Full wwPDB X-ray Structure Validation Report ⓘ

Dec 15, 2020 – 11:26 am GMT

PDB ID	:	6RTI
Title	:	X-ray structure of human glutamate carboxypeptidase II (GCPII) in complex with aptamer A9g
Authors	:	Motlova, L.; Kolenko, P.; Barinka, C.
Deposited on	:	2019-05-24
Resolution	:	2.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see references ⓘ) were used in the production of this report:

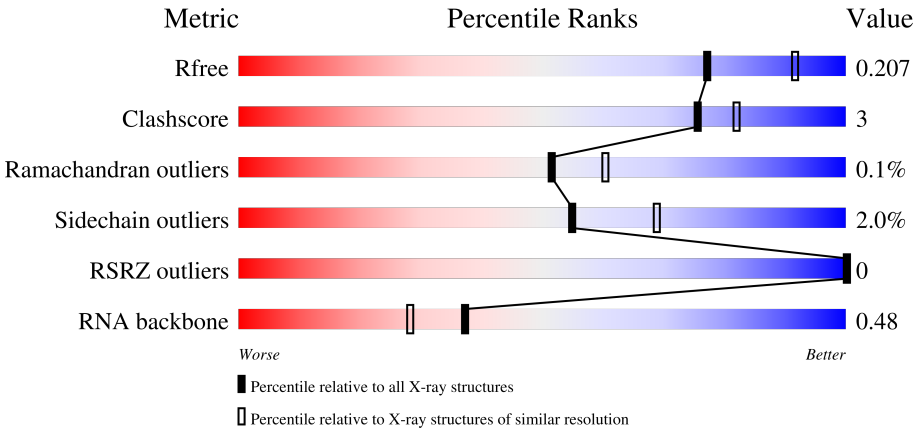
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.15.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.15.1

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 2.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)
RNA backbone	3102	1032 (2.60-1.80)

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	707	91% 7% ••
2	X	43	30% 60% 9%
3	B	3	100%
3	D	3	33% 67%

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Mol	Chain	Length	Quality of chain
3	G	3	33% 67%
4	C	2	100%
4	E	2	50% 50%
4	H	2	100%
5	F	4	25% 75%

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 7271 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.

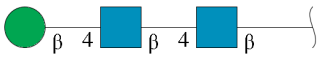
- Molecule 1 is a protein called Glutamate carboxypeptidase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	693	Total	C	N	O	S	0	15	0
			5575	3583	933	1040	19			

- Molecule 2 is a RNA chain called Aptamer A9g, RNA (43-MER).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	X	43	Total	C	F	N	O	P	0	3	0
			974	438	22	176	293	45			

- Molecule 3 is an oligosaccharide called 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
3	B	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	D	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	G	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 4 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
4	C	2	Total C N O 28 16 2 10	0	0	0
4	E	2	Total C N O 28 16 2 10	0	0	0
4	H	2	Total C N O 28 16 2 10	0	0	0

- Molecule 5 is an oligosaccharide called 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
5	F	4	Total C N O 50 28 2 20	0	0	0

- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	2	Total Zn 2 2	0	0

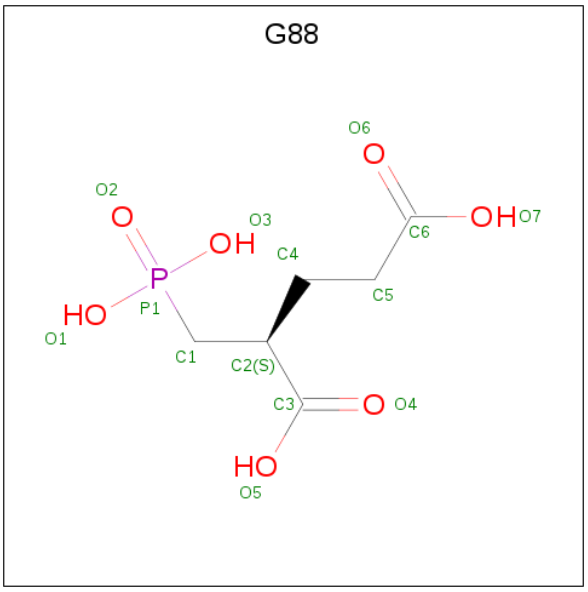
- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total Cl 1 1	0	0

- Molecule 8 is CALCIUM ION (three-letter code: CA) (formula: Ca).

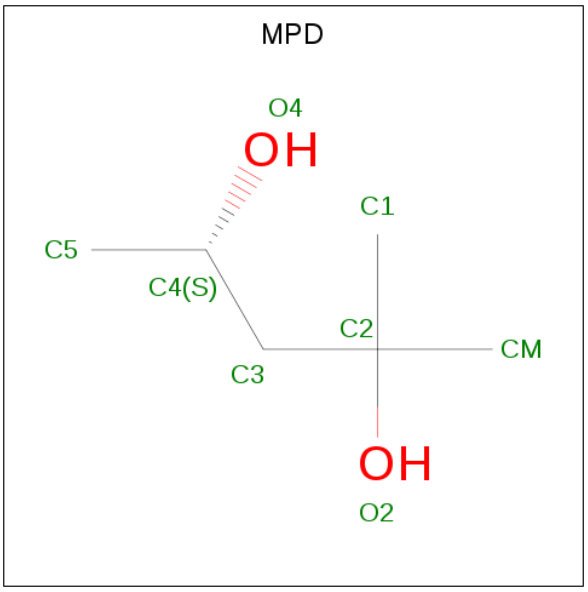
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total Ca 1 1	0	0

- Molecule 9 is (2S)-2-(PHOSPHONOMETHYL)PENTANEDIOIC ACID (three-letter code: G88) (formula: $C_6H_{11}O_7P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	A	1	Total	C	O	P	0	0
			14	6	7	1		

- Molecule 10 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total	C	O	0	0
			8	6	2		
10	A	1	Total	C	O	0	0
			8	6	2		

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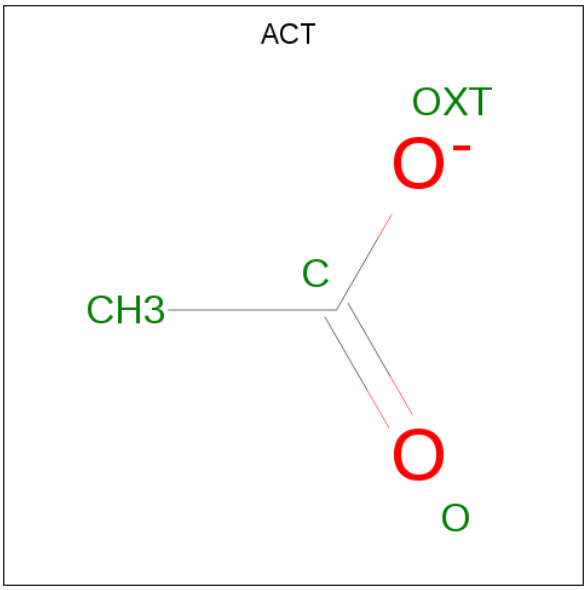
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	1	Total C O 8 6 2	0	0
10	X	1	Total C O 8 6 2	0	0
10	X	1	Total C O 8 6 2	0	0
10	X	1	Total C O 8 6 2	0	0

- Molecule 11 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



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

- Molecule 12 is water.

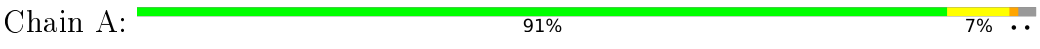
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	321	Total O 321 321	0	1
12	X	80	Total O 80 80	0	1

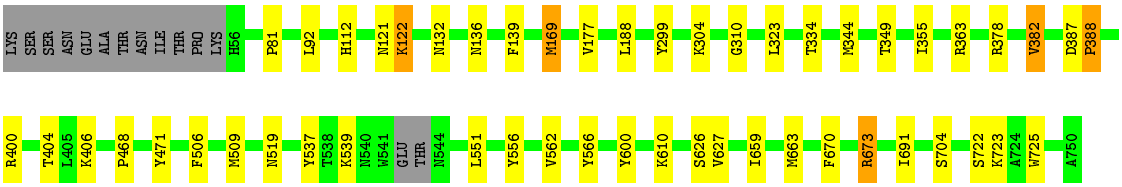
3 Residue-property plots (i)

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: Glutamate carboxypeptidase 2

Chain A:



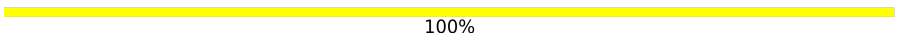


• Molecule 2: Aptamer A9g, RNA (43-MER)

Chain X:

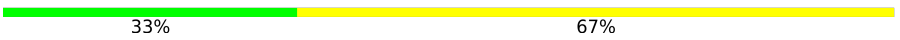
• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain B:



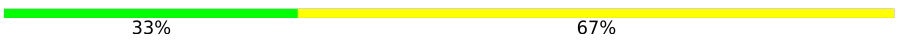
• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:



