Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2023 – 03:17 pm GMT

PDB ID	:	7ZE9
Title	:	Structure of an AA16 LPMO-like protein
Authors	:	Huang, Z.; Banerjee, S.; Muderspach, S.J.; Sun, P.; van Berkel, W.J.H.; Kabel, M.A.; Lo Leggio, L.
Deposited on	:	2022-03-30
Resolution	:	2.65 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:

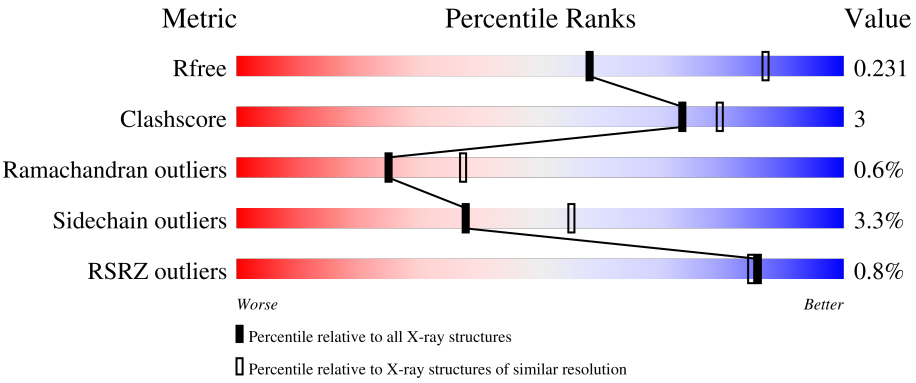
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.32.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.1

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 2.65 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	1426 (2.66-2.62)
Clashscore	141614	1472 (2.66-2.62)
Ramachandran outliers	138981	1446 (2.66-2.62)
Sidechain outliers	138945	1446 (2.66-2.62)
RSRZ outliers	127900	1408 (2.66-2.62)

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	AAA	188	81% · · 14%
1	BBB	188	78% 7% · 14%
1	CCC	188	81% 7% · 11%
2	AaA	7	100%
2	BaB	7	29% 71%

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Mol	Chain	Length	Quality of chain
3	CaC	5	100%

2 Entry composition

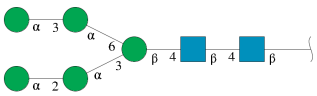
There are 7 unique types of molecules in this entry. The entry contains 4243 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Chitin-binding type-4 domain-containing protein.

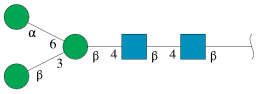
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	162	Total	C	N	O	S	0	0	0
			1259	796	209	247	7			
1	BBB	162	Total	C	N	O	S	0	0	0
			1259	796	209	247	7			
1	CCC	168	Total	C	N	O	S	0	0	0
			1297	819	215	256	7			

- Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-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.



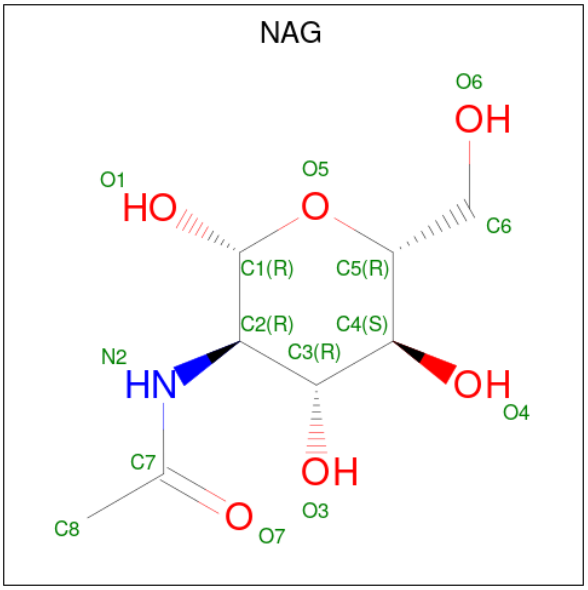
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	AaA	7	Total	C	N	O	0	0	0
			83	46	2	35			
2	BaB	7	Total	C	N	O	0	0	0
			83	46	2	35			

- Molecule 3 is an oligosaccharide called beta-D-mannopyranose-(1-3)-[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
3	CaC	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).

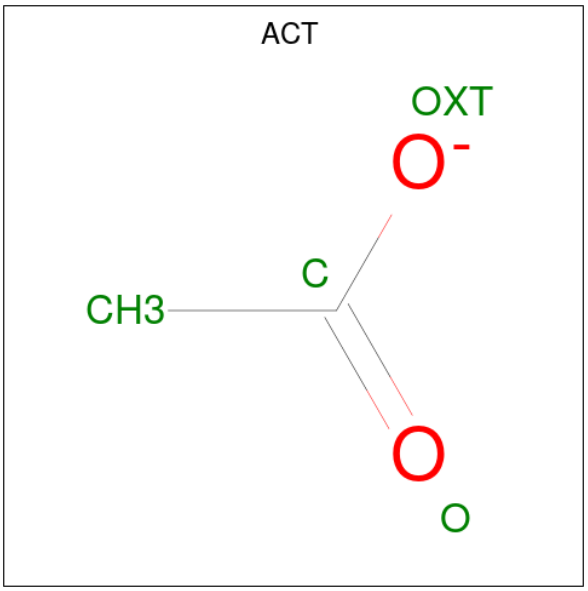


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	AAA	1	Total	C	N	O	0	0
			14	8	1	5		
4	BBB	1	Total	C	N	O	0	0
			14	8	1	5		
4	CCC	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	AAA	1	Total	Cu	0	0
			1	1		
5	BBB	1	Total	Cu	0	0
			1	1		
5	CCC	1	Total	Cu	0	0
			1	1		

- Molecule 6 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



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

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	AAA	52	Total O 52 52	0	0
7	BBB	40	Total O 41 41	0	1
7	CCC	59	Total O 59 59	0	0

3 Residue-property plots (i)

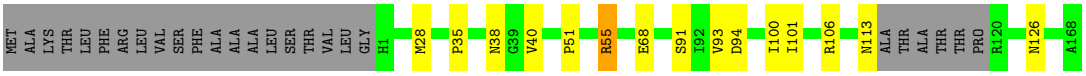
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Chitin-binding type-4 domain-containing protein

Chain AAA:

• Molecule 1: Chitin-binding type-4 domain-containing protein

Chain BBB:

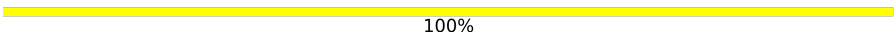


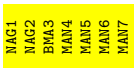
• Molecule 1: Chitin-binding type-4 domain-containing protein

Chain CCC:

• Molecule 2: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-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 AaA:





• Molecule 2: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-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 BaB:

• Molecule 3: beta-D-mannopyranose-(1-3)-[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 CaC:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	152.42Å 52.15Å 88.86Å 90.00° 105.67° 90.00°	Depositor
Resolution (Å)	85.55 – 2.65 85.55 – 2.65	Depositor EDS
% Data completeness (in resolution range)	99.1 (85.55-2.65) 99.1 (85.55-2.65)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.30 (at 2.65Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.178 , 0.233 0.184 , 0.231	Depositor DCC
R_{free} test set	967 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å^2)	52.1	Xtriage
Anisotropy	0.334	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 44.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	4243	wwPDB-VP
Average B, all atoms (Å^2)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.17% 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: ACT, BMA, HIC, NAG, MAN, CU

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	AAA	0.68	0/1282	0.81	0/1748
1	BBB	0.66	0/1282	0.83	0/1748
1	CCC	0.68	0/1322	0.83	0/1807
All	All	0.67	0/3886	0.82	0/5303

