Full wwPDB X-ray Structure Validation Report (i)

Sep 10, 2023 – 06:27 PM EDT

PDB ID	:	4KGJ
Title	:	Crystal structure of human alpha-L-iduronidase complex with 5-fluoro-alpha-L-idopyranosyluronic acid fluoride
Authors	:	Bie, H.; Yin, J.; He, X.; Kermode, A.R.; Goddard-Borger, E.D.; Withers, S.G.; James, M.N.G.
Deposited on	:	2013-04-29
Resolution	:	2.99 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:

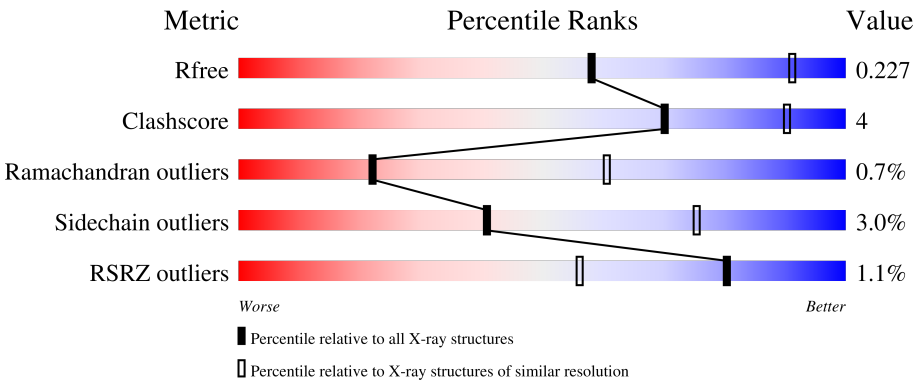
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.99 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	627	% 83% 11% • 5%
1	B	627	% 85% 11% •
2	C	2	50% 50%
2	E	2	100%
3	D	5	20% 60% 20%

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Mol	Chain	Length	Quality of chain
4	F	9	11% 89%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	C	2	-	-	-	X
5	NAG	A	901	-	-	-	X
6	GOL	A	910	-	-	X	-

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 9975 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 Alpha-L-iduronidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	595	4746	3036	854	842	14	0	2	0
1	B	607	4840	3093	874	859	14	0	3	0

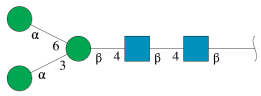
There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	33	GLN	HIS	SEE REMARK 999	UNP P35475
A	63	PRO	GLN	SEE REMARK 999	UNP P35475
A	105	GLN	ARG	SEE REMARK 999	UNP P35475
B	33	GLN	HIS	SEE REMARK 999	UNP P35475
B	63	PRO	GLN	SEE REMARK 999	UNP P35475
B	105	GLN	ARG	SEE REMARK 999	UNP P35475

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

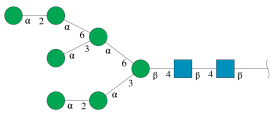
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	C	2	28	16	2	10	0	0	0
2	E	2	28	16	2	10	0	0	0

- Molecule 3 is an oligosaccharide called 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.



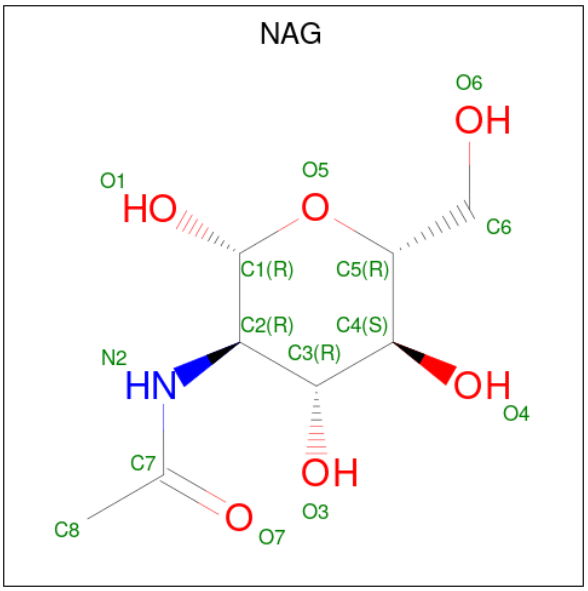
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	D	5	61	34	2	25	0	0	0

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	F	9	105	58	2	45	0	0	0

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

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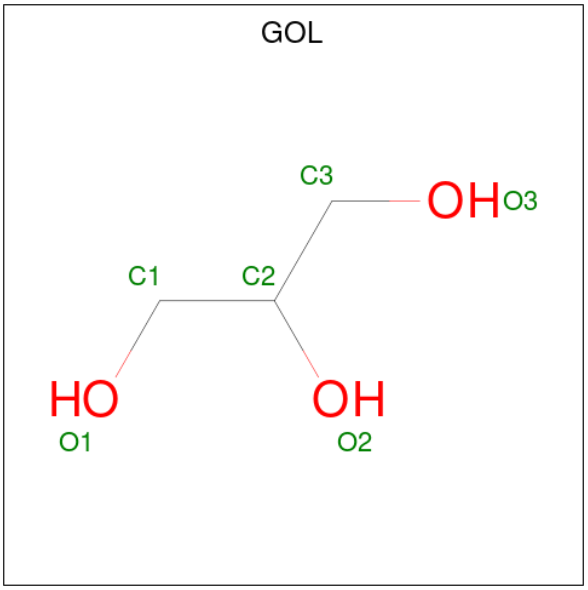
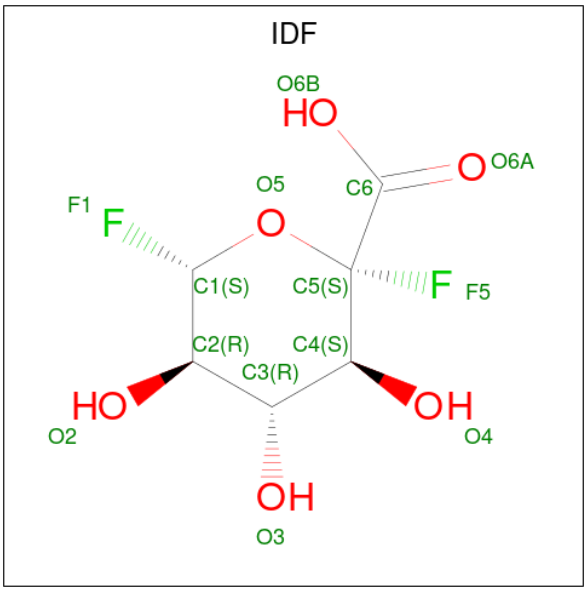
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	B	1	14	8	1	5	0	0

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



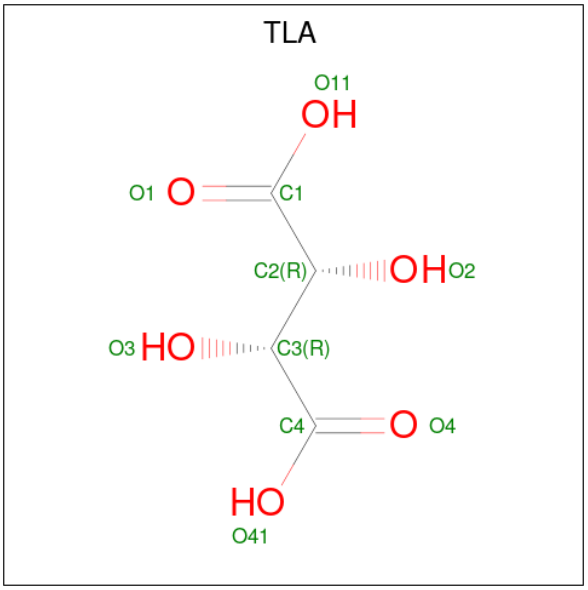
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O			
6	A	1	6	3	3		0	0
			Total	C	O			
6	A	1	6	3	3		0	0
			Total	C	O			
6	B	1	6	3	3		0	0
			Total	C	O			
6	B	1	6	3	3		0	0
			Total	C	O			
6	B	1	6	3	3		0	0
			Total	C	O			
6	B	1	6	3	3		0	0
			Total	C	O			
6	B	1	6	3	3		0	0