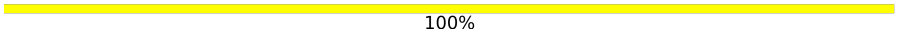
• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:



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

Chain C:

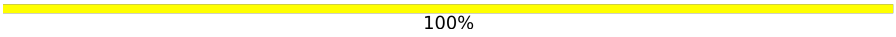


• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:

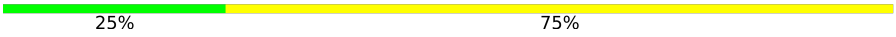
• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:



• Molecule 5: 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:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	121.10Å 121.10Å 216.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	105.66 – 2.20 105.66 – 2.20	Depositor EDS
% Data completeness (in resolution range)	100.0 (105.66-2.20) 100.0 (105.66-2.20)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.72 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.192 , 0.217 0.202 , 0.207	Depositor DCC
R_{free} test set	4036 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å^2)	36.2	Xtriage
Anisotropy	0.507	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 39.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	7271	wwPDB-VP
Average B, all atoms (Å^2)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.86% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, BMA, NAG, CL, G88, CA, MPD, CFZ, ACT, UFT, MAN

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	0.65	0/5787	0.77	1/7840 (0.0%)
2	X	0.39	0/603	0.74	0/938
All	All	0.63	0/6390	0.76	1/8778 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	673	ARG	CG-CD-NE	-5.24	100.80	111.80

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5575	0	5436	29	0
2	X	974	0	476	12	0
3	B	39	0	34	0	0
3	D	39	0	34	0	0
3	G	39	0	34	0	0
4	C	28	0	25	0	0
4	E	28	0	25	0	0
4	H	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	F	50	0	43	0	0
6	A	2	0	0	0	0
7	A	1	0	0	0	0
8	A	1	0	0	0	0
9	A	14	0	8	0	0
10	A	24	0	42	0	0
10	X	24	0	42	0	0
11	A	4	0	3	0	0
12	A	321	0	0	1	0
12	X	80	0	0	1	0
All	All	7271	0	6227	40	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 3.

All (40) 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)
2:X:9[A]:A:N6	12:X:201:HOH:O	1.93	1.02
2:X:7[B]:G:H5"	2:X:8[B]:A:H5'	1.49	0.93
1:A:122[A]:LYS:H	1:A:122[A]:LYS:HE3	1.34	0.91
1:A:122[A]:LYS:H	1:A:122[A]:LYS:CE	2.05	0.69
2:X:7[B]:G:H5'	2:X:8[B]:A:H8	1.59	0.67
1:A:132:ASN:HD21	1:A:136:ASN:HB2	1.64	0.62
1:A:400:ARG:O	1:A:404:THR:HG23	2.00	0.61
1:A:363[B]:ARG:HD2	12:A:1303:HOH:O	1.98	0.60
1:A:610:LYS:HE2	2:X:9[B]:A:C2	2.42	0.55
1:A:177:VAL:HG12	1:A:188:LEU:CD1	2.37	0.53
1:A:310:GLY:HA2	1:A:334:THR:HG23	1.91	0.52
2:X:9[A]:A:H8	2:X:9[A]:A:H5'	1.76	0.51
1:A:121:ASN:HA	1:A:122[A]:LYS:HE3	1.92	0.50
2:X:7[B]:G:H4'	2:X:8[B]:A:OP2	2.11	0.50
1:A:659:ILE:O	1:A:663[B]:MET:HG3	2.12	0.50
2:X:23:CFZ:H2'	2:X:24:UFT:O4'	2.12	0.50
1:A:177:VAL:HG12	1:A:188:LEU:HD11	1.94	0.49
1:A:132:ASN:ND2	1:A:136:ASN:HB2	2.29	0.47
1:A:169:MET:HA	1:A:344:MET:O	2.14	0.46
1:A:691:ILE:O	1:A:704:SER:HA	2.15	0.46
2:X:7[B]:G:H5'	2:X:8[B]:A:C8	2.47	0.45
1:A:506:PHE:HB3	1:A:509:MET:HG3	1.97	0.45
2:X:9[A]:A:H5'	2:X:9[A]:A:C8	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:PRO:HA	1:A:382:VAL:O	2.17	0.44
2:X:7[B]:G:H5"	2:X:8[B]:A:C5'	2.35	0.44
1:A:551:LEU:HD22	1:A:556:TYR:HB2	1.99	0.43
1:A:387:ASP:HA	1:A:388:PRO:HA	1.88	0.42
1:A:139:PHE:CE1	1:A:304:LYS:HG3	2.54	0.42
1:A:468:PRO:HA	1:A:471:TYR:CD1	2.55	0.41
1:A:670:PHE:HD1	1:A:673:ARG:HG3	1.85	0.41
1:A:627:VAL:HG21	1:A:725:TRP:CE3	2.55	0.41
1:A:673:ARG:NH1	1:A:673:ARG:HG2	2.36	0.41
2:X:17:UFT:O2	2:X:31:A:C2	2.74	0.41
1:A:468:PRO:HA	1:A:471:TYR:CE1	2.56	0.41
2:X:33:UFT:O5'	2:X:33:UFT:H6	2.21	0.41
1:A:562:VAL:HA	1:A:566:TYR:HB2	2.03	0.40
1:A:299:TYR:HB2	1:A:323:LEU:HD21	2.04	0.40
1:A:112:HIS:HA	1:A:355:ILE:O	2.22	0.40
1:A:92:LEU:HG	1:A:378:ARG:HD2	2.04	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	704/707 (100%)	683 (97%)	20 (3%)	1 (0%)	51 60

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	382	VAL

5.3.2 Protein sidechains

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	605/603 (100%)	592 (98%)	13 (2%)	53 67

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	122[A]	LYS
1	A	122[B]	LYS
1	A	169	MET
1	A	349	THR
1	A	388	PRO
1	A	406	LYS
1	A	519	ASN
1	A	537	TYR
1	A	539	LYS
1	A	600	TYR
1	A	626	SER
1	A	722	SER
1	A	723	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	X	17/43 (39%)	4 (23%)	0

All (4) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	X	12	A
2	X	25	A
2	X	27	A

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Mol	Chain	Res	Type
2	X	30	A

There are no RNA pucker outliers to report.

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

22 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	CFZ	X	15	2	15,21,22	1.11	0	17,30,33	1.07	1 (5%)
2	CFZ	X	34	2	15,21,22	1.31	1 (6%)	17,30,33	1.34	2 (11%)
2	CFZ	X	42	2	15,21,22	0.92	1 (6%)	17,30,33	1.05	1 (5%)
2	UFT	X	26	2	14,21,22	1.23	2 (14%)	14,30,33	1.16	1 (7%)
2	CFZ	X	5	2	15,21,22	0.83	1 (6%)	17,30,33	1.46	1 (5%)
2	UFT	X	17	2	14,21,22	1.36	3 (21%)	14,30,33	1.09	2 (14%)
2	CFZ	X	16	2	15,21,22	1.24	2 (13%)	17,30,33	1.34	1 (5%)
2	CFZ	X	37	2	15,21,22	0.97	1 (6%)	17,30,33	1.40	1 (5%)
2	UFT	X	35	2	14,21,22	1.27	3 (21%)	14,30,33	0.88	0
2	CFZ	X	43	2	15,21,22	1.00	1 (6%)	17,30,33	1.09	1 (5%)
2	UFT	X	21	2	14,21,22	0.99	1 (7%)	14,30,33	1.02	1 (7%)
2	UFT	X	33	2	14,21,22	1.48	4 (28%)	14,30,33	1.10	1 (7%)
2	CFZ	X	20	2	15,21,22	1.03	1 (6%)	17,30,33	1.84	4 (23%)
2	CFZ	X	41	2	15,21,22	1.00	1 (6%)	17,30,33	1.39	2 (11%)
2	UFT	X	39	2	14,21,22	1.27	1 (7%)	14,30,33	0.81	0
2	UFT	X	22	2	14,21,22	0.96	1 (7%)	14,30,33	0.82	0
2	CFZ	X	23	2	15,21,22	0.88	1 (6%)	17,30,33	1.43	1 (5%)
2	UFT	X	24	2	14,21,22	1.08	1 (7%)	14,30,33	1.01	0
2	UFT	X	29	2	14,21,22	1.20	2 (14%)	14,30,33	1.14	1 (7%)
2	CFZ	X	28	2	15,21,22	1.00	0	17,30,33	1.41	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	CFZ	X	6	2	15,21,22	0.87	1 (6%)	17,30,33	1.36	2 (11%)
2	UFT	X	40	2	14,21,22	1.32	1 (7%)	14,30,33	1.02	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	CFZ	X	15	2	-	1/5/25/26	0/2/2/2
2	CFZ	X	34	2	-	0/5/25/26	0/2/2/2
2	CFZ	X	42	2	-	0/5/25/26	0/2/2/2
2	UFT	X	26	2	-	4/5/25/26	0/2/2/2
2	CFZ	X	5	2	-	0/5/25/26	0/2/2/2
2	UFT	X	17	2	-	0/5/25/26	0/2/2/2
2	CFZ	X	16	2	-	0/5/25/26	0/2/2/2
2	CFZ	X	37	2	-	0/5/25/26	0/2/2/2
2	UFT	X	35	2	-	0/5/25/26	0/2/2/2
2	CFZ	X	43	2	-	0/5/25/26	0/2/2/2
2	UFT	X	21	2	-	0/5/25/26	0/2/2/2
2	UFT	X	33	2	-	0/5/25/26	0/2/2/2
2	CFZ	X	20	2	-	0/5/25/26	0/2/2/2
2	CFZ	X	41	2	-	0/5/25/26	0/2/2/2
2	UFT	X	39	2	-	0/5/25/26	0/2/2/2
2	UFT	X	22	2	-	0/5/25/26	0/2/2/2
2	CFZ	X	23	2	-	0/5/25/26	0/2/2/2
2	UFT	X	24	2	-	0/5/25/26	0/2/2/2
2	UFT	X	29	2	-	1/5/25/26	0/2/2/2
2	CFZ	X	28	2	-	2/5/25/26	0/2/2/2
2	CFZ	X	6	2	-	0/5/25/26	0/2/2/2
2	UFT	X	40	2	-	0/5/25/26	0/2/2/2

