wwPDB X-ray Structure Validation Summary Report (i)

Aug 6, 2020 – 11:03 AM BST

PDB ID	:	6GFF
Title	:	Structure of GARP (LRRC32) in complex with latent TGF-beta1 and MHG-8 Fab
Authors	:	Merceron, R.; Lienart, S.; Vanderaa, C.; Colau, D.; Stockis, J.; Van Der Woning, B.; De Haard, H.; Saunders, M.; Coulie, P.G.; Savvides, S.N.; Lucas, S.
Deposited on	:	2018-04-30
Resolution	:	3.10 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 following versions of software and data (see references (1)) were used in the production of this report:

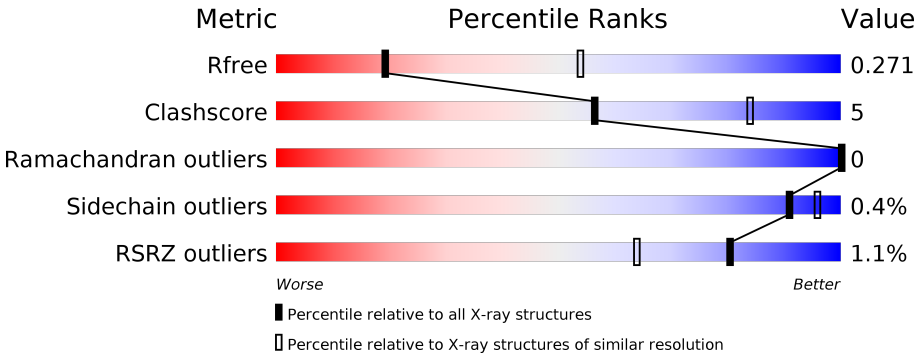
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

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 3.10 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	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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 on 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	249	% 61% 6% 33%
1	C	249	5% 77% 7% 16%
1	E	249	73% 16% 11%
1	G	249	76% 12% 12%
2	B	112	% 85% 15%
2	D	112	80% 18%

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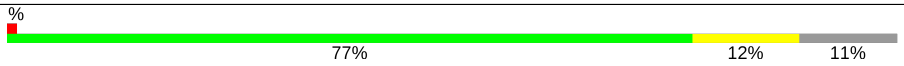
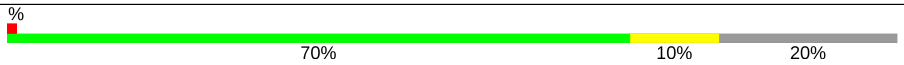
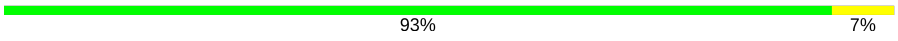
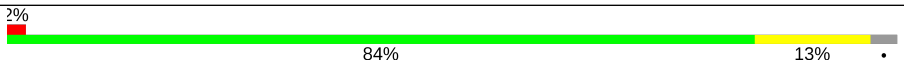
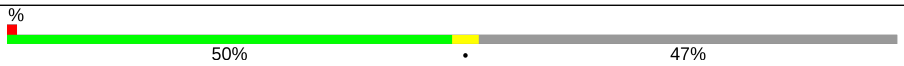
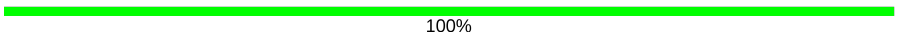
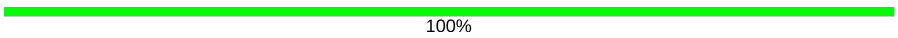
Mol	Chain	Length	Quality of chain
2	F	112	
2	H	112	
3	I	618	
3	J	618	
4	K	212	
4	M	212	
5	L	221	
5	N	221	
6	O	3	
6	P	3	
6	Q	3	
6	S	3	
6	T	3	
7	R	2	
8	U	4	

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 21668 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 Transforming growth factor beta-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	168	Total	C	N	O	S	0	0	0
			1070	676	194	195	5			
1	C	209	Total	C	N	O	S	0	0	0
			1410	884	259	260	7			
1	E	222	Total	C	N	O	S	0	0	0
			1666	1062	290	306	8			
1	G	218	Total	C	N	O	S	0	0	0
			1643	1042	289	305	7			

