Full wwPDB X-ray Structure Validation Report (i)

Jan 15, 2024 – 04:52 pm GMT

PDB ID	:	6YJU
Title	:	Crystal structure of MGAT5 (alpha-1,6-mannosylglycoprotein 6-beta-N-acetylglucosaminyltransferase V) luminal domain with a Lys329-Ile345 loop truncation, in complex with UDP and biantennary pentasaccharide M592
Authors	:	Wu, L.; Darby, J.F.; Gilio, A.K.; Davies, G.J.
Deposited on	:	2020-04-04
Resolution	:	1.96 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 (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:

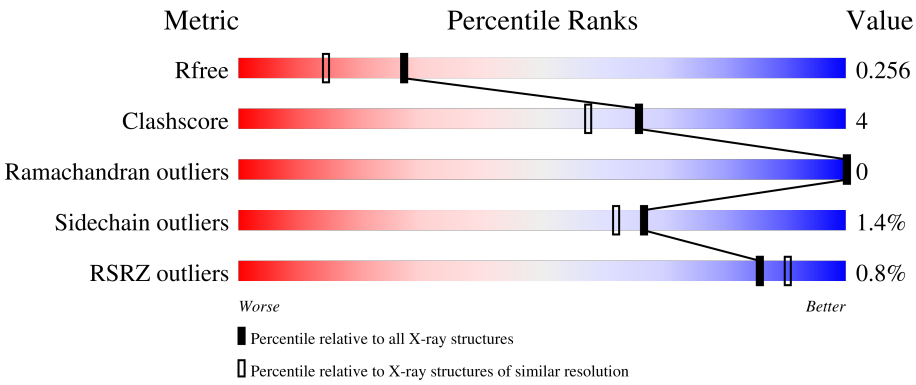
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.96 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	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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	515	% 89% 8% ·
1	BBB	515	% 87% 10% ·
2	A	4	100%
3	B	2	100%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 16720 atoms, of which 8219 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 Alpha-1,6-mannosylglycoprotein 6-beta-N-acetylglucosaminyl transferase A.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	AAA	502	8112	2611	4059	696	720	26	201	0	0
1	BBB	501	8106	2610	4056	694	720	26	199	0	0

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	?	-	LYS	deletion	UNP Q09328
AAA	?	-	LYS	deletion	UNP Q09328
AAA	?	-	VAL	deletion	UNP Q09328
AAA	?	-	VAL	deletion	UNP Q09328
AAA	?	-	GLY	deletion	UNP Q09328
AAA	?	-	ASN	deletion	UNP Q09328
AAA	?	-	ARG	deletion	UNP Q09328
AAA	?	-	SER	deletion	UNP Q09328
AAA	?	-	GLY	deletion	UNP Q09328
AAA	?	-	CYS	deletion	UNP Q09328
AAA	?	-	PRO	deletion	UNP Q09328
AAA	?	-	THR	deletion	UNP Q09328
AAA	?	-	VAL	deletion	UNP Q09328
AAA	330	GLY	ASP	conflict	UNP Q09328
AAA	331	GLY	ARG	conflict	UNP Q09328
AAA	332	GLY	ILE	conflict	UNP Q09328
BBB	?	-	LYS	deletion	UNP Q09328
BBB	?	-	LYS	deletion	UNP Q09328
BBB	?	-	VAL	deletion	UNP Q09328
BBB	?	-	VAL	deletion	UNP Q09328
BBB	?	-	GLY	deletion	UNP Q09328
BBB	?	-	ASN	deletion	UNP Q09328
BBB	?	-	ARG	deletion	UNP Q09328
BBB	?	-	SER	deletion	UNP Q09328

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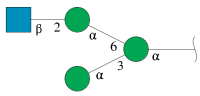
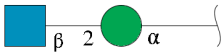
Chain	Residue	Modelled	Actual	Comment	Reference
BBB	?	-	GLY	deletion	UNP Q09328
BBB	?	-	CYS	deletion	UNP Q09328
BBB	?	-	PRO	deletion	UNP Q09328
BBB	?	-	THR	deletion	UNP Q09328
BBB	?	-	VAL	deletion	UNP Q09328
BBB	330	GLY	ASP	conflict	UNP Q09328
BBB	331	GLY	ARG	conflict	UNP Q09328
BBB	332	GLY	ILE	conflict	UNP Q09328

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



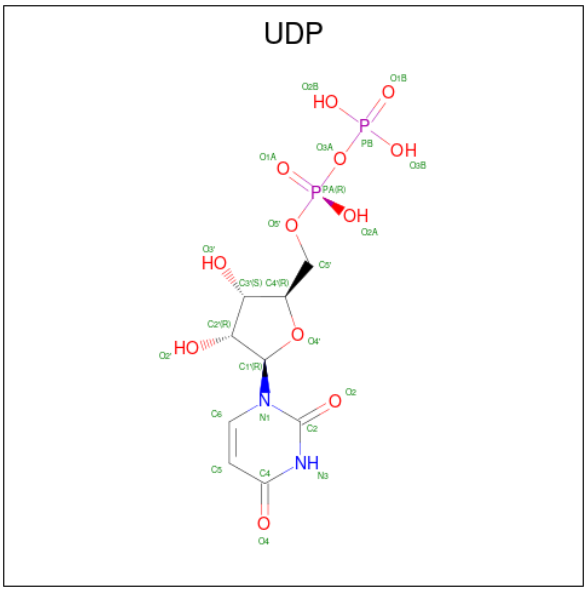
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	H	N	O			
2	A	4	93	26	45	1	21	13	0	0

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose.



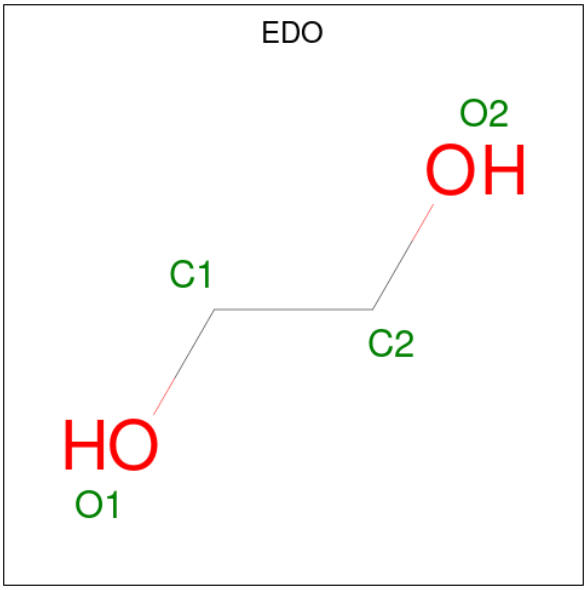
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	H	N	O			
3	B	2	51	14	25	1	11	7	0	0

- Molecule 4 is URIDINE-5'-DIPHOSPHATE (three-letter code: UDP) (formula: $C_9H_{14}N_2O_{12}P_2$) (labeled as "Ligand of Interest" by depositor).