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	AAA	1259	0	1163	6	0
1	BBB	1259	0	1163	7	0
1	CCC	1297	0	1202	7	0
2	AaA	83	0	70	0	0
2	BaB	83	0	70	0	0
3	CaC	61	0	52	0	0
4	AAA	14	0	13	0	0
4	BBB	14	0	13	0	0
4	CCC	14	0	13	0	0
5	AAA	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	BBB	1	0	0	0	0
5	CCC	1	0	0	0	0
6	CCC	4	0	3	0	0
7	AAA	52	0	0	2	0
7	BBB	41	0	0	1	0
7	CCC	59	0	0	2	0
All	All	4243	0	3762	20	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (20) 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:CCC:55:ARG:HD2	7:CCC:321:HOH:O	1.92	0.69
1:CCC:106:ARG:NH1	1:CCC:126:ASN:O	2.34	0.60
1:BBB:91:SER:CB	1:BBB:100:ILE:HD13	2.40	0.52
1:AAA:28:MET:O	1:AAA:55:ARG:NH2	2.45	0.50
1:AAA:35:PRO:HG2	1:AAA:38:ASN:HD22	1.77	0.49
1:BBB:35:PRO:HG2	1:BBB:38:ASN:HD22	1.76	0.49
1:BBB:94:ASP:HB2	1:BBB:101:ILE:HD11	1.94	0.48
1:CCC:28:MET:O	1:CCC:55:ARG:NH2	2.46	0.48
1:BBB:28:MET:O	1:BBB:55:ARG:NH2	2.47	0.47
1:CCC:84:HIS:HB3	7:CCC:341:HOH:O	2.17	0.45
1:BBB:55:ARG:HD2	7:BBB:315:HOH:O	2.15	0.45
1:CCC:167:LYS:O	1:CCC:168:ALA:C	2.55	0.45
1:AAA:55:ARG:HD2	7:AAA:329:HOH:O	2.19	0.43
1:BBB:106:ARG:NH1	1:BBB:126:ASN:O	2.48	0.43
1:AAA:113:ASN:ND2	7:AAA:303:HOH:O	2.53	0.42
1:AAA:106:ARG:NH1	1:AAA:126:ASN:O	2.45	0.42
1:CCC:6:VAL:O	1:CCC:75:PHE:HA	2.20	0.42
1:CCC:13:GLY:O	1:CCC:16:TYR:HB3	2.21	0.41
1:AAA:35:PRO:HG2	1:AAA:38:ASN:ND2	2.35	0.40
1:BBB:40:VAL:HG22	1:BBB:51:PRO:HG3	2.02	0.40

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	AAA	158/188 (84%)	156 (99%)	2 (1%)	0	100 100
1	BBB	158/188 (84%)	158 (100%)	0	0	100 100
1	CCC	166/188 (88%)	161 (97%)	2 (1%)	3 (2%)	8 11
All	All	482/564 (86%)	475 (98%)	4 (1%)	3 (1%)	25 37

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	CCC	114	ALA
1	CCC	120	ARG
1	CCC	115	THR

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	AAA	131/150 (87%)	126 (96%)	5 (4%)	33 50
1	BBB	131/150 (87%)	127 (97%)	4 (3%)	40 58
1	CCC	135/150 (90%)	131 (97%)	4 (3%)	41 59
All	All	397/450 (88%)	384 (97%)	13 (3%)	38 55

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	42	LYS
1	AAA	55	ARG
1	AAA	74	ASP
1	AAA	106	ARG
1	AAA	167	LYS
1	BBB	55	ARG
1	BBB	68	GLU
1	BBB	93	VAL
1	BBB	113	ASN
1	CCC	55	ARG
1	CCC	99	LYS
1	CCC	106	ARG
1	CCC	109	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

3 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
1	HIC	CCC	1	5,1	8,11,12	0.82	0	6,14,16	0.90	0
1	HIC	BBB	1	5,1	8,11,12	0.90	0	6,14,16	0.92	0
1	HIC	AAA	1	5,1	8,11,12	0.85	0	6,14,16	0.87	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
1	HIC	CCC	1	5,1	-	0/5/6/8	0/1/1/1
1	HIC	BBB	1	5,1	-	0/5/6/8	0/1/1/1
1	HIC	AAA	1	5,1	-	1/5/6/8	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	AAA	1	HIC	C-CA-CB-CG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

19 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	AaA	1	2,1	14,14,15	0.70	0	17,19,21	1.70	5 (29%)
2	NAG	AaA	2	2	14,14,15	0.58	0	17,19,21	1.38	1 (5%)
2	BMA	AaA	3	2	11,11,12	0.52	0	15,15,17	1.46	2 (13%)
2	MAN	AaA	4	2	11,11,12	0.44	0	15,15,17	1.57	2 (13%)
2	MAN	AaA	5	2	11,11,12	0.61	0	15,15,17	1.80	4 (26%)
2	MAN	AaA	6	2	11,11,12	0.73	0	15,15,17	2.62	3 (20%)
2	MAN	AaA	7	2	11,11,12	1.02	1 (9%)	15,15,17	1.60	3 (20%)
2	NAG	BaB	1	2,1	14,14,15	0.57	0	17,19,21	0.99	0
2	NAG	BaB	2	2	14,14,15	0.61	0	17,19,21	0.88	0
2	BMA	BaB	3	2	11,11,12	0.66	0	15,15,17	1.87	2 (13%)
2	MAN	BaB	4	2	11,11,12	0.66	0	15,15,17	2.04	6 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	MAN	BaB	5	2	11,11,12	0.36	0	15,15,17	1.86	4 (26%)
2	MAN	BaB	6	2	11,11,12	0.67	0	15,15,17	1.90	6 (40%)
2	MAN	BaB	7	2	11,11,12	1.13	1 (9%)	15,15,17	1.98	5 (33%)
3	NAG	CaC	1	3,1	14,14,15	0.71	1 (7%)	17,19,21	1.56	2 (11%)
3	NAG	CaC	2	3	14,14,15	0.47	0	17,19,21	1.17	2 (11%)
3	BMA	CaC	3	3	11,11,12	0.39	0	15,15,17	1.57	3 (20%)
3	BMA	CaC	4	3	11,11,12	1.53	2 (18%)	15,15,17	2.99	5 (33%)
3	MAN	CaC	5	3	11,11,12	0.84	0	15,15,17	1.92	3 (20%)

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	AaA	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	AaA	2	2	-	2/6/23/26	0/1/1/1
2	BMA	AaA	3	2	-	0/2/19/22	0/1/1/1
2	MAN	AaA	4	2	-	0/2/19/22	0/1/1/1
2	MAN	AaA	5	2	-	1/2/19/22	0/1/1/1
2	MAN	AaA	6	2	-	0/2/19/22	0/1/1/1
2	MAN	AaA	7	2	-	0/2/19/22	0/1/1/1
2	NAG	BaB	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	BaB	2	2	-	0/6/23/26	0/1/1/1
2	BMA	BaB	3	2	-	0/2/19/22	0/1/1/1
2	MAN	BaB	4	2	-	0/2/19/22	0/1/1/1
2	MAN	BaB	5	2	-	2/2/19/22	0/1/1/1
2	MAN	BaB	6	2	-	0/2/19/22	0/1/1/1
2	MAN	BaB	7	2	-	2/2/19/22	0/1/1/1
3	NAG	CaC	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	CaC	2	3	-	0/6/23/26	0/1/1/1
3	BMA	CaC	3	3	-	0/2/19/22	0/1/1/1
3	BMA	CaC	4	3	-	2/2/19/22	0/1/1/1
3	MAN	CaC	5	3	-	0/2/19/22	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	CaC	4	BMA	C2-C3	-3.83	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	BaB	7	MAN	C2-C3	2.84	1.56	1.52
2	AaA	7	MAN	C2-C3	2.40	1.56	1.52
3	CaC	4	BMA	C4-C3	2.26	1.58	1.52
3	CaC	1	NAG	O5-C1	-2.18	1.40	1.43

