Full wwPDB X-ray Structure Validation Report ⓘ

Jan 7, 2024 – 09:21 am GMT

PDB ID	:	6FIF
Title	:	Crystal structure of the BRI1 Gly644-Asp (bri1-6) mutant from Arabidopsis thaliana.
Authors	:	Hothorn, M.; Santiago, J.; Hohmann, U.
Deposited on	:	2018-01-18
Resolution	:	2.54 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:

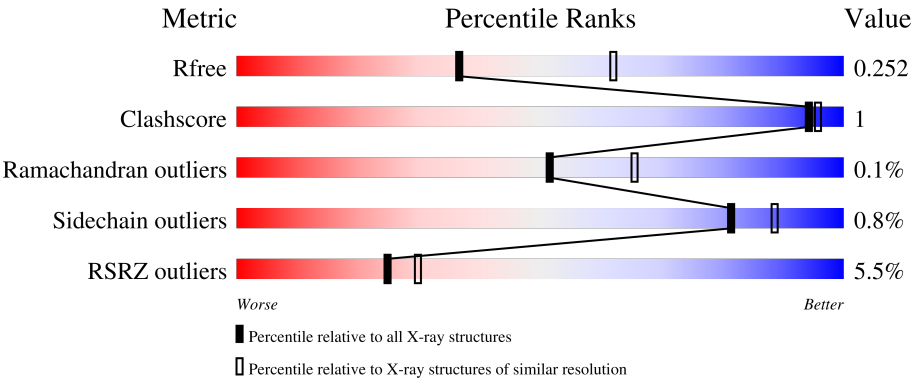
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.54 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	1284 (2.56-2.52)
Clashscore	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272 (2.56-2.52)

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	A	837	5%, 84%, 5%, 11%
2	B	2	50%, 50%
2	C	2	100%
3	D	3	33%, 67%
4	E	3	33%, 67%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	C	2	-	-	-	X
3	NAG	D	2	-	-	-	X
4	BMA	E	3	-	-	-	X

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 5846 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 BRASSINOSTEROID INSENSITIVE 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	744	Total	C	N	O	S	0	8	0
			5626	3559	928	1107	32			

There are 50 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	644	ASP	GLY	conflict	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	SER	-	expression tag	UNP O22476
A	798	ALA	-	expression tag	UNP O22476
A	799	TRP	-	expression tag	UNP O22476
A	800	SER	-	expression tag	UNP O22476
A	801	HIS	-	expression tag	UNP O22476
A	802	PRO	-	expression tag	UNP O22476
A	803	GLN	-	expression tag	UNP O22476
A	804	PHE	-	expression tag	UNP O22476
A	805	GLU	-	expression tag	UNP O22476
A	806	LYS	-	expression tag	UNP O22476
A	807	GLY	-	expression tag	UNP O22476
A	808	GLY	-	expression tag	UNP O22476
A	809	GLY	-	expression tag	UNP O22476
A	810	SER	-	expression tag	UNP O22476
A	811	GLY	-	expression tag	UNP O22476
A	812	GLY	-	expression tag	UNP O22476
A	813	GLY	-	expression tag	UNP O22476
A	814	SER	-	expression tag	UNP O22476

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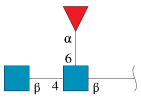
Chain	Residue	Modelled	Actual	Comment	Reference
A	815	GLY	-	expression tag	UNP O22476
A	816	GLY	-	expression tag	UNP O22476
A	817	SER	-	expression tag	UNP O22476
A	818	ALA	-	expression tag	UNP O22476
A	819	TRP	-	expression tag	UNP O22476
A	820	SER	-	expression tag	UNP O22476
A	821	HIS	-	expression tag	UNP O22476
A	822	PRO	-	expression tag	UNP O22476
A	823	GLN	-	expression tag	UNP O22476
A	824	PHE	-	expression tag	UNP O22476
A	825	GLU	-	expression tag	UNP O22476
A	826	LYS	-	expression tag	UNP O22476
A	827	GLY	-	expression tag	UNP O22476
A	828	ALA	-	expression tag	UNP O22476
A	829	HIS	-	expression tag	UNP O22476
A	830	HIS	-	expression tag	UNP O22476
A	831	HIS	-	expression tag	UNP O22476
A	832	HIS	-	expression tag	UNP O22476
A	833	HIS	-	expression tag	UNP O22476
A	834	HIS	-	expression tag	UNP O22476
A	835	HIS	-	expression tag	UNP O22476
A	836	HIS	-	expression tag	UNP O22476
A	837	HIS	-	expression tag	UNP O22476

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

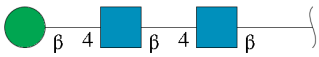
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	C	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



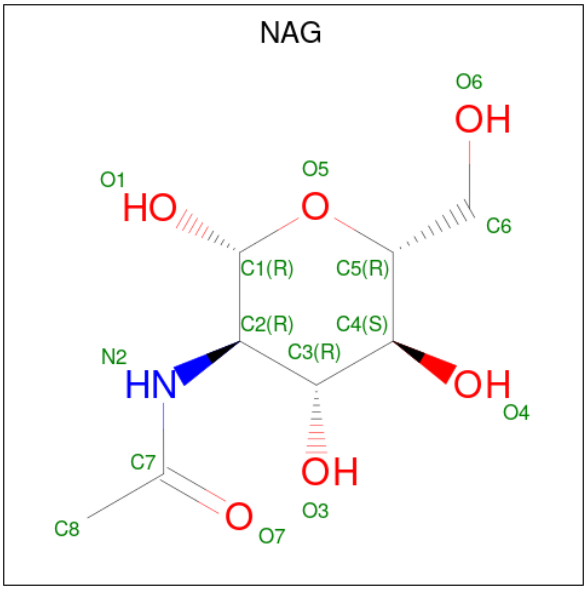
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
3	D	3	Total C N O 38 22 2 14	0	0	0

- Molecule 4 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
4	E	3	Total C N O 39 22 2 15	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	A	1	Total C N O 14 8 1 5	0	0
5	A	1	Total C N O 14 8 1 5	0	0