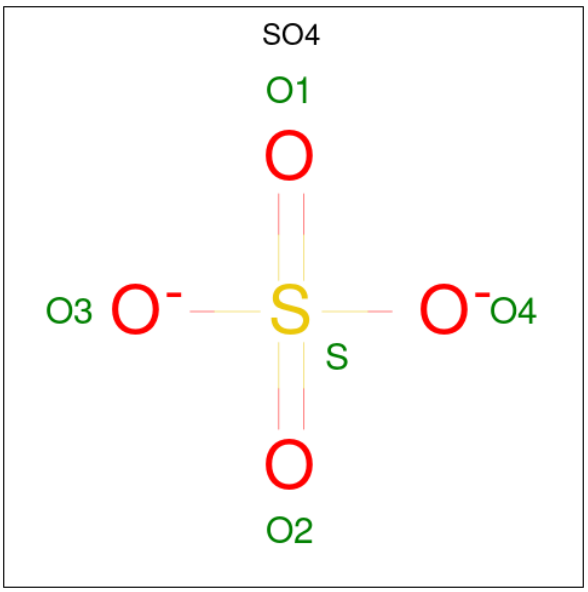
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	H	N	O	P		
4	AAA	1	36	9	11	2	12	2	2	0
			Total	C	H	N	O	P		
4	BBB	1	36	9	11	2	12	2	2	0

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
5	AAA	1	10	2	6	2	1	0
			Total	C	H	O		
5	BBB	1	10	2	6	2	1	0

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
6	AAA	1	5	4	1	0	0
			Total	O	S		
6	AAA	1	5	4	1	0	0
			Total	O	S		
6	AAA	1	5	4	1	0	0
			Total	O	S		
6	BBB	1	5	4	1	0	0
			Total	O	S		
6	BBB	1	5	4	1	0	0

- Molecule 7 is water.

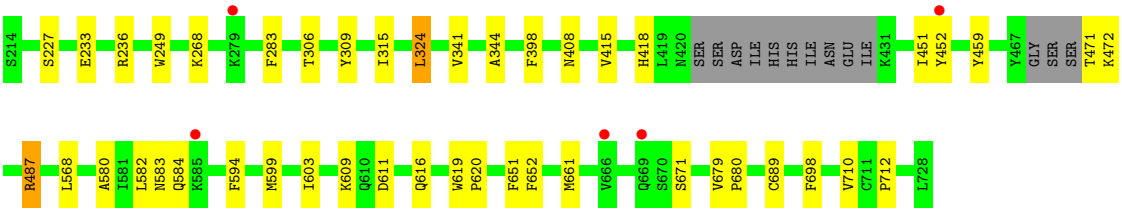
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	AAA	119	119	119	0	0
			Total	O		
7	BBB	122	122	122	0	0

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.

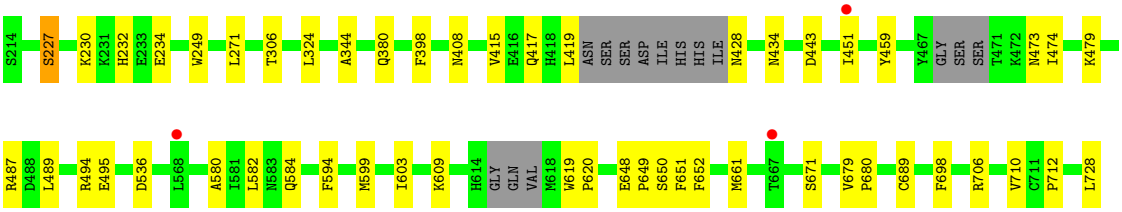
• Molecule 1: Alpha-1,6-mannosylglycoprotein 6-beta-N-acetylglucosaminyltransferase A

Chain AAA:



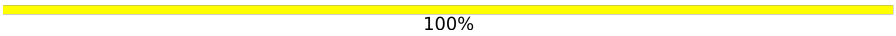
• Molecule 1: Alpha-1,6-mannosylglycoprotein 6-beta-N-acetylglucosaminyltransferase A

Chain BBB:



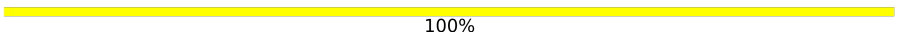
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose

Chain A:



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

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	46.60Å 69.55Å 90.94Å 107.48° 92.26° 106.22°	Depositor
Resolution (Å)	85.95 – 1.96 85.95 – 1.96	Depositor EDS
% Data completeness (in resolution range)	95.4 (85.95-1.96) 95.5 (85.95-1.96)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.83 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.200 , 0.252 0.206 , 0.256	Depositor DCC
R_{free} test set	3368 reflections (4.74%)	wwPDB-VP
Wilson B-factor (Å^2)	34.7	Xtriage
Anisotropy	0.236	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.41 , 46.3	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	16720	wwPDB-VP
Average B, all atoms (Å^2)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.60% 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: MAN, SO4, UDP, NAG, EDO

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	0.71	0/4158	0.83	0/5614
1	BBB	0.72	0/4154	0.85	0/5607
All	All	0.72	0/8312	0.84	0/11221

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 (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	AAA	4053	4059	4036	33	0
1	BBB	4050	4056	4032	34	0
2	A	48	45	42	1	0
3	B	26	25	24	0	0
4	AAA	25	11	11	0	0
4	BBB	25	11	11	1	0
5	AAA	4	6	6	0	0
5	BBB	4	6	6	0	0
6	AAA	15	0	0	0	0
6	BBB	10	0	0	0	0
7	AAA	119	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	BBB	122	0	0	4	0
All	All	8501	8219	8168	65	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 4.