- Molecule 2 is a protein called Transforming growth factor beta-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	112	Total	C	N	O	S	0	0	0
			849	548	139	152	10			
2	D	111	Total	C	N	O	S	0	0	0
			847	542	142	153	10			
2	F	112	Total	C	N	O	S	0	0	0
			850	545	143	152	10			
2	H	109	Total	C	N	O	S	0	0	0
			849	545	144	150	10			

- Molecule 3 is a protein called Leucine-rich repeat-containing protein 32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	I	551	Total	C	N	O	S	0	0	0
			4055	2579	693	765	18			
3	J	493	Total	C	N	O	S	0	0	0
			3533	2237	608	673	15			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	629	GLU	-	expression tag	UNP Q14392
I	630	ALA	-	expression tag	UNP Q14392
I	631	ALA	-	expression tag	UNP Q14392
I	632	GLU	-	expression tag	UNP Q14392
I	633	ASN	-	expression tag	UNP Q14392
I	634	LEU	-	expression tag	UNP Q14392
I	635	TYR	-	expression tag	UNP Q14392
I	636	PHE	-	expression tag	UNP Q14392
I	637	GLN	-	expression tag	UNP Q14392
J	629	GLU	-	expression tag	UNP Q14392
J	630	ALA	-	expression tag	UNP Q14392
J	631	ALA	-	expression tag	UNP Q14392
J	632	GLU	-	expression tag	UNP Q14392
J	633	ASN	-	expression tag	UNP Q14392
J	634	LEU	-	expression tag	UNP Q14392
J	635	TYR	-	expression tag	UNP Q14392
J	636	PHE	-	expression tag	UNP Q14392
J	637	GLN	-	expression tag	UNP Q14392

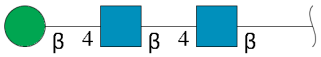
- Molecule 4 is a protein called MHG-8 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	K	212	Total	C	N	O	S	0	0	0
			1505	948	256	296	5			
4	M	104	Total	C	N	O	S	0	0	0
			715	450	123	140	2			

- Molecule 5 is a protein called MHG-8 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	L	214	Total	C	N	O	S	0	0	0
			1520	951	261	301	7			
5	N	118	Total	C	N	O	S	0	0	0
			883	550	149	179	5			

- Molecule 6 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
6	O	3	Total C N O 39 22 2 15	0	0	0
6	P	3	Total C N O 39 22 2 15	0	0	0
6	Q	3	Total C N O 39 22 2 15	0	0	0
6	S	3	Total C N O 39 22 2 15	0	0	0
6	T	3	Total C N O 39 22 2 15	0	0	0

- Molecule 7 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
7	R	2	Total C N O 28 16 2 10	0	0	0

- Molecule 8 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

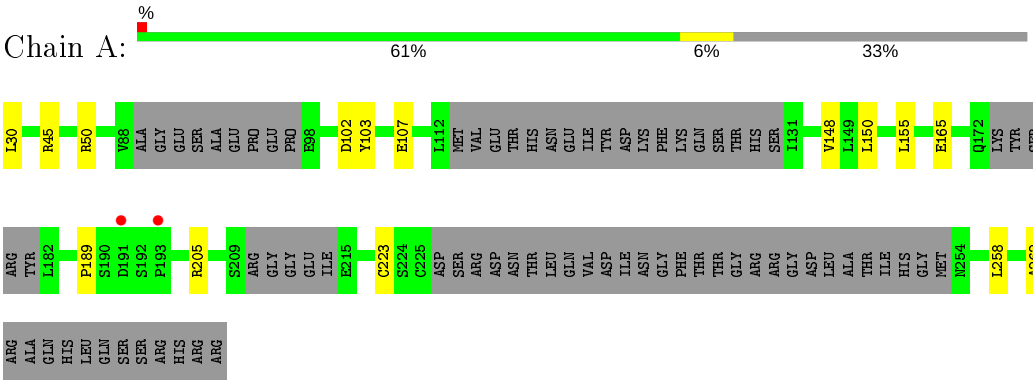
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
8	U	4	Total C N O 50 28 2 20	0	0	0

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.

