Full wwPDB X-ray Structure Validation Report (i)

Sep 25, 2023 – 12:11 PM EDT

PDB ID	:	5VU0
Title	:	Crystal structure of the complex between afucosylated/galactosylated human IgG1 Fc and Fc gamma receptor IIIa (CD16A) with Man5 N-glycans
Authors	:	Subedi, G.S.; Marcella, A.M.; Barb, A.W.
Deposited on	:	2017-05-18
Resolution	:	2.26 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:

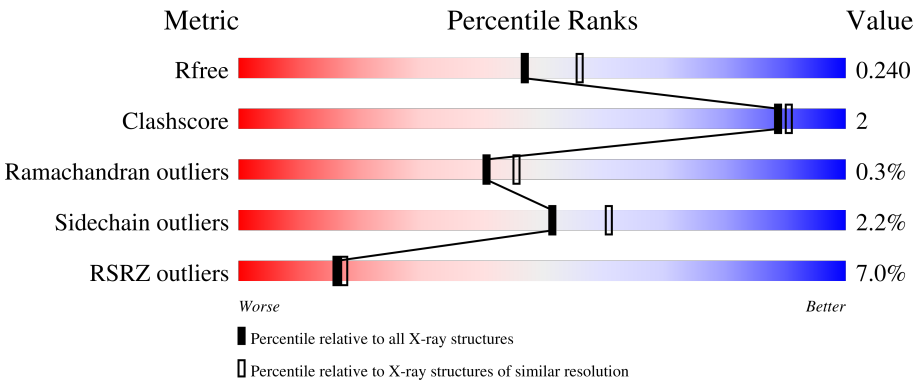
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 2.26 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	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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	217	3% 92% 7% •
1	B	217	5% 93% 6%
2	C	172	15% 85% 10% • •
3	D	8	88% 12%
3	E	8	88% 12%

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	D	8	-	-	-	X
3	NAG	E	8	-	-	-	X

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 5295 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 Immunoglobulin gamma-1 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	215	1706	1089	285	325	7	0	0	0
1	B	216	1718	1095	285	331	7	0	2	0

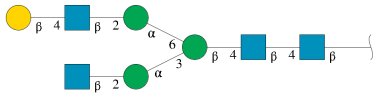
- Molecule 2 is a protein called Low affinity immunoglobulin gamma Fc region receptor III-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	165	1336	858	229	245	4	0	2	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	38	GLN	ASN	engineered mutation	UNP H0Y755
C	74	GLN	ASN	engineered mutation	UNP H0Y755
C	158	VAL	PHE	engineered mutation	UNP H0Y755
C	169	GLN	ASN	engineered mutation	UNP H0Y755

- Molecule 3 is an oligosaccharide called beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(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			
3	D	8	100	56	4	40	0	0	0

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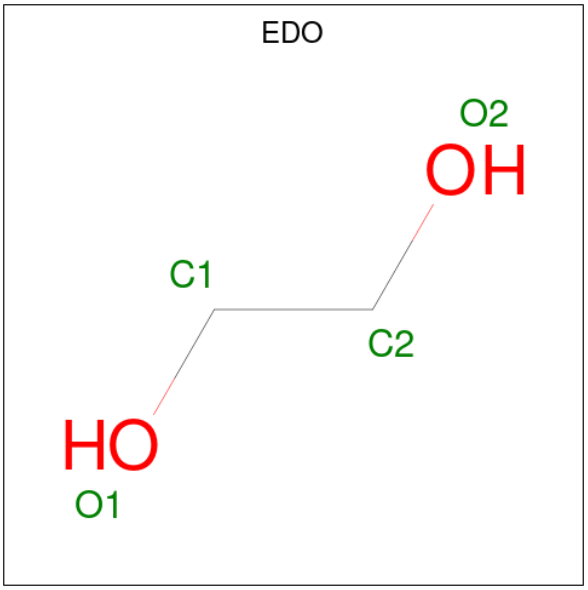
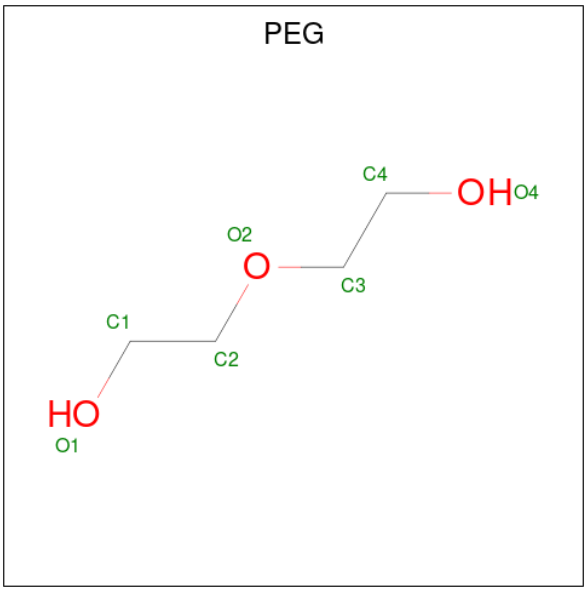
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	E	8	100	56	4	40	0	0	0

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O			
4	A	1	4	2	2		0	0
			Total	C	O			
4	A	1	4	2	2		0	0
			Total	C	O			
4	B	1	4	2	2		0	0
			Total	C	O			
4	C	1	4	2	2		0	0
			Total	C	O			
4	C	1	4	2	2		0	0

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).