All (65) 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:BBB:487:ARG:NH2	7:BBB:902:HOH:O	2.27	0.67
1:BBB:451:ILE:HD12	7:BBB:911:HOH:O	1.96	0.65
1:AAA:233:GLU:HG2	1:BBB:479:LYS:HD3	1.79	0.65
1:BBB:648:GLU:OE2	1:BBB:650:SER:OG	2.14	0.62
1:AAA:233:GLU:OE1	1:AAA:236:ARG:NH2	2.40	0.55
1:AAA:418:HIS:CG	1:AAA:487:ARG:HH12	2.25	0.54
1:AAA:611:ASP:OD2	1:AAA:616:GLN:HG3	2.08	0.54
1:AAA:452:TYR:CE1	1:AAA:568:LEU:HD22	2.43	0.53
1:AAA:283:PHE:CZ	1:AAA:341:VAL:HG21	2.44	0.53
1:BBB:249:TRP:CE2	1:BBB:306:THR:HG21	2.44	0.52
1:BBB:671:SER:HA	1:BBB:689:CYS:O	2.10	0.52
1:AAA:236:ARG:NH1	1:BBB:495:GLU:OE1	2.44	0.51
1:AAA:249:TRP:CE2	1:AAA:306:THR:HG21	2.46	0.51
1:AAA:671:SER:HA	1:AAA:689:CYS:O	2.11	0.50
1:AAA:283:PHE:CZ	2:A:1:MAN:H62	2.47	0.50
1:AAA:652:PHE:HB3	1:AAA:698:PHE:CD1	2.47	0.50
1:BBB:271:LEU:HD21	1:BBB:324:LEU:CD1	2.41	0.50
1:BBB:489:LEU:HD22	4:BBB:801:UDP:C6	2.47	0.50
1:AAA:324:LEU:HD12	1:AAA:324:LEU:O	2.12	0.49
1:AAA:268:LYS:NZ	7:AAA:905:HOH:O	2.45	0.49
1:AAA:451:ILE:CG2	7:AAA:984:HOH:O	2.59	0.49
1:BBB:415:VAL:HG23	1:BBB:594:PHE:HB3	1.95	0.48
1:BBB:652:PHE:HB3	1:BBB:698:PHE:CD1	2.48	0.48
1:BBB:619:TRP:HA	1:BBB:620:PRO:C	2.33	0.48
1:AAA:418:HIS:CD2	1:AAA:487:ARG:NH1	2.82	0.48
1:BBB:419:LEU:HD21	1:BBB:494:ARG:HG2	1.96	0.48
1:AAA:341:VAL:HG23	7:AAA:941:HOH:O	2.12	0.48
1:AAA:661:MET:CE	1:AAA:710:VAL:HG21	2.44	0.48
1:BBB:651:PHE:HB2	1:BBB:712:PRO:HB2	1.96	0.47
1:AAA:283:PHE:CE2	1:AAA:341:VAL:HG21	2.49	0.47
1:AAA:398:PHE:O	1:AAA:408:ASN:HB3	2.14	0.46
1:BBB:419:LEU:CD2	1:BBB:494:ARG:HG2	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BBB:474:ILE:CD1	1:BBB:474:ILE:N	2.79	0.46
1:AAA:324:LEU:HD12	1:AAA:324:LEU:C	2.35	0.45
1:AAA:451:ILE:HG23	7:AAA:984:HOH:O	2.16	0.45
1:BBB:609:LYS:HB3	1:BBB:619:TRP:CG	2.51	0.45
1:BBB:599:MET:O	1:BBB:603:ILE:HG22	2.17	0.45
1:BBB:398:PHE:O	1:BBB:408:ASN:HB3	2.17	0.45
1:AAA:415:VAL:HG23	1:AAA:594:PHE:HB3	1.98	0.45
1:AAA:344:ALA:HB3	7:AAA:921:HOH:O	2.18	0.44
1:BBB:417:GLN:HE21	1:BBB:419:LEU:H	1.64	0.44
1:AAA:651:PHE:HB2	1:AAA:712:PRO:HB2	1.99	0.44
1:BBB:494:ARG:HD3	7:BBB:1015:HOH:O	2.17	0.43
1:BBB:661:MET:HE3	1:BBB:710:VAL:HG21	2.00	0.43
1:AAA:309:TYR:N	1:AAA:315:ILE:HD11	2.34	0.43
1:AAA:661:MET:HE3	1:AAA:710:VAL:HG21	2.00	0.43
1:AAA:609:LYS:HB3	1:AAA:619:TRP:CD1	2.54	0.43
1:BBB:443:ASP:OD1	1:BBB:473:ASN:CB	2.67	0.43
1:BBB:580:ALA:O	1:BBB:584:GLN:HG3	2.19	0.42
1:BBB:661:MET:CE	1:BBB:710:VAL:HG21	2.48	0.42
1:BBB:661:MET:HE1	1:BBB:710:VAL:HG11	2.02	0.42
1:AAA:472:LYS:O	1:AAA:472:LYS:HG2	2.19	0.42
1:AAA:619:TRP:HA	1:AAA:620:PRO:C	2.39	0.42
1:BBB:459:TYR:HB3	1:BBB:582:LEU:HD11	2.02	0.42
1:AAA:599:MET:O	1:AAA:603:ILE:HG22	2.20	0.41
1:AAA:580:ALA:O	1:AAA:584:GLN:HG3	2.20	0.41
1:AAA:679:VAL:HA	1:AAA:680:PRO:C	2.41	0.41
1:BBB:227:SER:HA	1:BBB:230:LYS:HE3	2.01	0.41
1:BBB:474:ILE:N	1:BBB:474:ILE:HD12	2.36	0.41
1:BBB:652:PHE:HB3	1:BBB:698:PHE:CE1	2.55	0.41
1:AAA:459:TYR:HB3	1:AAA:582:LEU:HD11	2.02	0.41
1:BBB:232:HIS:HB3	1:BBB:234:GLU:OE1	2.21	0.40
1:BBB:728:LEU:HD23	1:BBB:728:LEU:HA	1.91	0.40
1:BBB:344:ALA:HB3	7:BBB:941:HOH:O	2.21	0.40
1:BBB:679:VAL:HA	1:BBB:680:PRO:C	2.42	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	496/515 (96%)	480 (97%)	16 (3%)	0	100	100
1	BBB	493/515 (96%)	479 (97%)	14 (3%)	0	100	100
All	All	989/1030 (96%)	959 (97%)	30 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	444/456 (97%)	439 (99%)	5 (1%)	73	71
1	BBB	444/456 (97%)	437 (98%)	7 (2%)	62	58
All	All	888/912 (97%)	876 (99%)	12 (1%)	67	62