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	X	17	UFT	O4'-C1'	3.55	1.46	1.41
2	X	20	CFZ	O4'-C1'	3.10	1.45	1.41
2	X	40	UFT	O4'-C1'	3.07	1.45	1.41
2	X	39	UFT	O4'-C1'	2.99	1.45	1.41
2	X	43	CFZ	O4'-C1'	2.98	1.45	1.41
2	X	34	CFZ	C2'-C1'	-2.93	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	X	33	UFT	C2'-C3'	-2.64	1.49	1.52
2	X	16	CFZ	O4'-C1'	2.51	1.44	1.41
2	X	23	CFZ	O4'-C1'	2.51	1.44	1.41
2	X	35	UFT	O4'-C1'	2.46	1.44	1.41
2	X	41	CFZ	O4'-C1'	2.46	1.44	1.41
2	X	26	UFT	O4'-C1'	2.39	1.44	1.41
2	X	29	UFT	C2'-C3'	-2.35	1.49	1.52
2	X	21	UFT	C2-N3	-2.30	1.33	1.38
2	X	33	UFT	O4'-C1'	2.28	1.44	1.41
2	X	29	UFT	C2-N3	-2.28	1.33	1.38
2	X	42	CFZ	O4'-C1'	2.20	1.44	1.41
2	X	33	UFT	C2-N3	-2.19	1.33	1.38
2	X	37	CFZ	O4'-C1'	2.14	1.44	1.41
2	X	26	UFT	F2'-C2'	-2.13	1.35	1.40
2	X	22	UFT	O4'-C1'	2.12	1.44	1.41
2	X	35	UFT	C2-N3	-2.11	1.34	1.38
2	X	24	UFT	C2-N3	-2.10	1.34	1.38
2	X	6	CFZ	O4'-C1'	2.08	1.44	1.41
2	X	35	UFT	C2'-C1'	-2.08	1.50	1.53
2	X	17	UFT	F2'-C2'	-2.08	1.35	1.40
2	X	16	CFZ	C2'-C1'	-2.06	1.50	1.53
2	X	33	UFT	C2'-C1'	-2.02	1.50	1.53
2	X	17	UFT	C2-N3	-2.00	1.34	1.38
2	X	5	CFZ	O4'-C1'	2.00	1.43	1.41

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	X	20	CFZ	C2-N3-C4	4.71	121.12	116.34
2	X	37	CFZ	C2-N3-C4	4.49	120.89	116.34
2	X	5	CFZ	C2-N3-C4	4.40	120.80	116.34
2	X	6	CFZ	C2-N3-C4	4.22	120.62	116.34
2	X	23	CFZ	C2-N3-C4	4.06	120.45	116.34
2	X	16	CFZ	C2-N3-C4	4.01	120.40	116.34
2	X	34	CFZ	C2-N3-C4	3.94	120.34	116.34
2	X	28	CFZ	C2-N3-C4	3.87	120.26	116.34
2	X	41	CFZ	C2-N3-C4	3.82	120.21	116.34
2	X	43	CFZ	C2-N3-C4	3.38	119.76	116.34
2	X	42	CFZ	C2-N3-C4	3.08	119.46	116.34
2	X	15	CFZ	C2-N3-C4	3.05	119.43	116.34
2	X	17	UFT	C3'-C2'-C1'	2.83	106.56	103.13
2	X	20	CFZ	N4-C4-N3	2.66	120.70	116.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	X	6	CFZ	N4-C4-N3	2.39	120.27	116.49
2	X	20	CFZ	C2'-C3'-C4'	-2.37	99.34	102.40
2	X	33	UFT	O3'-C3'-C4'	2.33	117.78	111.05
2	X	20	CFZ	C5-C4-N3	-2.31	119.05	121.72
2	X	26	UFT	O4'-C4'-C5'	2.22	116.68	109.37
2	X	21	UFT	C2'-C3'-C4'	-2.20	99.56	102.40
2	X	29	UFT	C2'-C3'-C4'	-2.13	99.66	102.40
2	X	41	CFZ	N4-C4-N3	2.05	119.73	116.49
2	X	34	CFZ	N4-C4-N3	2.04	119.72	116.49
2	X	17	UFT	F2'-C2'-C1'	-2.00	104.91	109.08

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	X	26	UFT	C2'-C1'-N1-C6
2	X	26	UFT	O4'-C1'-N1-C6
2	X	26	UFT	C3'-C4'-C5'-O5'
2	X	29	UFT	O4'-C1'-N1-C6
2	X	28	CFZ	C2'-C1'-N1-C6
2	X	28	CFZ	O4'-C1'-N1-C6
2	X	26	UFT	O4'-C4'-C5'-O5'
2	X	15	CFZ	O4'-C4'-C5'-O5'

There are no ring outliers.

4 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	X	17	UFT	1	0
2	X	33	UFT	1	0
2	X	23	CFZ	1	0
2	X	24	UFT	1	0

5.5 Carbohydrates (i)

19 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	B	1	1,3	14,14,15	0.44	0	17,19,21	1.17	1 (5%)
3	NAG	B	2	3	14,14,15	0.37	0	17,19,21	1.71	4 (23%)
3	BMA	B	3	3	11,11,12	0.36	0	15,15,17	1.25	2 (13%)
4	NAG	C	1	1,4	14,14,15	0.49	0	17,19,21	1.22	2 (11%)
4	NAG	C	2	4	14,14,15	0.36	0	17,19,21	1.52	2 (11%)
3	NAG	D	1	1,3	14,14,15	0.47	0	17,19,21	1.15	3 (17%)
3	NAG	D	2	3	14,14,15	0.33	0	17,19,21	1.05	0
3	BMA	D	3	3	11,11,12	0.52	0	15,15,17	2.13	3 (20%)
4	NAG	E	1	1,4	14,14,15	0.67	0	17,19,21	1.01	0
4	NAG	E	2	4	14,14,15	0.56	0	17,19,21	1.49	2 (11%)
5	NAG	F	1	1,5	14,14,15	0.40	0	17,19,21	0.95	1 (5%)
5	NAG	F	2	5	14,14,15	0.36	0	17,19,21	0.65	0
5	BMA	F	3	5	11,11,12	0.36	0	15,15,17	0.94	1 (6%)
5	MAN	F	4	5	11,11,12	0.60	0	15,15,17	2.32	5 (33%)
3	NAG	G	1	1,3	14,14,15	0.66	0	17,19,21	0.86	0
3	NAG	G	2	3	14,14,15	0.38	0	17,19,21	1.47	3 (17%)
3	BMA	G	3	3	11,11,12	0.60	0	15,15,17	1.48	3 (20%)
4	NAG	H	1	1,4	14,14,15	0.37	0	17,19,21	1.13	1 (5%)
4	NAG	H	2	4	14,14,15	0.47	0	17,19,21	1.49	2 (11%)