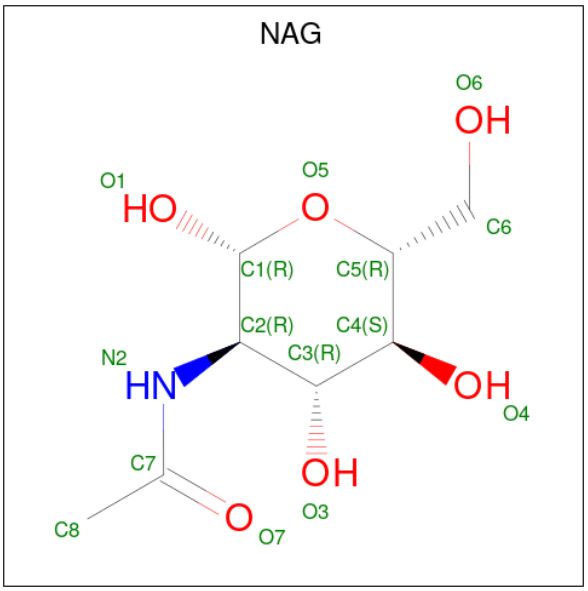


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 7 4 3	0	0
5	A	1	Total C O 7 4 3	0	0
5	A	1	Total C O 7 4 3	0	0
5	B	1	Total C O 7 4 3	0	0

- Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	5	Total Na 5 5	0	0
6	B	4	Total Na 4 4	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	C	1	12	7	1	4	0	0
			Total	C	N	O		
7	C	1	12	7	1	4	0	0

- Molecule 8 is water.

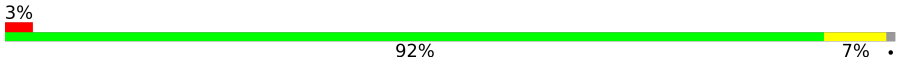
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
8	A	113	113	113	0	0
			Total	O		
8	B	88	88	88	0	0
			Total	O		
8	C	53	53	53	0	0

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.

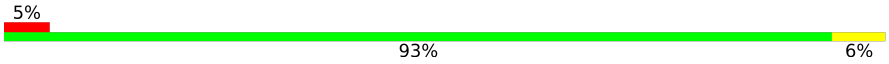
• Molecule 1: Immunoglobulin gamma-1 heavy chain

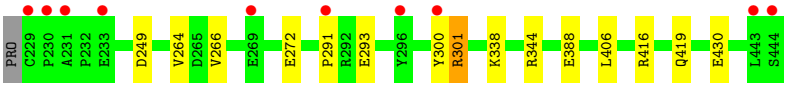
Chain A:



• Molecule 1: Immunoglobulin gamma-1 heavy chain

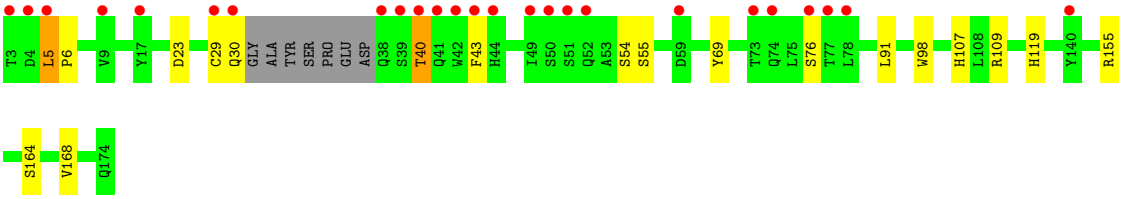
Chain B:





• Molecule 2: Low affinity immunoglobulin gamma Fc region receptor III-A

Chain C:



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

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

anose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	124.07Å 48.85Å 134.93Å 90.00° 103.77° 90.00°	Depositor
Resolution (Å)	10.00 – 2.26 9.99 – 2.26	Depositor EDS
% Data completeness (in resolution range)	97.3 (10.00-2.26) 98.6 (9.99-2.26)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.08 (at 2.26Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.192 , 0.237 0.198 , 0.240	Depositor DCC
R_{free} test set	1975 reflections (5.41%)	wwPDB-VP
Wilson B-factor (Å^2)	38.4	Xtriage
Anisotropy	0.167	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 42.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	5295	wwPDB-VP
Average B, all atoms (Å^2)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.45% 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: NAG, NA, PEG, EDO, MAN, BMA, GAL

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	0.98	3/1754 (0.2%)	0.99	4/2392 (0.2%)
1	B	0.97	1/1772 (0.1%)	0.94	4/2419 (0.2%)
2	C	0.85	1/1379 (0.1%)	0.95	4/1873 (0.2%)
All	All	0.94	5/4905 (0.1%)	0.96	12/6684 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	23	ASP	CB-CG	5.50	1.63	1.51
1	A	381	TRP	CB-CG	-5.46	1.40	1.50
1	A	430	GLU	CD-OE1	5.29	1.31	1.25
1	A	384	ASN	C-O	5.21	1.33	1.23
1	B	430	GLU	CD-OE1	5.13	1.31	1.25

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	344	ARG	NE-CZ-NH2	-10.04	115.28	120.30
1	B	344	ARG	NE-CZ-NH1	7.67	124.13	120.30
1	A	344	ARG	NE-CZ-NH1	7.11	123.86	120.30
1	A	255	ARG	NE-CZ-NH2	-6.73	116.94	120.30
1	A	255	ARG	NE-CZ-NH1	6.63	123.61	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	249	ASP	CB-CG-OD1	6.36	124.02	118.30
1	B	301	ARG	NE-CZ-NH2	-5.97	117.31	120.30
2	C	155	ARG	NE-CZ-NH1	5.84	123.22	120.30
2	C	29	CYS	CA-CB-SG	-5.69	103.76	114.00
1	A	280	ASP	CB-CG-OD1	5.43	123.19	118.30
2	C	109	ARG	NE-CZ-NH2	-5.35	117.62	120.30
2	C	109	ARG	NE-CZ-NH1	5.21	122.91	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	385	GLY	Peptide

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	1706	0	1665	6	0
1	B	1718	0	1671	6	0
2	C	1336	0	1280	6	0
3	D	100	0	85	2	0
3	E	100	0	85	3	0
4	A	8	0	12	0	0
4	B	4	0	6	0	0
4	C	8	0	12	1	0
5	A	21	0	30	2	0
5	B	7	0	10	0	0
6	A	5	0	0	0	0
6	B	4	0	0	0	0
7	C	24	0	20	0	0
8	A	113	0	0	0	1
8	B	88	0	0	0	0
8	C	53	0	0	0	0
All	All	5295	0	4876	19	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 2.