- Molecule 7 is 5-fluoro-alpha-L-idopyranosyluronic acid fluoride (three-letter code: IDF) (formula: $C_6H_8F_2O_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	F	O		
7	A	1	14	6	2	6	0	0
			Total	C	F	O		
7	B	1	14	6	2	6	0	0

- Molecule 8 is L(+)-TARTARIC ACID (three-letter code: TLA) (formula: $C_4H_6O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
8	B	1	10	4	6	0	0
			Total	C	O		
8	B	1	10	4	6	0	0

- Molecule 9 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
9	B	1	1	1	0	0

- Molecule 10 is water.

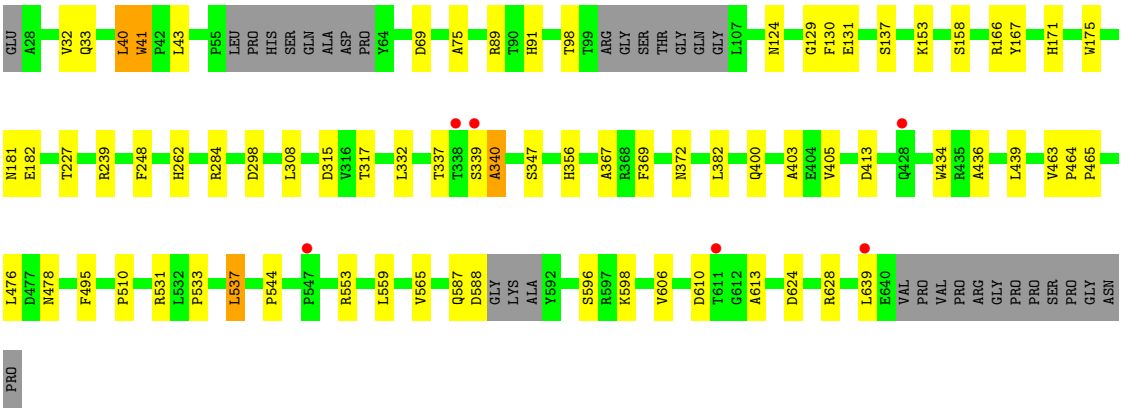
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
10	A	17	17	17	0	0
			Total	O		
10	B	31	31	31	0	0

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.

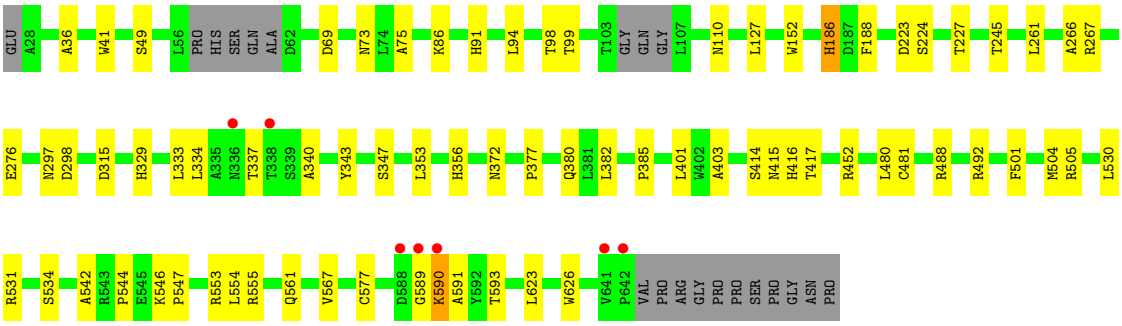
• Molecule 1: Alpha-L-iduronidase

Chain A:



• Molecule 1: Alpha-L-iduronidase

Chain B:



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

Chain C:

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

Chain E: 100%

NAG1
NAG2

• Molecule 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 D: 20% 60% 20%

NAG1
NAG2
BMA3
MAN4
MAN5

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

Chain F: 11% 89%

NAG1
NAG2
BMA3
MAN4
MAN5
MAN6
MAN7
MAN8
MAN9

4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α, β, γ	259.34Å 259.34Å 71.38Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	38.05 – 2.99 38.02 – 2.99	Depositor EDS
% Data completeness (in resolution range)	99.7 (38.05-2.99) 99.7 (38.02-2.99)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.19	Depositor
$< I/\sigma(I) >$ [1]	3.64 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.178 , 0.227 0.177 , 0.227	Depositor DCC
R_{free} test set	1803 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	43.0	Xtriage
Anisotropy	0.831	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 40.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.022 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	9975	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.10% 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: TLA, NAG, CL, BMA, MAN, GOL, IDF

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.33	0/4891	0.53	0/6682
1	B	0.33	0/4988	0.54	0/6815
All	All	0.33	0/9879	0.54	0/13497