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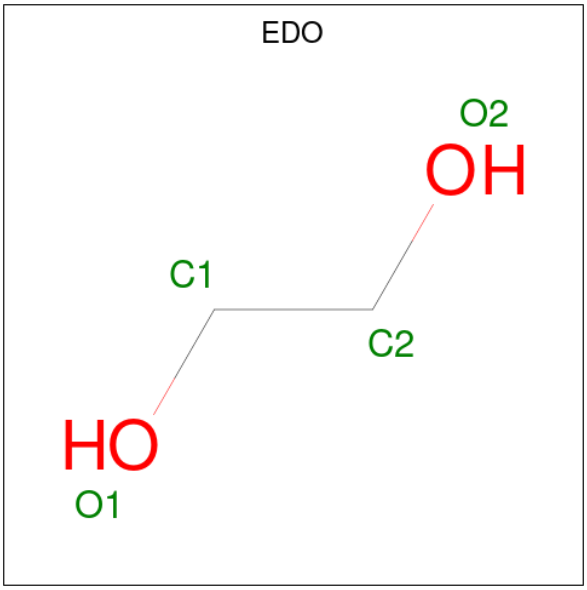
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N O 14 8 1 5	0	0
5	A	1	Total C N O 14 8 1 5	0	0

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 4 2 2	0	0

- Molecule 7 is water.

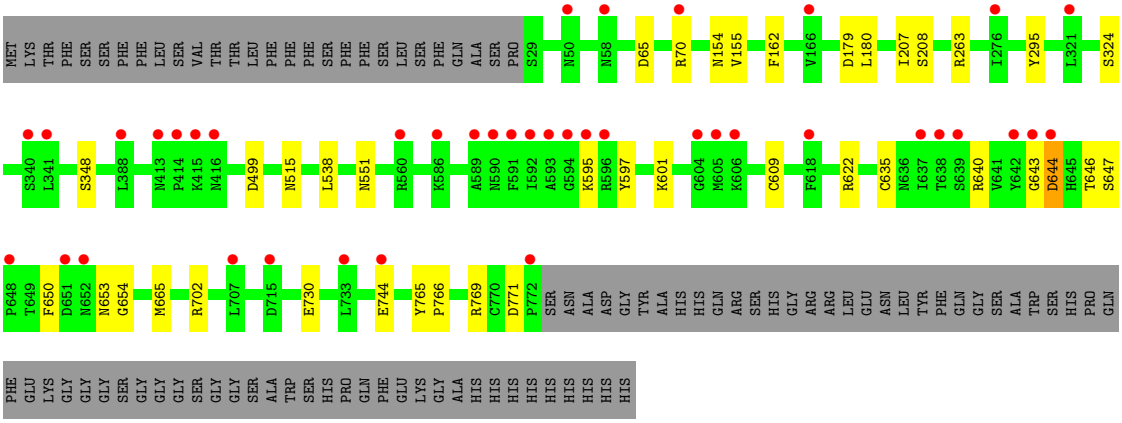
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	27	Total O 27 27	0	0

3 Residue-property plots (i)

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: Protein BRASSINOSTEROID INSENSITIVE 1

Chain A:

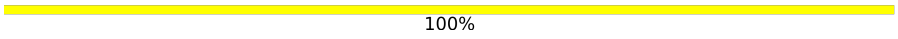


• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain B:

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

Chain C:

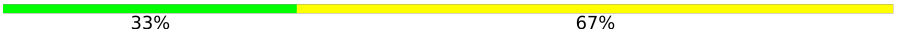


• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:

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

Chain E:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	119.68Å 67.57Å 151.85Å 90.00° 100.65° 90.00°	Depositor
Resolution (Å)	19.89 – 2.54 19.88 – 2.54	Depositor EDS
% Data completeness (in resolution range)	98.7 (19.89-2.54) 99.0 (19.88-2.54)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	1.13 (at 2.53Å)	Xtriage
Refinement program	REFMAC 5.8.0189	Depositor
R, R_{free}	0.205 , 0.254 0.208 , 0.252	Depositor DCC
R_{free} test set	1898 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å^2)	65.6	Xtriage
Anisotropy	0.659	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 46.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	5846	wwPDB-VP
Average B, all atoms (Å^2)	91.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.74% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] 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: EDO, FUC, BMA, 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	1.00	5/5757 (0.1%)	0.94	11/7820 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	551	ASN	CG-ND2	8.10	1.53	1.32
1	A	744	GLU	CD-OE2	6.06	1.32	1.25
1	A	208	SER	CB-OG	-5.68	1.34	1.42
1	A	730	GLU	CG-CD	5.37	1.60	1.51
1	A	154	ASN	CG-ND2	5.01	1.45	1.32

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	622	ARG	NE-CZ-NH2	-8.04	116.28	120.30
1	A	665	MET	CG-SD-CE	7.19	111.71	100.20
1	A	179	ASP	CB-CG-OD1	7.04	124.63	118.30
1	A	771	ASP	CB-CG-OD2	-6.60	112.36	118.30
1	A	499	ASP	CB-CG-OD2	6.56	124.20	118.30
1	A	65[A]	ASP	CB-CG-OD1	5.80	123.52	118.30
1	A	65[B]	ASP	CB-CG-OD1	5.80	123.52	118.30
1	A	179	ASP	OD1-CG-OD2	-5.61	112.65	123.30
1	A	702	ARG	NE-CZ-NH1	5.43	123.01	120.30
1	A	70[A]	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	A	70[B]	ARG	NE-CZ-NH2	-5.18	117.71	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	5626	0	5536	15	0
2	B	28	0	25	1	0
2	C	28	0	25	0	0
3	D	38	0	33	0	0
4	E	39	0	34	0	0
5	A	56	0	52	0	0
6	A	4	0	6	0	0
7	A	27	0	0	0	0
All	All	5846	0	5711	15	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 1.