All (19) 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:B:301:ARG:HE	3:E:2:NAG:H81	1.49	0.76
1:A:386:GLN:HG3	1:A:387:PRO:HD2	1.83	0.60
1:B:264:VAL:CG1	3:E:2:NAG:H83	2.35	0.56
2:C:91:LEU:HD12	2:C:164:SER:HA	1.93	0.49
1:A:308:VAL:HG12	1:A:319:TYR:CE2	2.48	0.49
2:C:98:TRP:CZ3	2:C:168:VAL:HG21	2.47	0.49
1:B:266:VAL:HB	1:B:300:TYR:HB2	1.97	0.47
1:A:232:PRO:C	1:A:234:LEU:HG	2.35	0.46
1:B:264:VAL:HG11	3:E:2:NAG:H83	1.98	0.46
2:C:43:PHE:O	2:C:69:TYR:HA	2.17	0.45
1:B:406:LEU:C	1:B:406:LEU:HD12	2.36	0.44
1:A:351:LEU:HB2	1:A:366:THR:HB	1.99	0.44
1:A:386:GLN:HG3	1:A:387:PRO:CD	2.48	0.44
1:B:388:GLU:OE2	1:B:416:ARG:NH1	2.50	0.43
5:A:1012:PEG:H11	3:D:5:NAG:H3	2.02	0.42
5:A:1013:PEG:H21	3:D:5:NAG:H83	2.01	0.42
2:C:40:THR:OG1	2:C:54:SER:HA	2.19	0.42
2:C:98:TRP:HE1	4:C:203:EDO:C2	2.34	0.41
1:A:235:LEU:HD22	2:C:119[B]:HIS:HD2	1.86	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:A:1178:HOH:O	8:A:1178:HOH:O[2_755]	2.05	0.15

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	211/217 (97%)	206 (98%)	5 (2%)	0	100	100
1	B	216/217 (100%)	212 (98%)	4 (2%)	0	100	100
2	C	163/172 (95%)	153 (94%)	8 (5%)	2 (1%)	13	9
All	All	590/606 (97%)	571 (97%)	17 (3%)	2 (0%)	41	46

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	5	LEU
2	C	6	PRO

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	197/201 (98%)	196 (100%)	1 (0%)	88	92
1	B	199/201 (99%)	194 (98%)	5 (2%)	47	56
2	C	146/156 (94%)	140 (96%)	6 (4%)	30	36
All	All	542/558 (97%)	530 (98%)	12 (2%)	52	61

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

Mol	Chain	Res	Type
1	A	234	LEU
1	B	272	GLU
1	B	291	PRO
1	B	293	GLU
1	B	338	LYS
1	B	419	GLN
2	C	5	LEU
2	C	30	GLN
2	C	40	THR
2	C	55	SER
2	C	76	SER

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Mol	Chain	Res	Type
2	C	107	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	C	30	GLN
2	C	52	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)

16 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	D	1	1,3	14,14,15	1.05	1 (7%)	17,19,21	2.56	8 (47%)
3	NAG	D	2	3	14,14,15	1.00	1 (7%)	17,19,21	1.28	3 (17%)
3	BMA	D	3	3	11,11,12	0.48	0	15,15,17	1.24	2 (13%)
3	MAN	D	4	3	11,11,12	1.20	1 (9%)	15,15,17	1.67	5 (33%)
3	NAG	D	5	3	14,14,15	0.67	0	17,19,21	1.58	5 (29%)
3	GAL	D	6	3	11,11,12	2.09	4 (36%)	15,15,17	2.54	6 (40%)
3	MAN	D	7	3	11,11,12	0.95	0	15,15,17	2.10	7 (46%)
3	NAG	D	8	3	14,14,15	0.88	1 (7%)	17,19,21	1.28	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	NAG	E	1	1,3	14,14,15	0.61	0	17,19,21	1.51	3 (17%)
3	NAG	E	2	3	14,14,15	0.75	0	17,19,21	1.90	5 (29%)
3	BMA	E	3	3	11,11,12	1.02	1 (9%)	15,15,17	1.25	2 (13%)
3	MAN	E	4	3	11,11,12	0.69	0	15,15,17	1.38	1 (6%)
3	NAG	E	5	3	14,14,15	0.64	0	17,19,21	1.59	4 (23%)
3	GAL	E	6	3	11,11,12	1.43	2 (18%)	15,15,17	1.90	4 (26%)
3	MAN	E	7	3	11,11,12	0.65	0	15,15,17	2.25	5 (33%)
3	NAG	E	8	3	14,14,15	0.80	0	17,19,21	1.77	4 (23%)