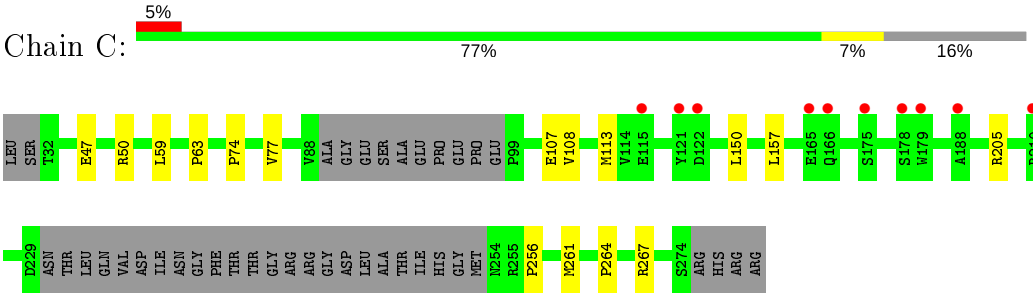
- Molecule 1: Transforming growth factor beta-1

Chain A:



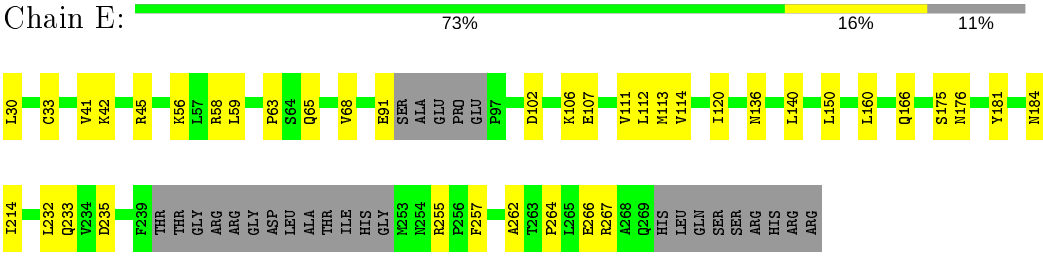
- Molecule 1: Transforming growth factor beta-1

Chain C:



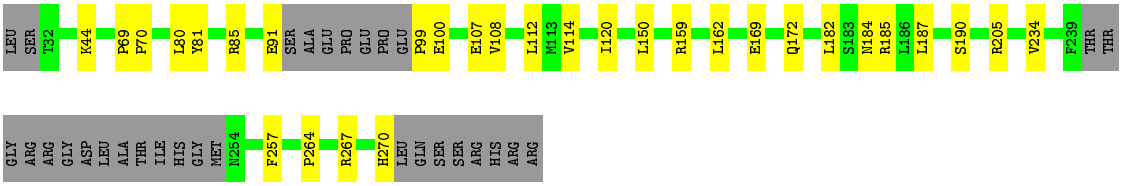
- Molecule 1: Transforming growth factor beta-1

Chain E:



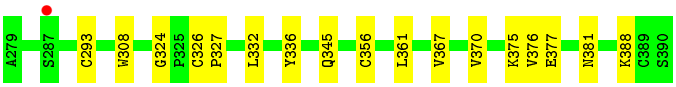
- Molecule 1: Transforming growth factor beta-1

Chain G:



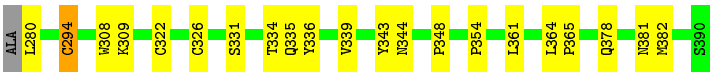
• Molecule 2: Transforming growth factor beta-1

Chain B:



• Molecule 2: Transforming growth factor beta-1

Chain D:



• Molecule 2: Transforming growth factor beta-1

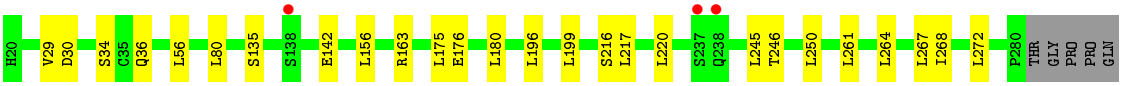
Chain F:

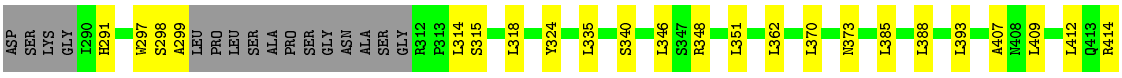
• Molecule 2: Transforming growth factor beta-1