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	227	SER
1	AAA	324	LEU
1	AAA	471	THR
1	AAA	487	ARG
1	AAA	583	ASN
1	BBB	227	SER
1	BBB	380	GLN
1	BBB	428	ASN

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Mol	Chain	Res	Type
1	BBB	434	ASN
1	BBB	536	ASP
1	BBB	649	PRO
1	BBB	706	ARG

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)

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

5.5 Carbohydrates (i)

6 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	MAN	A	1	2	12,12,12	0.62	0	17,17,17	0.76	0
2	MAN	A	2	2	11,11,12	1.09	1 (9%)	15,15,17	1.51	2 (13%)
2	NAG	A	3	2	14,14,15	0.91	0	17,19,21	1.41	1 (5%)
2	MAN	A	4	2	11,11,12	0.70	0	15,15,17	1.79	4 (26%)
3	MAN	B	1	3	12,12,12	1.03	1 (8%)	17,17,17	1.80	6 (35%)
3	NAG	B	2	3	14,14,15	1.27	1 (7%)	17,19,21	1.05	1 (5%)

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	MAN	A	1	2	-	0/2/22/22	0/1/1/1
2	MAN	A	2	2	-	0/2/19/22	0/1/1/1
2	NAG	A	3	2	-	1/6/23/26	0/1/1/1
2	MAN	A	4	2	-	1/2/19/22	0/1/1/1
3	MAN	B	1	3	-	0/2/22/22	0/1/1/1
3	NAG	B	2	3	-	1/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	2	NAG	C1-C2	3.31	1.57	1.52
2	A	2	MAN	O5-C5	2.46	1.48	1.43
3	B	1	MAN	O1-C1	2.29	1.46	1.39

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	2	MAN	O5-C5-C6	4.34	114.01	107.20
2	A	3	NAG	C1-O5-C5	-3.85	106.97	112.19
2	A	4	MAN	O2-C2-C1	3.83	116.99	109.15
3	B	1	MAN	O2-C2-C3	-3.27	102.79	110.35
3	B	1	MAN	O5-C5-C4	2.85	114.87	109.69
2	A	4	MAN	C2-C3-C4	2.73	115.62	110.89
2	A	4	MAN	C1-O5-C5	2.64	115.77	112.19
2	A	4	MAN	O4-C4-C5	-2.61	102.82	109.30
3	B	1	MAN	O5-C5-C6	2.58	112.86	106.44
3	B	1	MAN	C4-C3-C2	-2.37	106.69	110.82
3	B	1	MAN	O1-C1-C2	2.35	115.64	109.03
2	A	2	MAN	O3-C3-C4	-2.22	105.22	110.35
3	B	1	MAN	O5-C1-C2	-2.20	106.36	110.28
3	B	2	NAG	O4-C4-C3	-2.15	105.37	110.35

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	4	MAN	O5-C5-C6-O6
2	A	3	NAG	C3-C2-N2-C7
3	B	2	NAG	C3-C2-N2-C7

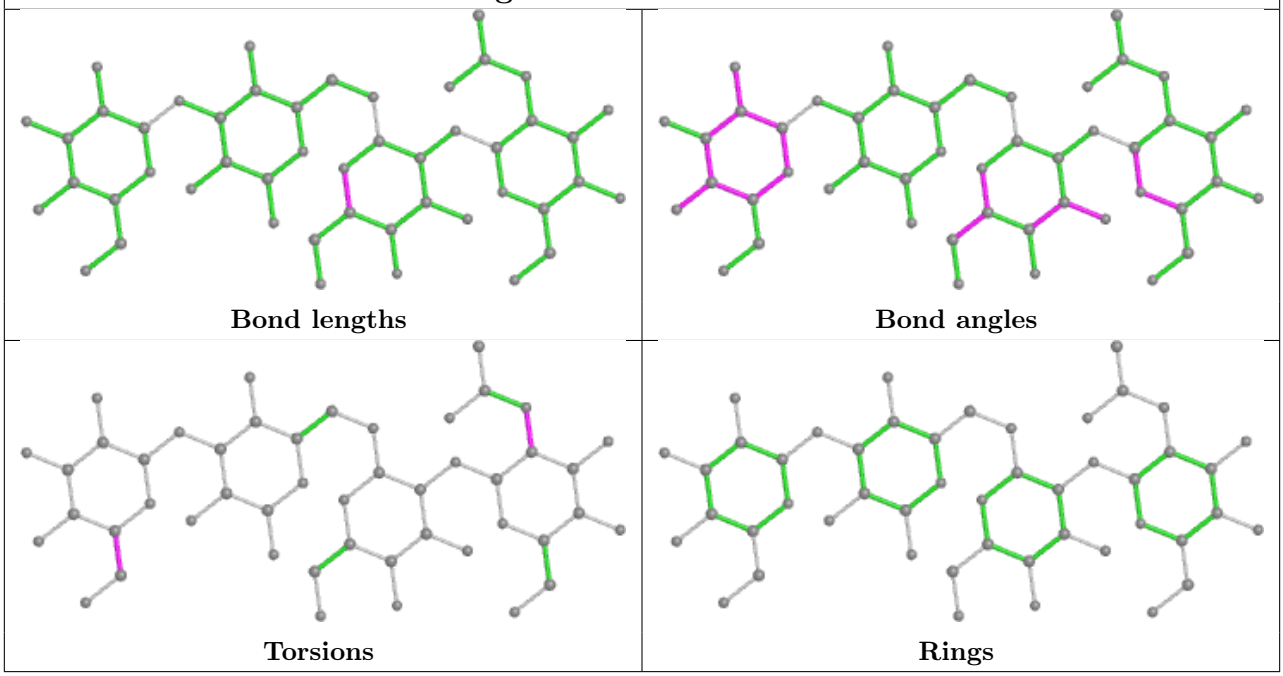
There are no ring outliers.