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	D	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	D	2	3	-	0/6/23/26	0/1/1/1
3	BMA	D	3	3	-	0/2/19/22	0/1/1/1
3	MAN	D	4	3	-	0/2/19/22	0/1/1/1
3	NAG	D	5	3	-	2/6/23/26	0/1/1/1
3	GAL	D	6	3	-	0/2/19/22	0/1/1/1
3	MAN	D	7	3	-	2/2/19/22	0/1/1/1
3	NAG	D	8	3	-	2/6/23/26	0/1/1/1
3	NAG	E	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	E	2	3	-	2/6/23/26	0/1/1/1
3	BMA	E	3	3	-	0/2/19/22	0/1/1/1
3	MAN	E	4	3	-	0/2/19/22	0/1/1/1
3	NAG	E	5	3	-	1/6/23/26	0/1/1/1
3	GAL	E	6	3	-	2/2/19/22	0/1/1/1
3	MAN	E	7	3	-	2/2/19/22	0/1/1/1
3	NAG	E	8	3	-	4/6/23/26	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	6	GAL	O2-C2	3.66	1.51	1.43
3	D	6	GAL	C1-C2	3.53	1.60	1.52
3	D	6	GAL	C2-C3	2.84	1.56	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	6	GAL	C1-C2	2.34	1.57	1.52
3	D	4	MAN	O2-C2	-2.33	1.38	1.43
3	D	1	NAG	C2-N2	2.31	1.50	1.46
3	D	2	NAG	C2-N2	-2.27	1.42	1.46
3	E	3	BMA	C2-C3	2.20	1.55	1.52
3	D	6	GAL	O4-C4	2.16	1.48	1.43
3	D	8	NAG	C1-C2	2.05	1.55	1.52
3	E	6	GAL	C2-C3	2.01	1.55	1.52

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	7	MAN	C1-O5-C5	5.00	118.97	112.19
3	D	6	GAL	O2-C2-C1	4.78	118.92	109.15
3	D	1	NAG	O6-C6-C5	-4.69	95.20	111.29
3	D	1	NAG	C1-O5-C5	4.55	118.35	112.19
3	E	7	MAN	O2-C2-C1	-4.48	99.98	109.15
3	E	6	GAL	O2-C2-C1	4.36	118.08	109.15
3	D	6	GAL	O5-C5-C6	4.31	113.97	107.20
3	D	7	MAN	O2-C2-C1	3.98	117.29	109.15
3	E	2	NAG	O5-C1-C2	-3.97	105.02	111.29
3	D	1	NAG	O5-C5-C6	-3.85	101.17	107.20
3	E	2	NAG	C4-C3-C2	-3.82	105.42	111.02
3	D	1	NAG	C6-C5-C4	-3.71	104.32	113.00
3	D	6	GAL	C2-C3-C4	3.54	117.02	110.89
3	E	8	NAG	C1-O5-C5	3.37	116.75	112.19
3	D	6	GAL	O5-C5-C4	-3.36	102.66	110.83
3	E	1	NAG	C8-C7-N2	3.33	121.73	116.10
3	D	6	GAL	O4-C4-C3	3.32	118.03	110.35
3	E	4	MAN	O3-C3-C4	3.31	118.00	110.35
3	E	5	NAG	C6-C5-C4	3.25	120.62	113.00
3	D	7	MAN	O5-C5-C6	3.17	112.17	107.20
3	D	4	MAN	C1-O5-C5	3.17	116.48	112.19
3	E	8	NAG	O5-C5-C6	3.16	112.16	107.20
3	E	7	MAN	O2-C2-C3	3.14	116.43	110.14
3	E	1	NAG	C1-O5-C5	3.14	116.44	112.19
3	E	8	NAG	C8-C7-N2	3.10	121.35	116.10
3	D	8	NAG	O5-C5-C6	3.08	112.03	107.20
3	D	3	BMA	O5-C1-C2	3.07	115.50	110.77
3	E	3	BMA	C1-O5-C5	3.06	116.33	112.19
3	D	4	MAN	O2-C2-C3	-3.03	104.07	110.14
3	D	1	NAG	C1-C2-N2	-3.03	105.32	110.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	1	NAG	O5-C5-C4	3.03	118.19	110.83
3	D	5	NAG	O4-C4-C3	-3.02	103.36	110.35
3	E	8	NAG	C2-N2-C7	2.98	127.15	122.90
3	D	5	NAG	C8-C7-N2	2.97	121.13	116.10
3	E	6	GAL	O5-C5-C4	-2.95	103.65	110.83
3	D	7	MAN	O2-C2-C3	-2.83	104.48	110.14
3	E	7	MAN	O3-C3-C4	2.75	116.72	110.35
3	E	2	NAG	C2-N2-C7	2.72	126.77	122.90
3	D	4	MAN	C6-C5-C4	-2.71	106.65	113.00
3	D	2	NAG	O4-C4-C5	-2.70	102.59	109.30
3	D	7	MAN	O4-C4-C3	-2.66	104.20	110.35
3	E	5	NAG	O3-C3-C4	2.61	116.38	110.35
3	E	5	NAG	O4-C4-C3	-2.54	104.48	110.35
3	D	1	NAG	O5-C1-C2	2.52	115.27	111.29
3	D	7	MAN	C2-C3-C4	2.49	115.20	110.89
3	E	6	GAL	O5-C5-C6	2.49	111.10	107.20
3	D	6	GAL	C1-O5-C5	2.46	115.53	112.19
3	D	7	MAN	C1-O5-C5	2.45	115.51	112.19
3	E	7	MAN	C1-C2-C3	-2.36	106.77	109.67
3	D	5	NAG	O5-C1-C2	-2.32	107.63	111.29
3	D	4	MAN	O6-C6-C5	-2.28	103.46	111.29
3	E	1	NAG	C2-N2-C7	2.27	126.13	122.90
3	E	3	BMA	C2-C3-C4	2.26	114.81	110.89
3	D	2	NAG	C4-C3-C2	-2.25	107.71	111.02
3	D	8	NAG	C2-N2-C7	2.22	126.07	122.90
3	D	5	NAG	O7-C7-C8	-2.22	117.94	122.06
3	D	8	NAG	C4-C3-C2	2.19	114.23	111.02
3	E	2	NAG	O6-C6-C5	-2.18	103.81	111.29
3	E	6	GAL	C2-C3-C4	2.16	114.63	110.89
3	E	5	NAG	C2-N2-C7	-2.15	119.84	122.90
3	D	2	NAG	O6-C6-C5	-2.13	103.98	111.29
3	D	3	BMA	O4-C4-C3	-2.08	105.55	110.35
3	E	2	NAG	C8-C7-N2	2.07	119.60	116.10
3	D	4	MAN	C1-C2-C3	2.06	112.19	109.67
3	D	7	MAN	O3-C3-C4	-2.04	105.63	110.35
3	D	5	NAG	C2-N2-C7	2.03	125.80	122.90
3	D	1	NAG	O7-C7-C8	-2.03	118.29	122.06

