wwPDB X-ray Structure Validation Summary Report (i)

Oct 12, 2026 – 06:24 PM EDT

PDB ID	:	9YO3 / pdb_00009yo3
Title	:	Crystal structure of integrin a4b1 headpiece in complex with Firategrast (Mg)
Authors	:	Monroy, M.F.; Lin, F.Y.; Qiao, Q.
Deposited on	:	2025-10-13
Resolution	:	2.15 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 (i) 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 (i)) were used in the production of this report:

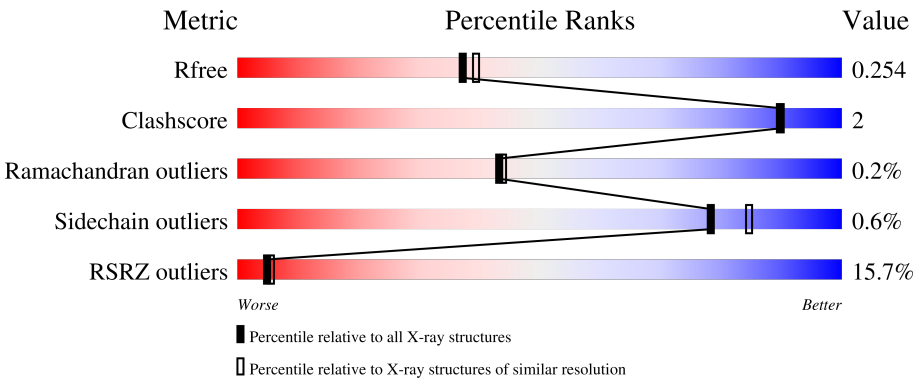
MolProbity	:	4-5-2 with Phenix2.2
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.2
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

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 2.15 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	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

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	597	5%, 94%
2	B	490	27%, 89%, 9%
3	C	3	100%
4	D	2	50%, 50%
5	E	4	50%, 50%

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 16309 atoms, of which 7912 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 Integrin alpha-4,Integrin alpha-V heavy chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	588	8968	2858	4437	785	866	22	0	0	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	PHE	TYR	conflict	UNP P13612
A	589	GLY	-	expression tag	UNP P06756
A	590	GLY	-	expression tag	UNP P06756
A	591	SER	-	expression tag	UNP P06756
A	592	GLU	-	expression tag	UNP P06756
A	593	ASN	-	expression tag	UNP P06756
A	594	LEU	-	expression tag	UNP P06756
A	595	TYR	-	expression tag	UNP P06756
A	596	PHE	-	expression tag	UNP P06756
A	597	GLN	-	expression tag	UNP P06756

- Molecule 2 is a protein called Integrin beta-1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
2	B	448	6768	2151	3316	579	692	30	0	0	0

There are 11 discrepancies between the modelled and reference sequences:

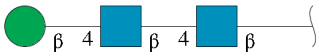
Chain	Residue	Modelled	Actual	Comment	Reference
B	92	HIS	THR	conflict	UNP P05556
B	195	THR	SER	conflict	UNP P05556
B	482	GLY	-	expression tag	UNP P05556
B	483	GLY	-	expression tag	UNP P05556
B	484	SER	-	expression tag	UNP P05556
B	485	GLU	-	expression tag	UNP P05556

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	486	ASN	-	expression tag	UNP P05556
B	487	LEU	-	expression tag	UNP P05556
B	488	TYR	-	expression tag	UNP P05556
B	489	PHE	-	expression tag	UNP P05556
B	490	GLN	-	expression tag	UNP P05556

- Molecule 3 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
			Total	C	H	N	O			
3	C	3	63	22	24	2	15	0	0	0

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

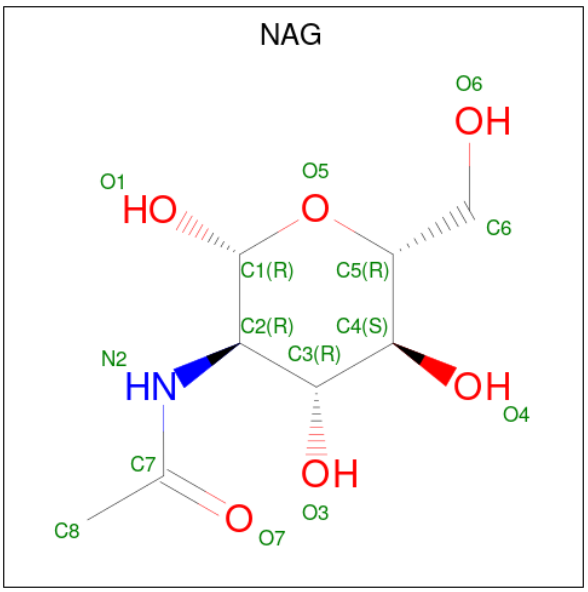
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	H	N	O			
4	D	2	46	16	18	2	10	0	0	0

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-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
			Total	C	H	N	O			
5	E	4	81	28	31	2	20	0	0	0

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula:

