Full wwPDB X-ray Structure Validation Report (i)

Jun 22, 2024 – 09:06 PM EDT

PDB ID	:	4XL1
Title	:	Complex of Notch1 (EGF11-13) bound to Delta-like 4 (N-EGF1)
Authors	:	Luca, V.C.; Jude, K.M.; Garcia, K.C.
Deposited on	:	2015-01-13
Resolution	:	2.30 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:

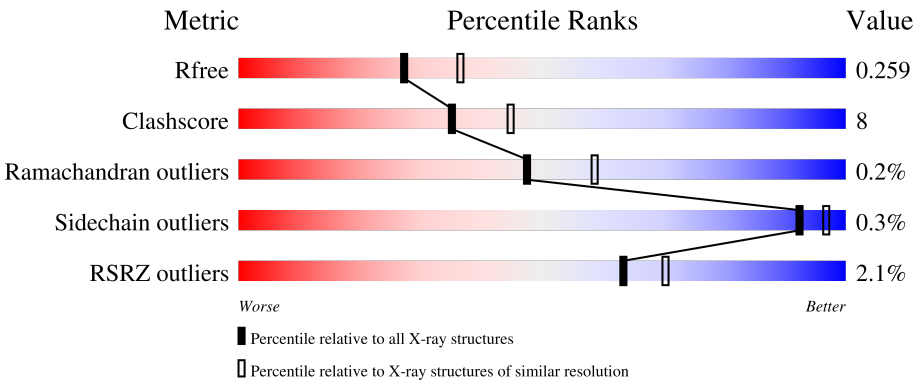
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	118	.% 85% 13% •
1	D	118	3% 89% 10% •
2	B	230	3% 81% 17% •
2	E	230	.% 83% 17%
3	C	2	100%

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Mol	Chain	Length	Quality of chain
3	F	2	100%

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
3	NAG	C	2	-	-	-	X

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 5865 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 Neurogenic locus notch homolog protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	115	860	517	147	177	19	0	1	0
1	D	117	885	533	148	185	19	0	3	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	411	PRO	-	expression tag	UNP Q07008
A	527	SER	-	expression tag	UNP Q07008
A	528	GLY	-	expression tag	UNP Q07008
D	411	PRO	-	expression tag	UNP Q07008
D	527	SER	-	expression tag	UNP Q07008
D	528	GLY	-	expression tag	UNP Q07008

- Molecule 2 is a protein called Delta-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	227	1794	1116	321	340	17	0	1	0
2	E	229	1797	1117	322	341	17	0	0	0

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	25	GLY	-	expression tag	UNP D3ZHH1
B	26	SER	-	expression tag	UNP D3ZHH1
B	28	SER	GLY	engineered mutation	UNP D3ZHH1
B	107	LEU	PHE	engineered mutation	UNP D3ZHH1
B	206	PRO	LEU	engineered mutation	UNP D3ZHH1
B	253	ALA	-	expression tag	UNP D3ZHH1

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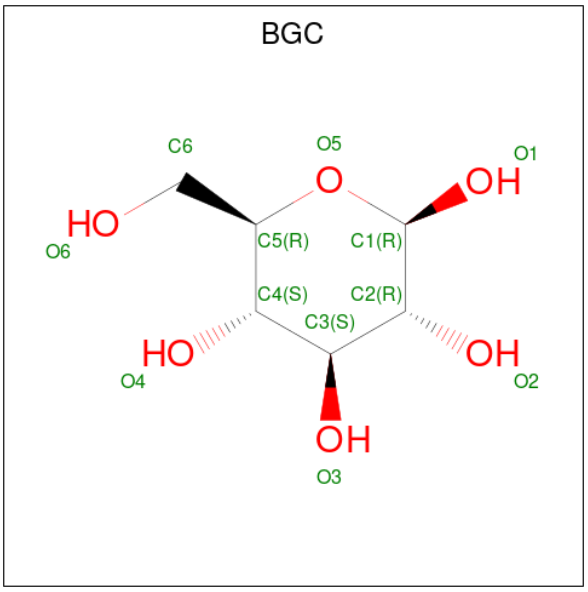
Chain	Residue	Modelled	Actual	Comment	Reference
B	254	ALA	-	expression tag	UNP D3ZHH1
E	25	GLY	-	expression tag	UNP D3ZHH1
E	26	SER	-	expression tag	UNP D3ZHH1
E	28	SER	GLY	engineered mutation	UNP D3ZHH1
E	107	LEU	PHE	engineered mutation	UNP D3ZHH1
E	206	PRO	LEU	engineered mutation	UNP D3ZHH1
E	253	ALA	-	expression tag	UNP D3ZHH1
E	254	ALA	-	expression tag	UNP D3ZHH1

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

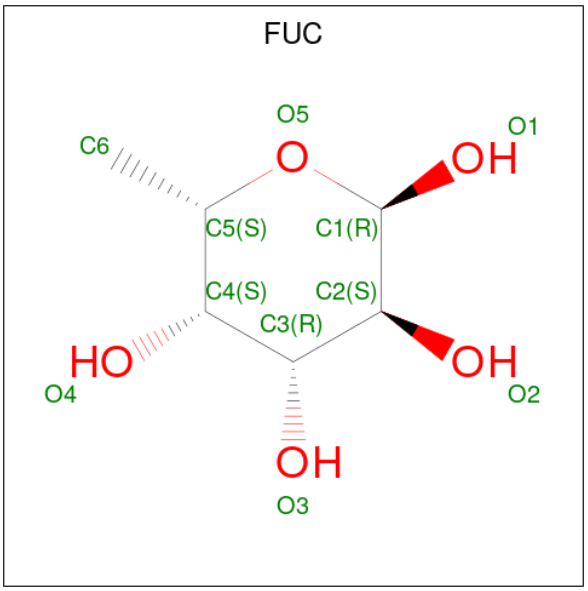
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	C	2	28	16	2	10	0	0	0
			Total	C	N	O			
3	F	2	28	16	2	10	0	0	0