All (15) 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:595:LYS:O	1:A:646:THR:HG23	1.62	0.99
1:A:595:LYS:O	1:A:646:THR:CG2	2.40	0.68
1:A:597:TYR:HD1	1:A:646:THR:H	1.40	0.66
1:A:601:LYS:HB3	1:A:640:ARG:CB	2.33	0.58
1:A:155:VAL:HG23	1:A:180:LEU:HD23	1.90	0.53
1:A:155:VAL:CG2	1:A:180:LEU:HD23	2.38	0.53
1:A:295:TYR:CE2	2:B:1:NAG:H82	2.46	0.51
1:A:650:PHE:CE1	1:A:654:GLY:HA3	2.49	0.47
1:A:207:ILE:HG23	1:A:207:ILE:O	2.13	0.47
1:A:609:CYS:HB2	1:A:635:CYS:HA	1.99	0.44
1:A:515:ASN:HA	1:A:538:LEU:HA	2.01	0.43
1:A:643:GLY:C	1:A:644:ASP:OD1	2.56	0.43
1:A:644:ASP:OD1	1:A:644:ASP:N	2.53	0.41
1:A:765:TYR:CG	1:A:766:PRO:HA	2.55	0.41
1:A:324:SER:HA	1:A:348:SER:O	2.20	0.41

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	750/837 (90%)	696 (93%)	53 (7%)	1 (0%)	51 65

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	647	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	648/733 (88%)	643 (99%)	5 (1%)	81 88

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	162	PHE
1	A	263	ARG
1	A	644	ASP
1	A	653	ASN
1	A	769	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	204	HIS
1	A	249	HIS

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

10 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	1,2	14,14,15	0.51	0	17,19,21	1.46	3 (17%)
2	NAG	B	2	2	14,14,15	0.82	1 (7%)	17,19,21	0.92	0
2	NAG	C	1	1,2	14,14,15	0.63	0	17,19,21	1.22	2 (11%)
2	NAG	C	2	2	14,14,15	0.58	0	17,19,21	1.21	1 (5%)
3	NAG	D	1	1,3	14,14,15	0.46	0	17,19,21	0.82	1 (5%)
3	NAG	D	2	3	14,14,15	1.21	1 (7%)	17,19,21	3.98	5 (29%)
3	FUC	D	3	3	10,10,11	0.49	0	14,14,16	0.71	0
4	NAG	E	1	1,4	14,14,15	1.51	1 (7%)	17,19,21	0.99	1 (5%)
4	NAG	E	2	4	14,14,15	0.36	0	17,19,21	0.70	0
4	BMA	E	3	4	11,11,12	0.42	0	15,15,17	0.84	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	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	2	2	-	2/6/23/26	0/1/1/1
2	NAG	C	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	C	2	2	-	1/6/23/26	0/1/1/1
3	NAG	D	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	D	2	3	-	3/6/23/26	0/1/1/1
3	FUC	D	3	3	-	-	0/1/1/1
4	NAG	E	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	E	2	4	-	0/6/23/26	0/1/1/1
4	BMA	E	3	4	-	0/2/19/22	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	1	NAG	C1-C2	5.04	1.59	1.52
3	D	2	NAG	C2-N2	-2.95	1.41	1.46
2	B	2	NAG	C1-C2	2.17	1.55	1.52

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	2	NAG	C8-C7-N2	-11.28	96.99	116.10
3	D	2	NAG	C2-N2-C7	8.26	134.66	122.90
3	D	2	NAG	O7-C7-C8	7.01	135.08	122.06
2	C	2	NAG	C1-O5-C5	4.04	117.67	112.19
4	E	1	NAG	C1-C2-N2	-3.15	105.11	110.49
3	D	2	NAG	O7-C7-N2	2.95	127.38	121.95
2	B	1	NAG	O7-C7-N2	2.73	126.97	121.95
2	B	1	NAG	O5-C1-C2	-2.63	107.13	111.29
2	B	1	NAG	O5-C5-C6	2.53	111.17	107.20
2	C	1	NAG	C3-C4-C5	2.40	114.52	110.24
4	E	3	BMA	O5-C5-C6	2.27	110.76	107.20
3	D	2	NAG	O3-C3-C2	2.08	113.76	109.47
3	D	1	NAG	O5-C5-C6	2.02	110.38	107.20
2	C	1	NAG	O5-C5-C4	-2.01	105.93	110.83

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	2	NAG	C1-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
2	C	1	NAG	C4-C5-C6-O6
2	C	1	NAG	O5-C5-C6-O6
2	B	2	NAG	C4-C5-C6-O6
3	D	2	NAG	O7-C7-N2-C2
2	B	2	NAG	O5-C5-C6-O6
2	C	2	NAG	O5-C5-C6-O6
3	D	2	NAG	C8-C7-N2-C2

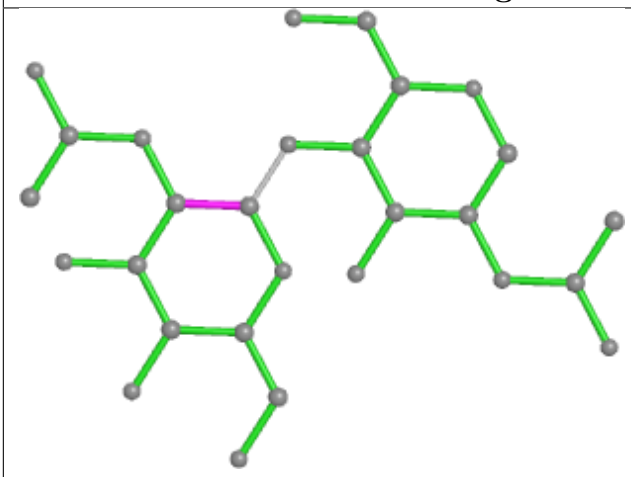
There are no ring outliers.