1 monomer is involved in 1 short contact:

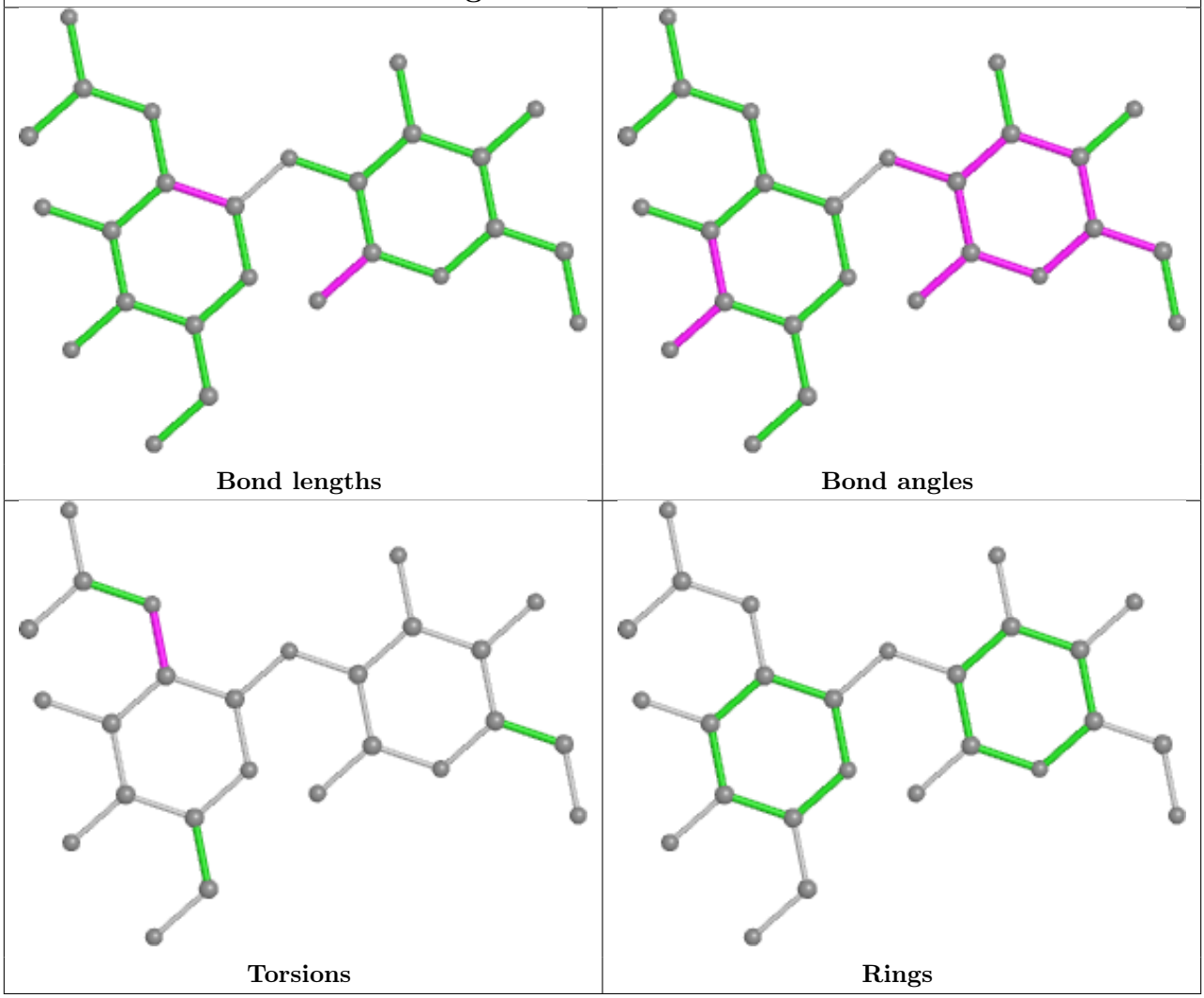
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1	MAN	1	0

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 A



Oligosaccharide Chain B



5.6 Ligand geometry (i)

9 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	$\#\|Z\| > 2$
4	UDP	BBB	801	-	24,26,26	1.07	2 (8%)	37,40,40	1.76	6 (16%)
5	EDO	AAA	806	-	3,3,3	0.14	0	2,2,2	0.22	0
6	SO4	AAA	809	-	4,4,4	0.26	0	6,6,6	0.16	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	SO4	BBB	805	-	4,4,4	0.33	0	6,6,6	0.06	0
5	EDO	BBB	804	-	3,3,3	0.38	0	2,2,2	0.36	0
4	UDP	AAA	801	-	24,26,26	0.98	2 (8%)	37,40,40	1.71	6 (16%)
6	SO4	AAA	807	-	4,4,4	0.36	0	6,6,6	0.05	0
6	SO4	BBB	806	-	4,4,4	0.30	0	6,6,6	0.19	0
6	SO4	AAA	808	-	4,4,4	0.32	0	6,6,6	0.13	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
5	EDO	BBB	804	-	-	1/1/1/1	-
4	UDP	AAA	801	-	-	5/16/32/32	0/2/2/2
5	EDO	AAA	806	-	-	1/1/1/1	-
4	UDP	BBB	801	-	-	4/16/32/32	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	BBB	801	UDP	C2-N3	-2.55	1.33	1.38
4	AAA	801	UDP	C4-N3	-2.15	1.34	1.38
4	AAA	801	UDP	C2-N3	-2.11	1.34	1.38
4	BBB	801	UDP	C4-N3	-2.10	1.34	1.38

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	BBB	801	UDP	C4-N3-C2	-4.96	120.03	126.58
4	BBB	801	UDP	N3-C2-N1	4.38	120.71	114.89
4	AAA	801	UDP	C4-N3-C2	-4.31	120.89	126.58
4	AAA	801	UDP	C5-C4-N3	4.27	121.23	114.84
4	BBB	801	UDP	C5-C4-N3	4.05	120.89	114.84
4	AAA	801	UDP	N3-C2-N1	3.96	120.14	114.89
4	BBB	801	UDP	O2-C2-N1	-3.32	118.38	122.79
4	AAA	801	UDP	O3B-PB-O2B	3.14	119.65	107.64
4	BBB	801	UDP	O4-C4-C5	-2.86	120.12	125.16
4	AAA	801	UDP	O4-C4-C5	-2.42	120.90	125.16
4	BBB	801	UDP	O5'-C5'-C4'	2.26	116.76	108.99
4	AAA	801	UDP	C4'-O4'-C1'	-2.07	104.92	109.47