- Molecule 4 is beta-D-glucopyranose (three-letter code: BGC) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	A	1	11	6	5	0	0
			Total	C	O		
4	A	1	11	6	5	0	0
			Total	C	O		
4	A	1	11	6	5	0	0
			Total	C	O		
4	D	1	11	6	5	0	0
			Total	C	O		
4	D	1	11	6	5	0	0
			Total	C	O		
4	D	1	11	6	5	0	0

- Molecule 5 is alpha-L-fucopyranose (three-letter code: FUC) (formula: $C_6H_{12}O_5$).

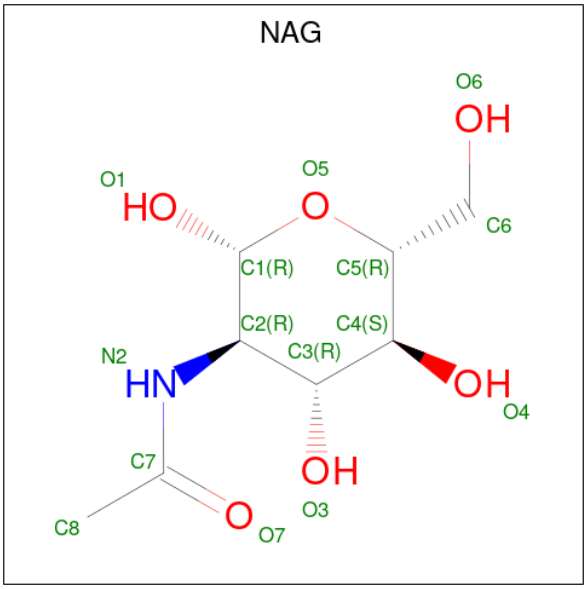


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
5	A	1	10	6	4	0	0
			Total	C	O		
5	D	1	10	6	4	0	0

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
6	A	3	3	3	0	0
			Total	Ca		
6	D	3	3	3	0	0

- Molecule 7 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		
7	B	1	14	8	1	5	0	0
			Total	C	N	O		
7	B	1	14	8	1	5	0	0
			Total	C	N	O		
7	E	1	14	8	1	5	0	0
			Total	C	N	O		
7	E	1	14	8	1	5	0	0

- Molecule 8 is water.

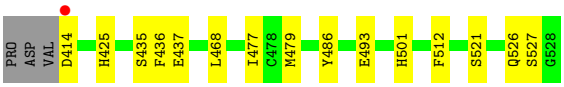
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
8	A	74	74	74	0	0
			Total	O		
8	B	99	99	99	0	0
			Total	O		
8	D	57	57	57	0	0
			Total	O		
8	E	95	95	95	0	0

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.

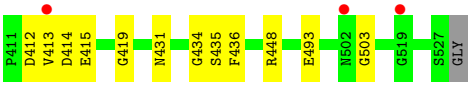
• Molecule 1: Neurogenic locus notch homolog protein 1

Chain A:



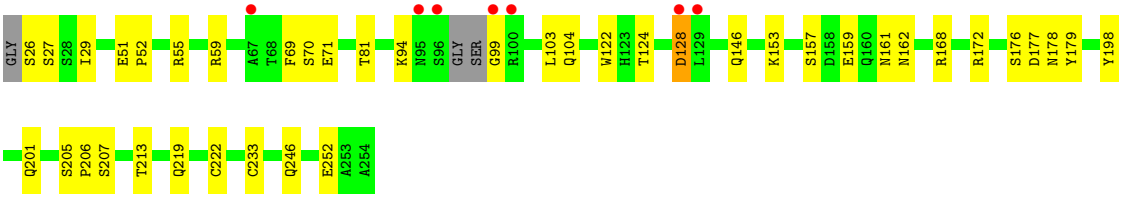
• Molecule 1: Neurogenic locus notch homolog protein 1

Chain D:



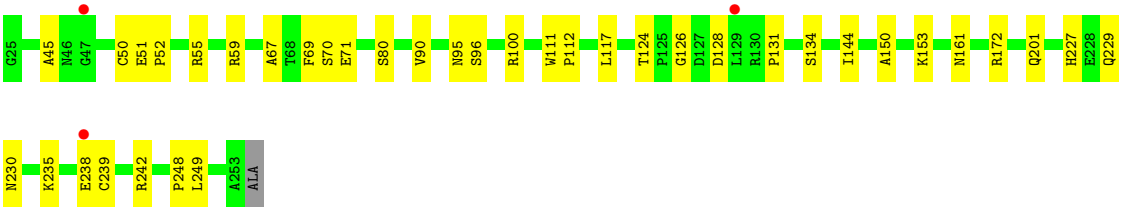
• Molecule 2: Delta-like protein

Chain B:



• Molecule 2: Delta-like protein

Chain E:



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

Chain C: 100%

NAG1
NAG2

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

Chain F: 100%

NAG1
NAG2

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	77.81Å 93.70Å 99.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.56 – 2.30 49.56 – 2.30	Depositor EDS
% Data completeness (in resolution range)	97.7 (49.56-2.30) 91.3 (49.56-2.30)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.51 (at 2.29Å)	Xtriage
Refinement program	PHENIX DEV-1839	Depositor
R, R_{free}	0.218 , 0.259 0.218 , 0.259	Depositor DCC
R_{free} test set	1594 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å^2)	36.8	Xtriage
Anisotropy	0.828	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 43.5	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	0.94	EDS
Total number of atoms	5865	wwPDB-VP
Average B, all atoms (Å^2)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.04% 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: FUC, BGC, NAG, CA, MLY

