Full wwPDB X-ray Structure Validation Report (i)

Jan 15, 2024 – 02:19 pm GMT

PDB ID	:	6YJR
Title	:	Crystal structure of unliganded MGAT5 (alpha-1,6-mannosylglycoprotein 6-beta-N-acetylglucosaminyltransferase V) luminal domain.
Authors	:	Wu, L.; Darby, J.F.; Gilio, A.K.; Davies, G.J.
Deposited on	:	2020-04-04
Resolution	:	2.20 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:

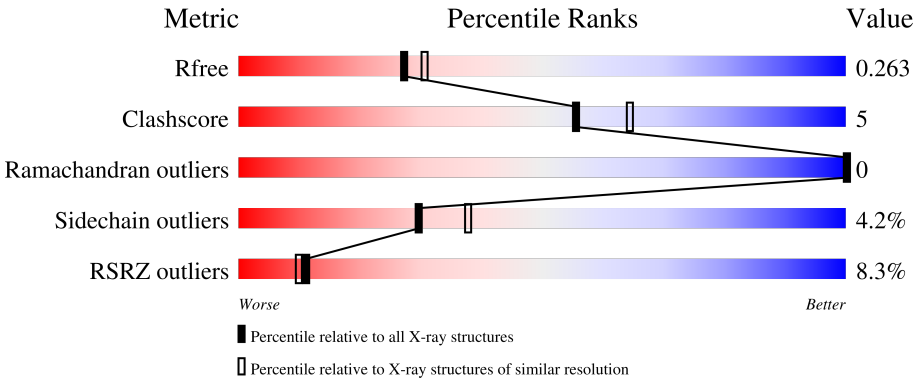
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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	528	5% 80% 13% • 6%
1	BBB	528	11% 78% 14% • 7%
2	A	2	100%
2	B	2	50% 50%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 15909 atoms, of which 7857 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.

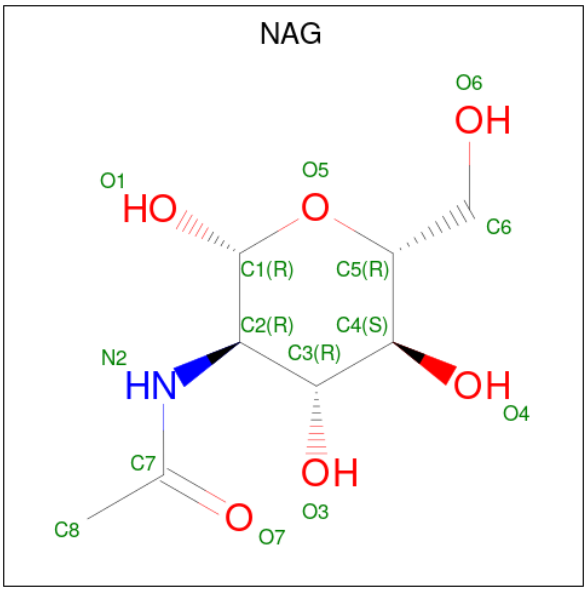
- Molecule 1 is a protein called Alpha-1,6-mannosylglycoprotein 6-beta-N-acetylglucosaminyl transferase A.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	AAA	495	Total	C	H	N	O	S	219	0	0
			7881	2541	3916	690	709	25			
1	BBB	493	Total	C	H	N	O	S	223	0	0
			7774	2505	3853	685	706	25			

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

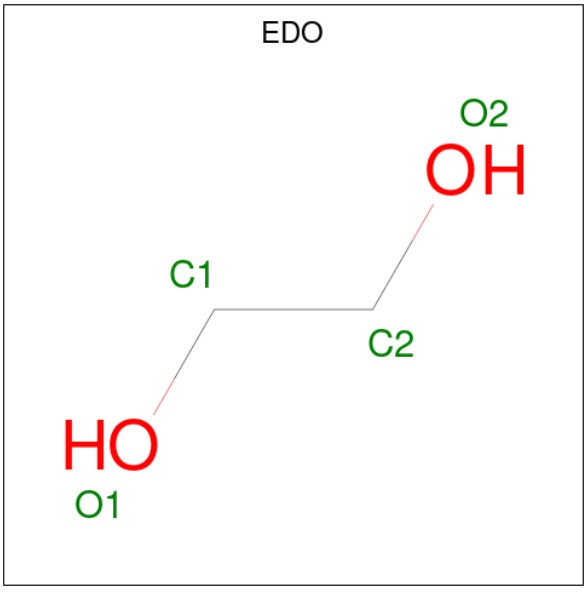
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	2	Total	C	H	N	O	5	0	0
			49	14	25	1	9			
2	B	2	Total	C	H	N	O	5	0	0
			49	14	25	1	9			

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	AAA	1	Total	C	H	N	O	3	0
			28	8	14	1	5		

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

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

- Molecule 5 is water.