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	A	4746	0	4640	38	0
1	B	4840	0	4740	33	0
2	C	28	0	25	0	0
2	E	28	0	25	0	0
3	D	61	0	52	1	0
4	F	105	0	88	0	0
5	A	14	0	13	0	0
5	B	14	0	13	0	0
6	A	12	0	16	4	0
6	B	30	0	40	4	0
7	A	14	0	7	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B	14	0	7	0	0
8	B	20	0	8	1	0
9	B	1	0	0	0	0
10	A	17	0	0	0	0
10	B	31	0	0	0	0
All	All	9975	0	9674	71	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 (71) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:315:ASP:HB2	1:A:478:ASN:OD1	1.82	0.78
1:A:284:ARG:HH12	1:A:339:SER:HB2	1.53	0.72
1:B:333:LEU:O	1:B:337:THR:HG21	1.97	0.65
1:B:501:PHE:HA	1:B:504:MET:HE3	1.80	0.64
1:A:356:HIS:HB2	6:A:910:GOL:H2	1.79	0.62
1:B:334:LEU:HD21	1:B:343:TYR:HB3	1.82	0.61
1:B:356:HIS:HB2	6:B:913:GOL:H31	1.82	0.61
1:A:298:ASP:HA	1:A:347:SER:HB3	1.82	0.60
1:B:266:ALA:O	1:B:267:ARG:HB2	1.99	0.60
1:A:131:GLU:OE2	1:A:181:ASN:HB2	2.03	0.59
1:B:590:LYS:HG3	1:B:591:ALA:H	1.67	0.59
1:A:369:PHE:HE2	1:A:382:LEU:HD12	1.71	0.55
1:B:98:THR:OG1	1:B:110:ASN:HB3	2.06	0.55
1:A:369:PHE:HD1	6:A:910:GOL:H11	1.72	0.55
1:A:369:PHE:CD1	6:A:910:GOL:H11	2.42	0.54
1:A:171:HIS:CD2	1:A:175:TRP:HE1	2.26	0.54
1:B:86:LYS:HE2	1:B:127:LEU:HD11	1.90	0.53
1:A:284:ARG:NH1	1:A:339:SER:HB2	2.23	0.52
1:B:73:ASN:HB2	1:B:353:LEU:HD21	1.91	0.52
1:B:94:LEU:HD12	1:B:152:TRP:CH2	2.45	0.52
1:A:559:LEU:HD11	1:A:565:VAL:HG23	1.93	0.50
1:A:75:ALA:HA	1:A:124:ASN:OD1	2.12	0.49
1:A:434:TRP:CZ3	1:A:463:VAL:HG13	2.48	0.48
1:A:544:PRO:HD2	1:A:628:ARG:HH22	1.79	0.48
1:B:372:ASN:HA	1:B:377:PRO:HB3	1.96	0.48
1:B:542:ALA:O	1:B:544:PRO:HD3	2.13	0.48
1:A:40:LEU:HD13	1:A:41:TRP:CZ2	2.49	0.47
1:A:43:LEU:HB2	1:A:400:GLN:HB2	1.94	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:276:GLU:OE1	1:B:329:HIS:NE2	2.48	0.47
1:A:339:SER:O	1:A:340:ALA:C	2.53	0.47
1:A:332:LEU:HD21	1:A:413:ASP:HB2	1.97	0.47
1:A:367:ALA:HB3	1:A:382:LEU:HB2	1.96	0.47
1:A:434:TRP:CH2	1:A:436:ALA:HB2	2.50	0.47
1:B:452:ARG:O	1:B:531:ARG:NH1	2.48	0.47
1:B:382:LEU:HD21	1:B:504:MET:HB3	1.97	0.46
1:A:369:PHE:CE2	1:A:382:LEU:HD12	2.50	0.46
1:A:495:PHE:CE1	3:D:1:NAG:H82	2.50	0.46
1:A:624:ASP:OD2	1:A:628:ARG:HB2	2.15	0.46
1:A:317:THR:HA	1:A:533:PRO:HG3	1.98	0.46
1:A:587:GLN:HE22	1:A:613:ALA:HB1	1.81	0.45
1:B:553:ARG:O	1:B:555:ARG:NH1	2.49	0.45
1:A:182:GLU:OE2	1:A:262:HIS:HD2	2.00	0.45
1:B:403:ALA:H	6:B:914:GOL:H32	1.83	0.44
1:A:153:LYS:HD2	1:A:248:PHE:CE2	2.52	0.44
1:B:75:ALA:HB2	6:B:917:GOL:H32	1.99	0.44
1:A:369:PHE:HA	6:A:910:GOL:H32	1.98	0.44
1:B:186:HIS:HB3	1:B:188:PHE:CD2	2.52	0.44
1:A:565:VAL:HG22	1:A:606:VAL:HG22	1.99	0.44
1:A:166:ARG:HD3	1:A:167:TYR:CZ	2.53	0.43
1:A:89:ARG:HA	1:A:129:GLY:HA3	2.00	0.43
1:B:36:ALA:HA	1:B:401:LEU:HD22	2.01	0.43
1:B:223:ASP:OD1	1:B:224:SER:N	2.52	0.42
1:B:315:ASP:HA	1:B:385:PRO:HG2	2.00	0.42
1:B:298:ASP:HA	1:B:347:SER:HB3	2.00	0.42
1:A:98:THR:HG22	1:A:137:SER:OG	2.20	0.42
1:B:49:SER:HB3	1:B:347:SER:HB2	2.01	0.42
1:B:86:LYS:HE3	8:B:919:TLA:H2	1.99	0.42
1:A:464:PRO:HA	1:A:465:PRO:HD3	1.95	0.42
1:B:577[A]:CYS:SG	1:B:626:TRP:HZ3	2.43	0.42
1:B:414:SER:C	1:B:416:HIS:H	2.22	0.42
1:B:261:LEU:O	1:B:297:ASN:HA	2.18	0.42
1:A:372:ASN:HB2	1:A:495:PHE:CZ	2.55	0.41
1:B:380:GLN:OE1	1:B:505:ARG:NH2	2.51	0.41
1:A:439:LEU:HB2	1:A:537:LEU:HD12	2.03	0.41
1:B:488:ARG:HA	1:B:492:ARG:HG3	2.02	0.41
1:B:530:LEU:HB3	1:B:534:SER:OG	2.20	0.41
1:A:33:GLN:O	1:A:403:ALA:HA	2.21	0.41
1:B:546:LYS:HB3	1:B:547:PRO:HD2	2.02	0.41
1:A:476:LEU:HG	1:A:510:PRO:HB3	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:555:ARG:NH2	6:B:917:GOL:O2	2.54	0.40
1:A:32:VAL:HG22	1:A:405:VAL:HG22	2.03	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	A	589/627 (94%)	546 (93%)	40 (7%)	3 (0%)	29	68
1	B	604/627 (96%)	570 (94%)	29 (5%)	5 (1%)	19	57
All	All	1193/1254 (95%)	1116 (94%)	69 (6%)	8 (1%)	22	60

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	340	ALA
1	B	186	HIS
1	B	340	ALA
1	B	589	GLY
1	A	40	LEU
1	B	590	LYS
1	A	337	THR
1	B	415	ASN

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	505/527 (96%)	489 (97%)	16 (3%)	39	74
1	B	515/527 (98%)	501 (97%)	14 (3%)	44	77
All	All	1020/1054 (97%)	990 (97%)	30 (3%)	41	76

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	TRP
1	A	69	ASP
1	A	91	HIS
1	A	130	PHE
1	A	158	SER
1	A	227	THR
1	A	239	ARG
1	A	308	LEU
1	A	531	ARG
1	A	537	LEU
1	A	553	ARG
1	A	588	ASP
1	A	596	SER
1	A	598	LYS
1	A	610	ASP
1	A	639	LEU
1	B	41	TRP
1	B	69	ASP
1	B	91	HIS
1	B	99	THR
1	B	227	THR
1	B	245	THR
1	B	417	THR
1	B	480	LEU
1	B	481	CYS
1	B	554	LEU
1	B	561	GLN
1	B	567	VAL
1	B	593	THR
1	B	623	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	GLN
1	A	125	GLN
1	A	171	HIS
1	A	281	GLN
1	A	587	GLN
1	A	603	ASN
1	B	147	GLN

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)

18 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	C	1	2,1	14,14,15	0.54	0	17,19,21	1.30	2 (11%)
2	NAG	C	2	2	14,14,15	0.60	0	17,19,21	0.78	0
3	NAG	D	1	3,1	14,14,15	0.56	0	17,19,21	1.28	2 (11%)
3	NAG	D	2	3	14,14,15	0.57	0	17,19,21	1.11	1 (5%)
3	BMA	D	3	3	11,11,12	0.41	0	15,15,17	0.85	0
3	MAN	D	4	3	11,11,12	0.60	0	15,15,17	0.95	1 (6%)
3	MAN	D	5	3	11,11,12	0.55	0	15,15,17	1.45	2 (13%)
2	NAG	E	1	2,1	14,14,15	0.59	0	17,19,21	1.06	1 (5%)
2	NAG	E	2	2	14,14,15	0.52	0	17,19,21	1.25	2 (11%)
4	NAG	F	1	4,1	14,14,15	0.60	0	17,19,21	1.10	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	NAG	F	2	4	14,14,15	0.61	0	17,19,21	1.00	1 (5%)
4	BMA	F	3	4	11,11,12	0.58	0	15,15,17	1.14	1 (6%)
4	MAN	F	4	4	11,11,12	0.60	0	15,15,17	0.97	1 (6%)
4	MAN	F	5	4	11,11,12	0.57	0	15,15,17	0.85	1 (6%)
4	MAN	F	6	4	11,11,12	0.61	0	15,15,17	0.79	0
4	MAN	F	7	4	11,11,12	0.55	0	15,15,17	1.32	1 (6%)
4	MAN	F	8	4	11,11,12	0.54	0	15,15,17	0.90	1 (6%)
4	MAN	F	9	4	11,11,12	0.65	0	15,15,17	1.08	1 (6%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	C	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	2/6/23/26	0/1/1/1
3	NAG	D	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	D	2	3	-	1/6/23/26	0/1/1/1
3	BMA	D	3	3	-	2/2/19/22	0/1/1/1
3	MAN	D	4	3	-	0/2/19/22	0/1/1/1
3	MAN	D	5	3	-	2/2/19/22	0/1/1/1
2	NAG	E	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	E	2	2	-	0/6/23/26	0/1/1/1
4	NAG	F	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	F	2	4	-	1/6/23/26	0/1/1/1
4	BMA	F	3	4	-	0/2/19/22	0/1/1/1
4	MAN	F	4	4	-	2/2/19/22	0/1/1/1
4	MAN	F	5	4	-	0/2/19/22	0/1/1/1
4	MAN	F	6	4	-	0/2/19/22	0/1/1/1
4	MAN	F	7	4	-	2/2/19/22	0/1/1/1
4	MAN	F	8	4	-	2/2/19/22	0/1/1/1
4	MAN	F	9	4	-	2/2/19/22	0/1/1/1