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	AaA	6	MAN	C1-O5-C5	7.56	122.44	112.19
3	CaC	4	BMA	C2-C3-C4	-6.44	99.75	110.89
3	CaC	4	BMA	O3-C3-C2	-5.92	98.66	109.99
3	CaC	4	BMA	O3-C3-C4	5.25	122.48	110.35
2	AaA	6	MAN	O5-C5-C6	4.94	114.96	107.20
2	BaB	4	MAN	C1-C2-C3	-4.94	103.59	109.67
2	BaB	3	BMA	C1-C2-C3	-4.84	103.72	109.67
2	BaB	7	MAN	O2-C2-C3	4.56	119.27	110.14
3	CaC	5	MAN	O5-C1-C2	4.35	117.48	110.77
2	AaA	5	MAN	C1-C2-C3	-4.25	104.44	109.67
2	AaA	4	MAN	C1-O5-C5	4.11	117.77	112.19
2	BaB	3	BMA	O5-C5-C6	4.02	113.50	107.20
2	BaB	5	MAN	C1-C2-C3	-3.89	104.89	109.67
2	BaB	6	MAN	C1-O5-C5	3.81	117.36	112.19
3	CaC	4	BMA	O2-C2-C3	-3.60	102.92	110.14
3	CaC	1	NAG	O3-C3-C2	3.42	116.55	109.47
2	AaA	7	MAN	O2-C2-C3	3.38	116.91	110.14
2	AaA	1	NAG	O4-C4-C3	-3.38	102.54	110.35
2	BaB	5	MAN	O5-C1-C2	-3.38	105.56	110.77
2	AaA	6	MAN	O5-C1-C2	3.34	115.92	110.77
3	CaC	3	BMA	O3-C3-C4	-3.33	102.66	110.35
2	AaA	3	BMA	O5-C5-C6	3.31	112.40	107.20
2	AaA	1	NAG	O5-C5-C6	3.14	112.13	107.20
2	BaB	7	MAN	C1-C2-C3	-3.13	105.82	109.67
2	BaB	4	MAN	O3-C3-C4	3.04	117.37	110.35
2	AaA	7	MAN	C2-C3-C4	2.98	116.05	110.89
3	CaC	5	MAN	O5-C5-C4	-2.94	103.67	110.83
2	AaA	2	NAG	C2-N2-C7	2.93	127.08	122.90
3	CaC	1	NAG	O7-C7-C8	-2.87	116.72	122.06
2	AaA	5	MAN	O5-C1-C2	-2.82	106.42	110.77
3	CaC	5	MAN	C1-O5-C5	2.82	116.01	112.19
2	BaB	4	MAN	C1-O5-C5	2.79	115.98	112.19
2	BaB	5	MAN	O5-C5-C6	2.77	111.55	107.20
2	AaA	5	MAN	C1-O5-C5	2.73	115.89	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	BaB	7	MAN	C1-O5-C5	2.70	115.85	112.19
2	AaA	5	MAN	O2-C2-C3	2.65	115.45	110.14
2	BaB	6	MAN	O5-C1-C2	2.65	114.86	110.77
2	BaB	6	MAN	O6-C6-C5	-2.63	102.28	111.29
2	BaB	6	MAN	C3-C4-C5	-2.57	105.65	110.24
3	CaC	3	BMA	O5-C5-C6	2.56	111.22	107.20
2	BaB	4	MAN	O5-C5-C6	2.50	111.13	107.20
2	AaA	1	NAG	O5-C1-C2	-2.49	107.35	111.29
2	AaA	4	MAN	C6-C5-C4	-2.47	107.21	113.00
3	CaC	4	BMA	C3-C4-C5	2.47	114.64	110.24
2	AaA	7	MAN	O5-C5-C6	2.46	111.07	107.20
2	BaB	5	MAN	C3-C4-C5	2.38	114.48	110.24
2	BaB	7	MAN	C3-C4-C5	-2.35	106.05	110.24
2	AaA	1	NAG	C8-C7-N2	2.33	120.04	116.10
3	CaC	3	BMA	C1-O5-C5	2.29	115.30	112.19
2	AaA	3	BMA	O5-C5-C4	-2.27	105.30	110.83
2	BaB	6	MAN	O2-C2-C1	2.26	113.78	109.15
2	BaB	7	MAN	O4-C4-C5	2.21	114.80	109.30
3	CaC	2	NAG	O5-C5-C6	2.21	110.67	107.20
2	BaB	4	MAN	O4-C4-C5	-2.18	103.88	109.30
2	BaB	4	MAN	O2-C2-C3	2.18	114.50	110.14
3	CaC	2	NAG	C3-C4-C5	-2.17	106.37	110.24
2	AaA	1	NAG	O7-C7-C8	-2.13	118.11	122.06
2	BaB	6	MAN	O3-C3-C2	2.11	114.03	109.99

There are no chirality outliers.

All (9) torsion outliers are listed below:

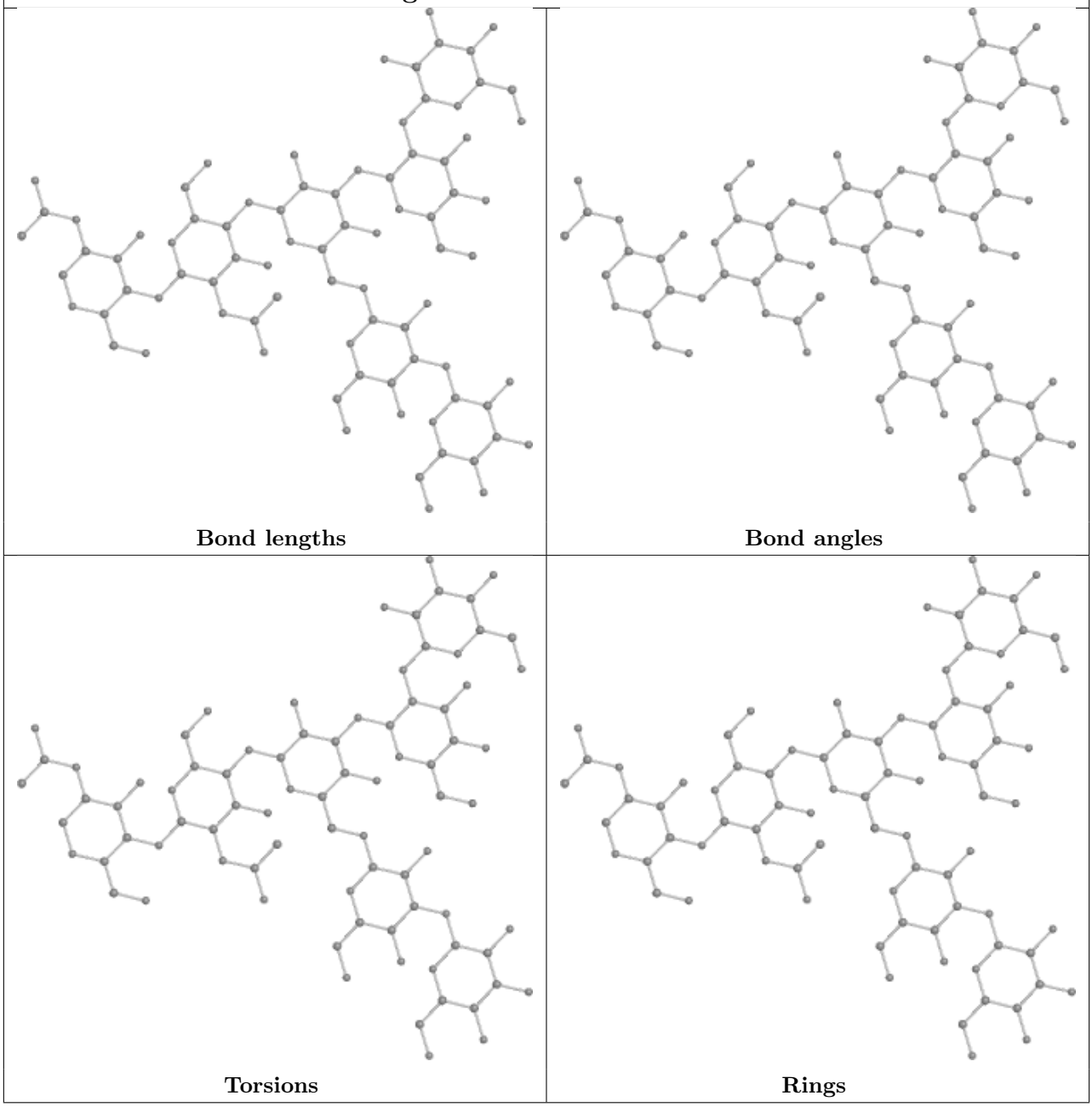
Mol	Chain	Res	Type	Atoms
3	CaC	4	BMA	O5-C5-C6-O6
3	CaC	4	BMA	C4-C5-C6-O6
2	BaB	7	MAN	O5-C5-C6-O6
2	BaB	5	MAN	C4-C5-C6-O6
2	AaA	2	NAG	C8-C7-N2-C2
2	AaA	2	NAG	O7-C7-N2-C2
2	BaB	5	MAN	O5-C5-C6-O6
2	BaB	7	MAN	C4-C5-C6-O6
2	AaA	5	MAN	C4-C5-C6-O6

There are no ring outliers.