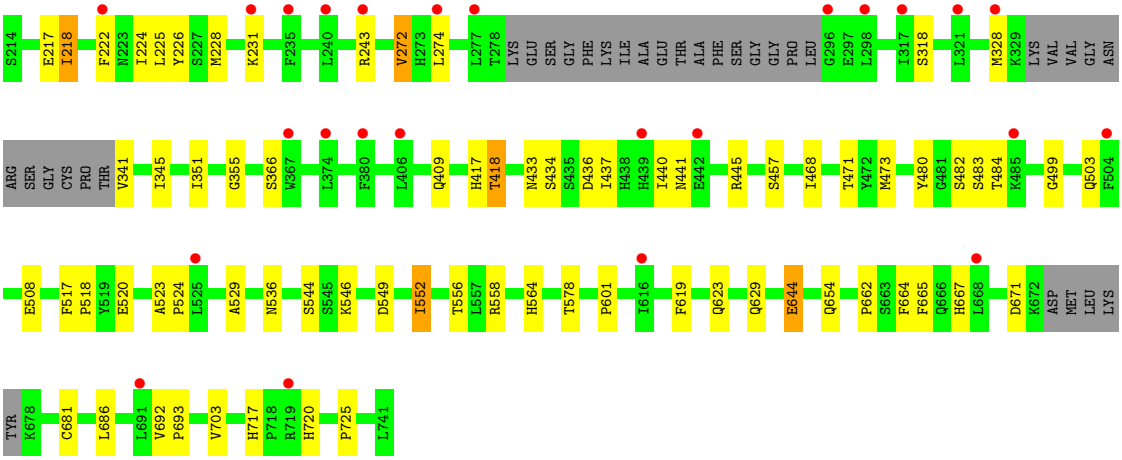
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	AAA	55	Total O 55 55	0	0
5	BBB	33	Total O 33 33	0	0

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.

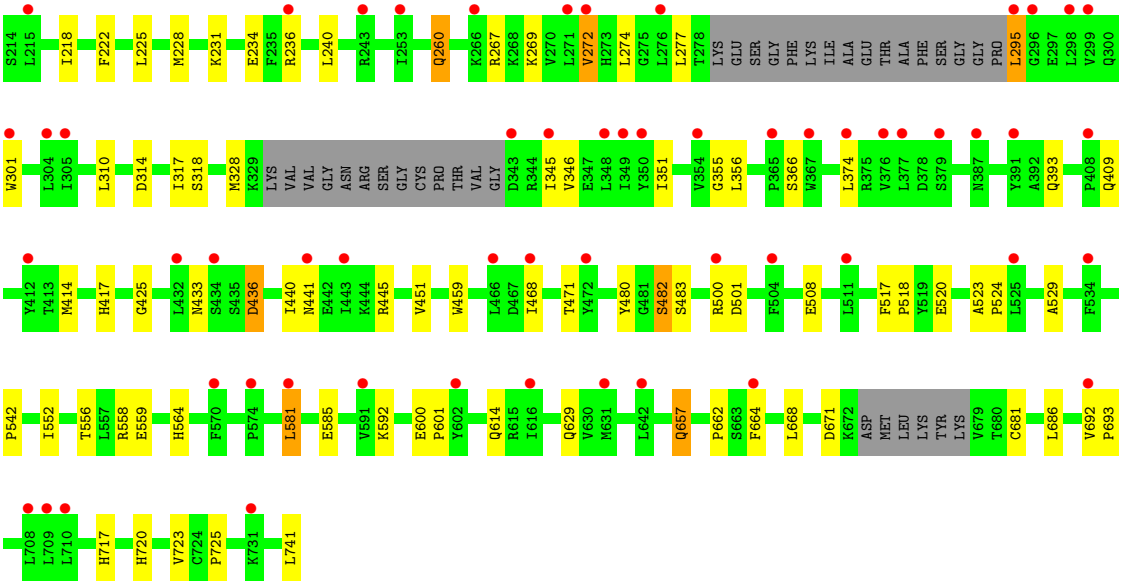
• Molecule 1: Alpha-1,6-mannosylglycoprotein 6-beta-N-acetylglucosaminyltransferase A

Chain AAA:



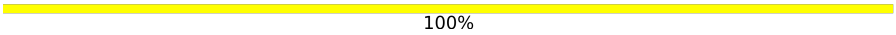
• Molecule 1: Alpha-1,6-mannosylglycoprotein 6-beta-N-acetylglucosaminyltransferase A

Chain BBB:



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

Chain A:



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

Chain B:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	59.81Å 100.42Å 207.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.81 – 2.20 48.81 – 2.20	Depositor EDS
% Data completeness (in resolution range)	57.1 (48.81-2.20) 57.1 (48.81-2.20)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.07 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.208 , 0.263 0.210 , 0.263	Depositor DCC
R_{free} test set	1866 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	45.2	Xtriage
Anisotropy	0.949	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 57.6	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	15909	wwPDB-VP
Average B, all atoms (Å^2)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.24% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: EDO, FUC, NAG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	AAA	0.68	0/4067	0.85	2/5500 (0.0%)
1	BBB	0.67	0/4020	0.85	0/5436
All	All	0.67	0/8087	0.85	2/10936 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AAA	441	ASN	CB-CA-C	-6.31	97.79	110.40
1	AAA	644	GLU	CB-CA-C	5.89	122.18	110.40

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	3965	3916	3866	37	1
1	BBB	3921	3853	3791	43	1
2	A	24	25	22	0	0
2	B	24	25	22	1	0
3	AAA	14	14	13	0	0
4	AAA	8	12	12	0	0
4	BBB	8	12	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	AAA	55	0	0	1	0
5	BBB	33	0	0	2	0
All	All	8052	7857	7738	80	1

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 5.