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	5	MAN	C1-O5-C5	4.32	118.05	112.19
4	F	7	MAN	C1-O5-C5	4.03	117.66	112.19
2	C	1	NAG	C1-O5-C5	3.60	117.06	112.19
4	F	3	BMA	C1-C2-C3	3.32	113.74	109.67
3	D	1	NAG	C4-C3-C2	2.97	115.36	111.02
2	E	2	NAG	C2-N2-C7	2.88	127.01	122.90
4	F	4	MAN	C1-O5-C5	2.84	116.03	112.19
2	E	1	NAG	O5-C5-C6	2.84	111.65	107.20
4	F	2	NAG	C1-O5-C5	2.77	115.94	112.19
4	F	5	MAN	C1-O5-C5	2.66	115.80	112.19
3	D	2	NAG	C1-O5-C5	2.66	115.80	112.19
4	F	9	MAN	C1-C2-C3	2.57	112.83	109.67
4	F	1	NAG	O5-C1-C2	-2.36	107.56	111.29
3	D	5	MAN	O5-C5-C6	2.35	110.88	107.20
3	D	1	NAG	O5-C1-C2	-2.27	107.71	111.29
4	F	8	MAN	C1-O5-C5	2.26	115.25	112.19
2	C	1	NAG	O5-C1-C2	-2.23	107.77	111.29
3	D	4	MAN	C1-O5-C5	2.23	115.21	112.19
2	E	2	NAG	O5-C5-C6	2.00	110.34	107.20

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	F	9	MAN	O5-C5-C6-O6
4	F	7	MAN	C4-C5-C6-O6
4	F	7	MAN	O5-C5-C6-O6
2	C	2	NAG	C4-C5-C6-O6
4	F	8	MAN	C4-C5-C6-O6
2	E	1	NAG	O5-C5-C6-O6
3	D	3	BMA	O5-C5-C6-O6
3	D	5	MAN	O5-C5-C6-O6
2	E	1	NAG	C4-C5-C6-O6
3	D	3	BMA	C4-C5-C6-O6
3	D	5	MAN	C4-C5-C6-O6
2	C	2	NAG	O5-C5-C6-O6
4	F	8	MAN	O5-C5-C6-O6
4	F	4	MAN	C4-C5-C6-O6
4	F	9	MAN	C4-C5-C6-O6
3	D	2	NAG	O5-C5-C6-O6
4	F	4	MAN	O5-C5-C6-O6
4	F	2	NAG	C4-C5-C6-O6

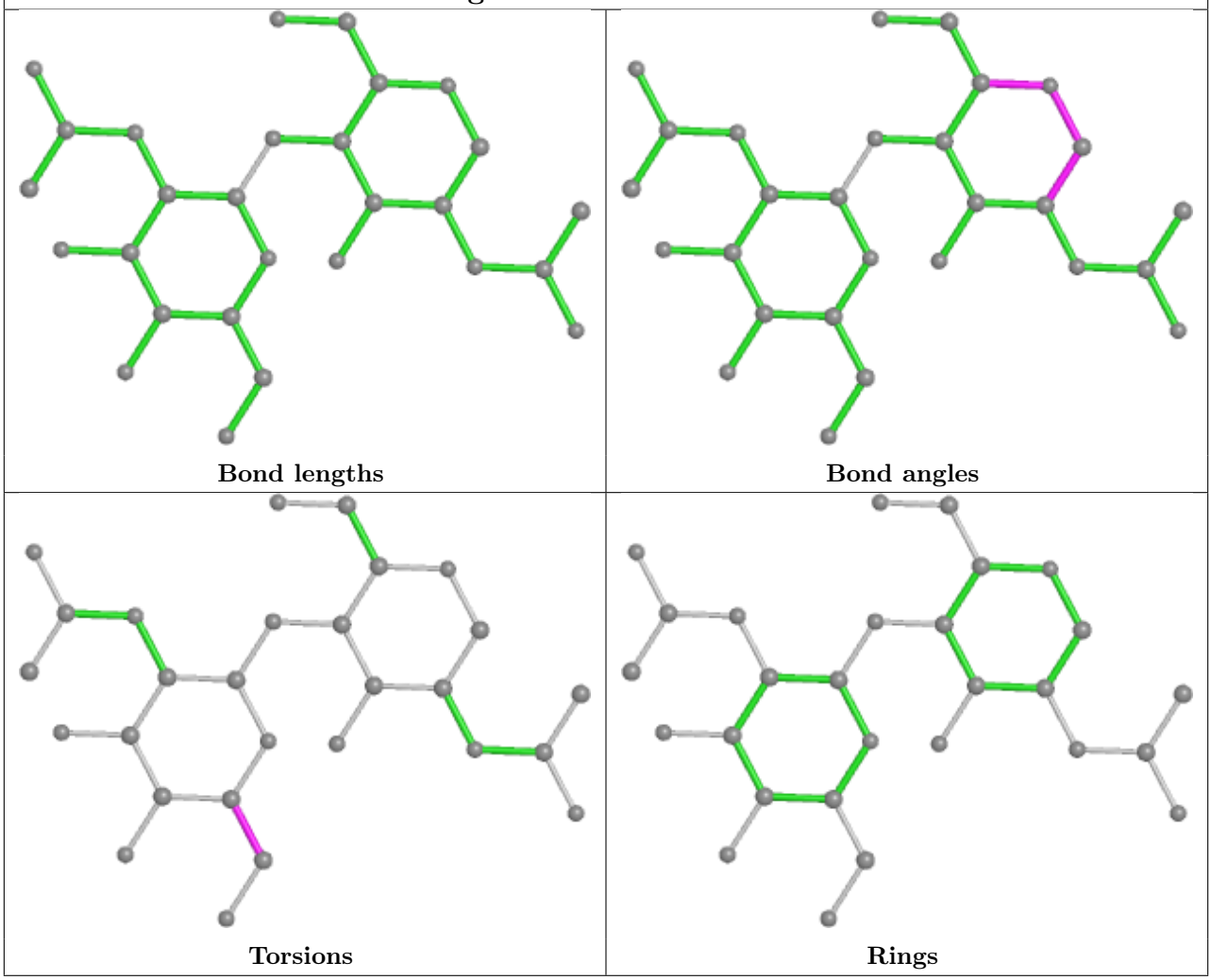
There are no ring outliers.