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	B	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	B	2	3	-	0/6/23/26	0/1/1/1
3	BMA	B	3	3	-	2/2/19/22	0/1/1/1
4	NAG	C	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	C	2	4	-	1/6/23/26	0/1/1/1
3	NAG	D	1	1,3	-	0/6/23/26	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
4	NAG	E	1	1,4	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	E	2	4	-	2/6/23/26	0/1/1/1
5	NAG	F	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	F	2	5	-	0/6/23/26	0/1/1/1
5	BMA	F	3	5	-	0/2/19/22	0/1/1/1
5	MAN	F	4	5	-	2/2/19/22	0/1/1/1
3	NAG	G	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	G	2	3	-	0/6/23/26	0/1/1/1
3	BMA	G	3	3	-	1/2/19/22	0/1/1/1
4	NAG	H	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	H	2	4	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	F	4	MAN	C1-C2-C3	5.90	116.92	109.67
3	D	3	BMA	O5-C1-C2	5.46	119.20	110.77
4	H	2	NAG	O5-C1-C2	4.74	118.77	111.29
4	C	2	NAG	C1-O5-C5	4.44	118.20	112.19
3	B	2	NAG	O5-C1-C2	4.26	118.01	111.29
5	F	4	MAN	O5-C1-C2	4.26	117.34	110.77
4	E	2	NAG	O5-C5-C6	4.22	113.82	107.20
3	D	3	BMA	C1-O5-C5	4.08	117.72	112.19
3	D	3	BMA	C1-C2-C3	3.89	114.45	109.67
5	F	4	MAN	C1-O5-C5	3.44	116.85	112.19
3	G	3	BMA	C1-O5-C5	3.34	116.72	112.19
3	G	2	NAG	C3-C4-C5	3.12	115.81	110.24
3	B	2	NAG	C4-C3-C2	3.11	115.57	111.02
3	B	1	NAG	O4-C4-C3	-2.93	103.58	110.35
4	C	2	NAG	C3-C4-C5	2.92	115.45	110.24
4	C	1	NAG	C8-C7-N2	2.76	120.77	116.10
3	B	3	BMA	O5-C1-C2	2.73	114.99	110.77
3	D	1	NAG	O4-C4-C3	-2.73	104.05	110.35
4	E	2	NAG	C4-C3-C2	2.66	114.92	111.02
3	B	2	NAG	O5-C5-C4	-2.66	104.36	110.83
4	H	1	NAG	O5-C5-C6	2.63	111.33	107.20
3	G	2	NAG	C1-C2-N2	2.56	114.86	110.49
4	H	2	NAG	C1-O5-C5	2.53	115.62	112.19
3	G	3	BMA	O5-C1-C2	2.43	114.53	110.77
5	F	4	MAN	O5-C5-C6	2.38	110.93	107.20
5	F	4	MAN	C3-C4-C5	-2.26	106.21	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	G	2	NAG	O5-C1-C2	-2.23	107.76	111.29
5	F	1	NAG	O5-C1-C2	2.23	114.81	111.29
3	G	3	BMA	O3-C3-C2	-2.19	105.80	109.99
3	B	2	NAG	O5-C5-C6	2.16	110.59	107.20
3	B	3	BMA	C1-O5-C5	2.12	115.06	112.19
4	C	1	NAG	O5-C5-C6	2.09	110.48	107.20
3	D	1	NAG	C1-O5-C5	2.07	114.99	112.19
5	F	3	BMA	C1-O5-C5	2.06	114.99	112.19
3	D	1	NAG	C3-C4-C5	2.01	113.82	110.24

There are no chirality outliers.

All (10) torsion outliers are listed below:

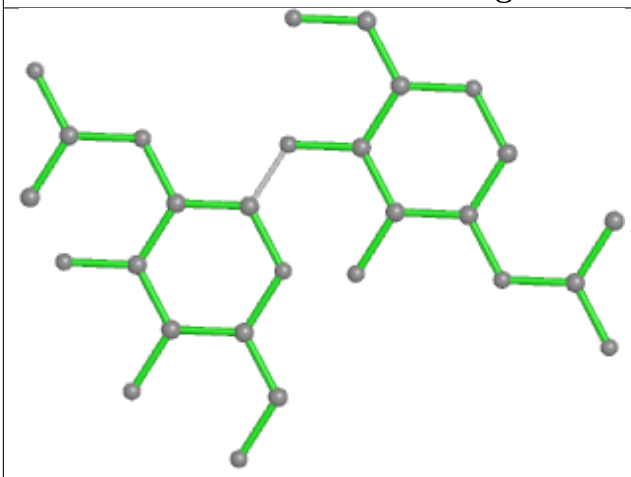
Mol	Chain	Res	Type	Atoms
5	F	4	MAN	O5-C5-C6-O6
4	C	1	NAG	C8-C7-N2-C2
4	C	1	NAG	O7-C7-N2-C2
4	E	2	NAG	O5-C5-C6-O6
5	F	4	MAN	C4-C5-C6-O6
4	E	2	NAG	C4-C5-C6-O6
4	C	2	NAG	C4-C5-C6-O6
3	G	3	BMA	O5-C5-C6-O6
3	B	3	BMA	C4-C5-C6-O6
3	B	3	BMA	O5-C5-C6-O6

There are no ring outliers.

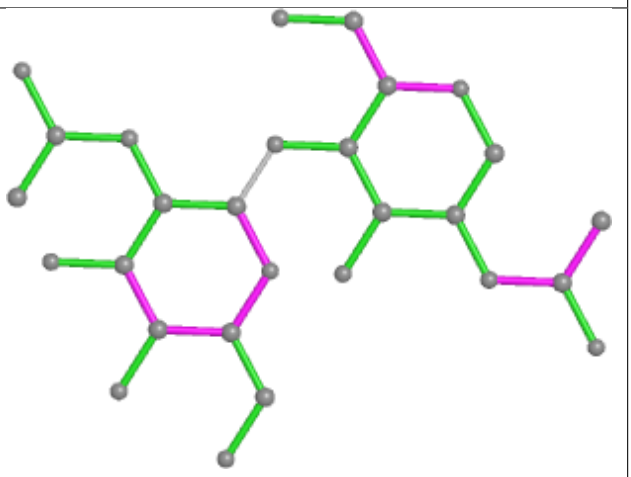
No monomer is involved in short contacts.