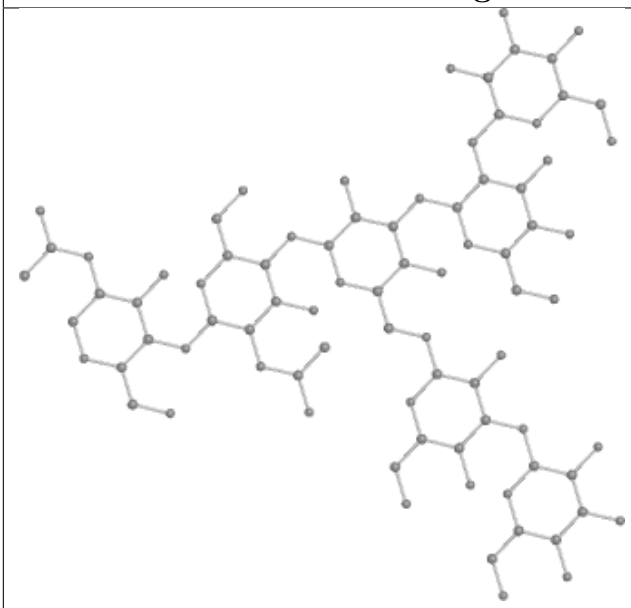
No monomer is involved in short contacts.