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	0/875	0.54	0/1183
1	D	0.28	0/907	0.51	0/1229
2	B	0.27	0/1776	0.52	0/2416
2	E	0.25	0/1780	0.48	0/2422
All	All	0.27	0/5338	0.51	0/7250

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	860	0	758	14	0
1	D	885	0	773	14	0
2	B	1794	0	1673	33	0
2	E	1797	0	1676	28	0
3	C	28	0	25	2	0
3	F	28	0	25	0	0
4	A	33	0	30	1	0
4	D	33	0	30	0	0
5	A	10	0	10	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	10	0	10	0	0
6	A	3	0	0	0	0
6	D	3	0	0	0	0
7	B	28	0	26	0	0
7	E	28	0	26	0	0
8	A	74	0	0	6	0
8	B	99	0	0	9	1
8	D	57	0	0	3	0
8	E	95	0	0	8	1
All	All	5865	0	5062	87	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 8.

All (87) 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:D:415[A]:GLU:OE1	1:D:431[A]:ASN:OD1	1.85	0.93
1:D:415[A]:GLU:OE1	1:D:435:SER:O	1.97	0.82
1:D:413:VAL:O	1:D:415[A]:GLU:OE2	2.00	0.79
2:B:177:ASP:O	8:B:459:HOH:O	2.01	0.77
2:E:153:MLY:HH12	2:E:172:ARG:HH22	1.48	0.77
1:D:414:ASP:OD1	1:D:431[B]:ASN:ND2	2.22	0.72
2:B:168:ARG:HG2	2:B:168:ARG:HH11	1.53	0.72
2:B:59:ARG:NH1	8:B:485:HOH:O	2.26	0.67
4:A:601:BGC:O6	8:A:734:HOH:O	2.12	0.67
2:B:157:SER:OG	8:B:458:HOH:O	2.11	0.67
2:E:55:ARG:NH2	2:E:128:ASP:OD1	2.28	0.67
2:B:162:ASN:O	8:B:463:HOH:O	2.13	0.66
2:B:168:ARG:HG2	2:B:168:ARG:NH1	2.11	0.65
2:B:26:SER:N	8:B:443:HOH:O	2.28	0.65
1:A:437:GLU:OE2	8:A:701:HOH:O	2.14	0.64
1:D:493:GLU:OE2	8:D:724:HOH:O	2.15	0.64
2:E:150:ALA:O	8:E:478:HOH:O	2.14	0.64
2:B:161:ASN:HB2	2:E:161:ASN:HB2	1.79	0.64
1:D:503:GLY:O	8:D:744:HOH:O	2.15	0.64
1:A:425:HIS:HE1	8:A:725:HOH:O	1.81	0.64
2:E:50:CYS:O	8:E:449:HOH:O	2.15	0.64
2:E:124:THR:HG21	2:E:131:PRO:HB3	1.81	0.63
1:A:526:GLN:N	1:A:526:GLN:OE1	2.32	0.63
2:B:201:GLN:HG3	2:B:207:SER:HB2	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:229:GLN:O	2:E:242:ARG:NH1	2.31	0.61
2:B:178:ASN:HB2	8:B:459:HOH:O	2.01	0.60
1:D:415[A]:GLU:HB2	1:D:436:PHE:HB3	1.82	0.60
2:B:70:SER:HB2	2:E:70:SER:HB2	1.84	0.60
2:E:248:PRO:O	8:E:401:HOH:O	2.17	0.59
1:A:501:HIS:ND1	1:A:526:GLN:HA	2.17	0.59
2:E:80:SER:O	8:E:444:HOH:O	2.16	0.59
2:E:201:GLN:NE2	8:E:406:HOH:O	2.32	0.58
1:D:412[A]:ASP:OD1	1:D:434:GLY:HA2	2.03	0.58
1:D:413:VAL:O	1:D:415[A]:GLU:CD	2.44	0.55
1:D:435:SER:OG	1:D:436:PHE:N	2.38	0.54
1:A:414:ASP:N	8:A:761:HOH:O	2.39	0.54
1:D:412[A]:ASP:OD1	1:D:413:VAL:N	2.40	0.54
2:B:59:ARG:NH2	8:B:462:HOH:O	2.41	0.54
1:A:493:GLU:HB3	1:A:512:PHE:HB3	1.90	0.54
2:E:117:LEU:O	2:E:144:ILE:HD12	2.08	0.54
2:B:27:SER:OG	8:B:480:HOH:O	2.17	0.53
2:B:55:ARG:NH1	2:B:124:THR:O	2.42	0.52
2:E:90:VAL:O	8:E:402:HOH:O	2.19	0.52
1:D:448:ARG:NH1	8:D:722:HOH:O	2.23	0.52
1:D:415[B]:GLU:HB2	1:D:436:PHE:HB3	1.92	0.52
1:A:479:MET:HG2	5:A:603:FUC:H62	1.92	0.52
2:B:81:THR:HG22	2:B:103:LEU:HD21	1.94	0.50
1:A:521:SER:O	1:A:527:SER:OG	2.25	0.49
2:E:59:ARG:HD3	8:E:491:HOH:O	2.14	0.47
2:B:168:ARG:HH11	2:B:168:ARG:CG	2.26	0.46
2:B:29:ILE:HG21	2:B:104:GLN:NE2	2.30	0.46
1:A:486:TYR:OH	8:A:763:HOH:O	2.20	0.46
3:C:1:NAG:O3	3:C:2:NAG:O5	2.26	0.46
2:E:95:ASN:ND2	8:E:411:HOH:O	2.49	0.46
1:A:425:HIS:CE1	8:A:725:HOH:O	2.61	0.46
2:E:69:PHE:O	2:E:71:GLU:HG2	2.15	0.45
2:B:201:GLN:OE1	2:B:205:SER:OG	2.31	0.45
2:E:126:GLY:HA3	2:E:134:SER:OG	2.16	0.45
1:A:435:SER:OG	1:A:436:PHE:N	2.48	0.45
2:B:27:SER:HA	2:B:179:TYR:CD2	2.52	0.45
1:A:512:PHE:O	1:A:512:PHE:CD1	2.70	0.44
2:B:153:MLY:HE2	2:B:172:ARG:HH12	1.82	0.44
1:A:468:LEU:HD11	1:A:477:ILE:HD11	1.99	0.44
2:B:128:ASP:N	2:B:128:ASP:OD1	2.50	0.44
2:B:176:SER:HB2	2:B:179:TYR:HD2	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:51:GLU:HA	2:E:52:PRO:HA	1.86	0.43
1:A:512:PHE:CD1	1:A:512:PHE:C	2.92	0.43
2:B:99:GLY:N	8:B:475:HOH:O	2.50	0.43
2:B:222:CYS:SG	2:B:233:CYS:N	2.91	0.43
2:B:122:TRP:CH2	2:E:67:ALA:HB1	2.54	0.43
2:E:238:GLU:HG3	2:E:239:CYS:N	2.33	0.43
2:B:146:GLN:HG2	2:E:45:ALA:HB1	2.01	0.43
2:E:55:ARG:HH21	2:E:128:ASP:CG	2.22	0.42
2:E:248:PRO:O	2:E:249:LEU:HB2	2.19	0.42
2:B:51:GLU:HA	2:B:52:PRO:HA	1.83	0.42
2:E:111:TRP:HA	2:E:112:PRO:HD2	1.91	0.42
2:B:213:THR:HG23	2:B:219:GLN:HB2	2.02	0.41
2:E:227:HIS:HB3	2:E:230:ASN:HB2	2.01	0.41
2:E:235:MLY:HH13	2:E:235:MLY:HD2	1.80	0.41
2:B:69:PHE:O	2:B:71:GLU:HG2	2.21	0.40
2:B:159:GLU:OE1	3:C:1:NAG:H3	2.21	0.40
2:B:246:GLN:HG2	2:B:252:GLU:O	2.22	0.40
2:B:153:MLY:HH23	2:B:172:ARG:HH22	1.87	0.40
2:B:198:TYR:CG	2:B:206:PRO:HB3	2.56	0.40
2:E:96:SER:HA	2:E:100:ARG:HE	1.86	0.40
2:E:96:SER:HA	2:E:100:ARG:NE	2.36	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)
8:B:412:HOH:O	8:E:426:HOH:O[3_554]	2.17	0.03