1 monomer is involved in 1 short contact:

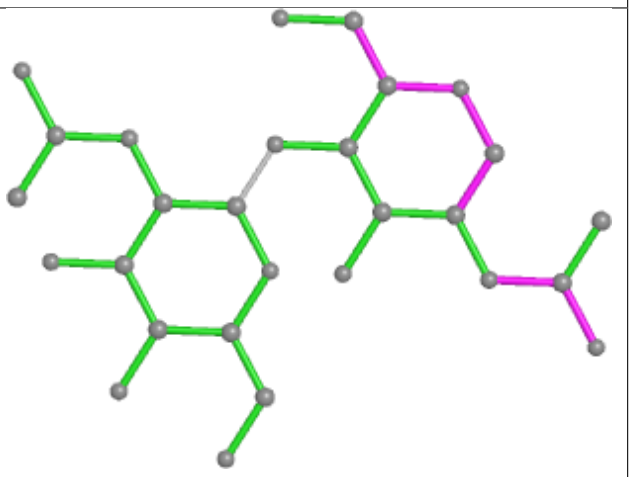
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1	NAG	1	0

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

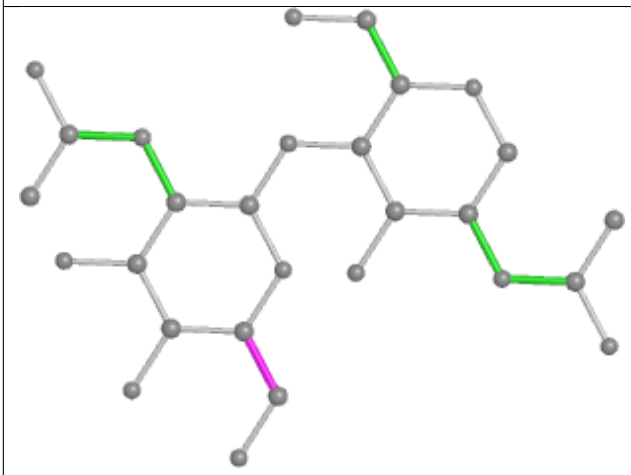
Oligosaccharide Chain B



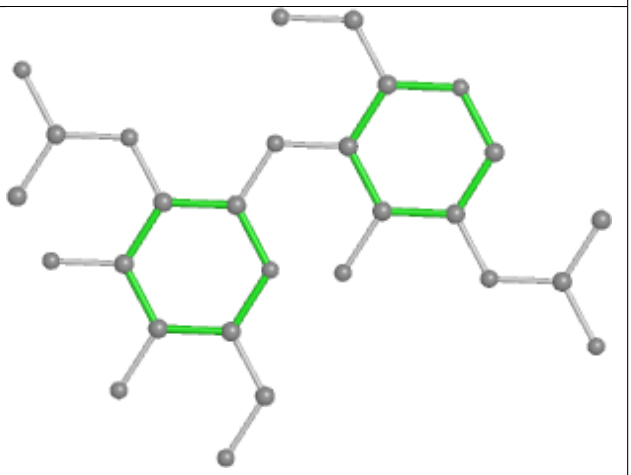
Bond lengths



Bond angles

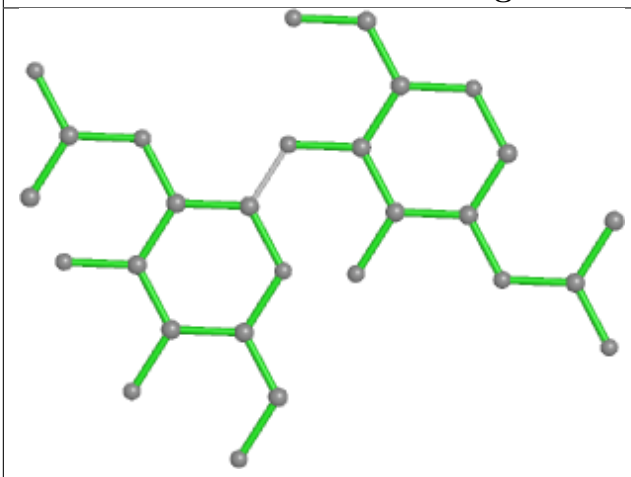


Torsions

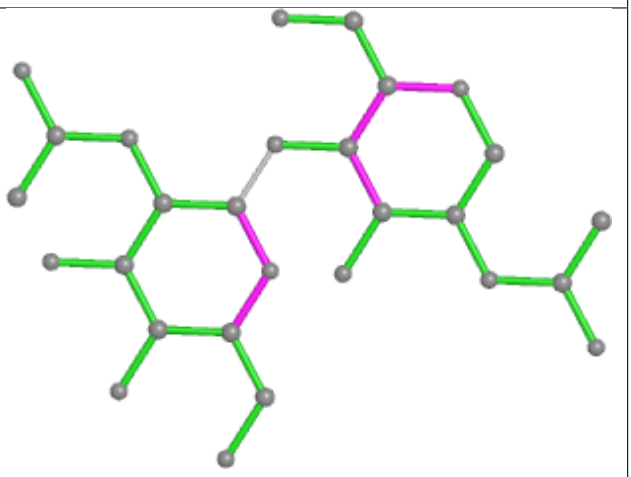


Rings

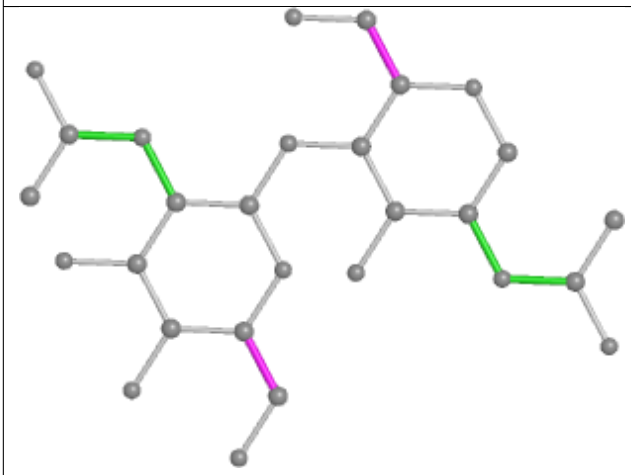
Oligosaccharide Chain C



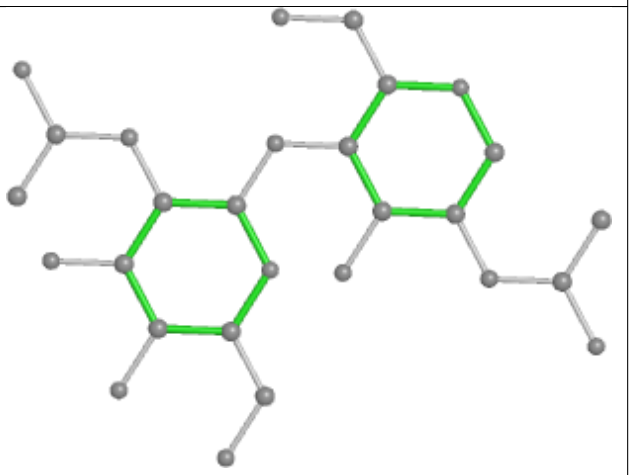
Bond lengths



Bond angles

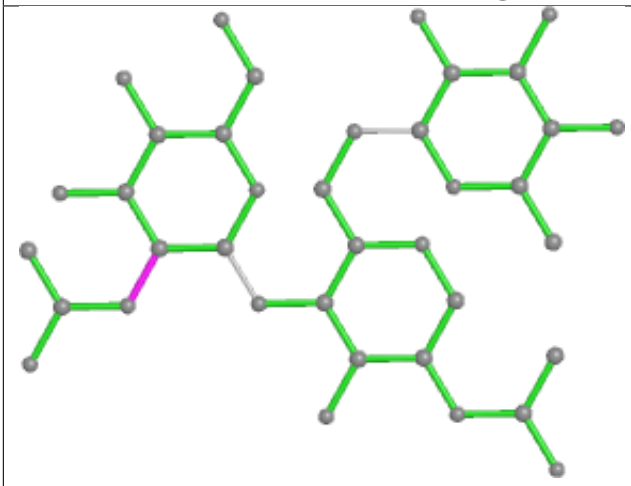


Torsions

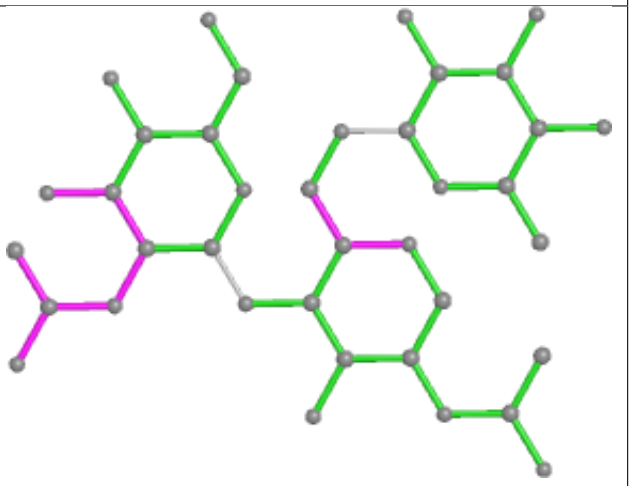


Rings

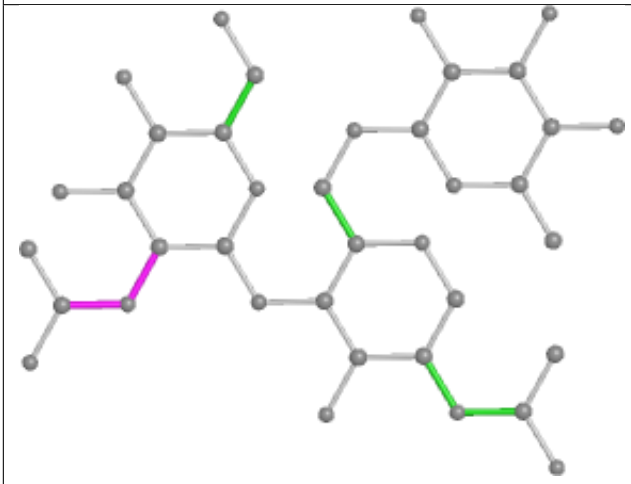
Oligosaccharide Chain D



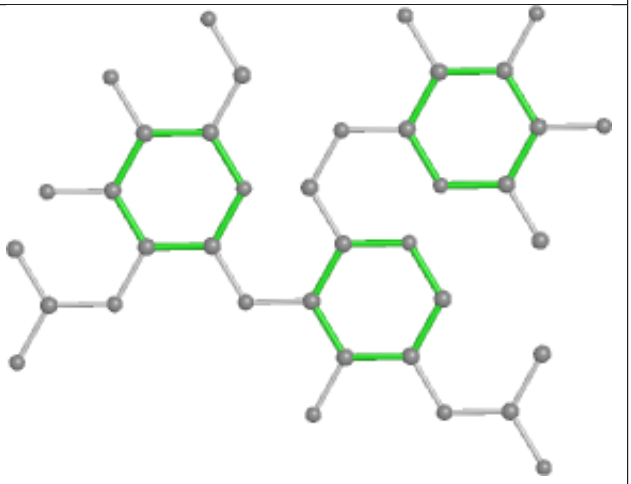
Bond lengths



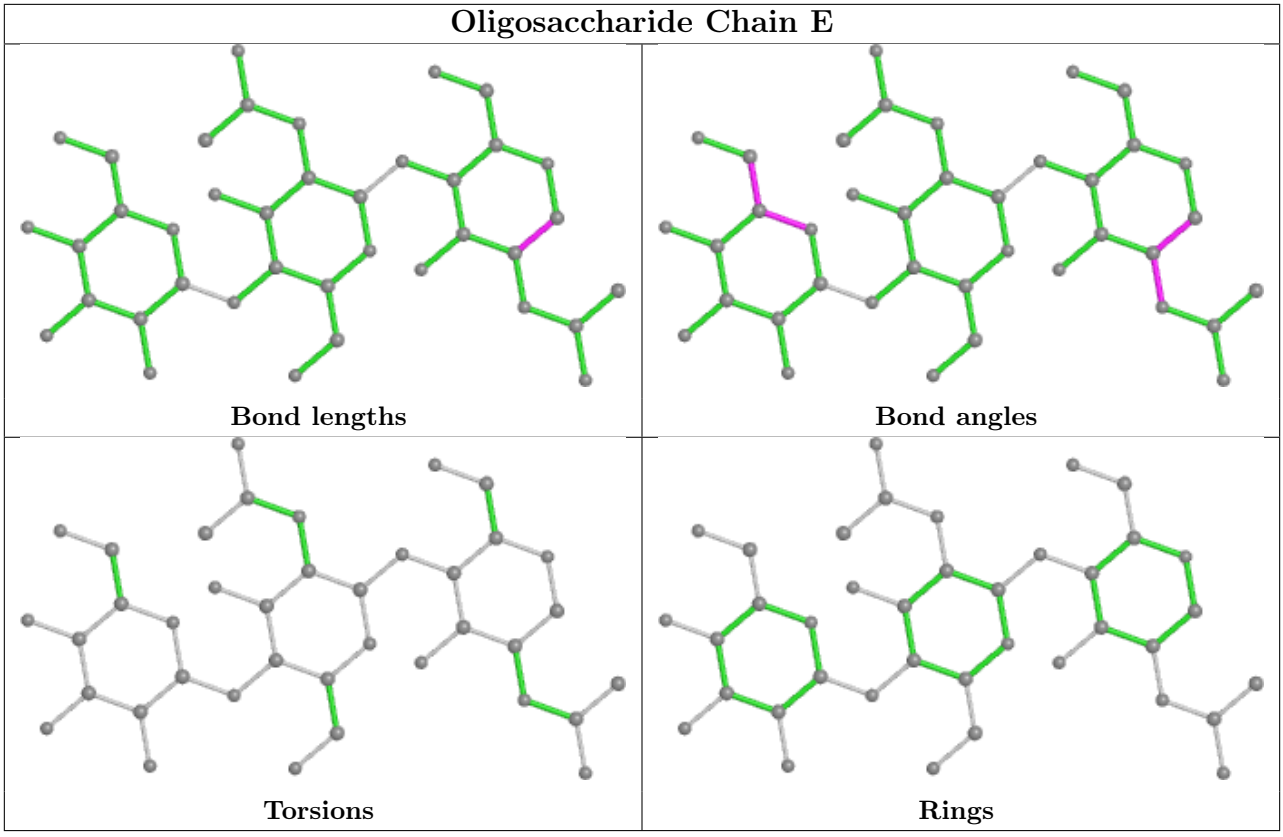
Bond angles



Torsions



Rings



5.6 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	$\#\|Z\| > 2$
6	EDO	A	915	-	3,3,3	0.82	0	2,2,2	0.51	0
