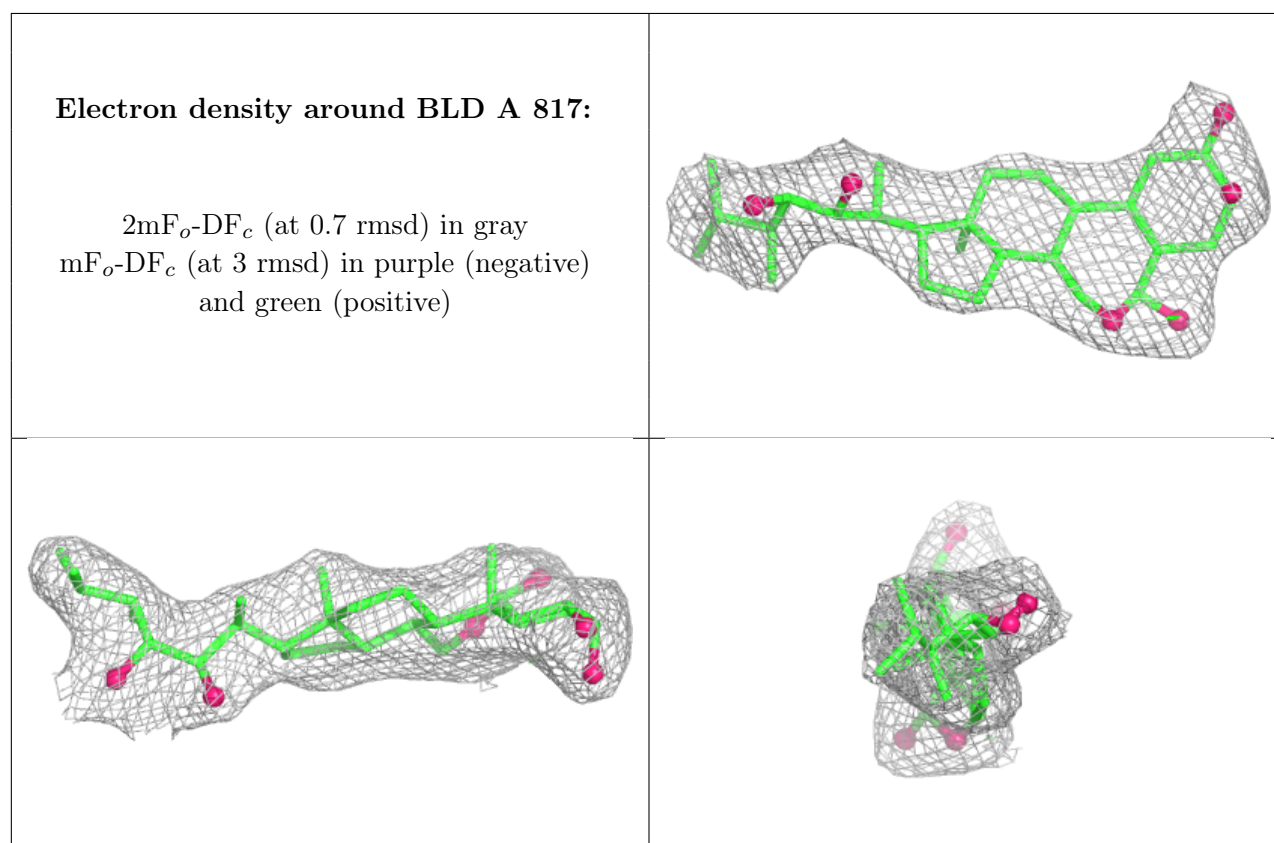


5.4 Ligands [i](#)

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	A	816	14/15	0.61	0.24	94,118,127,130	0
3	NAG	A	811	14/15	0.66	0.16	100,112,120,120	0
3	NAG	A	806	14/15	0.74	0.19	66,90,95,102	0
3	NAG	A	801	14/15	0.82	0.17	72,92,107,113	0
4	BLD	A	817	34/34	0.96	0.10	46,60,70,80	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



5.5 Other polymers [i](#)

There are no such residues in this entry.