1 monomer is involved in 1 short contact:

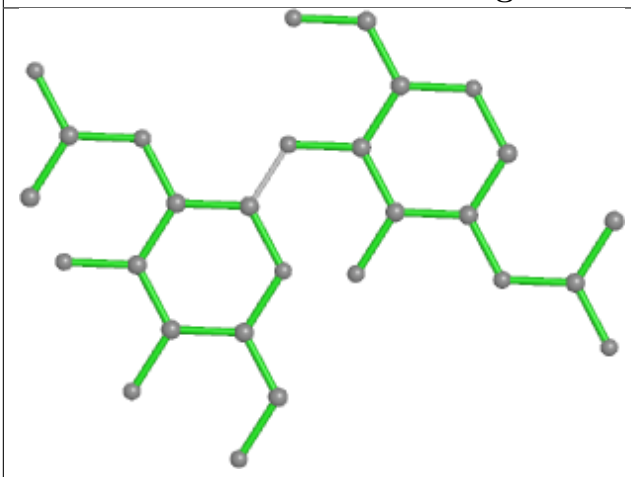
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	1	NAG	1	0

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

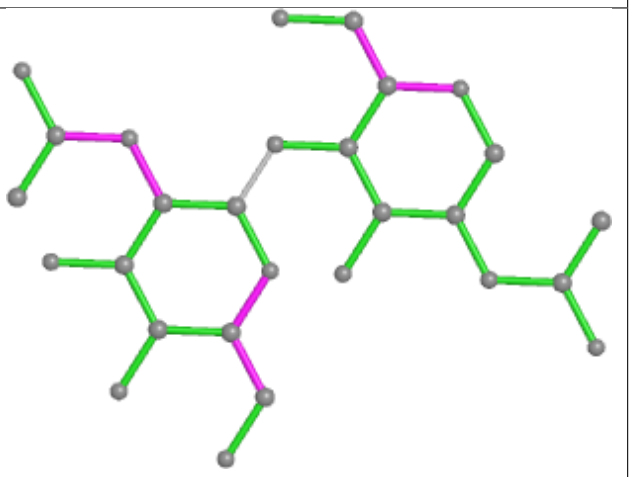
Oligosaccharide Chain C



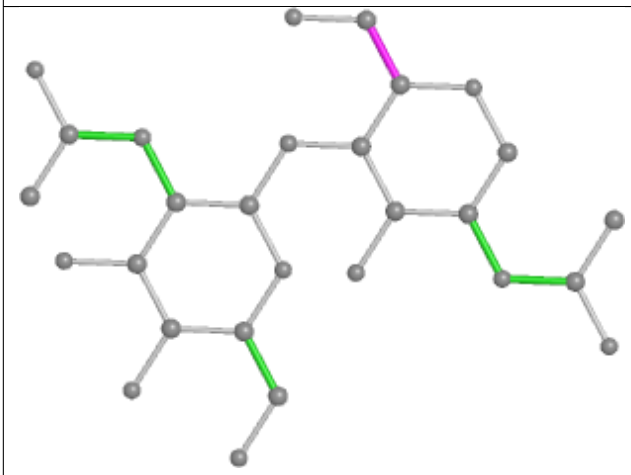
Oligosaccharide Chain E



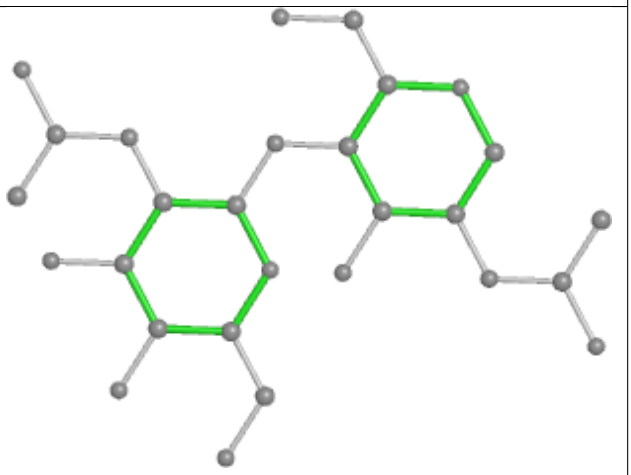
Bond lengths



Bond angles

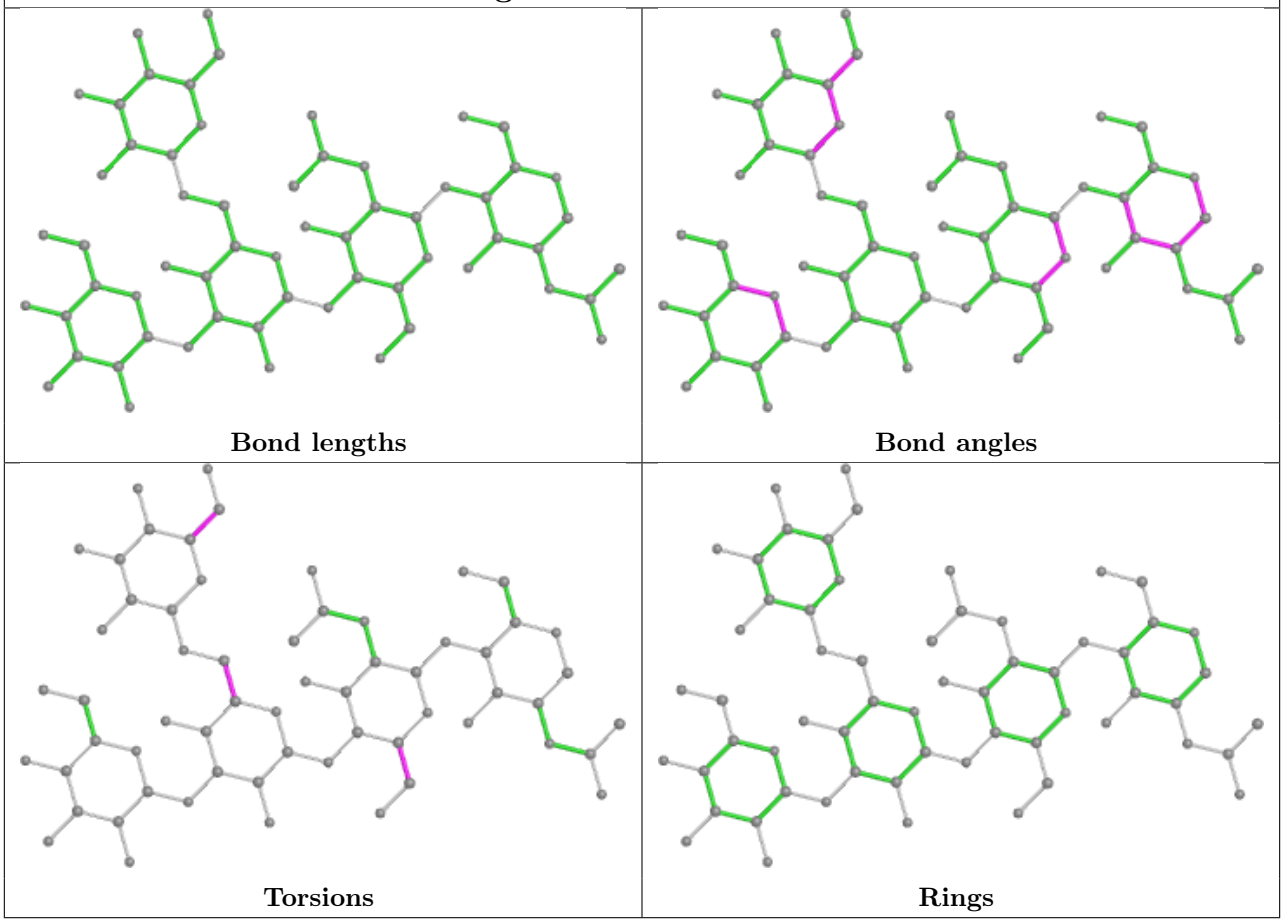


Torsions

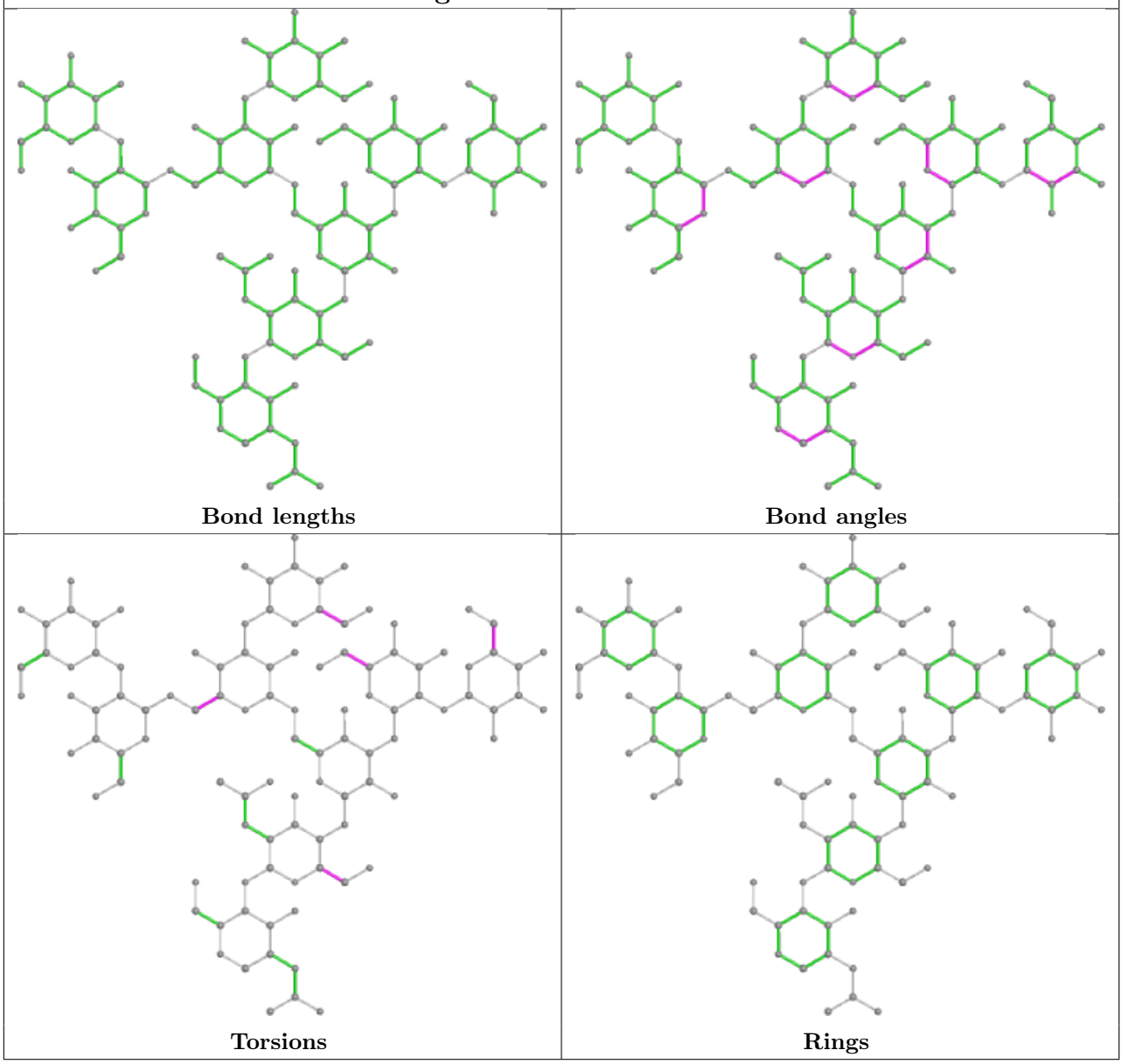


Rings

Oligosaccharide Chain D



Oligosaccharide Chain F



5.6 Ligand geometry (i)

Of 14 ligands modelled in this entry, 1 is monoatomic - leaving 13 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	$\#\|Z\| > 2$
5	NAG	A	901	1	14,14,15	0.49	0	17,19,21	1.20	2 (11%)
5	NAG	B	901	1	14,14,15	0.49	0	17,19,21	1.16	3 (17%)
7	IDF	B	920	-	10,14,14	2.61	4 (40%)	12,22,22	1.38	3 (25%)
6	GOL	A	909	-	5,5,5	0.21	0	5,5,5	0.39	0
6	GOL	B	915	-	5,5,5	0.22	0	5,5,5	0.41	0
6	GOL	B	917	-	5,5,5	0.28	0	5,5,5	0.42	0
8	TLA	B	918	-	9,9,9	1.14	0	12,12,12	0.93	1 (8%)