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	7	MAN	C4-C5-C6-O6
3	D	1	NAG	C4-C5-C6-O6
3	D	7	MAN	O5-C5-C6-O6
3	D	8	NAG	O5-C5-C6-O6
3	D	1	NAG	O5-C5-C6-O6
3	D	8	NAG	C4-C5-C6-O6
3	D	5	NAG	C8-C7-N2-C2
3	D	5	NAG	O7-C7-N2-C2
3	E	1	NAG	C8-C7-N2-C2
3	E	1	NAG	O7-C7-N2-C2
3	E	2	NAG	C8-C7-N2-C2
3	E	2	NAG	O7-C7-N2-C2
3	E	8	NAG	C8-C7-N2-C2
3	E	8	NAG	O7-C7-N2-C2
3	E	7	MAN	C4-C5-C6-O6
3	E	6	GAL	C4-C5-C6-O6
3	E	1	NAG	C4-C5-C6-O6
3	E	6	GAL	O5-C5-C6-O6
3	E	8	NAG	O5-C5-C6-O6
3	E	7	MAN	O5-C5-C6-O6
3	E	1	NAG	O5-C5-C6-O6
3	E	8	NAG	C4-C5-C6-O6
3	E	5	NAG	C4-C5-C6-O6

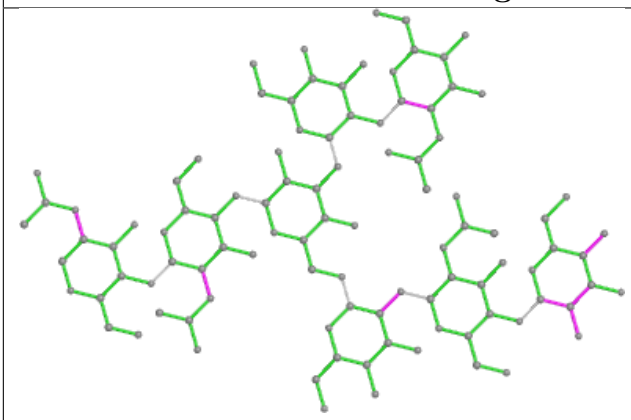
There are no ring outliers.

2 monomers are involved in 5 short contacts:

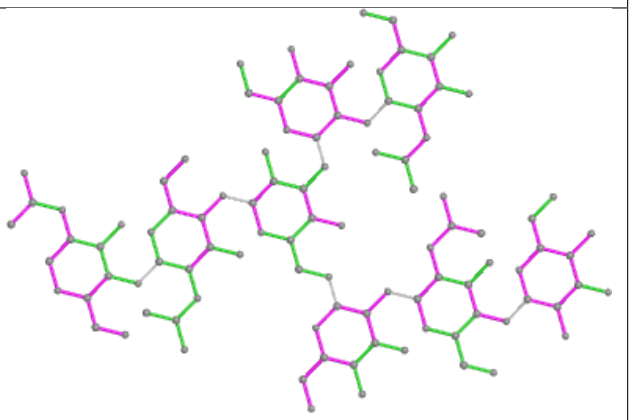
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	5	NAG	2	0
3	E	2	NAG	3	0