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

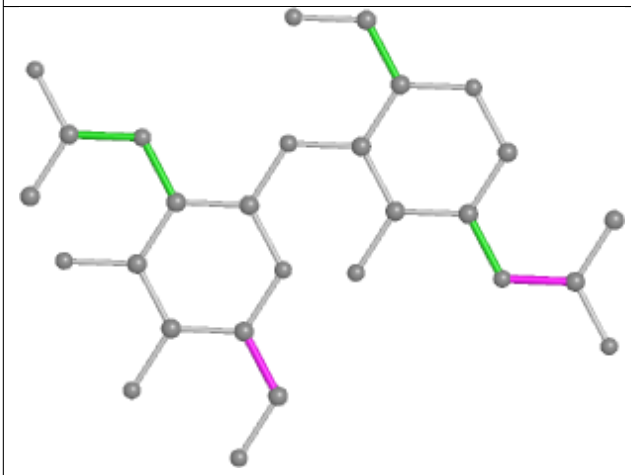
Oligosaccharide Chain C



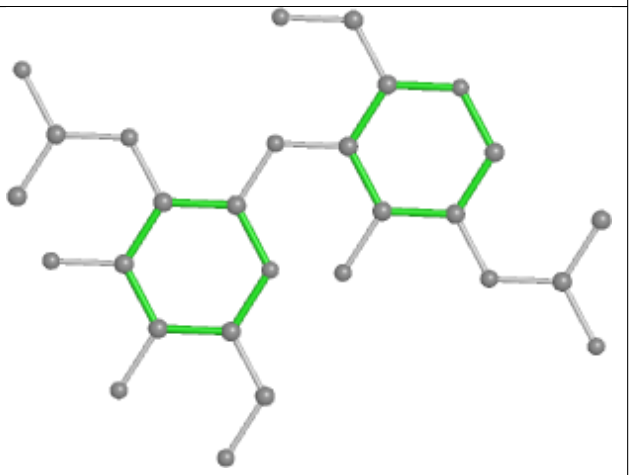
Bond lengths



Bond angles

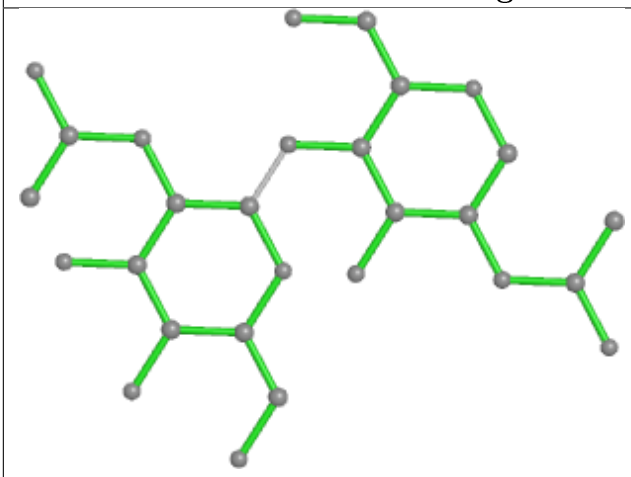


Torsions

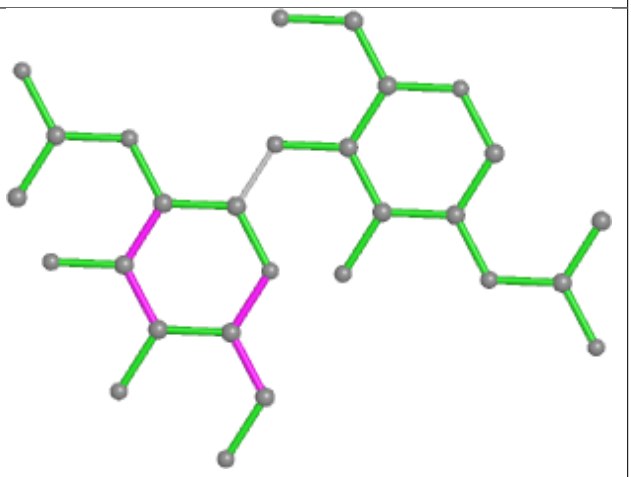


Rings

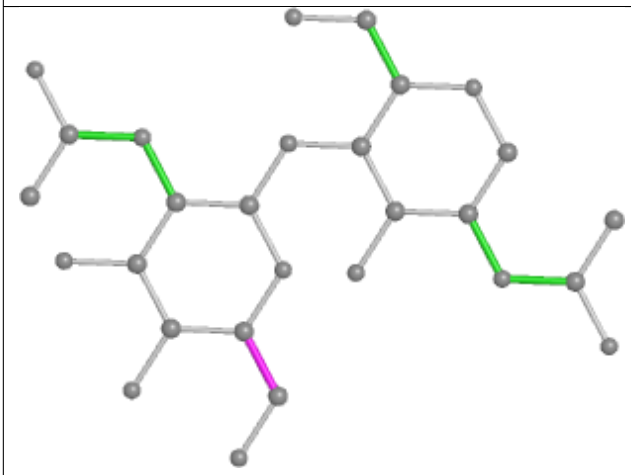
Oligosaccharide Chain E



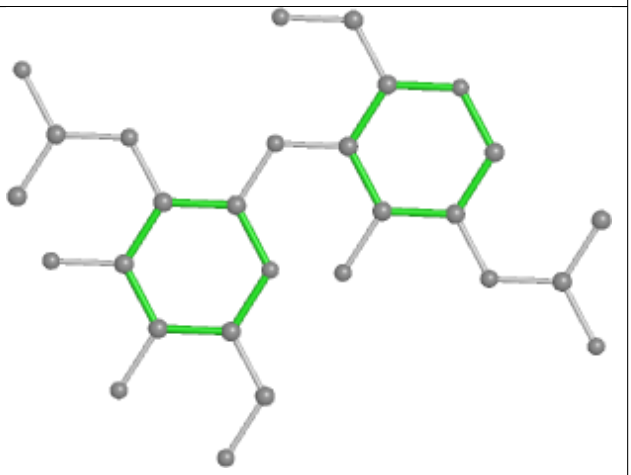
Bond lengths



Bond angles

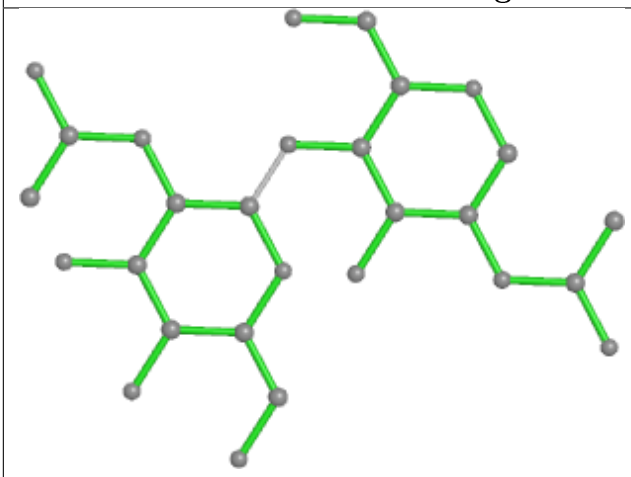


Torsions

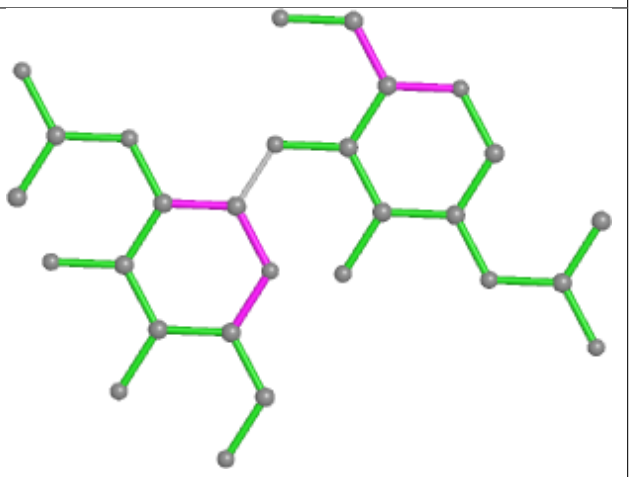


Rings

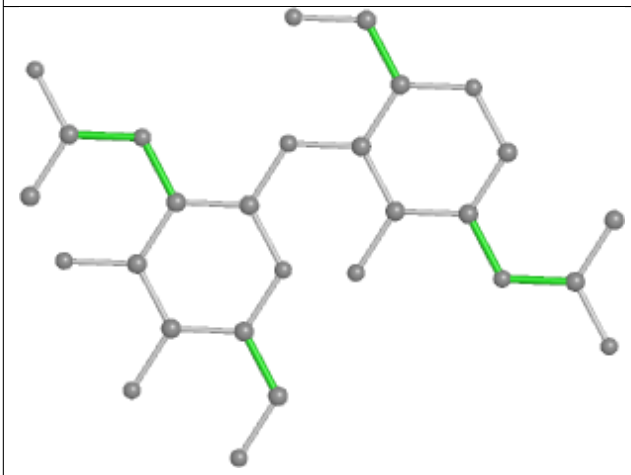
Oligosaccharide Chain H



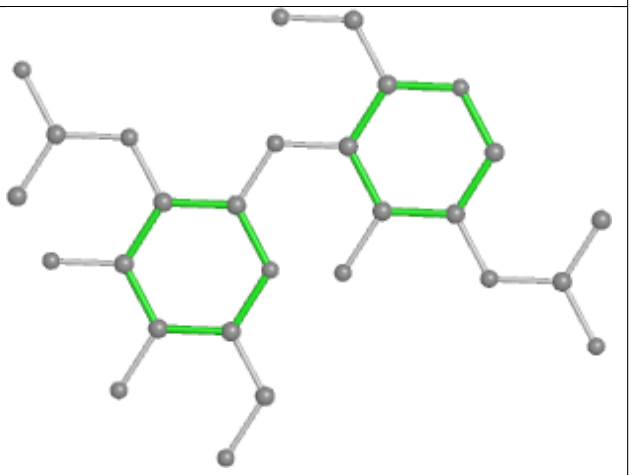
Bond lengths



Bond angles

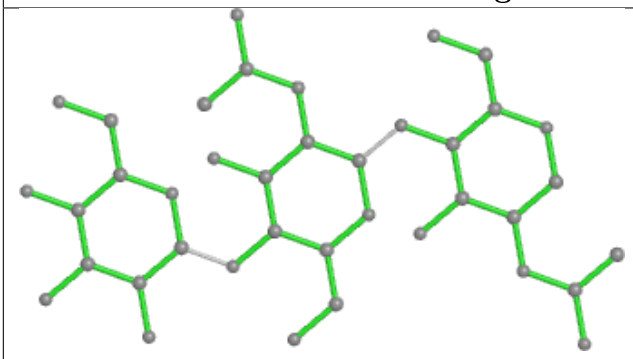


Torsions

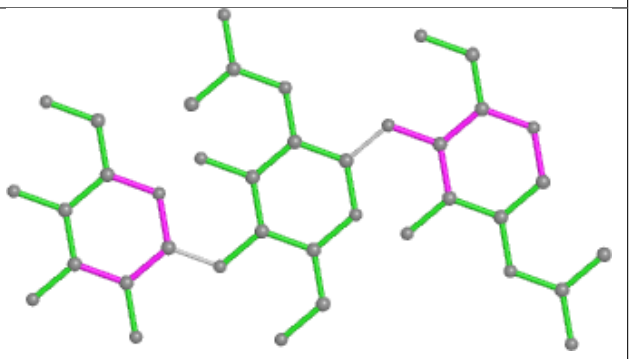


Rings

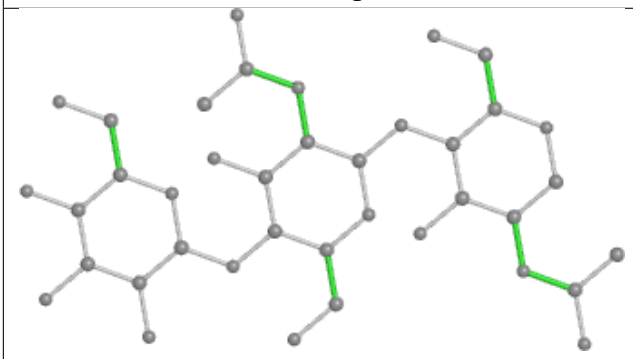
Oligosaccharide Chain D



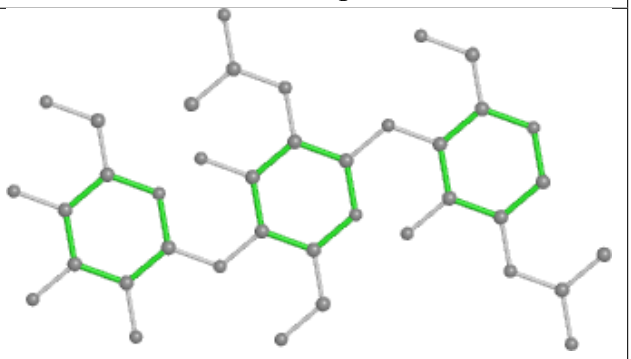
Bond lengths



Bond angles

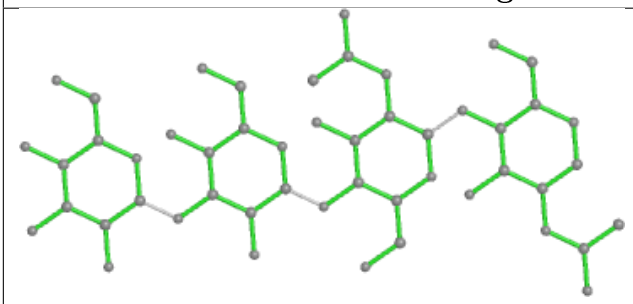


Torsions

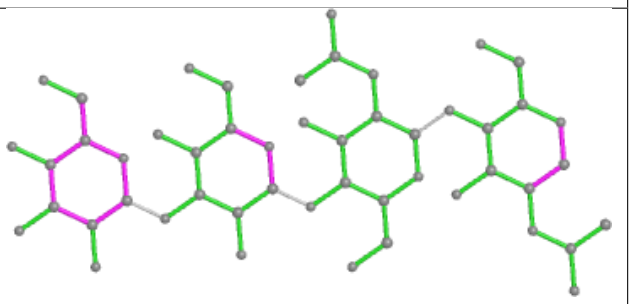


Rings

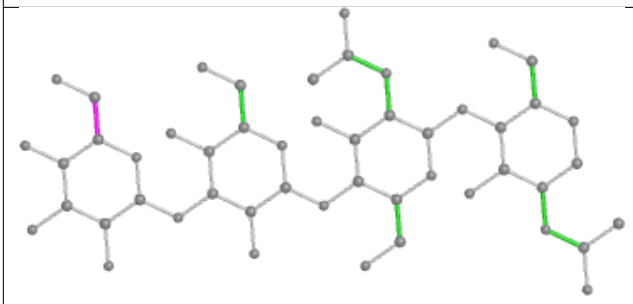
Oligosaccharide Chain F



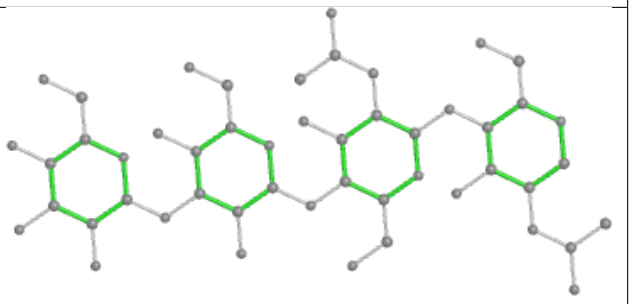
Bond lengths



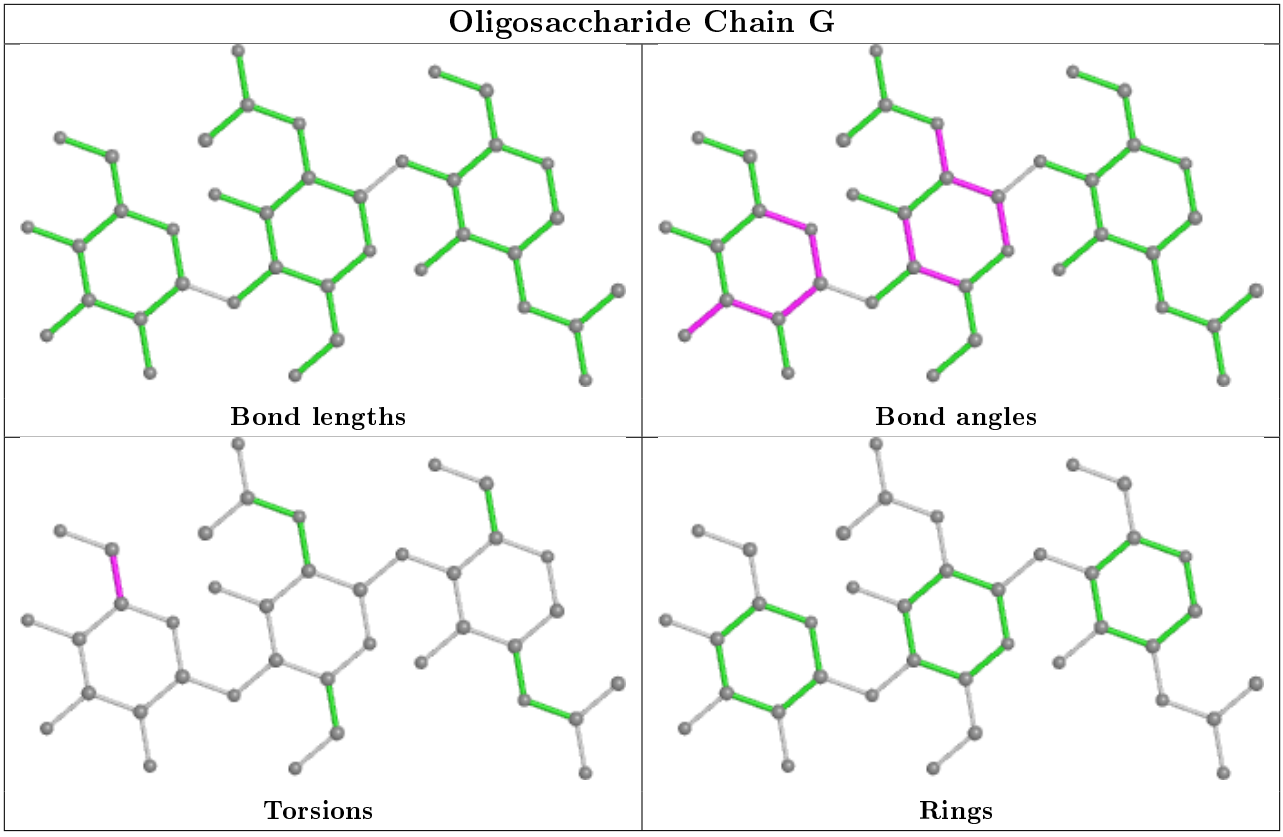
Bond angles



Torsions



Rings



5.6 Ligand geometry

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 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	$\#\|Z\| > 2$