All (80) 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:AAA:433:ASN:O	1:AAA:437:ILE:HG12	1.81	0.79
1:AAA:417:HIS:ND1	1:AAA:418:THR:HG23	1.98	0.78
1:BBB:657:GLN:O	1:BBB:657:GLN:HG3	1.86	0.74
1:BBB:581:LEU:HD23	5:BBB:913:HOH:O	1.93	0.68
1:BBB:295:LEU:HD12	5:BBB:932:HOH:O	1.98	0.64
1:AAA:529:ALA:O	1:AAA:601:PRO:HB3	1.98	0.63
1:AAA:231:LYS:O	1:AAA:231:LYS:HG2	2.00	0.62
1:BBB:657:GLN:O	1:BBB:657:GLN:CG	2.47	0.61
1:BBB:436:ASP:O	1:BBB:440:ILE:N	2.33	0.60
1:AAA:217:GLU:O	1:AAA:217:GLU:HG2	2.01	0.60
1:BBB:529:ALA:O	1:BBB:601:PRO:HB3	2.02	0.59
1:AAA:436:ASP:O	1:AAA:440:ILE:N	2.33	0.58
1:BBB:267:ARG:NE	1:BBB:314:ASP:OD1	2.35	0.57
1:AAA:549:ASP:HA	1:AAA:552:ILE:HD13	1.87	0.57
1:AAA:224:ILE:HD12	1:AAA:224:ILE:H	1.70	0.57
1:BBB:272:VAL:HG13	1:BBB:317:ILE:HA	1.87	0.56
1:AAA:484:THR:HG21	5:AAA:939:HOH:O	2.06	0.56
1:BBB:234:GLU:OE1	1:BBB:234:GLU:N	2.23	0.56
1:BBB:542:PRO:HB2	1:BBB:559:GLU:HB3	1.87	0.55
1:BBB:274:LEU:HD12	1:BBB:274:LEU:N	2.22	0.54
1:BBB:417:HIS:HB2	1:BBB:558:ARG:HD2	1.90	0.54
1:AAA:417:HIS:ND1	1:AAA:418:THR:CG2	2.70	0.52
1:BBB:409:GLN:NE2	1:BBB:662:PRO:HG2	2.25	0.52
1:BBB:272:VAL:HG22	1:BBB:274:LEU:HD11	1.91	0.51
1:BBB:272:VAL:HG23	1:BBB:301:TRP:CZ3	2.45	0.51
1:AAA:272:VAL:HG23	1:AAA:274:LEU:HD11	1.93	0.51
1:AAA:218:ILE:CG1	1:AAA:218:ILE:O	2.59	0.50
1:AAA:274:LEU:HD12	1:AAA:274:LEU:N	2.27	0.50
1:BBB:692:VAL:HA	1:BBB:693:PRO:C	2.32	0.50
1:BBB:436:ASP:CG	1:BBB:500:ARG:HH21	2.15	0.49
1:AAA:517:PHE:CG	1:AAA:518:PRO:HA	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BBB:269:LYS:HG3	1:BBB:346:VAL:HA	1.93	0.49
1:AAA:629:GLN:NE2	1:AAA:667:HIS:CE1	2.80	0.48
1:AAA:692:VAL:HA	1:AAA:693:PRO:C	2.34	0.48
1:BBB:664:PHE:HB2	1:BBB:725:PRO:HB2	1.95	0.48
1:BBB:523:ALA:N	1:BBB:524:PRO:CD	2.76	0.48
1:BBB:417:HIS:HB2	1:BBB:558:ARG:CD	2.43	0.48
1:AAA:717:HIS:CD2	1:AAA:720:HIS:HB2	2.49	0.48
1:AAA:409:GLN:NE2	1:AAA:662:PRO:HG2	2.30	0.46
1:BBB:218:ILE:HA	1:BBB:310:LEU:O	2.15	0.46
1:AAA:671:ASP:HB3	1:AAA:681:CYS:SG	2.56	0.46
1:BBB:717:HIS:CD2	1:BBB:720:HIS:HB2	2.50	0.46
1:BBB:433:ASN:OD1	1:BBB:436:ASP:OD1	2.34	0.46
1:BBB:517:PHE:CG	1:BBB:518:PRO:HA	2.50	0.46
1:AAA:445:ARG:HA	1:AAA:508:GLU:HA	1.98	0.45
1:BBB:592:LYS:HD2	2:B:2:FUC:H61	1.98	0.45
1:BBB:671:ASP:HB3	1:BBB:681:CYS:SG	2.56	0.45
1:BBB:480:TYR:HE2	1:BBB:482:SER:HG	1.61	0.45
1:AAA:468:ILE:O	1:AAA:471:THR:HB	2.17	0.45
1:BBB:445:ARG:HA	1:BBB:508:GLU:HA	1.99	0.45
1:AAA:664:PHE:HB2	1:AAA:725:PRO:HB2	1.99	0.44
1:BBB:225:LEU:O	1:BBB:228:MET:HB2	2.18	0.44
1:BBB:356:LEU:HD11	1:BBB:374:LEU:HD13	2.00	0.44
1:AAA:523:ALA:N	1:AAA:524:PRO:CD	2.80	0.44
1:AAA:520:GLU:HA	1:AAA:564:HIS:CD2	2.52	0.44
1:AAA:226:TYR:CE1	1:AAA:243:ARG:HG3	2.52	0.43
1:AAA:417:HIS:CE1	1:AAA:418:THR:HG23	2.51	0.43
1:BBB:260:GLN:HE22	1:BBB:614:GLN:HE21	1.66	0.43
1:BBB:668:LEU:HD13	1:BBB:723:VAL:HG12	2.01	0.43
1:BBB:468:ILE:O	1:BBB:471:THR:HB	2.18	0.43
1:AAA:536:ASN:O	1:AAA:578:THR:HA	2.18	0.43
1:BBB:222:PHE:HD1	1:BBB:225:LEU:HD23	1.84	0.43
1:AAA:222:PHE:HD1	1:AAA:225:LEU:HD23	1.84	0.42
1:BBB:328:MET:HA	1:BBB:345:ILE:CD1	2.49	0.42
1:AAA:328:MET:HA	1:AAA:345:ILE:CD1	2.49	0.42
1:BBB:523:ALA:HB3	1:BBB:524:PRO:HD3	2.00	0.42
1:AAA:686:LEU:HD23	1:AAA:686:LEU:HA	1.82	0.42
1:AAA:480:TYR:CE2	1:AAA:482:SER:HB2	2.55	0.41
1:AAA:544:SER:C	1:AAA:546:LYS:H	2.23	0.41
1:AAA:499:GLY:O	1:AAA:503:GLN:HG3	2.19	0.41
1:BBB:520:GLU:HA	1:BBB:564:HIS:CD2	2.55	0.41
1:AAA:351:ILE:HD11	1:AAA:355:GLY:C	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:225:LEU:O	1:AAA:228:MET:HB2	2.20	0.41
1:AAA:619:PHE:O	1:AAA:623:GLN:HB3	2.21	0.41
1:BBB:236:ARG:NH1	1:BBB:240:LEU:HD11	2.36	0.41
1:BBB:414:MET:O	1:BBB:425:GLY:HA2	2.21	0.41
1:BBB:686:LEU:HD23	1:BBB:686:LEU:HA	1.90	0.41
1:BBB:351:ILE:HD11	1:BBB:355:GLY:C	2.41	0.41
1:BBB:451:VAL:HG11	1:BBB:459:TRP:CZ2	2.56	0.40
1:AAA:692:VAL:HG11	1:AAA:703:VAL:HG12	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:480:TYR:OH	1:BBB:501:ASP:OD2[4_545]	2.00	0.20