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

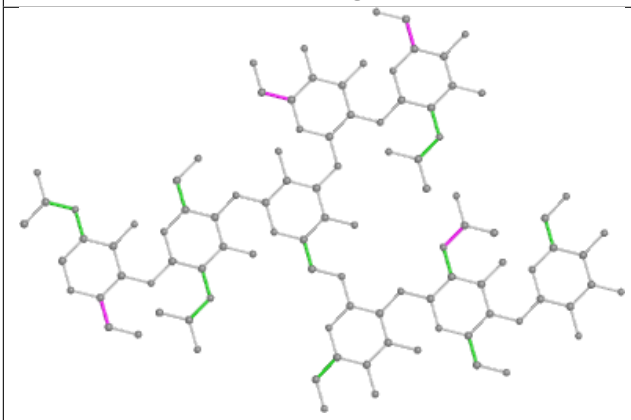
Oligosaccharide Chain D



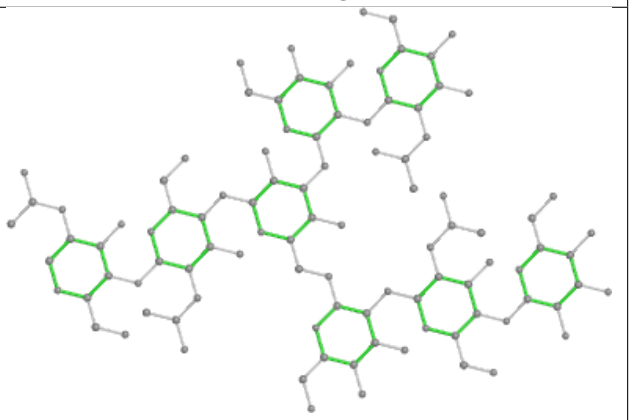
Bond lengths



Bond angles

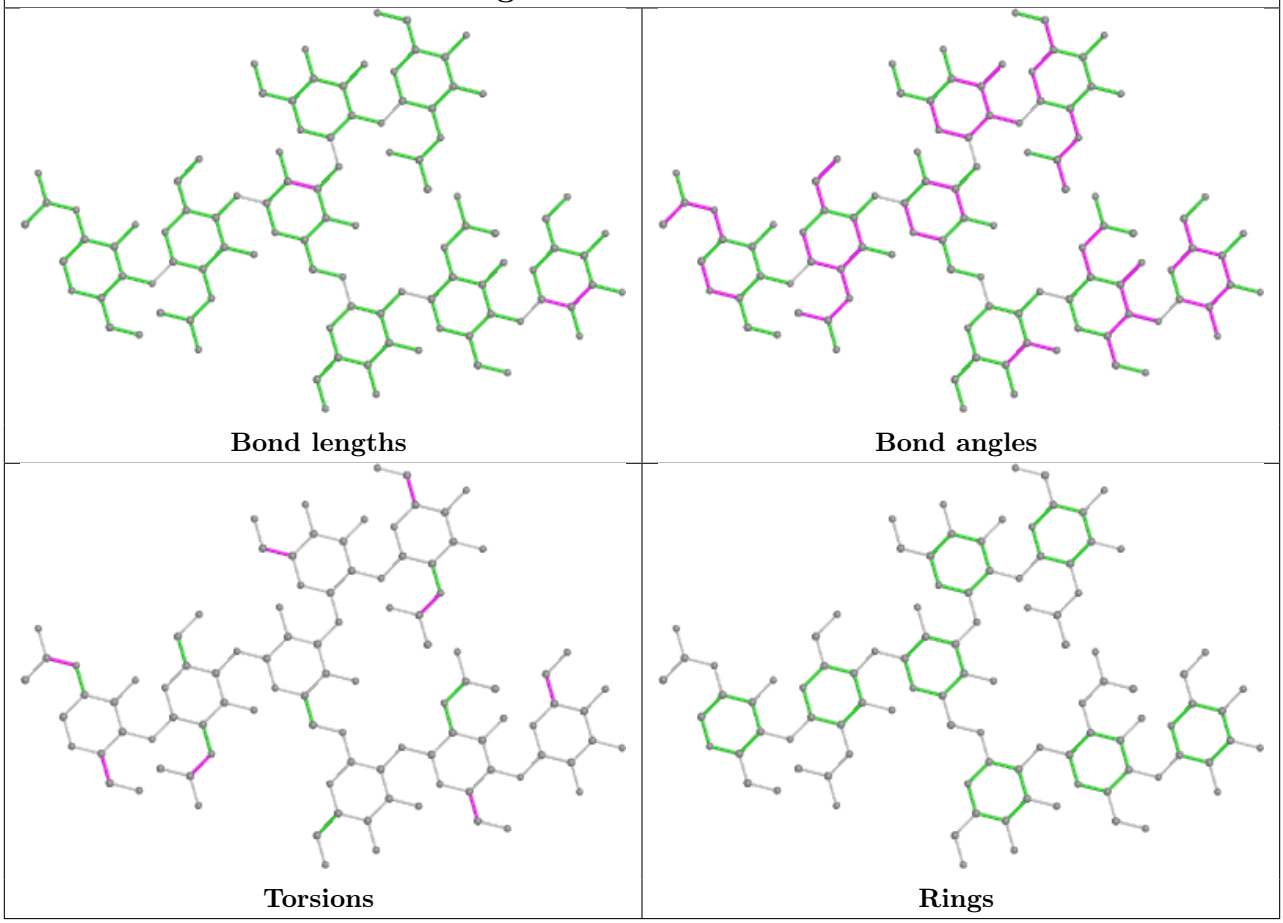


Torsions



Rings

Oligosaccharide Chain E



5.6 Ligand geometry (i)

Of 20 ligands modelled in this entry, 9 are monoatomic - leaving 11 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	C	201	2	11,12,15	1.78	3 (27%)	13,16,21	3.37	6 (46%)
4	EDO	C	204	-	3,3,3	0.95	0	2,2,2	0.31	0
7	NAG	C	202	2	11,12,15	1.50	1 (9%)	13,16,21	2.04	2 (15%)
5	PEG	A	1012	-	6,6,6	0.66	0	5,5,5	0.46	0
5	PEG	B	1010	-	6,6,6	0.36	0	5,5,5	1.07	0
4	EDO	A	1010	-	3,3,3	0.55	0	2,2,2	0.50	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	EDO	A	1009	-	3,3,3	0.87	0	2,2,2	0.47	0
4	EDO	B	1009	-	3,3,3	0.65	0	2,2,2	0.31	0
5	PEG	A	1011	-	6,6,6	0.51	0	5,5,5	0.41	0
5	PEG	A	1013	-	6,6,6	0.58	0	5,5,5	0.39	0
4	EDO	C	203	-	3,3,3	0.29	0	2,2,2	0.77	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
7	NAG	C	201	2	-	3/4/21/26	0/1/1/1
4	EDO	C	204	-	-	1/1/1/1	-
7	NAG	C	202	2	-	2/4/21/26	0/1/1/1
5	PEG	A	1012	-	-	1/4/4/4	-
5	PEG	B	1010	-	-	1/4/4/4	-
4	EDO	A	1010	-	-	0/1/1/1	-
4	EDO	A	1009	-	-	1/1/1/1	-
4	EDO	B	1009	-	-	1/1/1/1	-
5	PEG	A	1011	-	-	2/4/4/4	-
5	PEG	A	1013	-	-	0/4/4/4	-
4	EDO	C	203	-	-	1/1/1/1	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	202	NAG	C7-N2	-4.39	1.35	1.46
7	C	201	NAG	C7-N2	-4.30	1.35	1.46
7	C	201	NAG	O5-C1	-2.62	1.39	1.43
7	C	201	NAG	O5-C5	-2.30	1.38	1.43