5	NAG	A	903	1	14,14,15	0.61	0	17,19,21	1.22	2 (11%)
5	NAG	A	906	1	14,14,15	0.61	0	17,19,21	1.10	1 (5%)
5	NAG	A	911	1	14,14,15	0.60	0	17,19,21	1.21	1 (5%)
5	NAG	A	910	1	14,14,15	0.76	0	17,19,21	1.54	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
6	EDO	A	915	-	-	1/1/1/1	-
5	NAG	A	903	1	-	0/6/23/26	0/1/1/1
5	NAG	A	906	1	-	0/6/23/26	0/1/1/1
5	NAG	A	911	1	-	0/6/23/26	0/1/1/1
5	NAG	A	910	1	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	910	NAG	C4-C3-C2	4.06	116.97	111.02
5	A	910	NAG	O7-C7-C8	-2.56	117.31	122.06
5	A	911	NAG	C1-O5-C5	2.53	115.63	112.19
5	A	903	NAG	C1-C2-N2	-2.52	106.18	110.49
5	A	903	NAG	C1-O5-C5	2.43	115.49	112.19
5	A	906	NAG	C2-N2-C7	2.06	125.83	122.90

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	910	NAG	C1-C2-N2-C7
5	A	910	NAG	O5-C5-C6-O6
6	A	915	EDO	O1-C1-C2-O2
5	A	910	NAG	C4-C5-C6-O6
5	A	910	NAG	C3-C2-N2-C7

There are no ring outliers.

No monomer is involved in short contacts.

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