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	487/528 (92%)	464 (95%)	23 (5%)	0	100	100
1	BBB	485/528 (92%)	457 (94%)	28 (6%)	0	100	100
All	All	972/1056 (92%)	921 (95%)	51 (5%)	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	429/470 (91%)	413 (96%)	16 (4%)	34	43
1	BBB	419/470 (89%)	399 (95%)	20 (5%)	25	32
All	All	848/940 (90%)	812 (96%)	36 (4%)	30	38

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	218	ILE
1	AAA	272	VAL
1	AAA	318	SER
1	AAA	341	VAL
1	AAA	366	SER
1	AAA	418	THR
1	AAA	434	SER
1	AAA	457	SER
1	AAA	473	MET
1	AAA	483	SER
1	AAA	552	ILE
1	AAA	556	THR
1	AAA	558	ARG
1	AAA	644	GLU
1	AAA	654	GLN
1	AAA	665	PHE
1	BBB	231	LYS
1	BBB	260	GLN
1	BBB	272	VAL
1	BBB	277	LEU
1	BBB	295	LEU
1	BBB	318	SER
1	BBB	366	SER
1	BBB	393	GLN
1	BBB	436	ASP
1	BBB	441	ASN
1	BBB	482	SER
1	BBB	483	SER
1	BBB	552	ILE
1	BBB	556	THR
1	BBB	581	LEU
1	BBB	585	GLU
1	BBB	600	GLU

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Mol	Chain	Res	Type
1	BBB	629	GLN
1	BBB	657	GLN
1	BBB	741	LEU

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)

4 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	A	1	2,1	14,14,15	0.49	0	17,19,21	1.44	2 (11%)
2	FUC	A	2	2	10,10,11	0.89	0	14,14,16	1.95	3 (21%)
2	NAG	B	1	2,1	14,14,15	0.85	0	17,19,21	1.91	5 (29%)
2	FUC	B	2	2	10,10,11	0.81	0	14,14,16	1.56	3 (21%)

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	A	1	2,1	-	2/6/23/26	0/1/1/1
2	FUC	A	2	2	-	-	0/1/1/1
2	NAG	B	1	2,1	-	2/6/23/26	0/1/1/1
2	FUC	B	2	2	-	-	0/1/1/1

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	2	FUC	C1-C2-C3	-4.51	104.12	109.67
2	A	1	NAG	C1-C2-N2	-4.39	103.00	110.49
2	B	1	NAG	C3-C4-C5	-3.61	103.80	110.24
2	B	1	NAG	O4-C4-C5	3.52	118.05	109.30
2	B	1	NAG	O5-C5-C6	3.48	112.67	107.20
2	A	2	FUC	O5-C5-C4	-3.16	103.86	109.52
2	A	2	FUC	O2-C2-C3	3.02	116.19	110.14
2	B	1	NAG	C2-N2-C7	-2.77	118.96	122.90
2	B	2	FUC	O5-C5-C4	2.75	114.45	109.52
2	B	1	NAG	C1-O5-C5	2.60	115.72	112.19
2	B	2	FUC	O3-C3-C2	2.59	114.96	109.99
2	A	1	NAG	C4-C3-C2	2.58	114.81	111.02
2	B	2	FUC	O5-C1-C2	-2.56	106.81	110.77

There are no chirality outliers.

All (4) torsion outliers are listed below:

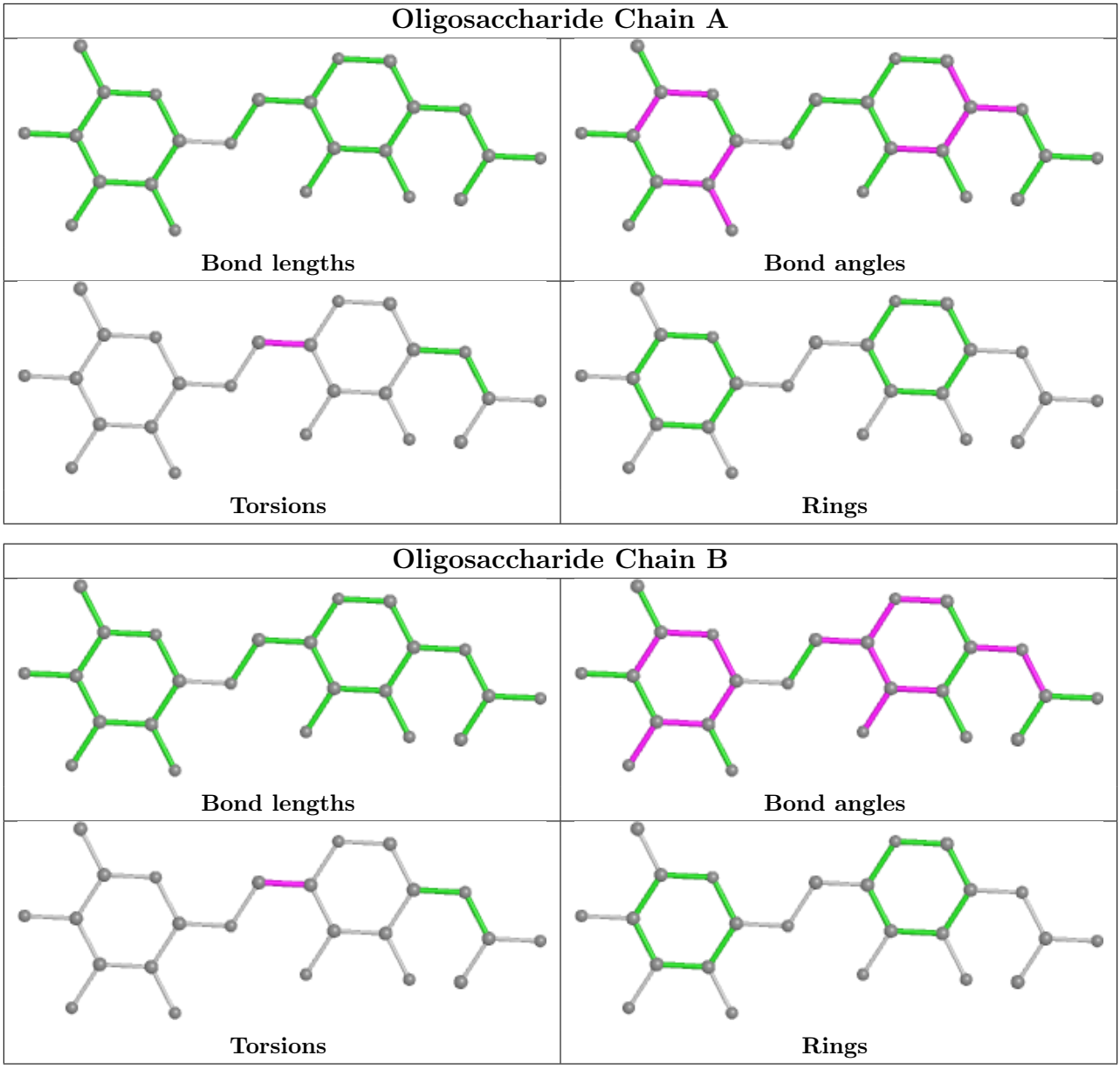
Mol	Chain	Res	Type	Atoms
2	B	1	NAG	O5-C5-C6-O6
2	B	1	NAG	C4-C5-C6-O6
2	A	1	NAG	O5-C5-C6-O6
2	A	1	NAG	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2	FUC	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.



5.6 Ligand geometry (i)

5 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	NAG	AAA	803	1	14,14,15	0.78	0	17,19,21	1.71	4 (23%)
4	EDO	AAA	804	-	3,3,3	0.18	0	2,2,2	0.34	0
4	EDO	BBB	804	-	3,3,3	0.11	0	2,2,2	0.20	0
4	EDO	BBB	803	-	3,3,3	0.17	0	2,2,2	0.15	0
4	EDO	AAA	805	-	3,3,3	0.32	0	2,2,2	0.33	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
3	NAG	AAA	803	1	-	2/6/23/26	0/1/1/1
4	EDO	AAA	804	-	-	1/1/1/1	-
4	EDO	BBB	804	-	-	1/1/1/1	-
4	EDO	BBB	803	-	-	1/1/1/1	-
4	EDO	AAA	805	-	-	1/1/1/1	-

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	AAA	803	NAG	O5-C5-C6	4.13	113.68	107.20
3	AAA	803	NAG	O7-C7-C8	-2.47	117.47	122.06
3	AAA	803	NAG	C1-O5-C5	2.18	115.15	112.19
3	AAA	803	NAG	O5-C1-C2	-2.01	108.11	111.29