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	C	201	NAG	C1-O5-C5	7.24	122.00	112.19
7	C	201	NAG	C4-C3-C2	6.32	120.28	111.02
7	C	201	NAG	O5-C1-C2	5.23	119.54	111.29
7	C	202	NAG	O5-C5-C6	5.16	115.30	107.20
7	C	202	NAG	C1-O5-C5	3.70	117.20	112.19
7	C	201	NAG	C6-C5-C4	-2.67	106.74	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	C	201	NAG	O6-C6-C5	-2.57	102.47	111.29
7	C	201	NAG	O3-C3-C4	-2.13	105.42	110.35

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	C	201	NAG	C1-C2-N2-C7
7	C	201	NAG	C3-C2-N2-C7
7	C	202	NAG	O5-C5-C6-O6
5	A	1012	PEG	O2-C3-C4-O4
5	A	1011	PEG	O2-C3-C4-O4
4	A	1009	EDO	O1-C1-C2-O2
4	C	203	EDO	O1-C1-C2-O2
7	C	202	NAG	C4-C5-C6-O6
5	B	1010	PEG	C4-C3-O2-C2
4	B	1009	EDO	O1-C1-C2-O2
4	C	204	EDO	O1-C1-C2-O2
7	C	201	NAG	O5-C5-C6-O6
5	A	1011	PEG	C1-C2-O2-C3

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1012	PEG	1	0
5	A	1013	PEG	1	0
4	C	203	EDO	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	215/217 (99%)	-0.16	7 (3%)	46	48	20, 35, 65, 134	1 (0%)
1	B	216/217 (99%)	0.02	10 (4%)	32	35	21, 42, 80, 122	0
2	C	165/172 (95%)	0.74	25 (15%)	2	2	33, 53, 107, 127	0
All	All	596/606 (98%)	0.15	42 (7%)	16	17	20, 42, 98, 134	1 (0%)

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	231	ALA	8.1
2	C	3	THR	8.0
2	C	40	THR	6.5
2	C	51	SER	5.6
1	B	444	SER	5.4
1	A	234	LEU	5.4
2	C	4	ASP	5.0
2	C	29	CYS	4.9
1	B	229	CYS	4.8
1	B	230	PRO	4.8
1	B	231	ALA	4.8
1	B	443	LEU	4.3
1	A	230	PRO	4.3
1	B	291	PRO	4.3
1	B	296	TYR	4.3
1	A	229	CYS	4.1
2	C	77	THR	4.0
1	B	300	TYR	3.8
2	C	38	GLN	3.5
2	C	73	THR	3.4
2	C	39	SER	3.3
1	A	232	PRO	3.3
2	C	30	GLN	2.8

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Mol	Chain	Res	Type	RSRZ
2	C	50	SER	2.8
2	C	17	TYR	2.8
1	A	235	LEU	2.7
2	C	41	GLN	2.6
2	C	140[A]	TYR	2.6
1	B	233	GLU	2.5
2	C	5	LEU	2.5
2	C	49	ILE	2.4
2	C	43	PHE	2.4
2	C	9	VAL	2.3
2	C	59	ASP	2.2
2	C	74	GLN	2.2
1	B	269	GLU	2.2
1	A	384	ASN	2.2
2	C	44	HIS	2.1
2	C	52	GLN	2.1
2	C	76	SER	2.1
2	C	42	TRP	2.0
2	C	78	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, 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	E	8	14/15	0.54	0.49	87,99,104,106	0
3	GAL	E	6	11/12	0.70	0.34	54,67,70,71	0
3	NAG	D	8	14/15	0.71	0.46	98,106,110,110	0
3	GAL	D	6	11/12	0.83	0.25	43,46,49,49	0
3	NAG	E	5	14/15	0.83	0.18	49,55,57,59	0
3	MAN	E	7	11/12	0.85	0.16	61,64,69,80	0
3	MAN	D	7	11/12	0.86	0.20	53,59,65,81	0
3	MAN	D	4	11/12	0.91	0.12	27,28,30,31	0
3	NAG	E	1	14/15	0.92	0.12	55,60,64,65	0