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	114/118 (97%)	112 (98%)	2 (2%)	0	100	100
1	D	118/118 (100%)	113 (96%)	4 (3%)	1 (1%)	19	23
2	B	218/230 (95%)	214 (98%)	4 (2%)	0	100	100
2	E	221/230 (96%)	216 (98%)	5 (2%)	0	100	100
All	All	671/696 (96%)	655 (98%)	15 (2%)	1 (0%)	47	64

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	419	GLY

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	99/101 (98%)	99 (100%)	0	100	100
1	D	103/101 (102%)	103 (100%)	0	100	100
2	B	194/194 (100%)	192 (99%)	2 (1%)	76	87
2	E	194/194 (100%)	194 (100%)	0	100	100
All	All	590/590 (100%)	588 (100%)	2 (0%)	92	97

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	94	LYS
2	B	128	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	425	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

12 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	MLY	B	63	2	9,10,11	0.54	0	6,11,13	1.00	0
2	MLY	E	215	2	9,10,11	0.52	0	6,11,13	0.85	0
2	MLY	E	235	2	9,10,11	0.50	0	6,11,13	0.91	0
2	MLY	B	235	2	9,10,11	0.50	0	6,11,13	0.94	0
2	MLY	B	189	2	9,10,11	0.53	0	6,11,13	0.90	0
2	MLY	E	63	2	9,10,11	0.53	0	6,11,13	0.91	0
2	MLY	B	190	2	9,10,11	0.59	0	6,11,13	0.78	0
2	MLY	E	189	2	9,10,11	0.54	0	6,11,13	0.91	0
2	MLY	E	190	2	9,10,11	0.44	0	6,11,13	1.02	0
2	MLY	B	153	2	9,10,11	0.52	0	6,11,13	0.89	0
2	MLY	E	153	2	9,10,11	0.54	0	6,11,13	0.83	0
2	MLY	B	215	2	9,10,11	0.54	0	6,11,13	0.81	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
2	MLY	B	63	2	-	4/8/9/11	-
2	MLY	E	215	2	-	3/8/9/11	-
2	MLY	E	235	2	-	2/8/9/11	-
2	MLY	B	235	2	-	3/8/9/11	-
2	MLY	B	189	2	-	3/8/9/11	-
2	MLY	E	63	2	-	3/8/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MLY	B	190	2	-	1/8/9/11	-
2	MLY	E	189	2	-	2/8/9/11	-
2	MLY	E	190	2	-	3/8/9/11	-
2	MLY	B	153	2	-	1/8/9/11	-
2	MLY	E	153	2	-	3/8/9/11	-
2	MLY	B	215	2	-	3/8/9/11	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	235	MLY	N-CA-CB-CG
2	B	235	MLY	C-CA-CB-CG
2	E	63	MLY	N-CA-CB-CG
2	E	63	MLY	C-CA-CB-CG
2	E	235	MLY	N-CA-CB-CG
2	E	235	MLY	C-CA-CB-CG
2	E	190	MLY	CD-CE-NZ-CH2
2	B	63	MLY	CD-CE-NZ-CH2
2	E	215	MLY	CD-CE-NZ-CH1
2	E	189	MLY	CG-CD-CE-NZ
2	B	63	MLY	CG-CD-CE-NZ
2	B	215	MLY	CA-CB-CG-CD
2	B	153	MLY	CG-CD-CE-NZ
2	B	189	MLY	CD-CE-NZ-CH2
2	E	190	MLY	CD-CE-NZ-CH1
2	E	215	MLY	CD-CE-NZ-CH2
2	B	215	MLY	CE-CD-CG-CB
2	E	153	MLY	CA-CB-CG-CD
2	E	215	MLY	CE-CD-CG-CB
2	B	63	MLY	CD-CE-NZ-CH1
2	E	189	MLY	CD-CE-NZ-CH2
2	B	235	MLY	CE-CD-CG-CB
2	B	215	MLY	CG-CD-CE-NZ
2	E	153	MLY	C-CA-CB-CG
2	B	63	MLY	CE-CD-CG-CB
2	E	63	MLY	CE-CD-CG-CB
2	B	189	MLY	CD-CE-NZ-CH1