6	GOL	B	916	-	5,5,5	0.27	0	5,5,5	0.35	0
6	GOL	B	914	-	5,5,5	0.25	0	5,5,5	0.32	0
6	GOL	B	913	-	5,5,5	0.34	0	5,5,5	0.27	0
8	TLA	B	919	-	9,9,9	1.14	0	12,12,12	1.12	2 (16%)
7	IDF	A	911	-	10,14,14	2.49	4 (40%)	12,22,22	1.43	2 (16%)
6	GOL	A	910	-	5,5,5	0.32	0	5,5,5	0.39	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	NAG	A	901	1	-	1/6/23/26	0/1/1/1
5	NAG	B	901	1	-	2/6/23/26	0/1/1/1
7	IDF	B	920	-	-	0/1/29/29	0/1/1/1
6	GOL	A	909	-	-	2/4/4/4	-
6	GOL	B	915	-	-	2/4/4/4	-
6	GOL	B	917	-	-	0/4/4/4	-
8	TLA	B	918	-	-	0/12/12/12	-
6	GOL	B	916	-	-	2/4/4/4	-
6	GOL	B	914	-	-	2/4/4/4	-
6	GOL	B	913	-	-	4/4/4/4	-
8	TLA	B	919	-	-	2/12/12/12	-
7	IDF	A	911	-	-	0/1/29/29	0/1/1/1
6	GOL	A	910	-	-	2/4/4/4	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	920	IDF	C2-C1	5.39	1.55	1.52
7	A	911	IDF	C2-C1	5.15	1.55	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	920	IDF	O6B-C6	-3.31	1.17	1.30
7	A	911	IDF	O6B-C6	-3.28	1.18	1.30
7	A	911	IDF	O6A-C6	3.22	1.32	1.22
7	B	920	IDF	O6A-C6	3.19	1.32	1.22
7	B	920	IDF	O5-C1	2.85	1.43	1.39
7	A	911	IDF	O5-C1	2.36	1.43	1.39