$C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	N	O		
6	A	1	24	8	10	1	5	0	0
			Total	C	H	N	O		
6	A	1	24	8	10	1	5	0	0
			Total	C	H	N	O		
6	A	1	24	8	10	1	5	0	0
			Total	C	H	N	O		
6	A	1	24	8	10	1	5	0	0
			Total	C	H	N	O		
6	B	1	24	8	10	1	5	0	0
			Total	C	H	N	O		
6	B	1	24	8	10	1	5	0	0

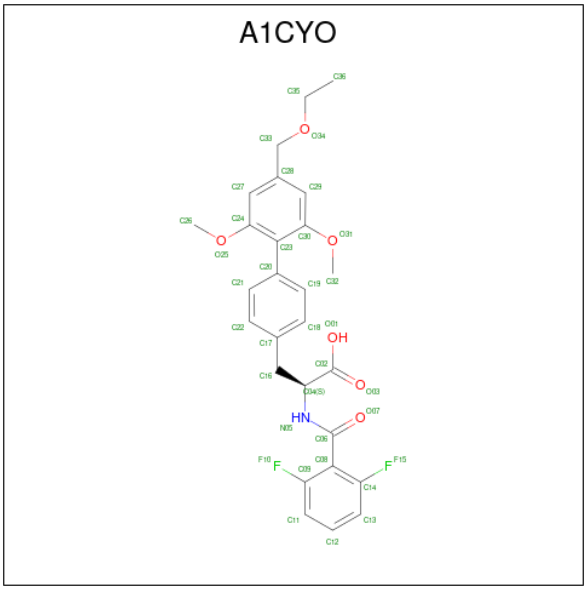
- Molecule 7 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
7	A	3	3	3	0	0
			Total	Ca		
7	B	2	2	2	0	0

- Molecule 8 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
8	B	1	1	1	0	0

- Molecule 9 is N-(2,6-difluorobenzoyl)-4-[4-(ethoxymethyl)-2,6-dimethoxyphenyl]-L-phenylalanine (CCD ID: A1CYO) (formula: $C_{27}H_{27}F_2NO_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	F	H	N	O		
9	B	1	62	27	2	26	1	6	0	0

- Molecule 10 is water.

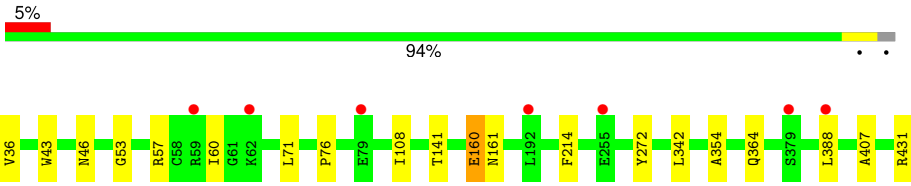
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
10	A	129	129	129	0	0
10	B	42	42	42	0	0

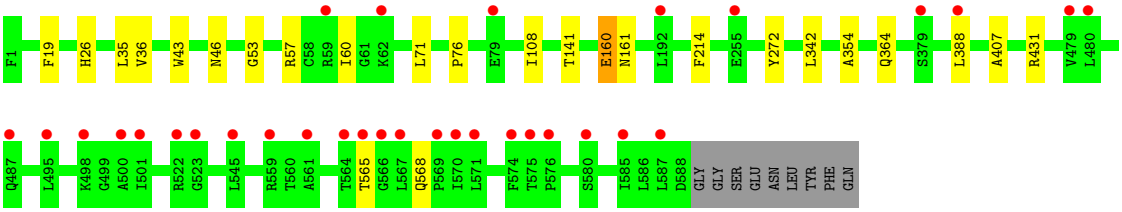
3 Residue-property plots (i)

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: Integrin alpha-4,Integrin alpha-V heavy chain

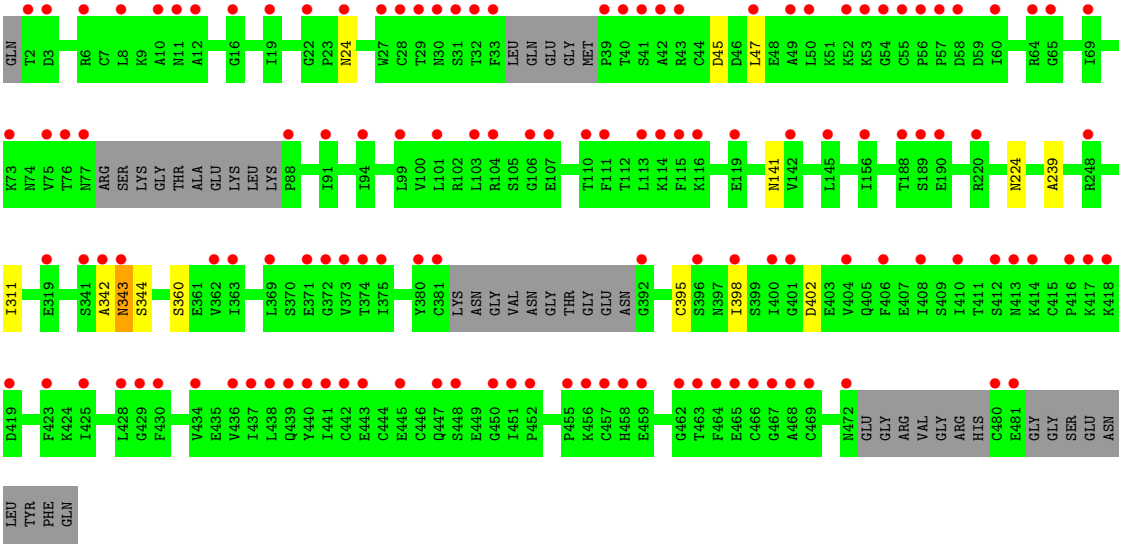
Chain A:





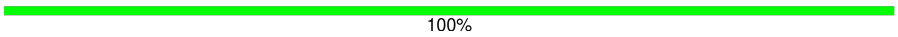
• Molecule 2: Integrin beta-1

Chain B:



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

Chain C:



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

Chain D:

• Molecule 5: alpha-D-mannopyranose-(1-6)-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	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	82.89Å 109.40Å 124.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	62.36 – 2.15 62.36 – 2.15	Depositor EDS
% Data completeness (in resolution range)	99.5 (62.36-2.15) 99.6 (62.36-2.15)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.17 (at 2.14Å)	Xtriage
Refinement program	PHENIX (1.19.2_4158)	Depositor
R, R_{free}	0.218 , 0.245 0.225 , 0.254	Depositor DCC
R_{free} test set	3133 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	44.3	Xtriage
Anisotropy	0.118	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.41 , 45.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	16309	wwPDB-VP
Average B, all atoms (Å^2)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.20% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, MG, A1CYO, BMA, CA, MAN

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	0.17	0/4624	0.38	0/6259
2	B	0.14	0/3512	0.33	0/4745
All	All	0.16	0/8136	0.36	0/11004

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	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	160	GLU	Peptide

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	4531	4437	4434	17	0
2	B	3452	3316	3313	12	0
3	C	39	24	34	0	0
4	D	28	18	25	3	0
5	E	50	31	43	0	0
6	A	56	40	52	2	0
6	B	28	20	26	0	0
7	A	3	0	0	0	0
7	B	2	0	0	0	0
8	B	1	0	0	0	0
9	B	36	26	0	0	0
10	A	129	0	0	0	0
10	B	42	0	0	1	0
All	All	8397	7912	7927	29	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 2.

The worst 5 of 29 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)
2:B:342:ALA:O	10:B:601:HOH:O	1.96	0.82
1:A:46:ASN:ND2	1:A:76:PRO:O	2.19	0.74
1:A:71:LEU:HB3	1:A:141:THR:HG21	1.78	0.65
1:A:35:LEU:CD1	1:A:108:ILE:HD13	2.28	0.63
1:A:35:LEU:HD11	1:A:108:ILE:HD13	1.83	0.59

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	586/597 (98%)	579 (99%)	5 (1%)	2 (0%)	36	34
2	B	438/490 (89%)	425 (97%)	13 (3%)	0	100	100
All	All	1024/1087 (94%)	1004 (98%)	18 (2%)	2 (0%)	43	44

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	214	PHE
1	A	161	ASN

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	487/496 (98%)	485 (100%)	2 (0%)	84	89
2	B	393/431 (91%)	390 (99%)	3 (1%)	73	79
All	All	880/927 (95%)	875 (99%)	5 (1%)	78	84

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

Mol	Chain	Res	Type
1	A	160	GLU
1	A	272	TYR
2	B	45	ASP
2	B	224	ASN
2	B	343	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	123	ASN
1	A	211	GLN
1	A	364	GLN
2	B	5	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	201	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

9 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	3,1	14,14,15	0.41	0	17,19,21	0.53	0
3	NAG	C	2	3	14,14,15	0.30	0	17,19,21	0.51	0
3	BMA	C	3	3	11,11,12	0.65	0	15,15,17	0.82	0
4	NAG	D	1	4	14,14,15	0.68	1 (7%)	17,19,21	0.61	0
4	NAG	D	2	4	14,14,15	0.17	0	17,19,21	0.36	0
5	NAG	E	1	5,1	14,14,15	0.20	0	17,19,21	0.57	0
5	NAG	E	2	5	14,14,15	0.25	0	17,19,21	0.62	0
5	BMA	E	3	5	11,11,12	1.08	1 (9%)	15,15,17	1.02	1 (6%)
5	MAN	E	4	5	11,11,12	0.75	0	15,15,17	1.70	2 (13%)

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	3,1	-	0/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	C	2	3	-	2/6/23/26	0/1/1/1
3	BMA	C	3	3	-	2/2/19/22	0/1/1/1
4	NAG	D	1	4	-	2/6/23/26	0/1/1/1
4	NAG	D	2	4	-	0/6/23/26	0/1/1/1
5	NAG	E	1	5,1	-	1/6/23/26	0/1/1/1
5	NAG	E	2	5	-	2/6/23/26	0/1/1/1
5	BMA	E	3	5	-	1/2/19/22	0/1/1/1
5	MAN	E	4	5	-	1/2/19/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1	NAG	O5-C1	-2.42	1.39	1.43
5	E	3	BMA	C1-C2	2.30	1.57	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	E	4	MAN	C1-O5-C5	5.47	119.51	112.19
5	E	3	BMA	O2-C2-C3	-2.65	104.66	110.15
5	E	4	MAN	O2-C2-C3	-2.16	105.68	110.15