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Mol	Chain	Res	Type	Atoms
2	E	153	MLY	CE-CD-CG-CB
2	E	190	MLY	CE-CD-CG-CB
2	B	190	MLY	CD-CE-NZ-CH2
2	B	189	MLY	CG-CD-CE-NZ

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	235	MLY	1	0
2	B	153	MLY	2	0
2	E	153	MLY	1	0

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	$\#\|Z\| > 2$
3	NAG	C	1	3,2	14,14,15	0.21	0	17,19,21	0.63	0
3	NAG	C	2	3	14,14,15	0.23	0	17,19,21	0.40	0
3	NAG	F	1	3,2	14,14,15	0.28	0	17,19,21	0.57	0
3	NAG	F	2	3	14,14,15	0.28	0	17,19,21	0.34	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	C	1	3,2	-	2/6/23/26	0/1/1/1
3	NAG	C	2	3	-	2/6/23/26	0/1/1/1
3	NAG	F	1	3,2	-	1/6/23/26	0/1/1/1
3	NAG	F	2	3	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	1	NAG	O5-C5-C6-O6
3	C	1	NAG	C4-C5-C6-O6
3	C	2	NAG	O5-C5-C6-O6
3	F	1	NAG	C4-C5-C6-O6
3	C	2	NAG	C4-C5-C6-O6

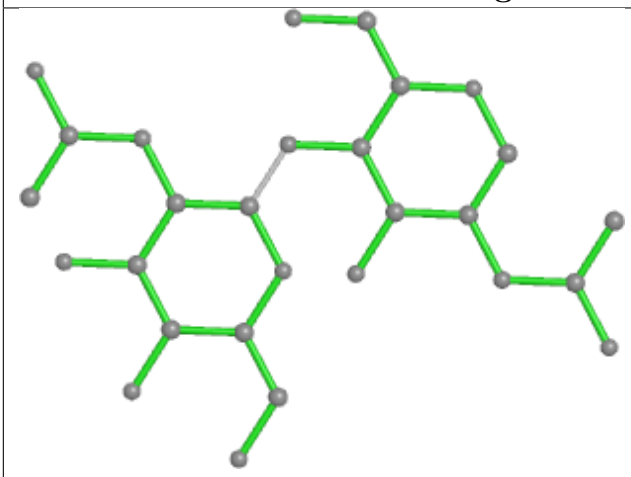
There are no ring outliers.

2 monomers are involved in 2 short contacts:

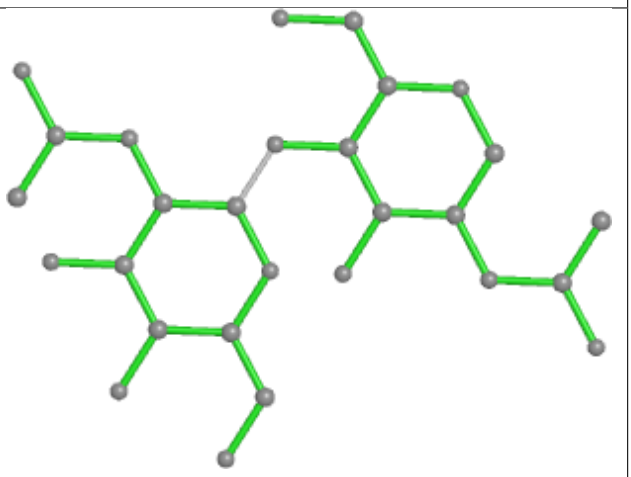
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	2	NAG	1	0
3	C	1	NAG	2	0