11	ACT	A	928	-	1,3,3	3.85	1 (100%)	0,3,3	0.00	-
9	G88	A	905	6	6,13,13	1.87	2 (33%)	9,18,18	2.60	1 (11%)
10	MPD	A	927	-	7,7,7	0.24	0	9,10,10	0.72	0
10	MPD	A	926	-	7,7,7	0.20	0	9,10,10	0.74	0
10	MPD	X	101	-	7,7,7	0.19	0	9,10,10	0.40	0
10	MPD	A	925	-	7,7,7	0.16	0	9,10,10	0.46	0
10	MPD	X	102	-	7,7,7	0.25	0	9,10,10	0.39	0
10	MPD	X	103	-	7,7,7	0.14	0	9,10,10	0.44	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
10	MPD	X	103	-	-	1/5/5/5	-
10	MPD	A	927	-	-	0/5/5/5	-
9	G88	A	905	6	-	1/8/14/14	-
10	MPD	A	926	-	-	1/5/5/5	-
10	MPD	X	101	-	-	2/5/5/5	-
10	MPD	A	925	-	-	0/5/5/5	-
10	MPD	X	102	-	-	0/5/5/5	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	928	ACT	CH3-C	3.85	1.53	1.48
9	A	905	G88	P1-O2	-3.69	1.42	1.50
9	A	905	G88	P1-O3	-2.16	1.50	1.54

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	A	905	G88	O2-P1-C1	-6.74	99.06	111.54

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	A	926	MPD	C2-C3-C4-O4
9	A	905	G88	C2-C1-P1-O3
10	X	101	MPD	C2-C3-C4-C5
10	X	103	MPD	C2-C3-C4-C5
10	X	101	MPD	C2-C3-C4-O4

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	693/707 (98%)	-0.16	0	100	100	28, 41, 69, 100	1 (0%)
2	X	21/43 (48%)	-0.45	0	100	100	40, 55, 66, 81	0
All	All	714/750 (95%)	-0.17	0	100	100	28, 41, 69, 100	1 (0%)

There are no RSRZ outliers to report.