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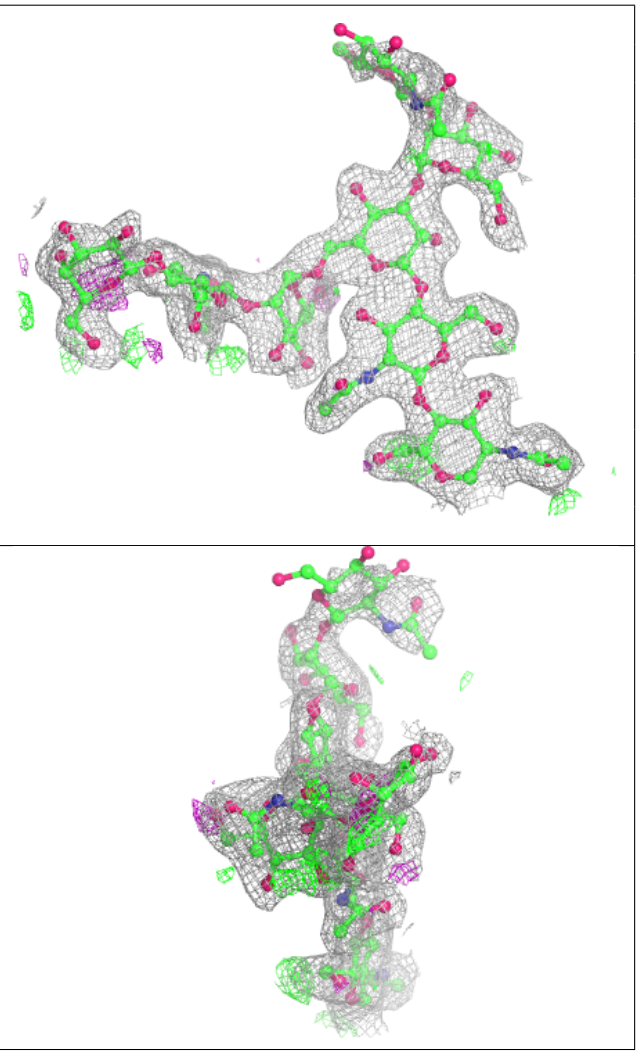
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NAG	E	2	14/15	0.92	0.12	50,53,54,54	0
3	NAG	D	5	14/15	0.93	0.13	30,33,36,38	0
3	BMA	E	3	11/12	0.93	0.13	47,52,53,54	0
3	MAN	E	4	11/12	0.94	0.14	53,55,58,58	0
3	NAG	D	2	14/15	0.95	0.10	27,27,29,30	0
3	NAG	D	1	14/15	0.95	0.09	27,28,30,33	0
3	BMA	D	3	11/12	0.96	0.08	31,31,36,42	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.

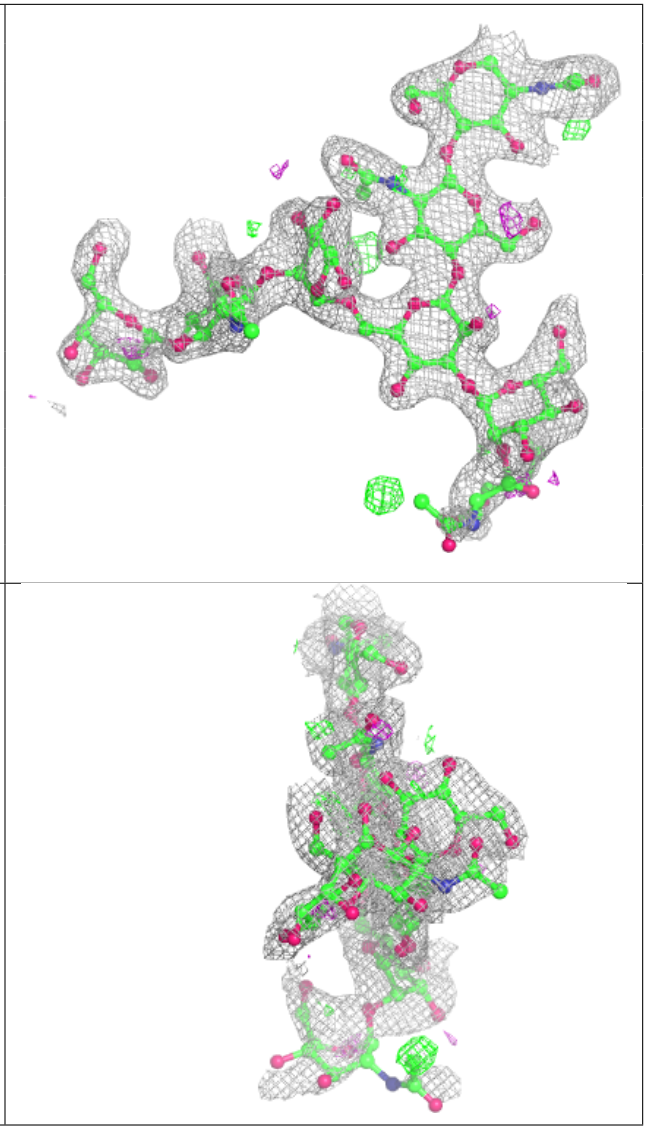
Electron density around Chain D:

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 E:

$2mF_o$-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	PEG	A	1012	7/7	0.59	0.38	40,49,51,51	0
4	EDO	A	1009	4/4	0.72	0.23	53,55,56,59	0
7	NAG	C	202	12/15	0.74	0.21	85,86,87,87	0
5	PEG	A	1013	7/7	0.80	0.21	57,59,62,63	0
7	NAG	C	201	12/15	0.83	0.16	37,39,42,45	0
6	NA	B	1013	1/1	0.85	0.27	46,46,46,46	0
5	PEG	A	1011	7/7	0.86	0.21	44,55,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	PEG	B	1010	7/7	0.87	0.28	38,41,50,55	0
6	NA	A	1017	1/1	0.90	0.14	34,34,34,34	0
4	EDO	B	1009	4/4	0.90	0.17	41,50,51,51	0
4	EDO	C	204	4/4	0.91	0.17	35,38,40,43	0
4	EDO	C	203	4/4	0.92	0.23	31,38,40,45	0
4	EDO	A	1010	4/4	0.92	0.17	34,35,35,35	0
6	NA	A	1014	1/1	0.93	0.25	43,43,43,43	0
6	NA	B	1014	1/1	0.93	0.10	39,39,39,39	0
6	NA	B	1011	1/1	0.94	0.12	40,40,40,40	0
6	NA	B	1012	1/1	0.94	0.16	33,33,33,33	0
6	NA	A	1016	1/1	0.96	0.20	36,36,36,36	0
6	NA	A	1015	1/1	0.97	0.12	38,38,38,38	0
6	NA	A	1018	1/1	0.97	0.22	40,40,40,40	0

6.5 Other polymers (i)

There are no such residues in this entry.