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

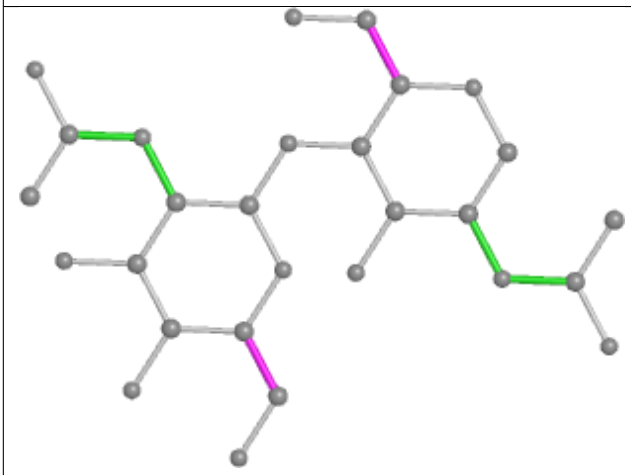
Oligosaccharide Chain C



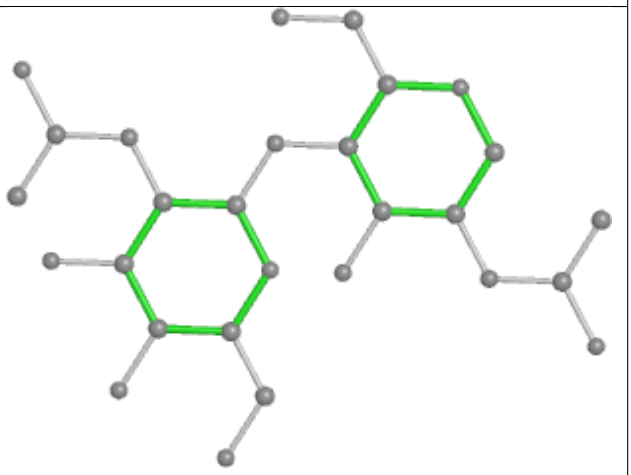
Bond lengths



Bond angles

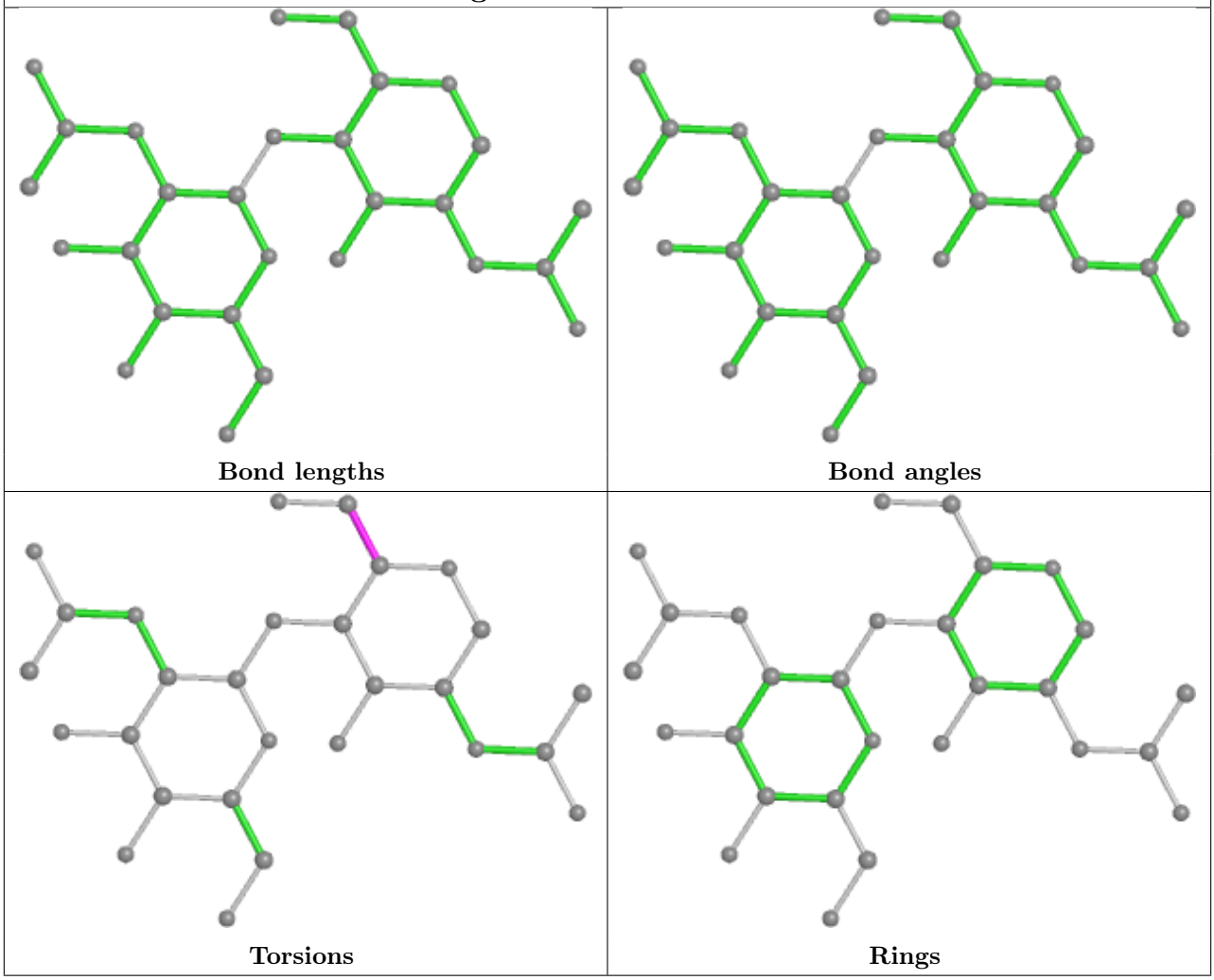


Torsions



Rings

Oligosaccharide Chain F



5.6 Ligand geometry (i)

Of 18 ligands modelled in this entry, 6 are monoatomic - leaving 12 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	$\#\|Z\| > 2$
7	NAG	B	302	2	14,14,15	0.30	0	17,19,21	0.78	1 (5%)
5	FUC	A	603	1	10,10,11	0.63	0	14,14,16	0.69	0
7	NAG	B	301	2	14,14,15	0.21	0	17,19,21	0.43	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	BGC	A	604	1	11,11,12	0.32	0	15,15,17	1.16	2 (13%)
4	BGC	D	601	1	11,11,12	0.20	0	15,15,17	0.90	1 (6%)
4	BGC	A	601	-	11,11,12	0.48	0	15,15,17	2.03	2 (13%)
4	BGC	D	602	1	11,11,12	0.31	0	15,15,17	0.77	0
7	NAG	E	301	2	14,14,15	0.35	0	17,19,21	0.53	0
4	BGC	D	604	1	11,11,12	0.28	0	15,15,17	1.21	2 (13%)
5	FUC	D	603	1	10,10,11	0.66	0	14,14,16	0.69	0
7	NAG	E	302	2	14,14,15	0.20	0	17,19,21	0.33	0
4	BGC	A	602	1	11,11,12	0.34	0	15,15,17	1.07	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
7	NAG	B	302	2	-	2/6/23/26	0/1/1/1
5	FUC	A	603	1	-	-	0/1/1/1
7	NAG	B	301	2	-	1/6/23/26	0/1/1/1
4	BGC	A	604	1	-	2/2/19/22	0/1/1/1
4	BGC	D	601	1	-	1/2/19/22	0/1/1/1
4	BGC	A	601	-	-	2/2/19/22	0/1/1/1
4	BGC	D	602	1	-	1/2/19/22	0/1/1/1
7	NAG	E	301	2	-	1/6/23/26	0/1/1/1
4	BGC	D	604	1	-	1/2/19/22	0/1/1/1
5	FUC	D	603	1	-	-	0/1/1/1
7	NAG	E	302	2	-	1/6/23/26	0/1/1/1
4	BGC	A	602	1	-	2/2/19/22	0/1/1/1

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	601	BGC	C1-O5-C5	5.81	120.07	112.19
4	A	604	BGC	C1-C2-C3	3.24	113.65	109.67
4	D	604	BGC	C1-C2-C3	3.15	113.54	109.67
4	A	602	BGC	O5-C5-C6	3.04	111.98	107.20
4	D	604	BGC	C1-O5-C5	2.94	116.18	112.19
7	B	302	NAG	C1-O5-C5	2.58	115.69	112.19