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	AAA	801	UDP	C5'-O5'-PA-O1A
4	AAA	801	UDP	C5'-O5'-PA-O3A
4	BBB	801	UDP	C3'-C4'-C5'-O5'
4	BBB	801	UDP	O4'-C4'-C5'-O5'
5	BBB	804	EDO	O1-C1-C2-O2
4	AAA	801	UDP	C5'-O5'-PA-O2A
5	AAA	806	EDO	O1-C1-C2-O2
4	AAA	801	UDP	PB-O3A-PA-O1A
4	BBB	801	UDP	PB-O3A-PA-O1A
4	AAA	801	UDP	PB-O3A-PA-O2A
4	BBB	801	UDP	PB-O3A-PA-O2A

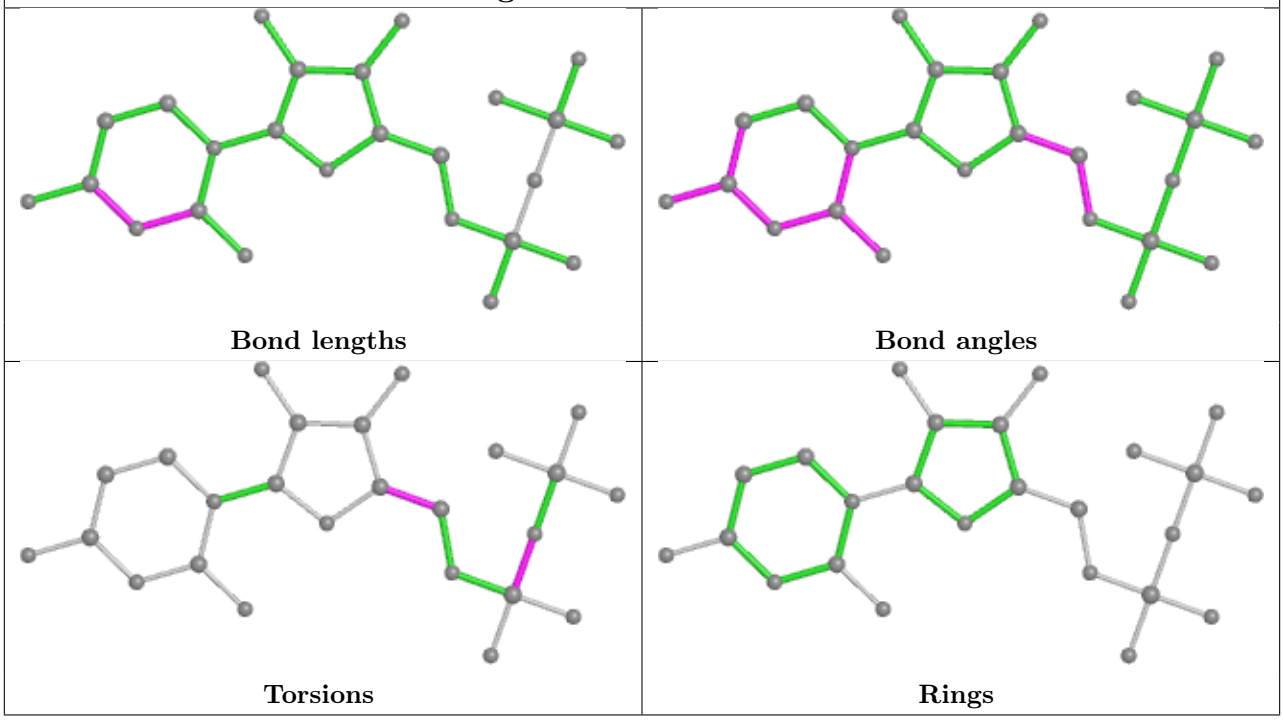
There are no ring outliers.

1 monomer is involved in 1 short contact:

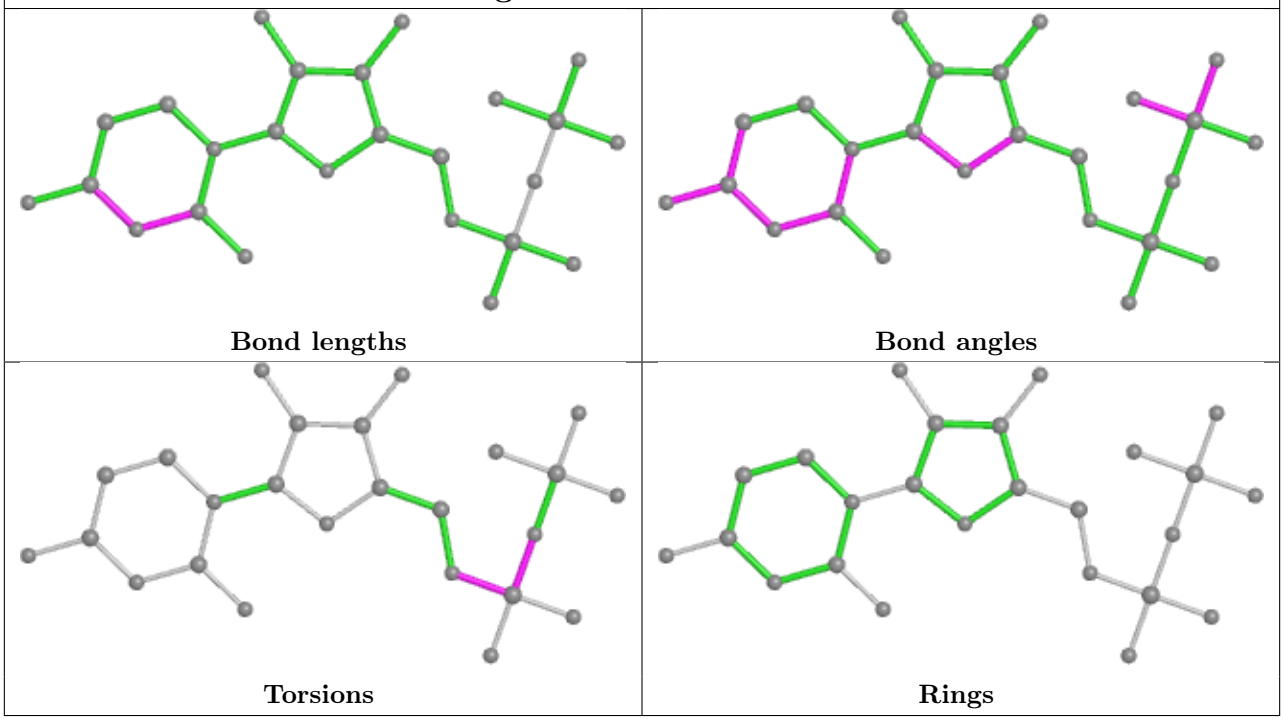
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	BBB	801	UDP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for 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 UDP BBB 801