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	901	NAG	C1-O5-C5	3.18	116.50	112.19
5	A	901	NAG	O5-C5-C6	2.64	111.34	107.20
5	B	901	NAG	C3-C4-C5	-2.61	105.58	110.24
7	A	911	IDF	C2-C3-C4	2.60	114.88	111.30
5	B	901	NAG	C1-O5-C5	2.47	115.54	112.19
7	B	920	IDF	C3-C2-C1	2.26	115.31	110.68
7	A	911	IDF	C3-C2-C1	2.25	115.29	110.68
8	B	919	TLA	O11-C1-C2	2.24	119.33	113.27
7	B	920	IDF	C2-C3-C4	2.15	114.26	111.30
8	B	918	TLA	O41-C4-C3	2.12	119.01	113.27
7	B	920	IDF	O4-C4-C3	-2.06	105.47	110.03
5	B	901	NAG	O5-C5-C6	2.03	110.39	107.20
8	B	919	TLA	O41-C4-C3	2.00	118.68	113.27

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	913	GOL	C1-C2-C3-O3
6	B	915	GOL	O1-C1-C2-C3
6	B	916	GOL	O1-C1-C2-C3
8	B	919	TLA	O1-C1-C2-O2
8	B	919	TLA	O11-C1-C2-O2
6	A	909	GOL	O1-C1-C2-O2
6	A	909	GOL	O1-C1-C2-C3
6	A	910	GOL	O1-C1-C2-C3
6	B	913	GOL	O1-C1-C2-C3
6	B	914	GOL	C1-C2-C3-O3
6	B	913	GOL	O2-C2-C3-O3
6	B	915	GOL	O1-C1-C2-O2
6	B	914	GOL	O2-C2-C3-O3
6	B	916	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
5	B	901	NAG	C4-C5-C6-O6
5	A	901	NAG	O5-C5-C6-O6
5	B	901	NAG	O5-C5-C6-O6
6	A	910	GOL	O1-C1-C2-O2
6	B	913	GOL	O1-C1-C2-O2

There are no ring outliers.

5 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	917	GOL	2	0
6	B	914	GOL	1	0
6	B	913	GOL	1	0
8	B	919	TLA	1	0
6	A	910	GOL	4	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	595/627 (94%)	-0.20	6 (1%)	82	59	25, 39, 65, 101	0
1	B	607/627 (96%)	-0.26	7 (1%)	79	54	22, 33, 59, 92	0
All	All	1202/1254 (95%)	-0.23	13 (1%)	80	56	22, 36, 64, 101	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	338	THR	5.4
1	B	589	GLY	4.8
1	A	338	THR	4.4
1	A	339	SER	4.0
1	B	336	ASN	2.9
1	B	588	ASP	2.8
1	B	590	LYS	2.8
1	A	428	GLN	2.5
1	A	611	THR	2.3
1	A	639	LEU	2.2
1	B	641	VAL	2.1
1	B	642	PRO	2.1
1	A	547	PRO	2.1

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

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

6.3 Carbohydrates (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

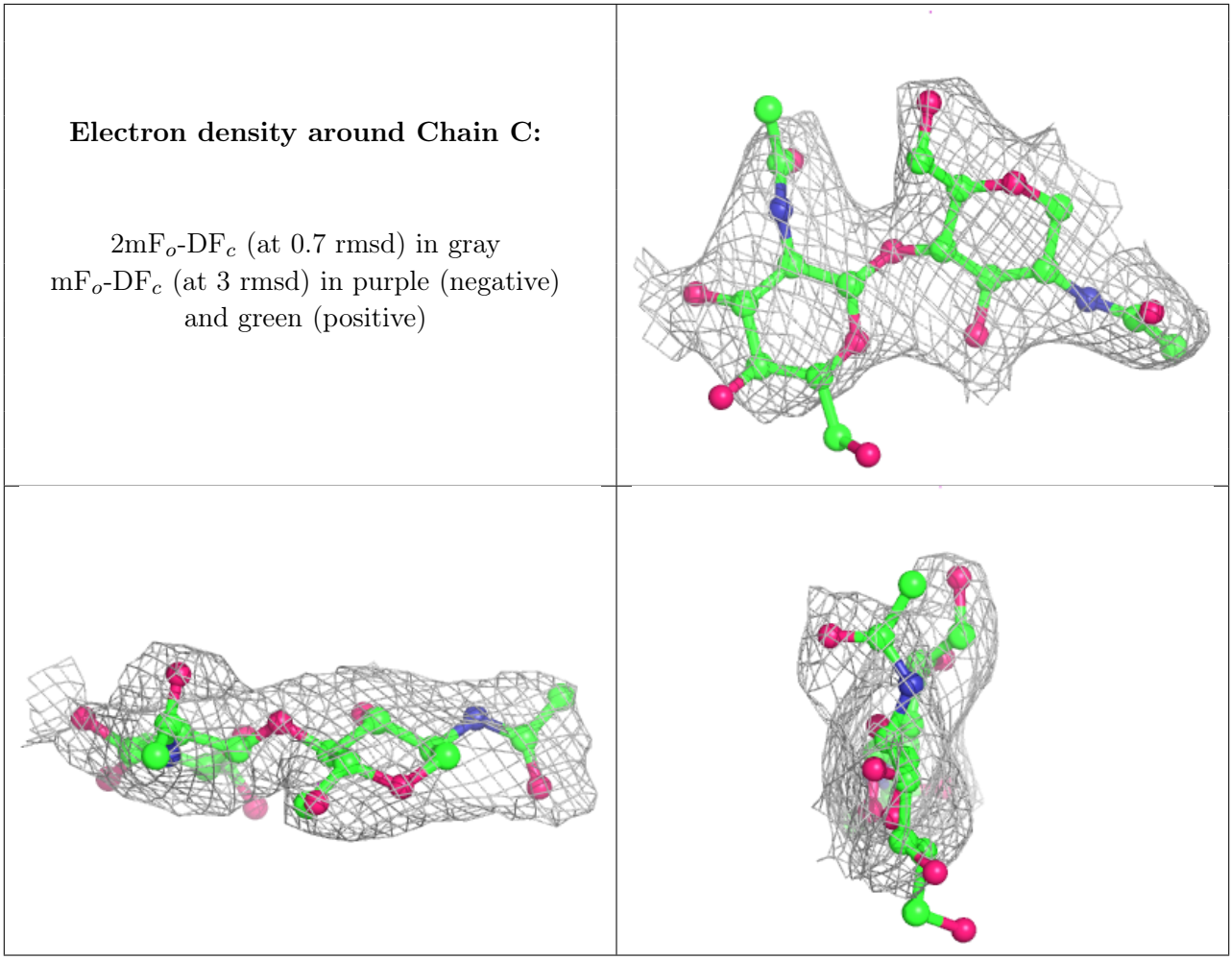
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	MAN	F	7	11/12	0.66	0.39	75,85,88,92	0
4	MAN	F	5	11/12	0.69	0.29	87,100,104,110	0
2	NAG	C	2	14/15	0.76	0.40	75,81,91,93	0
3	MAN	D	4	11/12	0.76	0.40	80,86,88,90	0
4	MAN	F	6	11/12	0.79	0.28	103,110,110,111	0
4	MAN	F	9	11/12	0.87	0.22	71,73,74,74	0
3	MAN	D	5	11/12	0.89	0.28	66,69,71,71	0
2	NAG	E	2	14/15	0.90	0.36	64,66,70,74	0
4	MAN	F	4	11/12	0.91	0.16	69,76,84,94	0
2	NAG	C	1	14/15	0.93	0.20	46,49,55,66	0
4	MAN	F	8	11/12	0.93	0.21	62,64,66,69	0
2	NAG	E	1	14/15	0.93	0.21	43,48,57,61	0
4	BMA	F	3	11/12	0.94	0.15	43,49,56,60	0
3	BMA	D	3	11/12	0.95	0.18	57,60,66,73	0
3	NAG	D	2	14/15	0.95	0.17	46,48,52,53	0
3	NAG	D	1	14/15	0.96	0.21	42,43,47,47	0
4	NAG	F	2	14/15	0.97	0.14	29,32,34,39	0
4	NAG	F	1	14/15	0.97	0.13	29,30,33,34	0