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	3	BMA	O5-C5-C6-O6
3	C	3	BMA	C4-C5-C6-O6
3	C	2	NAG	C4-C5-C6-O6
3	C	2	NAG	O5-C5-C6-O6
5	E	2	NAG	C8-C7-N2-C2

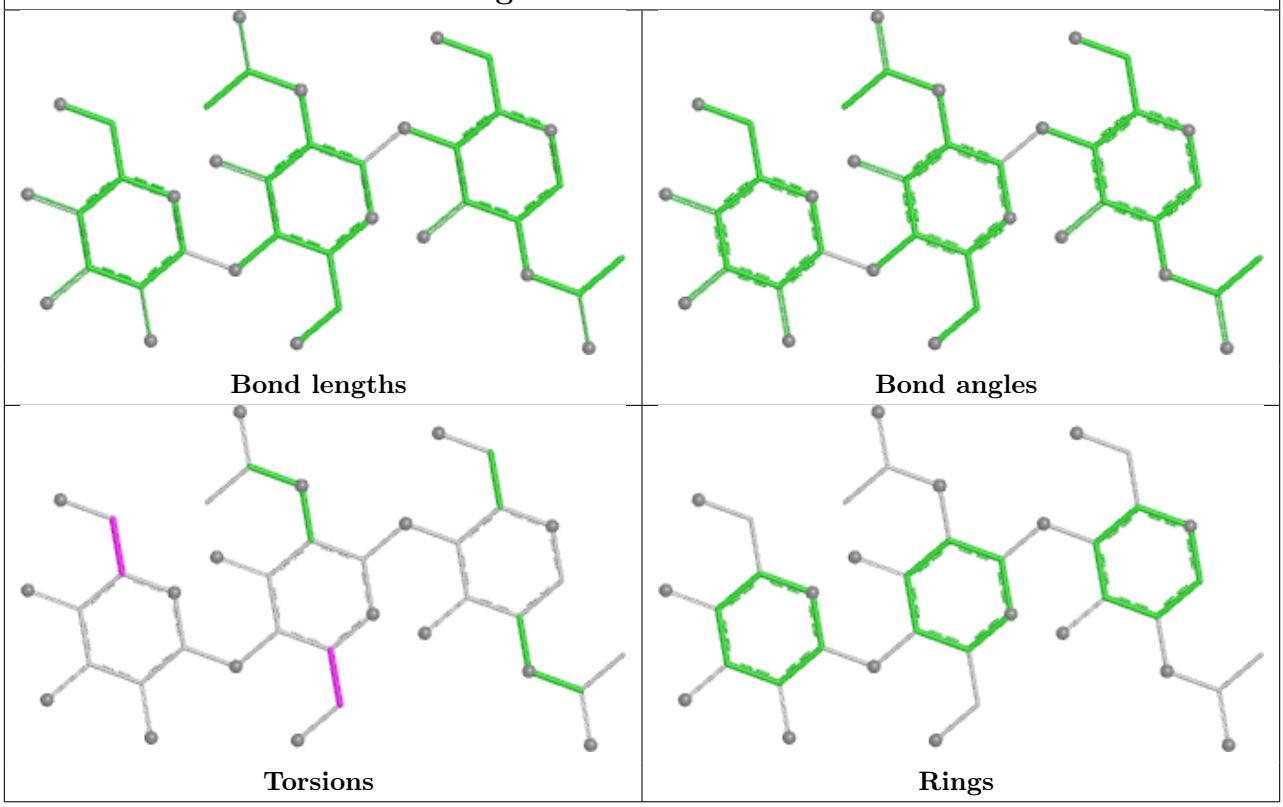
There are no ring outliers.

1 monomer is involved in 3 short contacts:

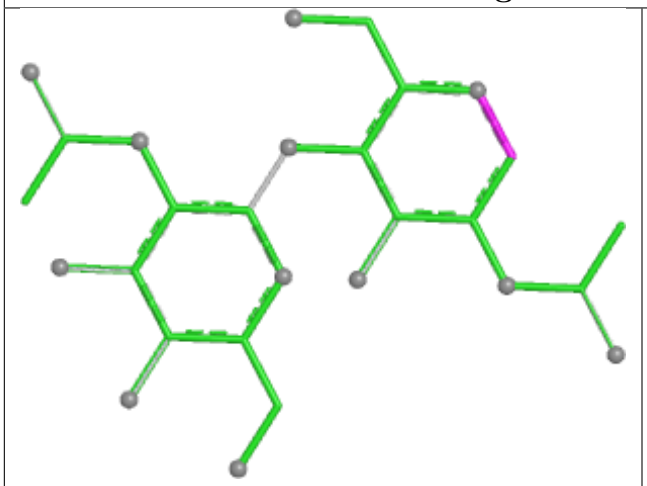
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	1	NAG	3	0