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

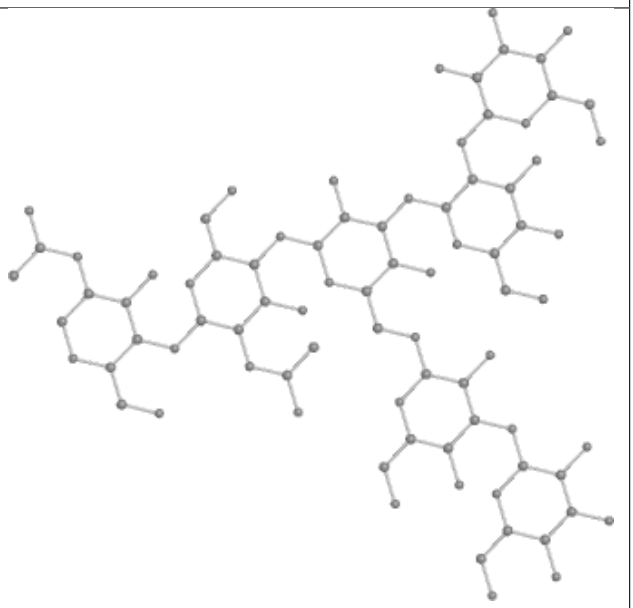
Oligosaccharide Chain AaA



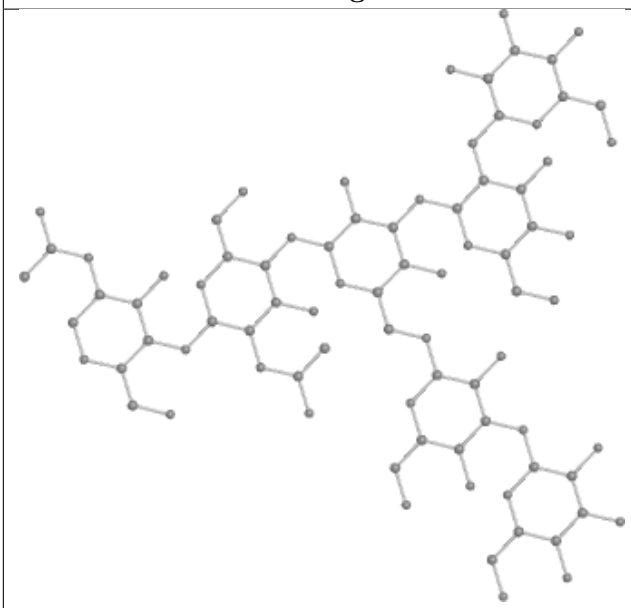
Oligosaccharide Chain BaB



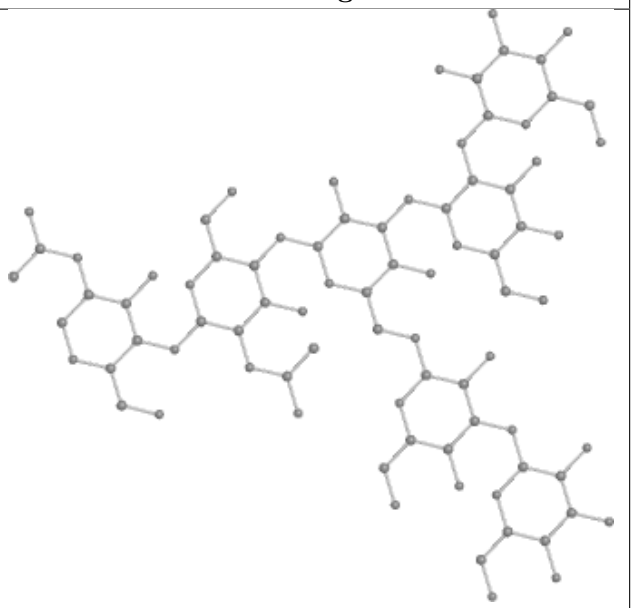
Bond lengths



Bond angles

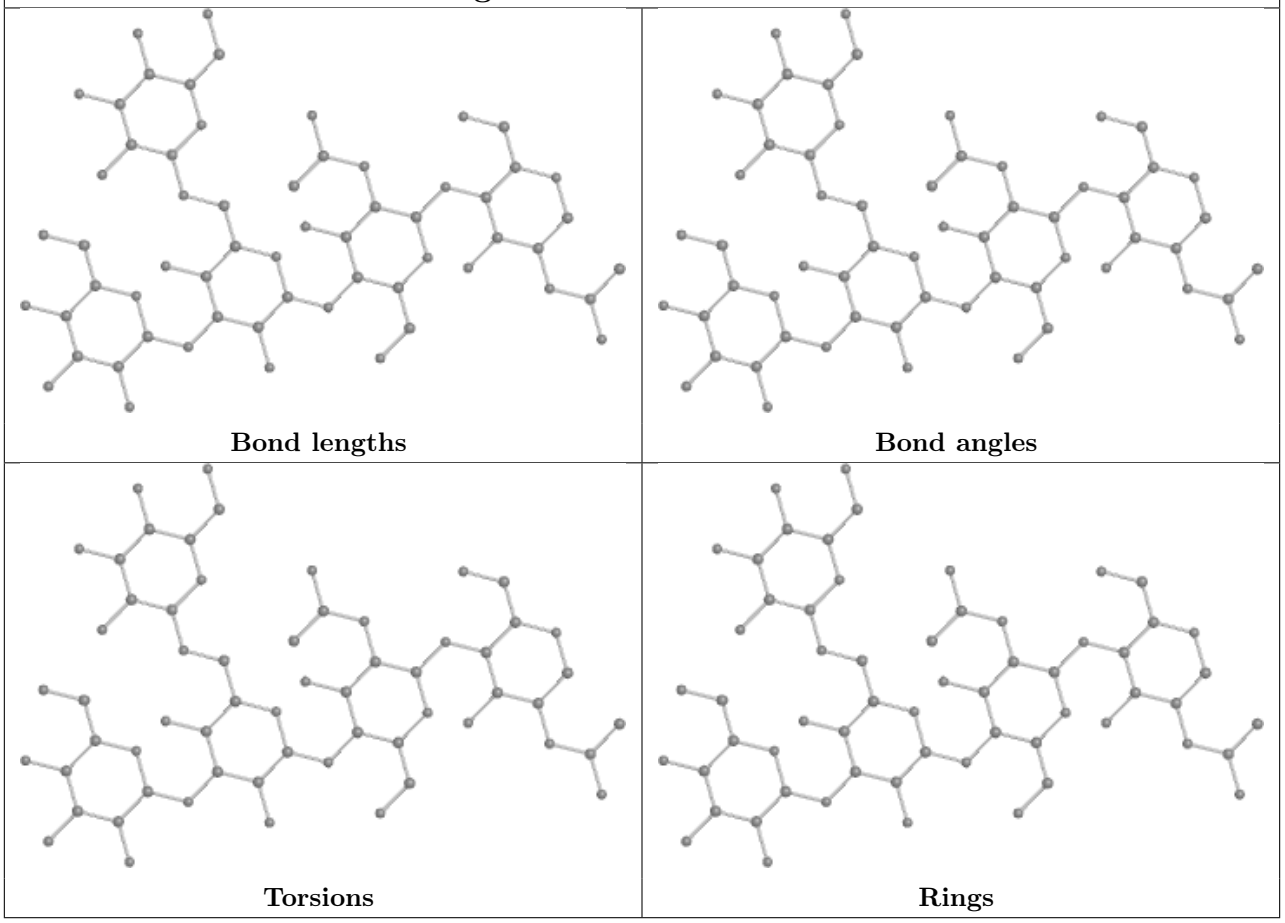


Torsions



Rings

Oligosaccharide Chain CaC



5.6 Ligand geometry (i)

Of 7 ligands modelled in this entry, 3 are monoatomic - leaving 4 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	$\#\|Z\| > 2$
4	NAG	BBB	201	1	14,14,15	0.61	0	17,19,21	1.14	1 (5%)
4	NAG	CCC	201	1	14,14,15	0.44	0	17,19,21	2.02	5 (29%)
4	NAG	AAA	201	1	14,14,15	0.38	0	17,19,21	1.93	5 (29%)
6	ACT	CCC	203	-	3,3,3	1.05	0	3,3,3	0.87	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
4	NAG	BBB	201	1	-	0/6/23/26	0/1/1/1
4	NAG	CCC	201	1	-	3/6/23/26	0/1/1/1
4	NAG	AAA	201	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	CCC	201	NAG	O5-C1-C2	3.98	117.57	111.29
4	AAA	201	NAG	C1-O5-C5	3.96	117.56	112.19
4	CCC	201	NAG	C1-O5-C5	3.73	117.25	112.19
4	AAA	201	NAG	C3-C4-C5	-3.44	104.11	110.24
4	CCC	201	NAG	C6-C5-C4	-3.37	105.12	113.00
4	AAA	201	NAG	C4-C3-C2	-3.11	106.46	111.02
4	CCC	201	NAG	O5-C5-C6	3.05	111.99	107.20
4	AAA	201	NAG	C2-N2-C7	2.47	126.42	122.90
4	BBB	201	NAG	C6-C5-C4	-2.29	107.64	113.00
4	AAA	201	NAG	O5-C5-C4	-2.09	105.73	110.83
4	CCC	201	NAG	C3-C4-C5	2.07	113.93	110.24

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	CCC	201	NAG	O5-C5-C6-O6
4	CCC	201	NAG	C4-C5-C6-O6
4	CCC	201	NAG	C3-C2-N2-C7

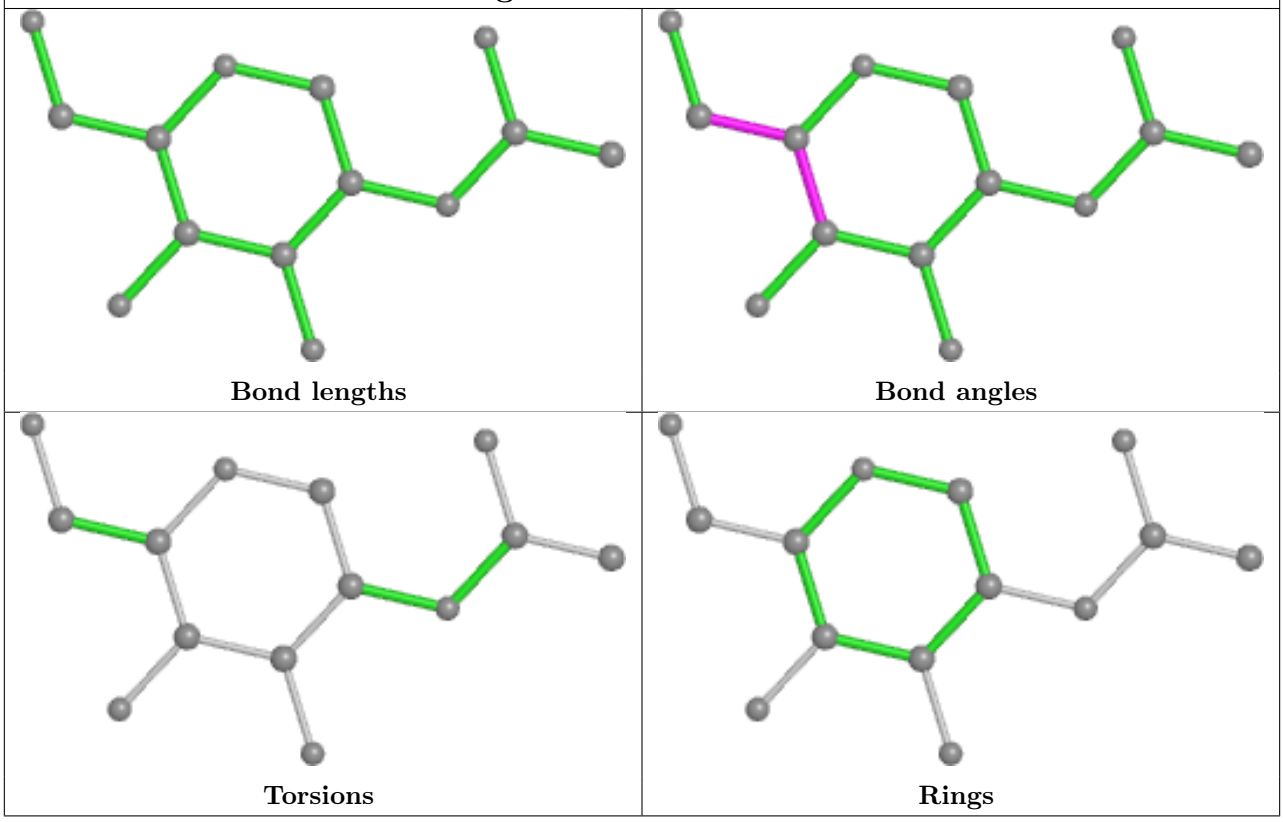
There are no ring outliers.

No monomer is involved in short contacts.

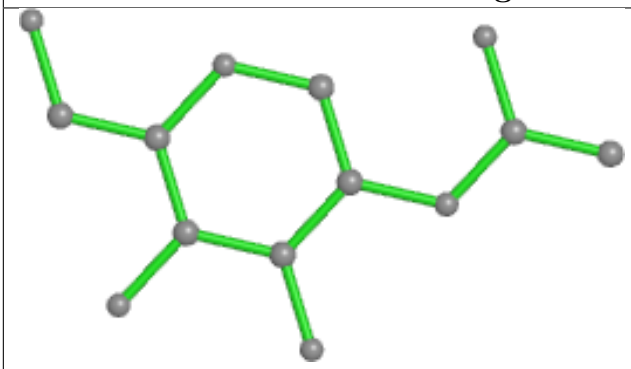
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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.