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, 95^{th} 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	744/837 (88%)	0.21	41 (5%) 25 30	50, 84, 141, 199	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	591	PHE	9.9
1	A	590	ASN	9.2
1	A	637	ILE	8.1
1	A	592	ILE	7.2
1	A	605	MET	7.1
1	A	593	ALA	6.3
1	A	594	GLY	6.2
1	A	414	PRO	5.7
1	A	604	GLY	4.7
1	A	586	LYS	4.5
1	A	415	LYS	4.5
1	A	772	PRO	4.0
1	A	595	LYS	3.9
1	A	276	ILE	3.7
1	A	638	THR	3.7
1	A	644	ASP	3.5
1	A	166	VAL	3.4
1	A	589	ALA	3.4
1	A	652	ASN	3.2
1	A	606	LYS	3.2
1	A	560	ARG	3.0
1	A	341	LEU	3.0
1	A	639	SER	2.8
1	A	340	SER	2.8
1	A	596	ARG	2.7
1	A	643	GLY	2.7
1	A	651	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	642	TYR	2.6
1	A	321	LEU	2.5
1	A	707	LEU	2.5
1	A	413	ASN	2.5
1	A	648	PRO	2.5
1	A	618	PHE	2.4
1	A	744	GLU	2.3
1	A	388	LEU	2.3
1	A	50	ASN	2.2
1	A	70[A]	ARG	2.2
1	A	58	ASN	2.1
1	A	416	ASN	2.1
1	A	733	LEU	2.1
1	A	715	ASP	2.0

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)