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	AAA	803	NAG	C4-C5-C6-O6
3	AAA	803	NAG	O5-C5-C6-O6
4	AAA	804	EDO	O1-C1-C2-O2
4	BBB	804	EDO	O1-C1-C2-O2
4	AAA	805	EDO	O1-C1-C2-O2
4	BBB	803	EDO	O1-C1-C2-O2

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	AAA	495/528 (93%)	0.56	25 (5%) 28 26	52, 69, 99, 116	0
1	BBB	493/528 (93%)	0.84	57 (11%) 4 4	57, 79, 109, 130	0
All	All	988/1056 (93%)	0.70	82 (8%) 11 10	52, 74, 106, 130	0

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	BBB	504	PHE	5.3
1	AAA	321	LEU	5.2
1	BBB	664	PHE	4.6
1	BBB	581	LEU	3.9
1	BBB	343	ASP	3.6
1	BBB	349	ILE	3.5
1	AAA	240	LEU	3.3
1	BBB	271	LEU	3.3
1	AAA	406	LEU	3.2
1	BBB	602	TYR	3.2
1	BBB	472	TYR	3.2
1	BBB	295	LEU	3.2
1	BBB	709	LEU	3.2
1	AAA	668	LEU	3.1
1	AAA	504	PHE	3.1
1	AAA	235	PHE	3.1
1	BBB	591	VAL	3.0
1	AAA	367	TRP	3.0
1	AAA	243	ARG	3.0
1	AAA	719	ARG	3.0
1	BBB	511	LEU	3.0
1	BBB	432	LEU	2.9
1	BBB	434	SER	2.9
1	AAA	616	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	BBB	253	ILE	2.8
1	AAA	328	MET	2.8
1	BBB	348	LEU	2.8
1	BBB	692	VAL	2.8
1	BBB	379	SER	2.8
1	BBB	215	LEU	2.7
1	AAA	380	PHE	2.7
1	BBB	296	GLY	2.6
1	BBB	466	LEU	2.6
1	BBB	443	ILE	2.6
1	BBB	304	LEU	2.5
1	BBB	525	LEU	2.5
1	BBB	305	ILE	2.5
1	BBB	391	TYR	2.5
1	AAA	442	GLU	2.5
1	BBB	710	LEU	2.4
1	AAA	317	ILE	2.4
1	BBB	468	ILE	2.4
1	BBB	570	PHE	2.4
1	BBB	387	ASN	2.4
1	BBB	236	ARG	2.4
1	BBB	642	LEU	2.4
1	BBB	408	PRO	2.4
1	BBB	574	PRO	2.4
1	BBB	276	LEU	2.3
1	BBB	365	PRO	2.3
1	AAA	274	LEU	2.3
1	BBB	500	ARG	2.3
1	BBB	354	VAL	2.3
1	BBB	376	VAL	2.3
1	BBB	301	TRP	2.3
1	BBB	534	PHE	2.2
1	BBB	441	ASN	2.2
1	BBB	367	TRP	2.2
1	BBB	731	LYS	2.2
1	BBB	374	LEU	2.2
1	BBB	708	LEU	2.2
1	BBB	631	MET	2.2
1	AAA	298	LEU	2.2
1	BBB	298	LEU	2.2
1	BBB	272	VAL	2.2
1	BBB	377	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	BBB	266	LYS	2.1
1	BBB	345	ILE	2.1
1	AAA	525	LEU	2.1
1	BBB	350	TYR	2.1
1	BBB	412	TYR	2.1
1	AAA	231	LYS	2.1
1	AAA	296	GLY	2.1
1	BBB	616	ILE	2.1
1	BBB	243	ARG	2.1
1	AAA	439	HIS	2.1
1	AAA	485	LYS	2.1
1	AAA	374	LEU	2.0
1	AAA	222	PHE	2.0
1	AAA	691	LEU	2.0
1	BBB	299	VAL	2.0
1	AAA	277	LEU	2.0

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

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

6.3 Carbohydrates (i)

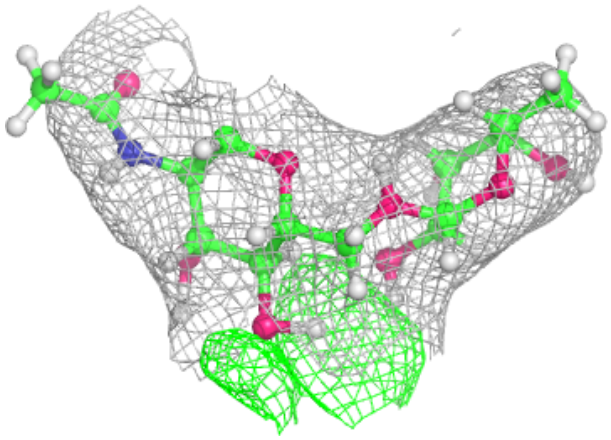
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