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

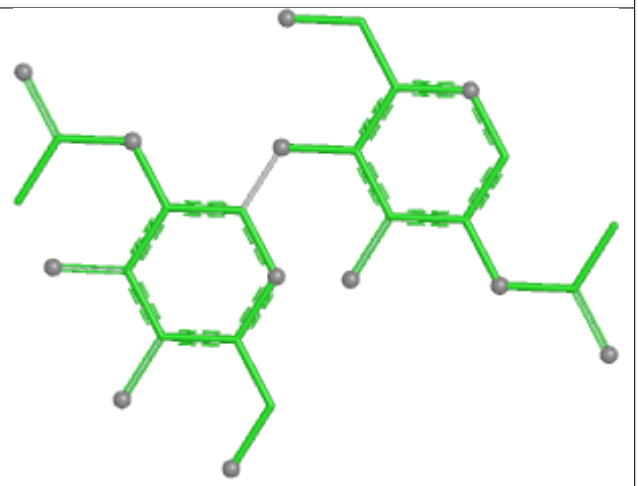
Oligosaccharide Chain C



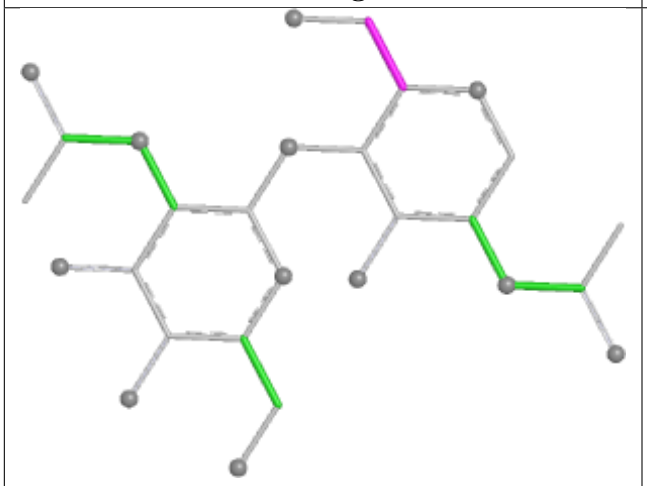
Oligosaccharide Chain D



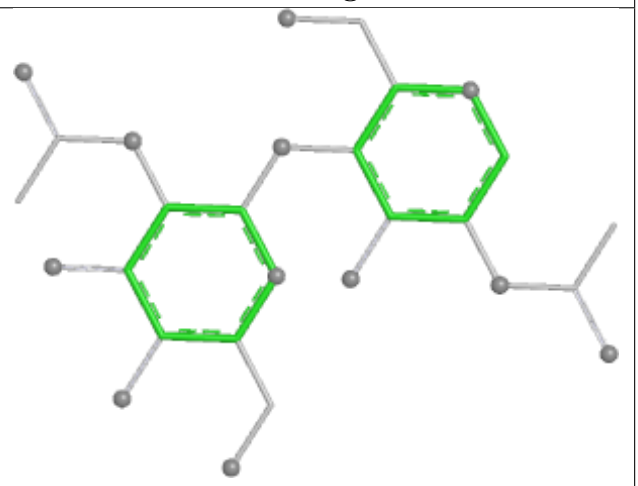
Bond lengths



Bond angles

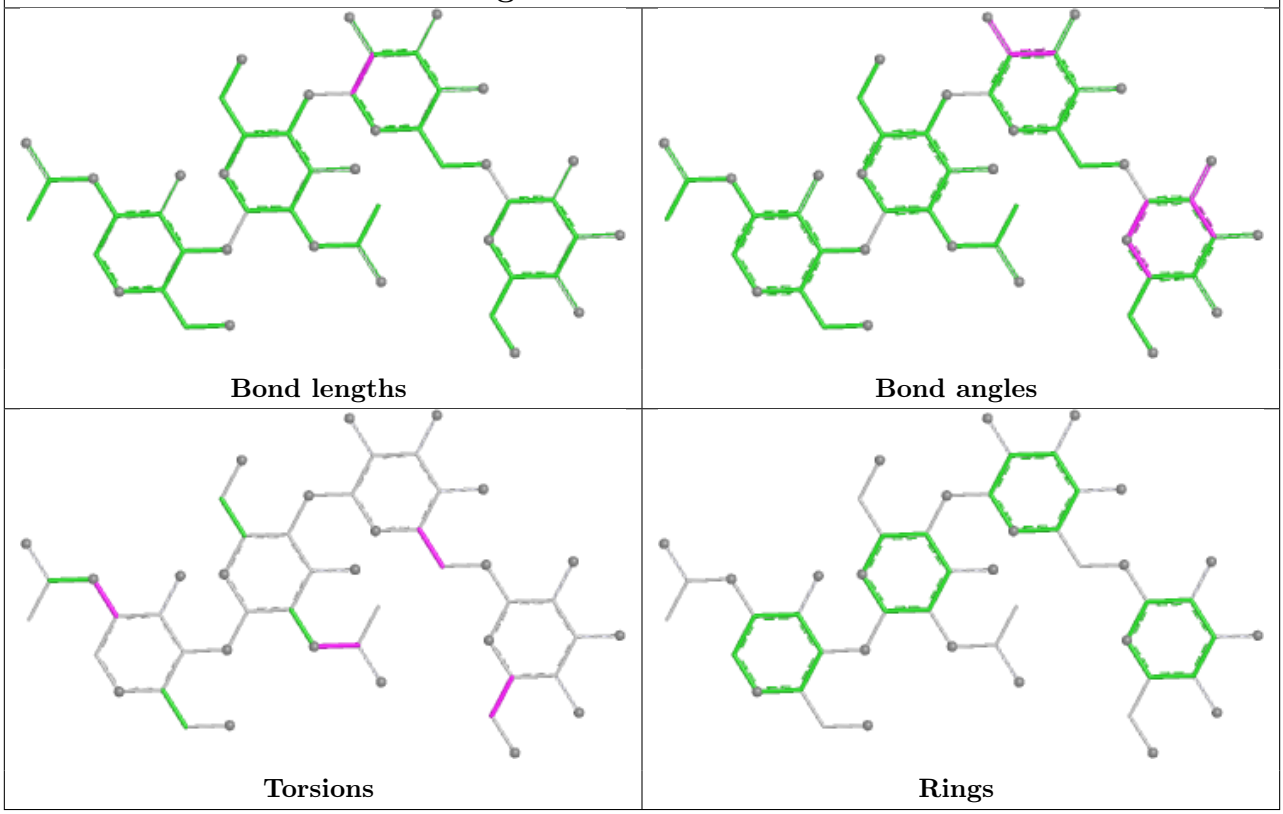


Torsions



Rings

Oligosaccharide Chain E



5.6 Ligand geometry (i)

Of 13 ligands modelled in this entry, 6 are monoatomic - leaving 7 for Mogul analysis.

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	NAG	B	504	2	14,14,15	0.68	0	17,19,21	0.89	1 (5%)
9	A1CYO	B	506	8	38,38,38	1.25	3 (7%)	52,52,52	1.35	7 (13%)
6	NAG	A	603	1	14,14,15	0.40	0	17,19,21	0.49	0
6	NAG	B	505	2	14,14,15	0.89	1 (7%)	17,19,21	1.14	1 (5%)
6	NAG	A	602	1	14,14,15	0.57	0	17,19,21	0.62	0
6	NAG	A	604	1	14,14,15	0.31	0	17,19,21	1.24	1 (5%)
6	NAG	A	601	-	14,14,15	0.63	1 (7%)	17,19,21	0.37	0

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	NAG	B	504	2	-	1/6/23/26	0/1/1/1