6.2 Non-standard residues in protein, DNA, RNA chains

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	CFZ	X	42	20/21	0.94	0.10	54,64,71,74	0
2	UFT	X	26	20/21	0.94	0.13	47,53,84,92	0
2	CFZ	X	20	20/21	0.94	0.13	48,67,75,76	0
2	CFZ	X	5	20/21	0.96	0.09	51,58,64,73	0
2	UFT	X	40	20/21	0.96	0.11	43,50,57,65	0
2	UFT	X	21	20/21	0.97	0.11	40,52,56,58	0
2	CFZ	X	37	20/21	0.97	0.09	56,59,62,63	0
2	CFZ	X	41	20/21	0.97	0.09	49,57,65,72	0
2	UFT	X	39	20/21	0.97	0.09	45,50,58,60	0
2	CFZ	X	6	20/21	0.97	0.09	50,59,64,67	0
2	CFZ	X	43	20/21	0.97	0.09	49,60,66,70	0
2	CFZ	X	15	20/21	0.98	0.11	36,43,46,47	0
2	UFT	X	22	20/21	0.98	0.10	37,42,44,46	0
2	CFZ	X	23	20/21	0.98	0.11	40,42,46,47	0
2	UFT	X	24	20/21	0.98	0.12	41,45,48,54	0
2	CFZ	X	28	20/21	0.98	0.11	37,38,43,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	UFT	X	35	20/21	0.98	0.10	44,54,57,58	0
2	UFT	X	17	20/21	0.98	0.12	35,37,40,42	0
2	UFT	X	29	20/21	0.99	0.13	36,39,47,48	0
2	CFZ	X	34	20/21	0.99	0.11	39,42,44,48	0
2	CFZ	X	16	20/21	0.99	0.12	38,41,45,45	0
2	UFT	X	33	20/21	0.99	0.12	39,42,44,45	0

6.3 Carbohydrates (i)

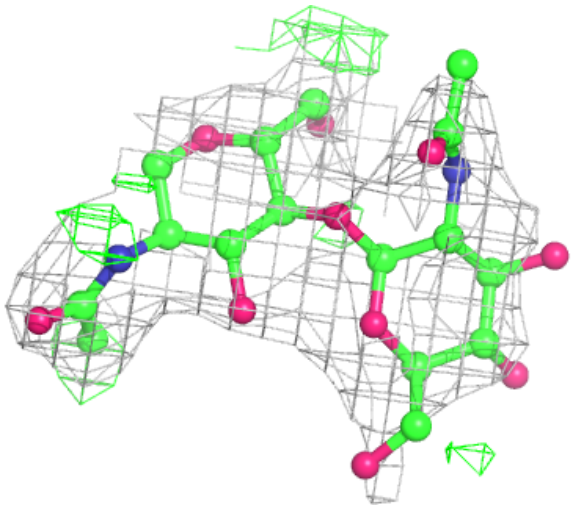
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

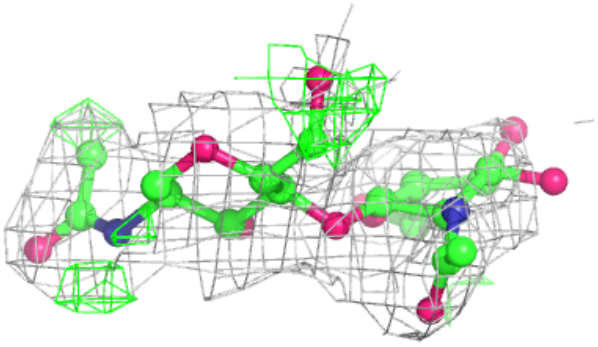
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	BMA	F	3	11/12	0.37	0.18	84,107,112,114	0
3	BMA	G	3	11/12	0.43	0.29	95,108,116,116	0
3	BMA	D	3	11/12	0.59	0.15	113,120,129,130	0
5	MAN	F	4	11/12	0.63	0.29	115,123,125,128	0
4	NAG	H	2	14/15	0.70	0.19	115,127,131,132	0
3	BMA	B	3	11/12	0.74	0.15	113,123,127,127	0
4	NAG	E	2	14/15	0.82	0.20	80,86,90,91	0
4	NAG	H	1	14/15	0.82	0.11	77,90,96,113	0
4	NAG	C	1	14/15	0.83	0.13	67,97,114,119	0
4	NAG	C	2	14/15	0.85	0.18	103,120,125,127	0
3	NAG	G	2	14/15	0.86	0.17	68,75,84,107	0
3	NAG	D	1	14/15	0.86	0.09	55,65,74,78	0
3	NAG	B	2	14/15	0.87	0.15	64,92,103,111	0
3	NAG	D	2	14/15	0.92	0.11	77,89,100,113	0
5	NAG	F	2	14/15	0.93	0.17	78,84,88,98	0
4	NAG	E	1	14/15	0.94	0.09	38,56,67,71	0
5	NAG	F	1	14/15	0.95	0.15	53,58,67,73	0
3	NAG	G	1	14/15	0.96	0.11	32,38,51,54	0
3	NAG	B	1	14/15	0.97	0.10	46,55,62,66	0

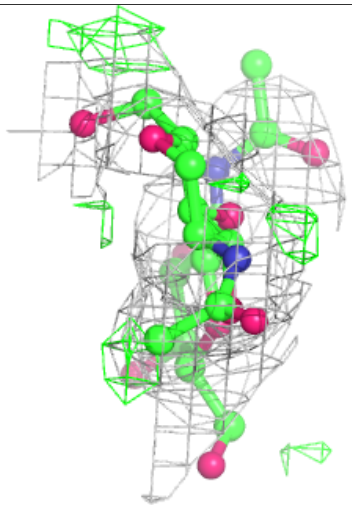
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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)

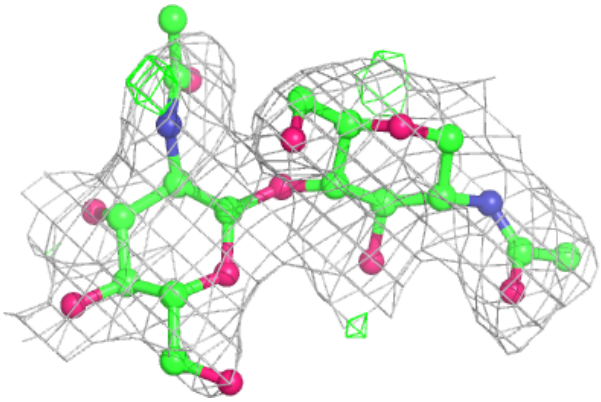


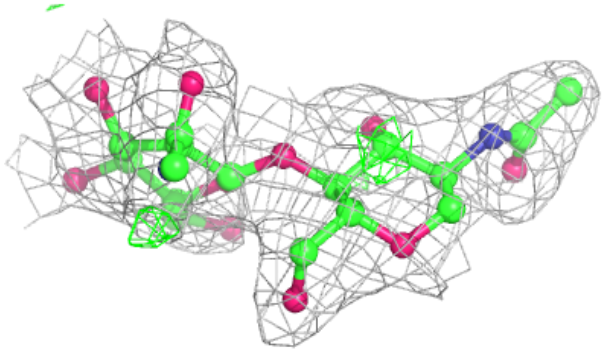


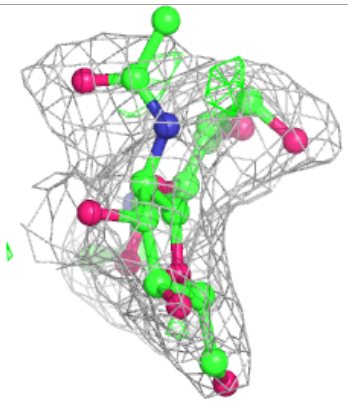


Electron density around Chain E:

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

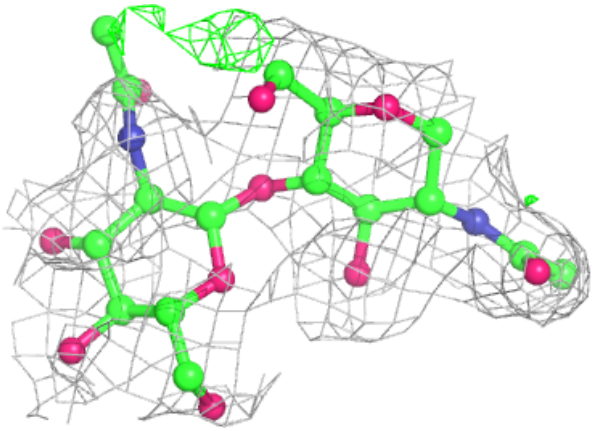


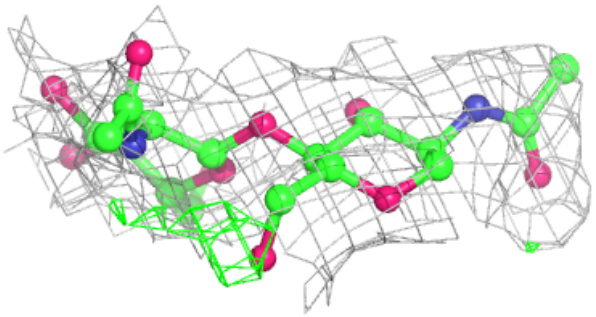


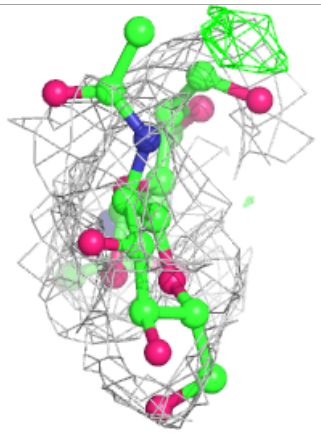


Electron density around Chain H:

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

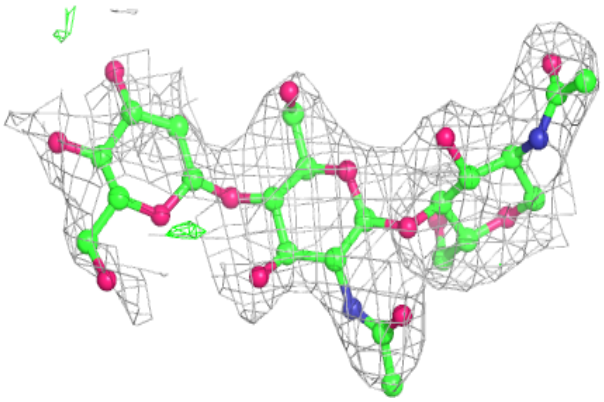


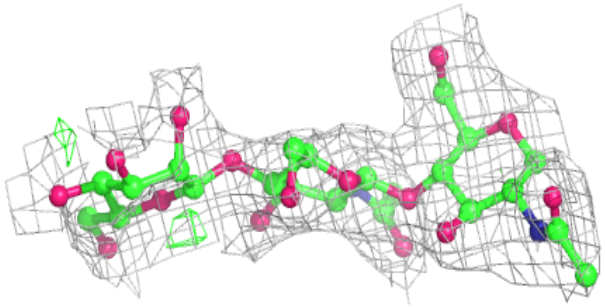


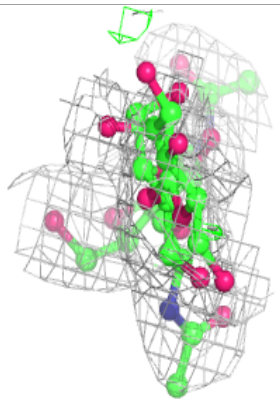


Electron density around Chain D:

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

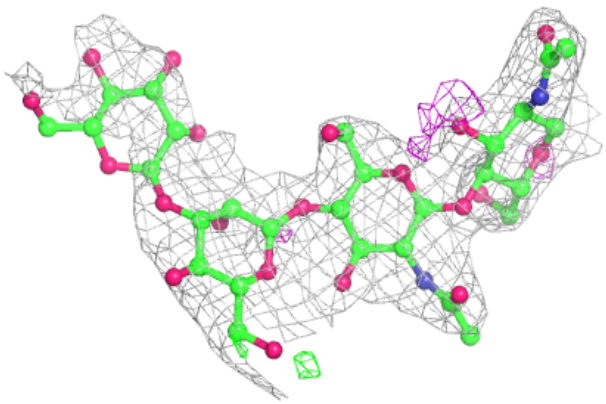


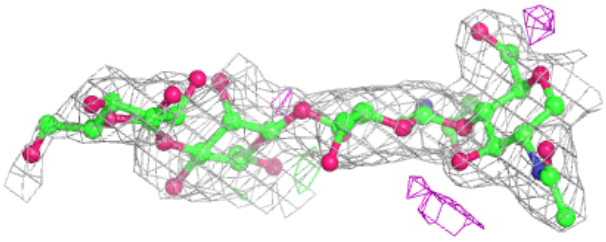


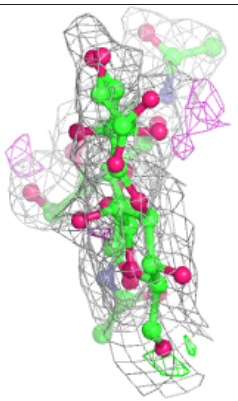


Electron density around Chain F:

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

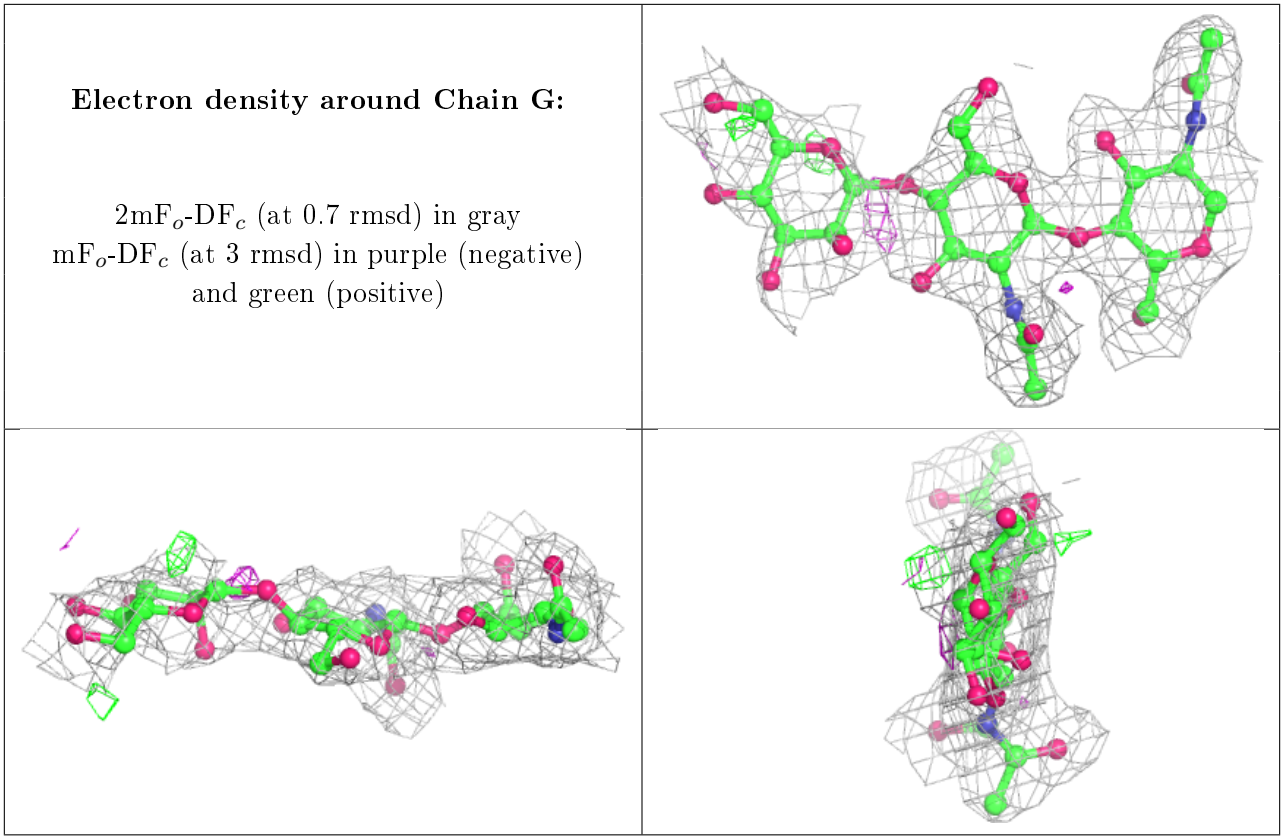






Electron density around Chain G:

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



6.4 Ligands

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
10	MPD	X	101	8/8	0.78	0.12	83,87,91,91	0
11	ACT	A	928	4/4	0.83	0.14	74,85,87,88	0
10	MPD	X	103	8/8	0.88	0.21	82,89,94,96	0
10	MPD	A	925	8/8	0.89	0.17	50,56,61,64	0
10	MPD	A	926	8/8	0.90	0.21	66,71,83,89	0
10	MPD	A	927	8/8	0.95	0.14	44,45,49,50	0
10	MPD	X	102	8/8	0.96	0.12	49,52,53,54	0
9	G88	A	905	14/14	0.98	0.13	34,36,38,38	0
7	CL	A	903	1/1	0.99	0.16	35,35,35,35	0
8	CA	A	904	1/1	0.99	0.17	32,32,32,32	0
6	ZN	A	901	1/1	1.00	0.18	34,34,34,34	0
6	ZN	A	902	1/1	1.00	0.19	33,33,33,33	0

6.5 Other polymers (i)

There are no such residues in this entry.