4	D	601	BGC	C1-C2-C3	2.49	112.72	109.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	601	BGC	C3-C4-C5	2.32	114.39	110.24
4	A	604	BGC	C1-O5-C5	2.08	115.01	112.19

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	B	302	NAG	O5-C5-C6-O6
4	A	602	BGC	O5-C5-C6-O6
4	A	601	BGC	O5-C5-C6-O6
4	A	604	BGC	O5-C5-C6-O6
7	B	302	NAG	C4-C5-C6-O6
4	A	602	BGC	C4-C5-C6-O6
4	A	601	BGC	C4-C5-C6-O6
4	A	604	BGC	C4-C5-C6-O6
4	D	604	BGC	O5-C5-C6-O6
4	D	601	BGC	O5-C5-C6-O6
4	D	602	BGC	O5-C5-C6-O6
7	B	301	NAG	O5-C5-C6-O6
7	E	302	NAG	O5-C5-C6-O6
7	E	301	NAG	O5-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	603	FUC	1	0
4	A	601	BGC	1	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	115/118 (97%)	-0.05	1 (0%)	84	88	36, 52, 94, 111	0
1	D	117/118 (99%)	0.02	3 (2%)	56	63	34, 49, 96, 123	0
2	B	221/230 (96%)	-0.09	7 (3%)	47	54	31, 45, 89, 112	0
2	E	223/230 (96%)	0.08	3 (1%)	77	81	27, 47, 92, 113	0
All	All	676/696 (97%)	-0.01	14 (2%)	63	70	27, 47, 94, 123	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	502	ASN	3.4
1	A	414	ASP	3.3
2	B	95	ASN	3.0
2	B	129	LEU	2.8
2	E	129	LEU	2.7
1	D	413	VAL	2.7
2	B	96	SER	2.6
2	E	47	GLY	2.5
2	B	99	GLY	2.5
2	B	100	ARG	2.4
2	B	128	ASP	2.2
1	D	519	GLY	2.2
2	E	238	GLU	2.1
2	B	67	ALA	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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	MLY	E	235	11/12	0.87	0.23	69,77,93,94	0
2	MLY	B	63	11/12	0.89	0.15	29,39,57,58	0
2	MLY	E	153	11/12	0.90	0.13	33,51,59,60	0
2	MLY	B	153	11/12	0.90	0.14	32,42,59,60	0
2	MLY	B	189	11/12	0.91	0.16	42,45,60,61	0
2	MLY	B	190	11/12	0.91	0.13	41,45,60,60	0
2	MLY	E	190	11/12	0.92	0.16	42,48,58,60	0
2	MLY	B	215	11/12	0.93	0.11	37,50,55,56	0
2	MLY	E	189	11/12	0.93	0.14	37,50,62,65	0
2	MLY	E	63	11/12	0.94	0.17	25,30,63,66	0
2	MLY	B	235	11/12	0.95	0.17	44,55,70,71	0
2	MLY	E	215	11/12	0.96	0.17	43,59,66,68	0