9	A1CYO	B	506	8	-	2/28/28/28	0/3/3/3
6	NAG	A	603	1	-	0/6/23/26	0/1/1/1
6	NAG	B	505	2	-	4/6/23/26	0/1/1/1
6	NAG	A	602	1	-	0/6/23/26	0/1/1/1
6	NAG	A	604	1	-	2/6/23/26	0/1/1/1
6	NAG	A	601	-	-	0/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	506	A1CYO	C06-N05	5.20	1.46	1.34
6	B	505	NAG	O5-C1	2.89	1.48	1.43
9	B	506	A1CYO	O31-C30	2.36	1.41	1.37
6	A	601	NAG	O5-C1	-2.30	1.39	1.43
9	B	506	A1CYO	O25-C24	2.28	1.40	1.37

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	604	NAG	C1-O5-C5	4.69	118.47	112.19
6	B	505	NAG	C1-O5-C5	4.43	118.12	112.19
9	B	506	A1CYO	O31-C30-C23	3.19	119.59	115.45
9	B	506	A1CYO	C09-C08-C14	2.82	119.78	114.93
9	B	506	A1CYO	O25-C24-C23	2.69	118.94	115.45

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	505	NAG	O5-C5-C6-O6
6	B	505	NAG	C4-C5-C6-O6
6	B	505	NAG	C8-C7-N2-C2
6	B	505	NAG	O7-C7-N2-C2
6	B	504	NAG	O5-C5-C6-O6

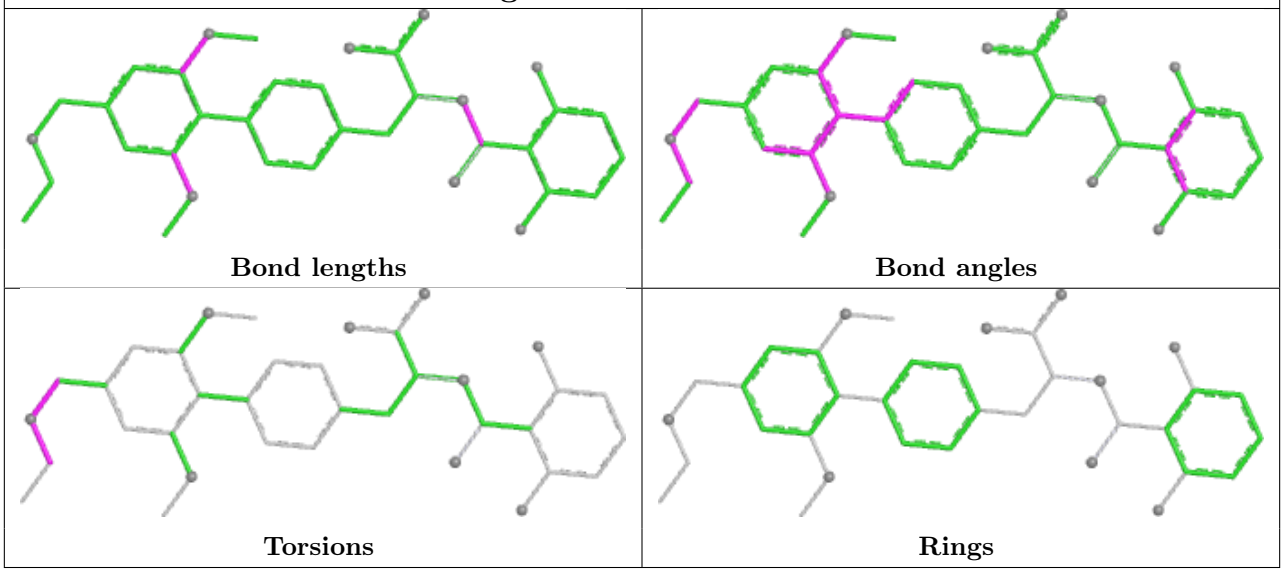
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	601	NAG	2	0