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

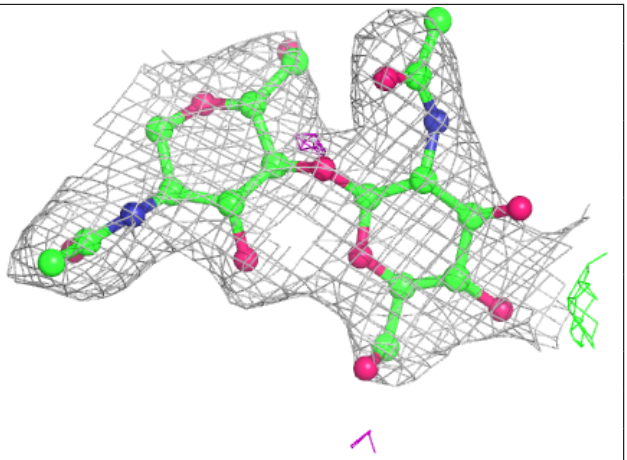
Electron density around Chain C:

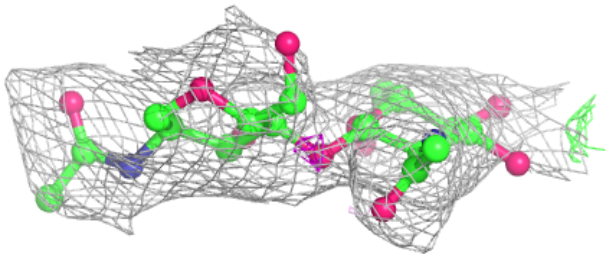
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

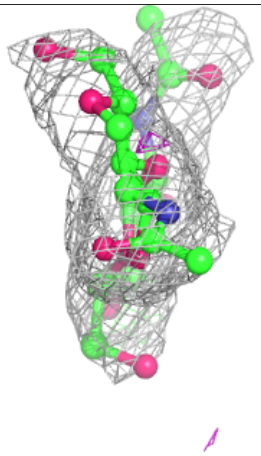


Electron density around Chain E:

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

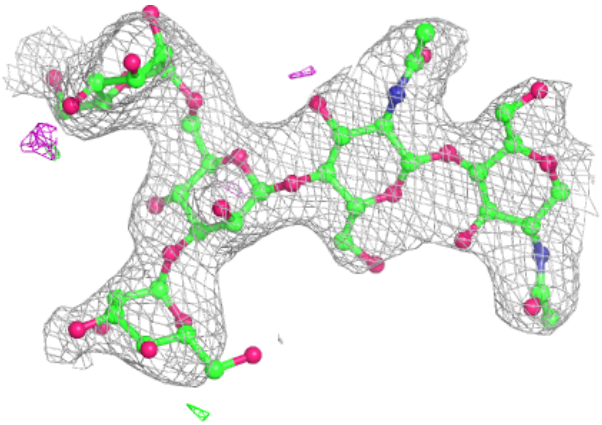


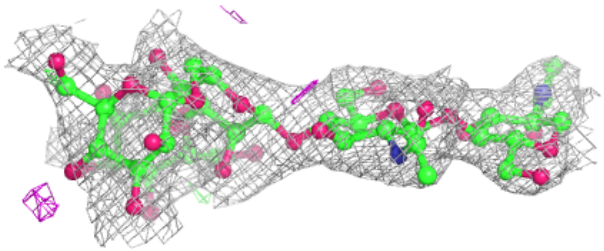


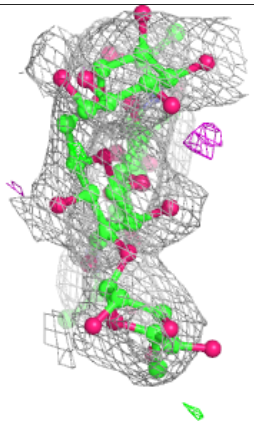


Electron density around Chain D:

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

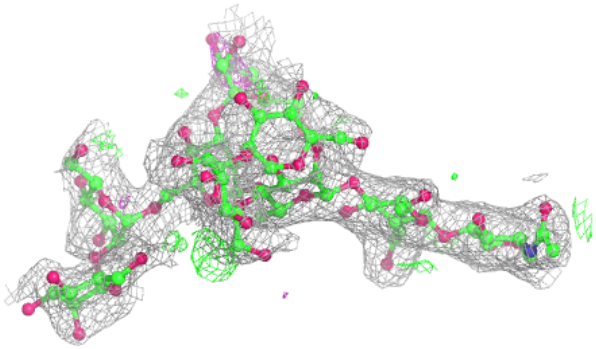


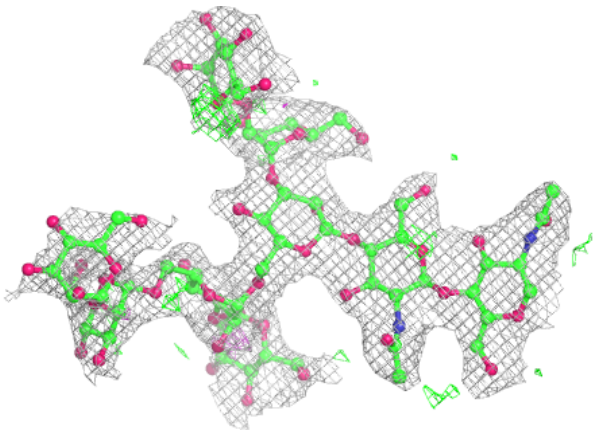


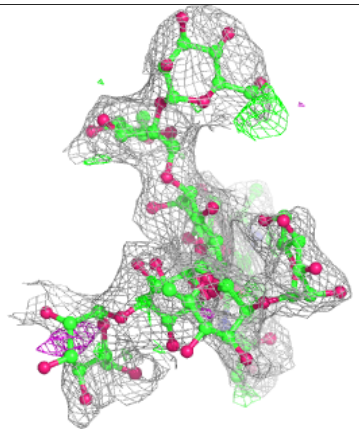


Electron density around Chain F:

$2mF_o$-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
5	NAG	A	901	14/15	0.78	0.41	67,72,76,77	0
8	TLA	B	919	10/10	0.86	0.22	72,75,82,83	0
7	IDF	A	911	14/14	0.88	0.20	55,58,60,61	0
6	GOL	A	909	6/6	0.92	0.26	50,53,55,55	0
6	GOL	B	913	6/6	0.92	0.23	51,54,54,55	0
6	GOL	B	917	6/6	0.93	0.24	33,37,38,40	0
6	GOL	B	915	6/6	0.93	0.17	48,48,48,48	0
6	GOL	B	916	6/6	0.93	0.25	51,53,54,55	0
6	GOL	B	914	6/6	0.94	0.20	41,43,43,44	0
7	IDF	B	920	14/14	0.94	0.15	49,51,53,54	0
8	TLA	B	918	10/10	0.94	0.20	48,50,52,53	0
5	NAG	B	901	14/15	0.94	0.27	40,42,47,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	GOL	A	910	6/6	0.95	0.16	45,48,49,51	0
9	CL	B	921	1/1	0.96	0.13	33,33,33,33	0

6.5 Other polymers (i)

There are no such residues in this entry.