Ligand UDP AAA 801



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	AAA	502/515 (97%)	0.12	5 (0%)	82	87	35, 53, 86, 114	0
1	BBB	501/515 (97%)	0.07	3 (0%)	89	93	34, 51, 82, 104	0
All	All	1003/1030 (97%)	0.10	8 (0%)	86	90	34, 52, 84, 114	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	BBB	568	LEU	3.8
1	AAA	669	GLN	3.8
1	BBB	667	THR	3.3
1	AAA	666	VAL	3.0
1	BBB	451	ILE	2.4
1	AAA	279	LYS	2.3
1	AAA	585	LYS	2.3
1	AAA	452	TYR	2.2

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

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

6.3 Carbohydrates (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	MAN	A	4	11/12	0.86	0.13	58,69,78,80	4

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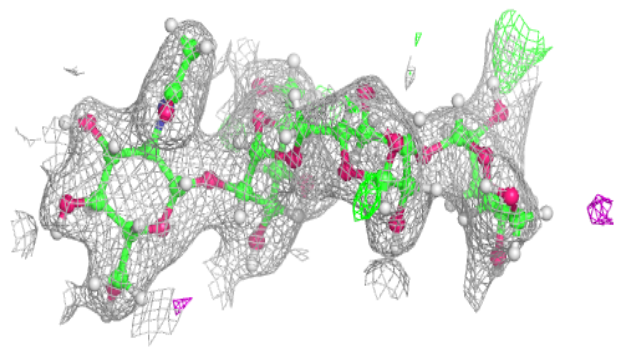
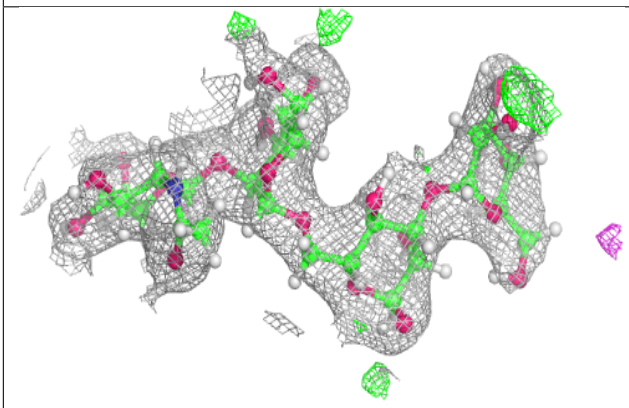
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	MAN	A	1	12/12	0.92	0.09	54,68,74,77	3
3	MAN	B	1	12/12	0.94	0.10	40,43,46,48	4
2	MAN	A	2	11/12	0.95	0.10	40,48,51,57	3
2	NAG	A	3	14/15	0.98	0.08	37,43,47,49	3
3	NAG	B	2	14/15	0.98	0.09	35,39,41,43	3

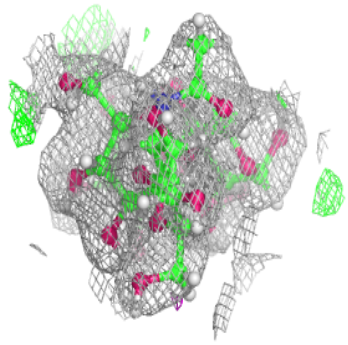
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain A:

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

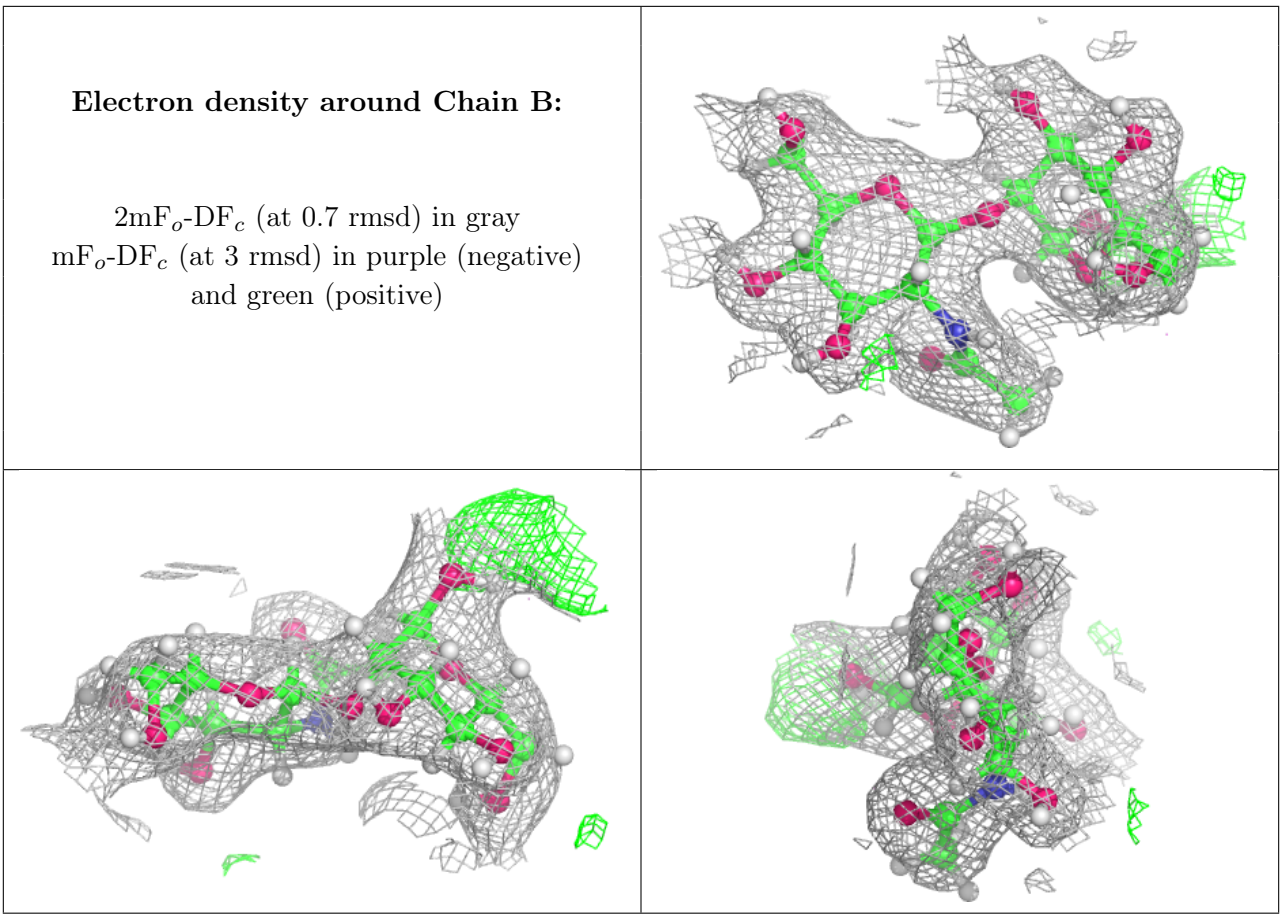






Electron density around Chain B:

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



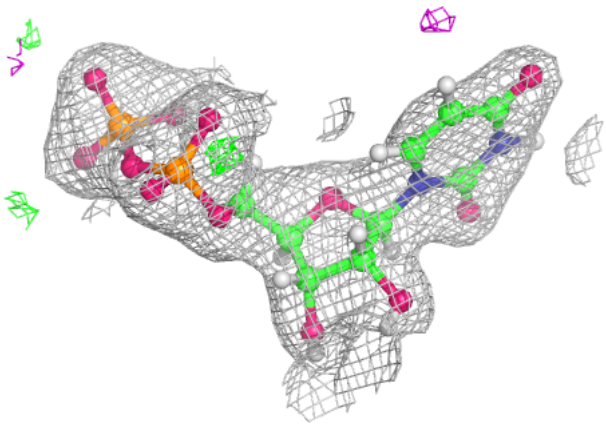
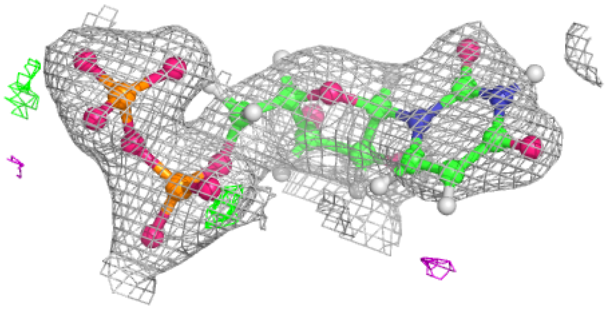
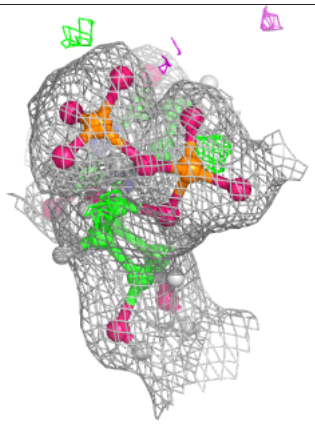
6.4 Ligands (i)

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	SO4	BBB	806	5/5	0.82	0.26	58,66,71,76	5
6	SO4	BBB	805	5/5	0.84	0.14	89,105,116,117	0
5	EDO	BBB	804	4/4	0.88	0.20	52,66,70,73	1
6	SO4	AAA	809	5/5	0.88	0.15	59,66,84,84	5
6	SO4	AAA	808	5/5	0.92	0.11	61,71,76,76	5
6	SO4	AAA	807	5/5	0.93	0.13	100,100,111,112	0
5	EDO	AAA	806	4/4	0.95	0.10	61,71,73,74	1
4	UDP	BBB	801	25/25	0.98	0.15	30,34,39,40	36
4	UDP	AAA	801	25/25	0.98	0.11	37,47,49,51	36

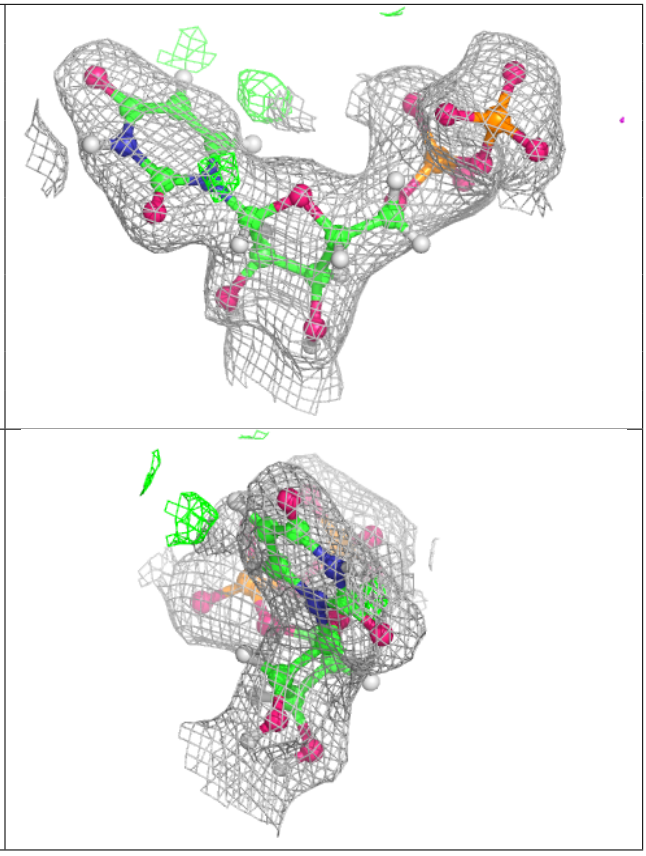
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different

orientation to approximate a three-dimensional view.

Electron density around UDP BBB 801: 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 UDP AAA 801:

$2mF_o$-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.