6.3 Carbohydrates (i)

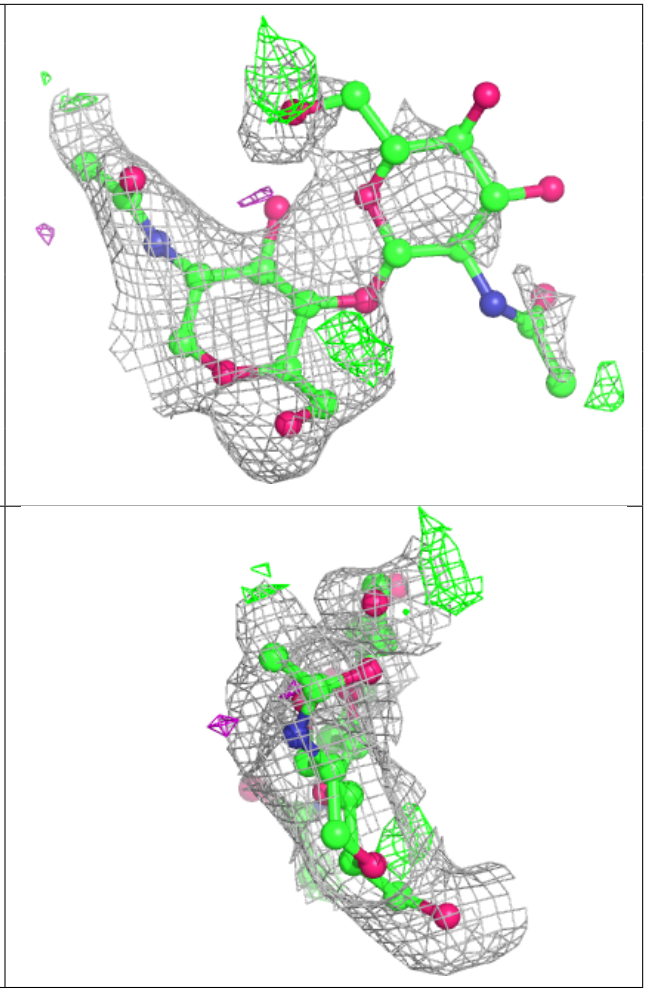
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NAG	C	2	14/15	0.47	0.45	91,96,98,101	14
3	NAG	C	1	14/15	0.81	0.16	61,69,82,86	0
3	NAG	F	1	14/15	0.82	0.15	42,53,58,62	0
3	NAG	F	2	14/15	0.87	0.24	58,71,75,77	14

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.

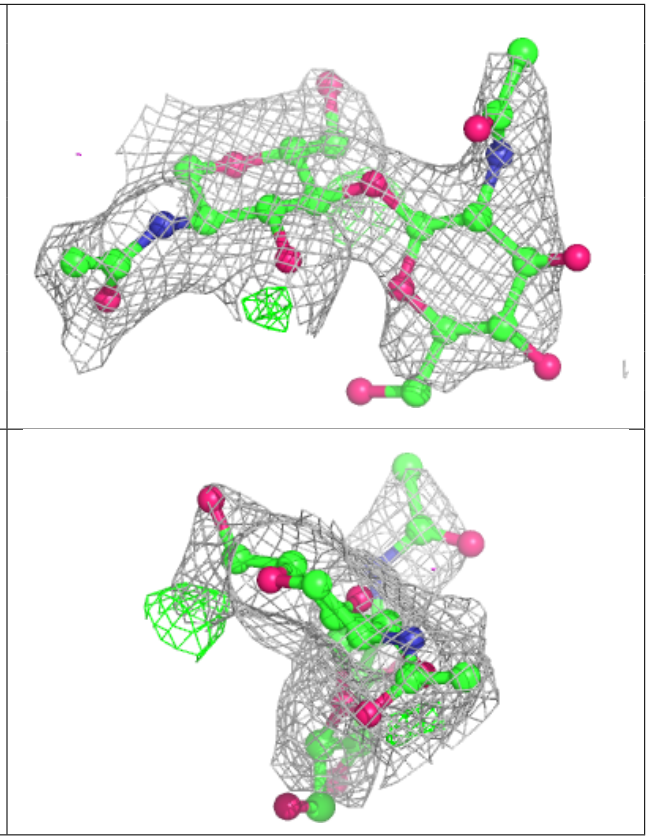
Electron density around Chain C:

$2mF_o$-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 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
6	CA	A	607	1/1	-0.30	0.16	90,90,90,90	1
6	CA	D	607	1/1	0.44	0.15	45,45,45,45	1
7	NAG	B	302	14/15	0.67	0.32	102,107,109,110	0
4	BGC	A	604	11/12	0.68	0.25	60,64,72,76	11
7	NAG	E	302	14/15	0.72	0.37	80,83,88,89	14
4	BGC	D	601	11/12	0.80	0.28	54,58,72,74	11
4	BGC	A	601	11/12	0.82	0.19	60,62,71,75	11
7	NAG	B	301	14/15	0.82	0.17	58,64,70,72	14
4	BGC	D	602	11/12	0.84	0.20	40,51,62,68	11
4	BGC	D	604	11/12	0.85	0.22	48,55,63,67	11
4	BGC	A	602	11/12	0.86	0.20	47,55,68,73	11
7	NAG	E	301	14/15	0.87	0.20	51,55,61,63	14
6	CA	A	606	1/1	0.87	0.10	35,35,35,35	1
6	CA	A	605	1/1	0.91	0.15	26,26,26,26	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	FUC	D	603	10/11	0.94	0.11	31,37,44,45	0
6	CA	D	606	1/1	0.96	0.09	40,40,40,40	0
5	FUC	A	603	10/11	0.96	0.10	23,31,38,42	0
6	CA	D	605	1/1	0.99	0.07	38,38,38,38	1

6.5 Other polymers (i)

There are no such residues in this entry.