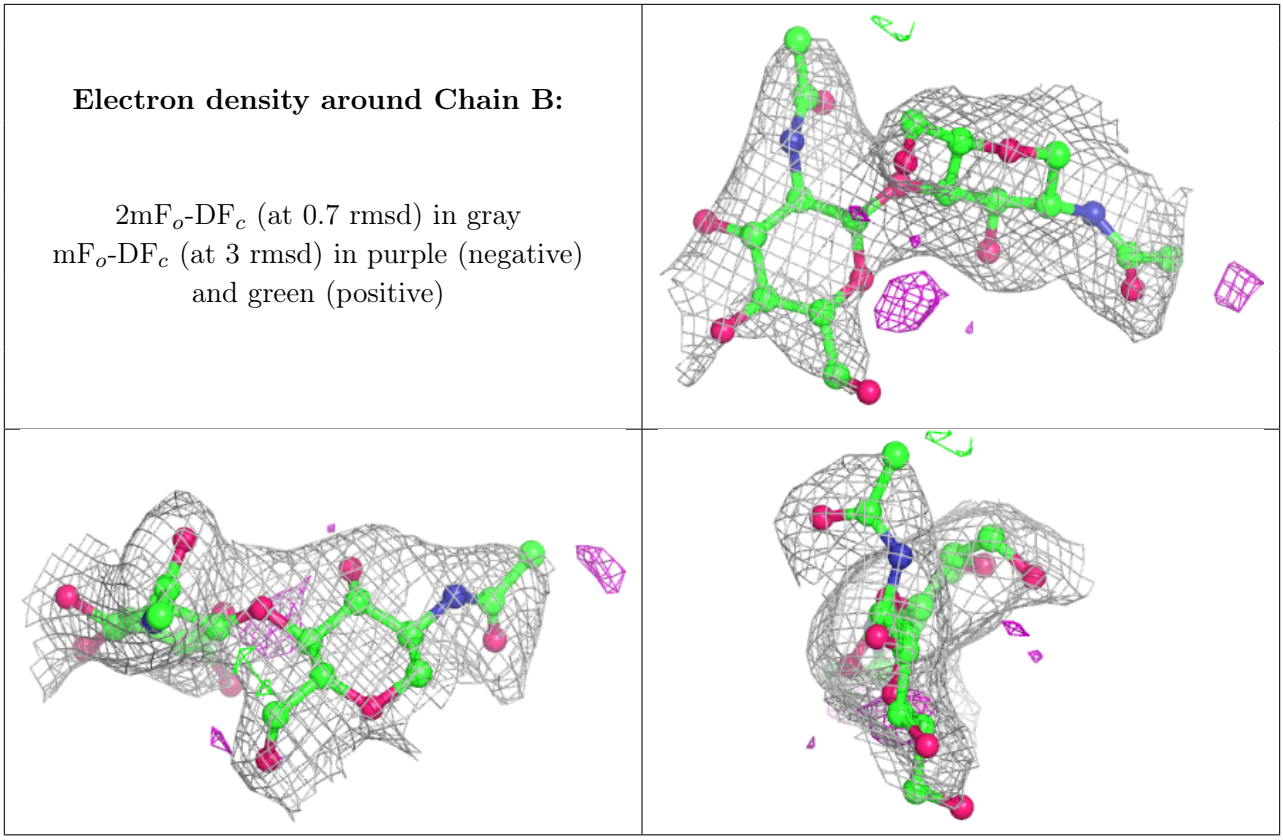
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
4	BMA	E	3	11/12	0.71	0.45	122,140,146,156	0
3	NAG	D	2	14/15	0.72	0.47	120,189,214,217	0
2	NAG	C	2	14/15	0.76	0.59	141,164,182,187	0
3	NAG	D	1	14/15	0.83	0.21	111,147,176,203	0
3	FUC	D	3	10/11	0.86	0.42	106,153,170,175	0
2	NAG	B	2	14/15	0.87	0.42	74,104,124,128	0
2	NAG	C	1	14/15	0.88	0.23	93,113,137,158	0
4	NAG	E	2	14/15	0.92	0.29	90,100,106,109	0
2	NAG	B	1	14/15	0.92	0.17	62,75,85,87	0
4	NAG	E	1	14/15	0.95	0.20	74,90,93,98	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.

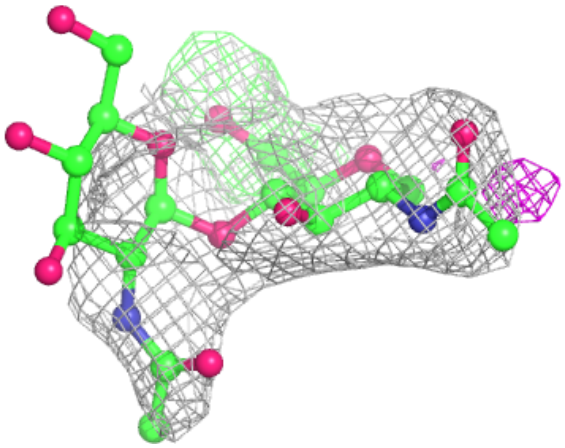
Electron density around Chain B:

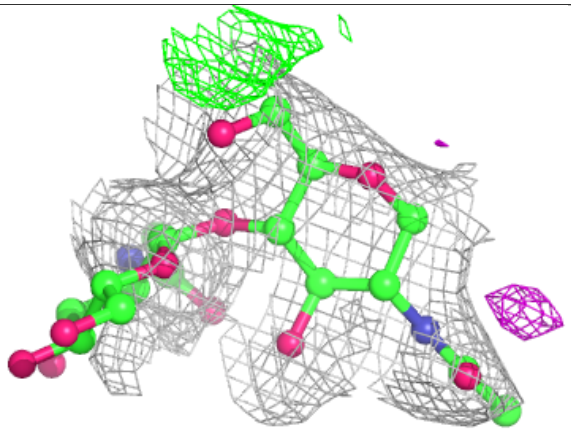
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

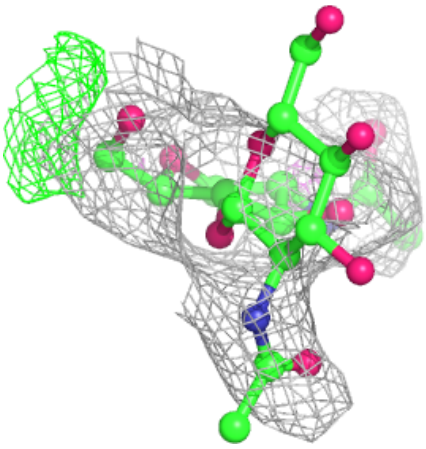


Electron density around Chain C:

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

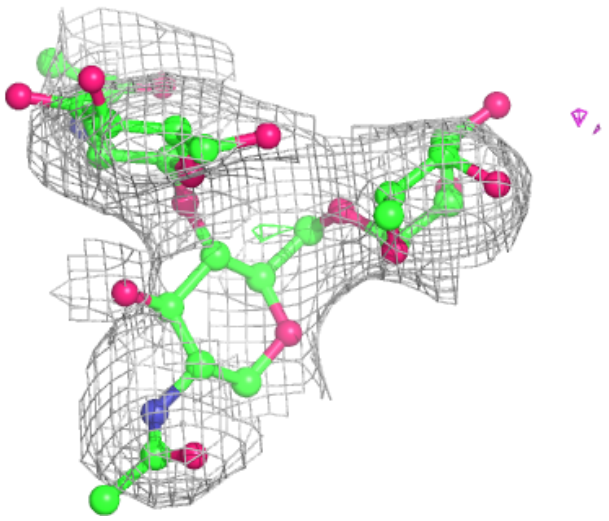


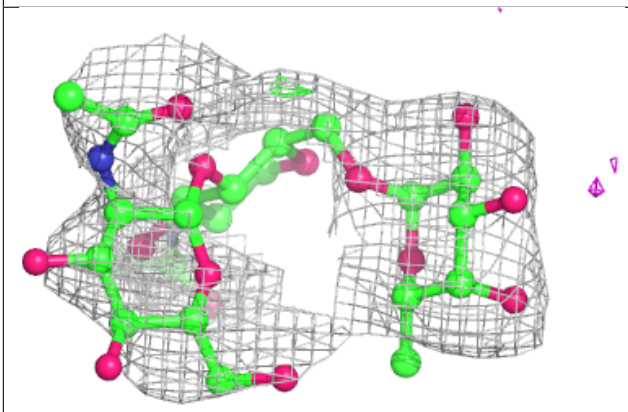


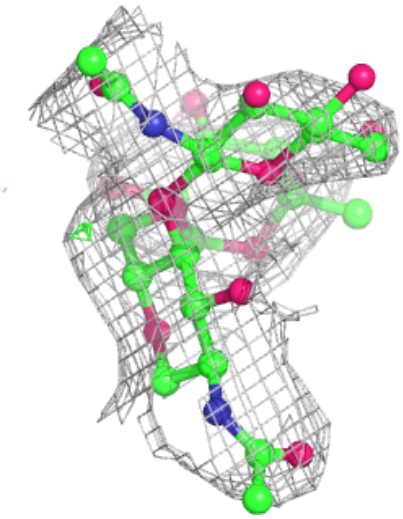


Electron density around Chain D:

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

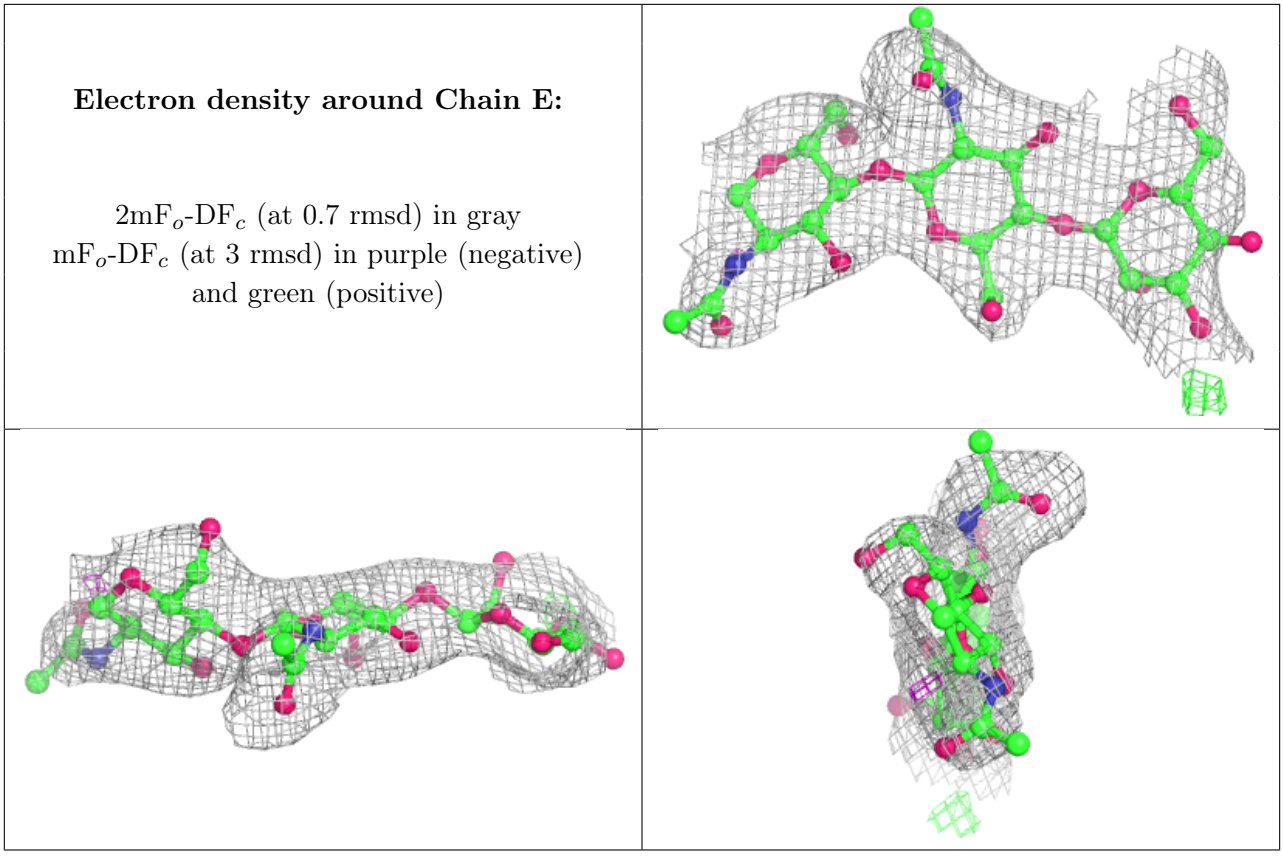






Electron density around Chain E:

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



6.4 Ligands

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, 95^{th} 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	A	910	14/15	0.81	0.43	130,148,167,187	0
5	NAG	A	911	14/15	0.82	0.45	136,152,162,163	0
5	NAG	A	903	14/15	0.85	0.43	92,118,136,140	0
5	NAG	A	906	14/15	0.86	0.41	105,116,130,133	0
6	EDO	A	915	4/4	0.93	0.16	63,70,71,71	0

6.5 Other polymers

There are no such residues in this entry.