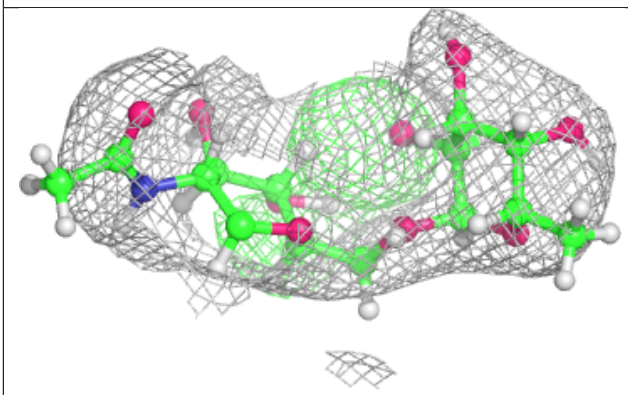
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	FUC	B	2	10/11	0.78	0.19	30,112,119,122	3
2	NAG	A	1	14/15	0.83	0.12	30,93,98,100	2
2	NAG	B	1	14/15	0.84	0.12	30,101,105,107	2
2	FUC	A	2	10/11	0.90	0.12	30,93,95,97	3

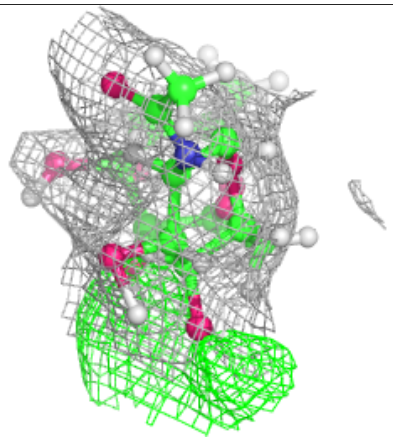
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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)

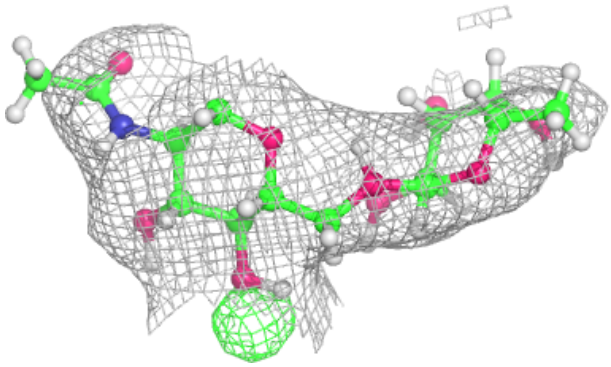


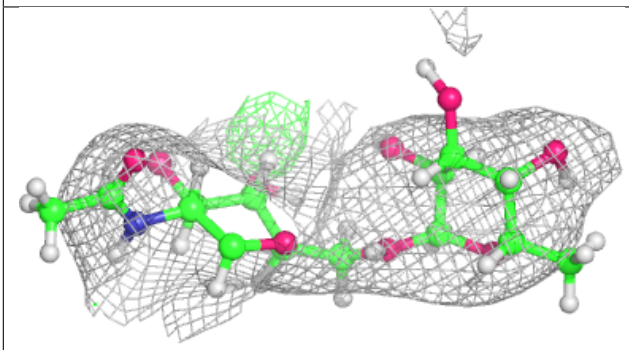


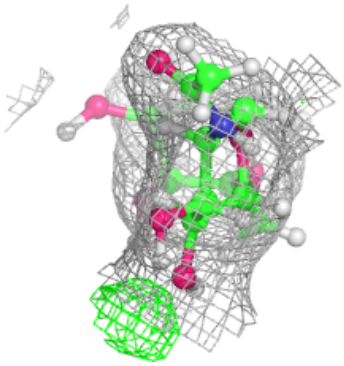


Electron density around Chain B:

$2mF_o$-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, 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
3	NAG	AAA	803	14/15	0.74	0.14	30,113,123,131	3
4	EDO	AAA	804	4/4	0.90	0.21	30,68,71,72	1
4	EDO	AAA	805	4/4	0.93	0.12	30,64,68,69	1
4	EDO	BBB	803	4/4	0.96	0.25	30,65,67,67	1
4	EDO	BBB	804	4/4	0.96	0.21	30,85,87,88	1

6.5 Other polymers (i)

There are no such residues in this entry.