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 then 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.

Ligand A1CYO B 506



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	588/597 (98%)	0.40	32 (5%)	31	35	34, 52, 80, 97	0
2	B	448/490 (91%)	1.23	131 (29%)	1	1	35, 84, 124, 136	0
All	All	1036/1087 (95%)	0.76	163 (15%)	5	5	34, 58, 112, 136	0

The worst 5 of 163 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	451	ILE	5.3
2	B	33	PHE	5.0
2	B	39	PRO	4.9
2	B	392	GLY	4.6
2	B	2	THR	4.5

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
4	NAG	D	2	14/15	0.34	0.22	68,72,83,86	0
5	MAN	E	4	11/12	0.35	0.19	67,72,87,87	0
4	NAG	D	1	14/15	0.46	0.21	63,68,82,84	0
5	BMA	E	3	11/12	0.50	0.17	61,64,76,82	0
3	BMA	C	3	11/12	0.50	0.17	65,69,83,87	0

Continued on next page...

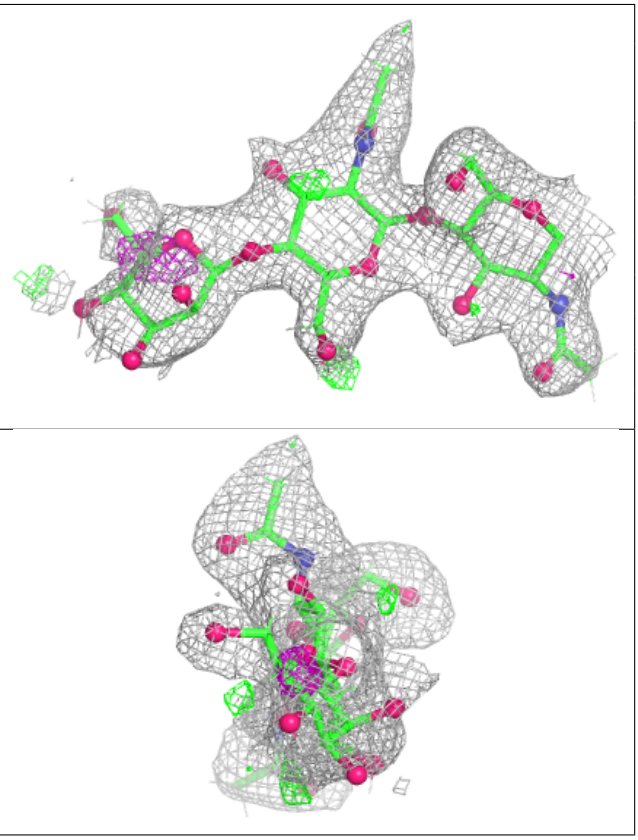
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NAG	C	2	14/15	0.66	0.14	60,65,76,79	0
5	NAG	E	2	14/15	0.83	0.13	52,58,70,70	0
5	NAG	E	1	14/15	0.86	0.11	55,59,70,76	0
3	NAG	C	1	14/15	0.88	0.10	49,58,68,70	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.

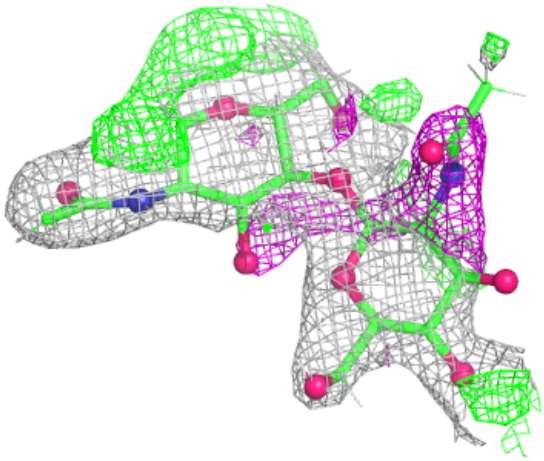
Electron density around Chain C:

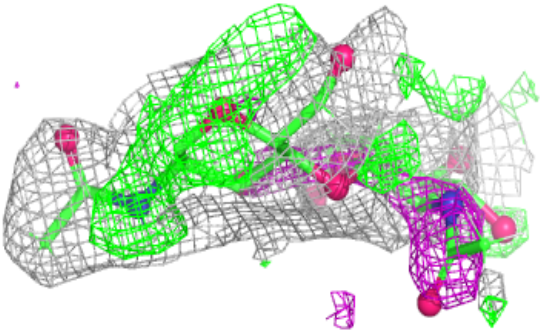
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)