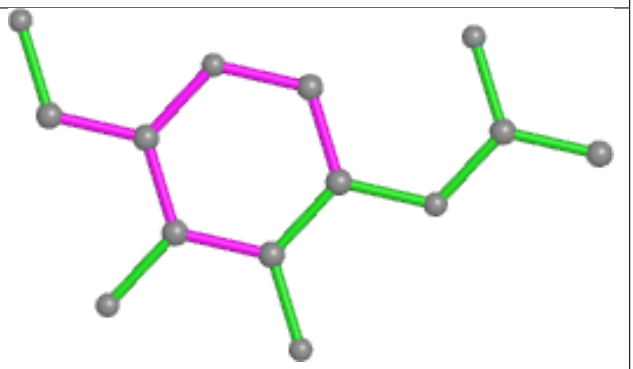
Ligand NAG BBB 201



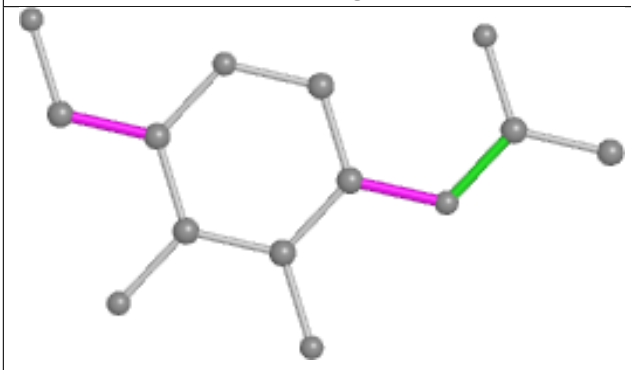
Ligand NAG CCC 201



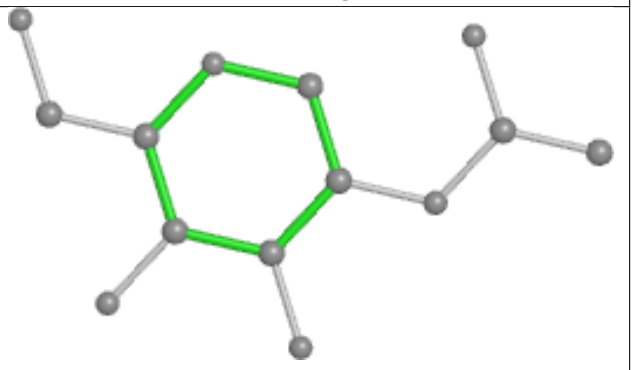
Bond lengths



Bond angles

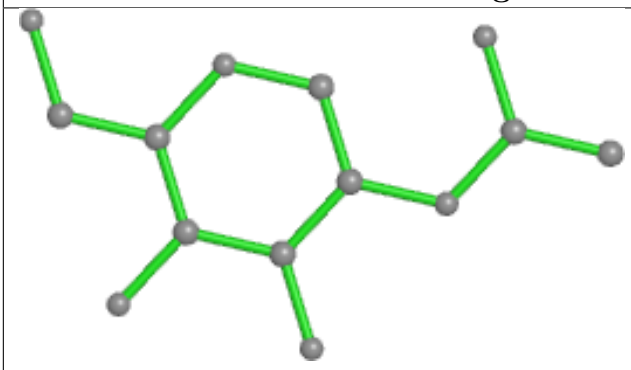


Torsions

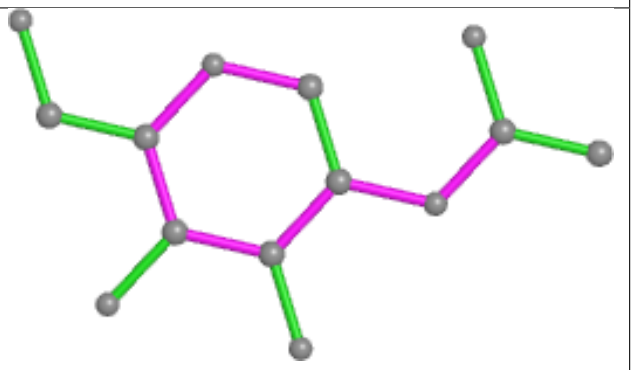


Rings

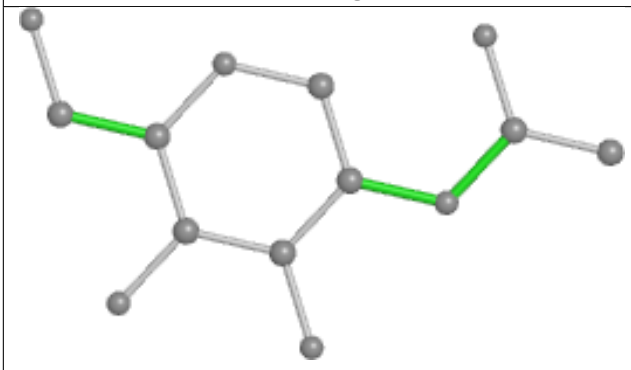
Ligand NAG AAA 201



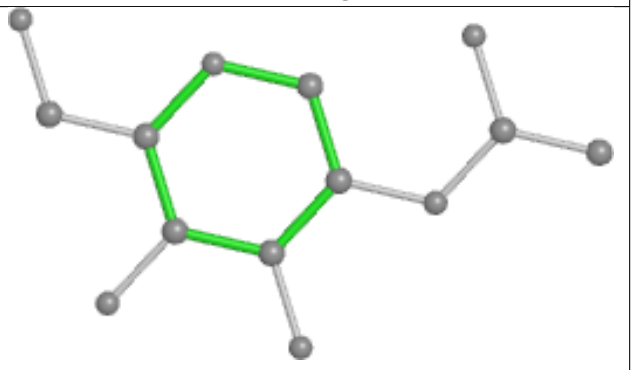
Bond lengths



Bond angles



Torsions



Rings

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	AAA	161/188 (85%)	0.17	1 (0%) 89 88	33, 50, 77, 101	0
1	BBB	161/188 (85%)	0.18	0 100 100	33, 47, 73, 98	0
1	CCC	167/188 (88%)	0.18	3 (1%) 68 66	36, 52, 90, 145	0
All	All	489/564 (86%)	0.18	4 (0%) 86 85	33, 50, 80, 145	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	168	ALA	3.7
1	CCC	115	THR	2.8
1	CCC	114	ALA	2.7
1	CCC	118	THR	2.5

6.2 Non-standard residues in protein, DNA, RNA chains

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
1	HIC	BBB	1	11/12	0.98	0.18	31,34,39,41	0
1	HIC	AAA	1	11/12	0.99	0.20	38,39,44,45	0
1	HIC	CCC	1	11/12	0.99	0.19	38,41,44,45	0

6.3 Carbohydrates

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,

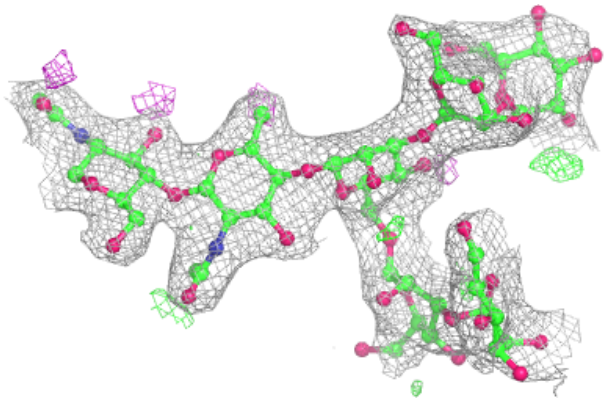
median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