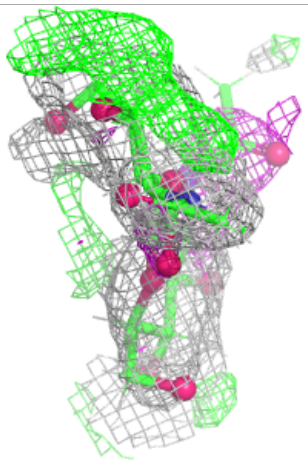


Electron density around Chain D:

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

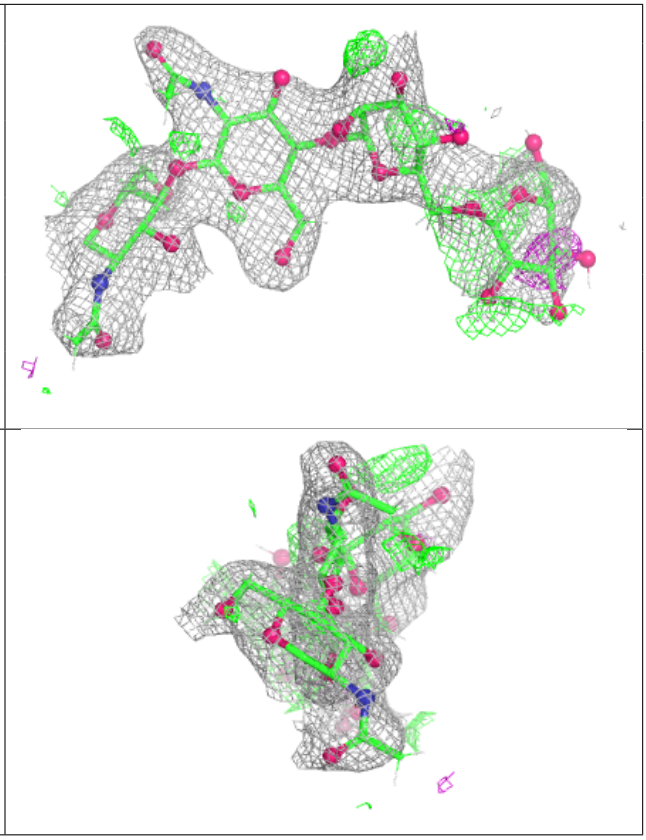






Electron density around Chain E:

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



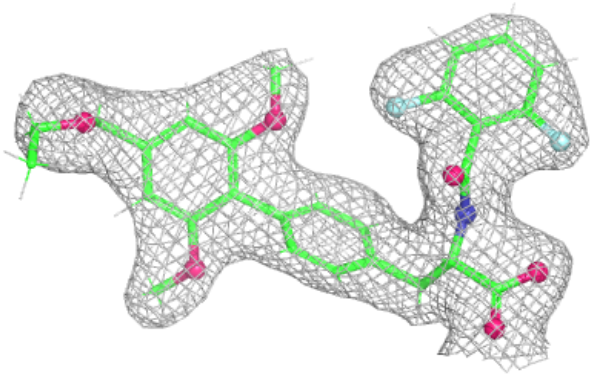
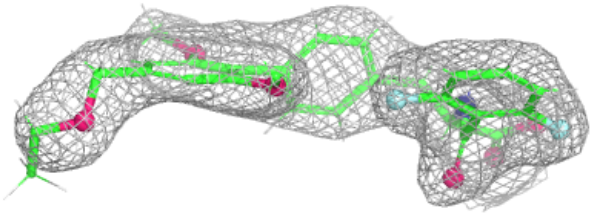
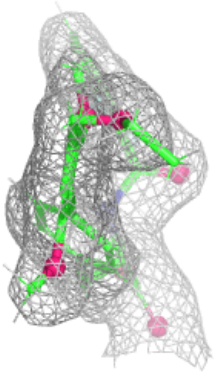
6.4 Ligands (i)

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
6	NAG	B	504	14/15	0.28	0.20	75,85,102,104	0
6	NAG	A	602	14/15	0.53	0.17	56,66,76,81	0
6	NAG	B	505	14/15	0.54	0.16	65,76,89,93	0
6	NAG	A	604	14/15	0.61	0.15	62,71,85,86	0
6	NAG	A	601	14/15	0.71	0.16	59,65,75,81	0
6	NAG	A	603	14/15	0.78	0.12	56,64,77,78	0
7	CA	B	502	1/1	0.88	0.14	72,72,72,72	0
9	A1CYO	B	506	36/36	0.93	0.09	39,49,62,62	0
7	CA	A	607	1/1	0.99	0.03	43,43,43,43	0
7	CA	B	501	1/1	0.99	0.05	36,36,36,36	0
7	CA	A	605	1/1	0.99	0.02	40,40,40,40	0
8	MG	B	503	1/1	0.99	0.09	37,37,37,37	0
7	CA	A	606	1/1	0.99	0.04	44,44,44,44	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.

Electron density around A1CYO B 506: $2mF_o$-DF_c (at 0.7 rmsd) in gray mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)	
	

6.5 Other polymers (i)

There are no such residues in this entry.