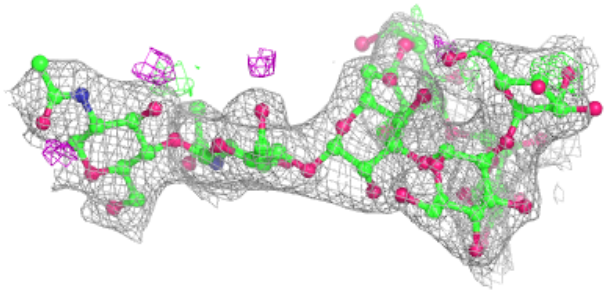
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	MAN	AaA	7	11/12	0.71	0.20	79,102,117,124	0
3	MAN	CaC	5	11/12	0.71	0.19	88,101,107,115	0
2	MAN	BaB	7	11/12	0.75	0.23	88,109,114,116	0
3	BMA	CaC	4	11/12	0.79	0.20	66,76,88,109	0
2	MAN	AaA	6	11/12	0.83	0.17	94,109,116,116	0
2	MAN	BaB	6	11/12	0.86	0.17	84,105,112,116	0
2	MAN	AaA	5	11/12	0.88	0.17	76,95,107,107	0
2	MAN	BaB	5	11/12	0.92	0.18	74,82,87,91	0
2	MAN	BaB	4	11/12	0.95	0.17	55,60,67,74	0
2	MAN	AaA	4	11/12	0.95	0.14	59,64,69,72	0
2	BMA	BaB	3	11/12	0.96	0.13	41,48,56,73	0
2	BMA	AaA	3	11/12	0.97	0.14	45,51,66,77	0
3	BMA	CaC	3	11/12	0.97	0.15	47,57,73,87	0
2	NAG	AaA	2	14/15	0.98	0.16	38,42,44,50	0
3	NAG	CaC	1	14/15	0.98	0.20	32,37,46,48	0
3	NAG	CaC	2	14/15	0.98	0.17	40,42,53,53	0
2	NAG	AaA	1	14/15	0.98	0.18	34,38,43,47	0
2	NAG	BaB	1	14/15	0.98	0.17	36,39,45,46	0
2	NAG	BaB	2	14/15	0.98	0.17	35,39,45,45	0

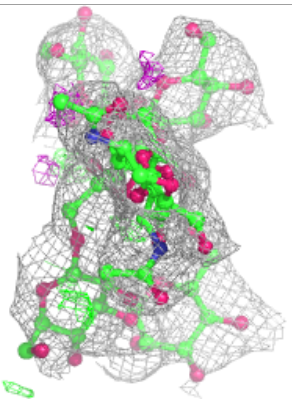
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain AaA:

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

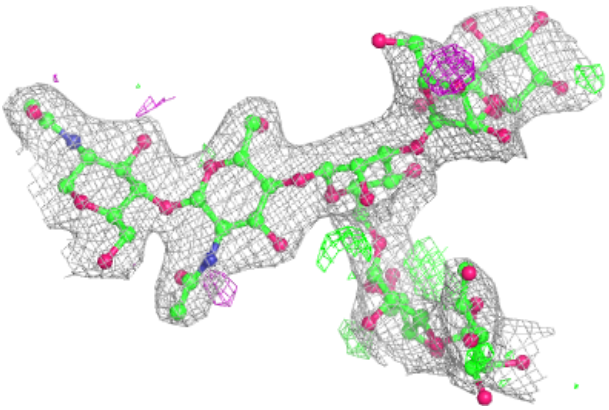


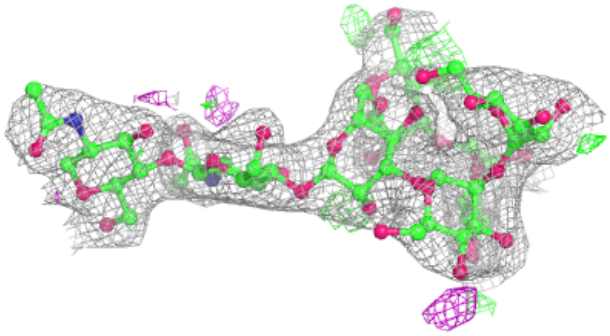


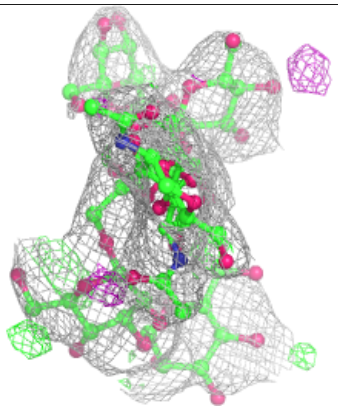


Electron density around Chain BaB:

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

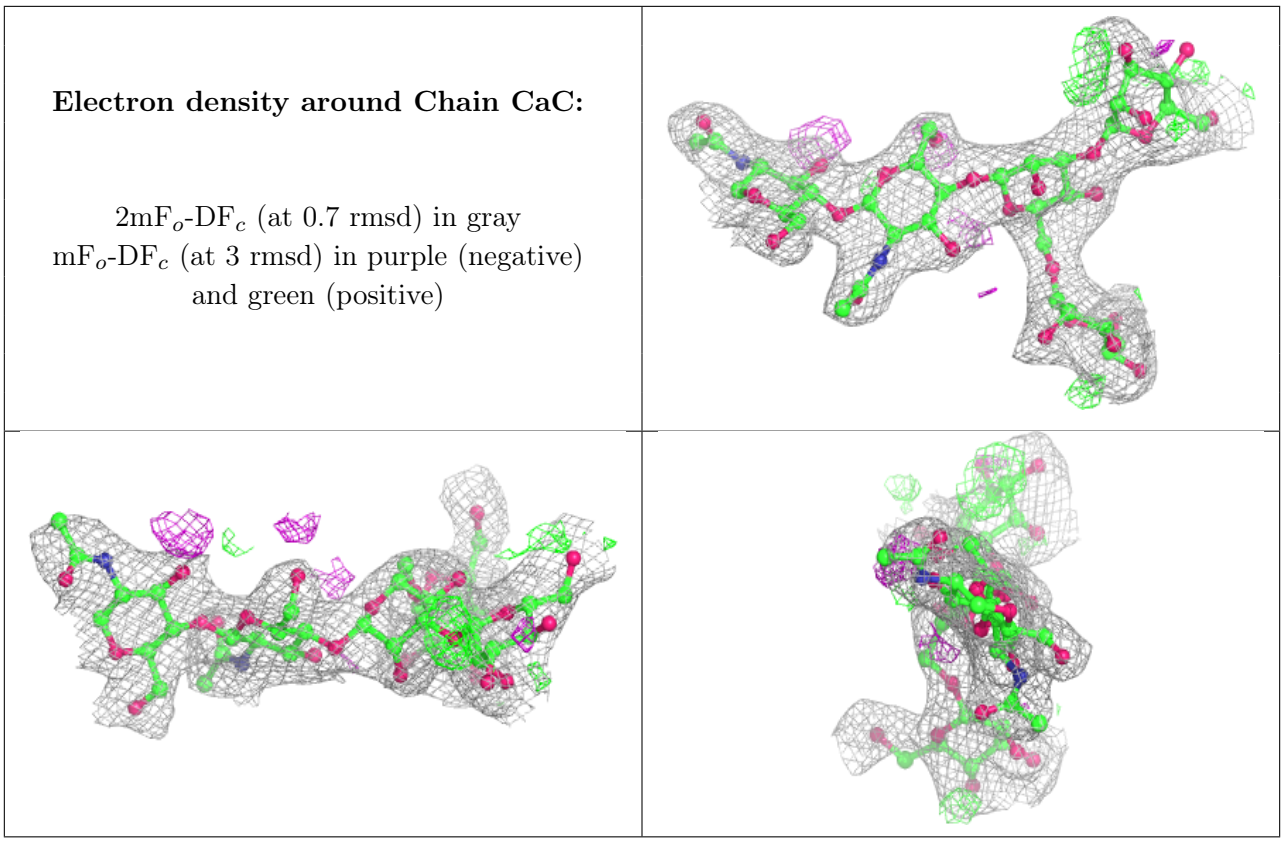






Electron density around Chain CaC:

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



6.4 Ligands

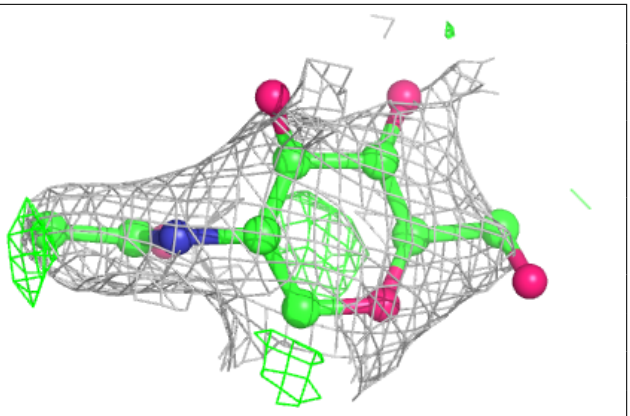
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

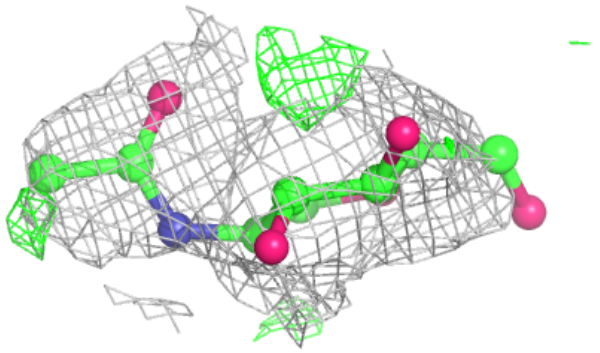
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	ACT	CCC	203	4/4	0.81	0.15	73,81,87,87	0
4	NAG	CCC	201	14/15	0.83	0.23	73,107,121,126	0
4	NAG	BBB	201	14/15	0.90	0.16	59,71,78,78	0
4	NAG	AAA	201	14/15	0.94	0.23	64,70,75,80	0
5	CU	BBB	202	1/1	0.99	0.17	44,44,44,44	0
5	CU	AAA	202	1/1	0.99	0.17	42,42,42,42	0
5	CU	CCC	202	1/1	1.00	0.18	42,42,42,42	0

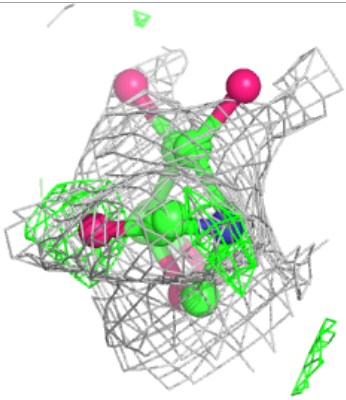
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAG CCC 201:

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

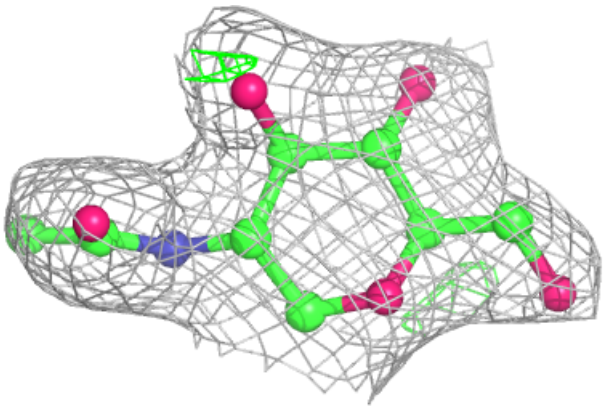


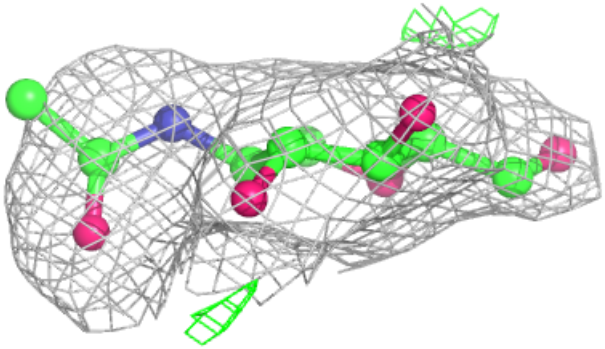


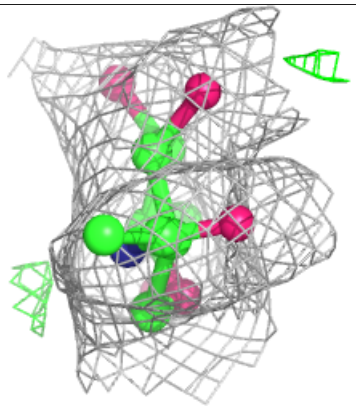


Electron density around NAG BBB 201:

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

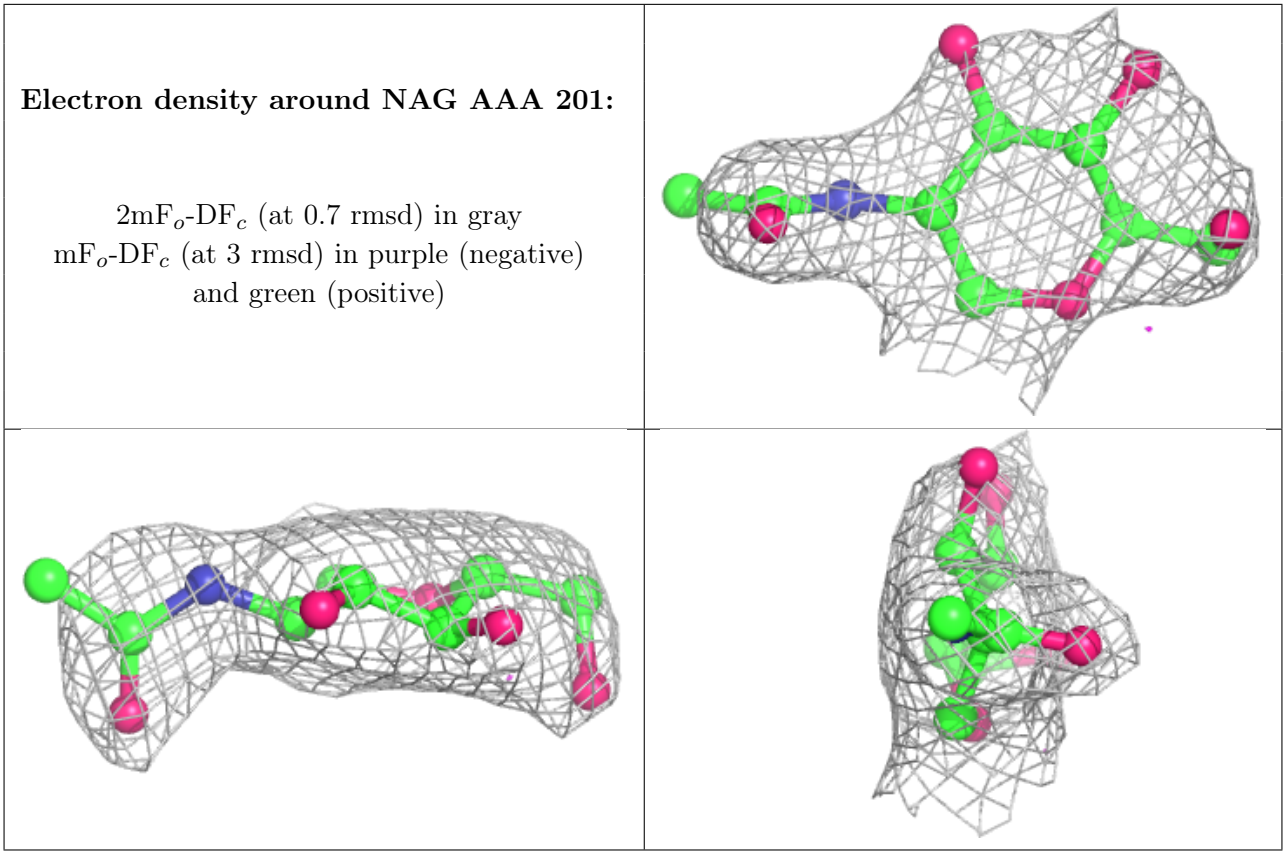






Electron density around NAG AAA 201:

$2mF_o$-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.