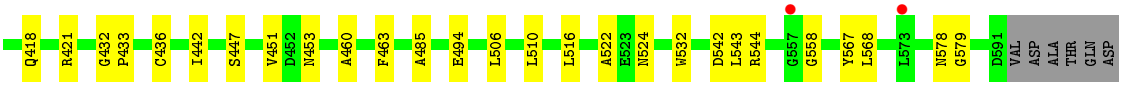
Chain H:

• Molecule 3: Leucine-rich repeat-containing protein 32

Chain I:

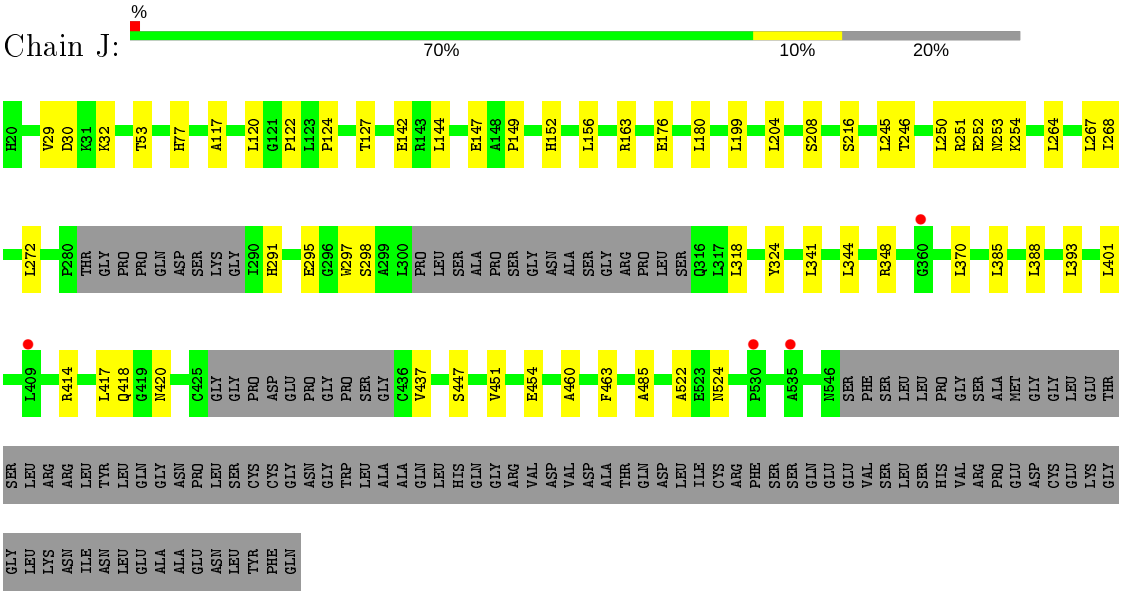






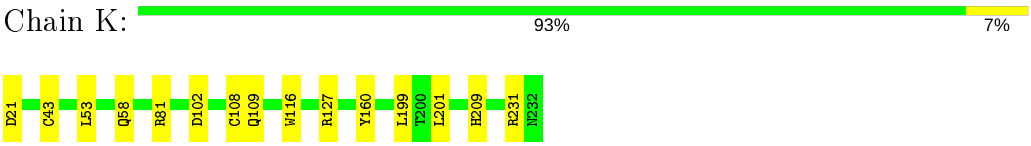
- Molecule 3: Leucine-rich repeat-containing protein 32

Chain J:



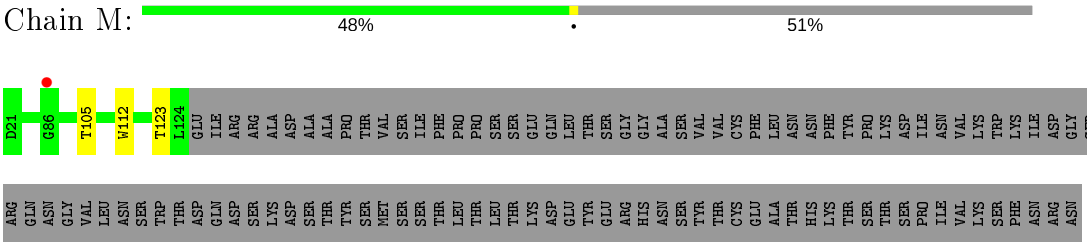
- Molecule 4: MHG-8 Fab light chain

Chain K:



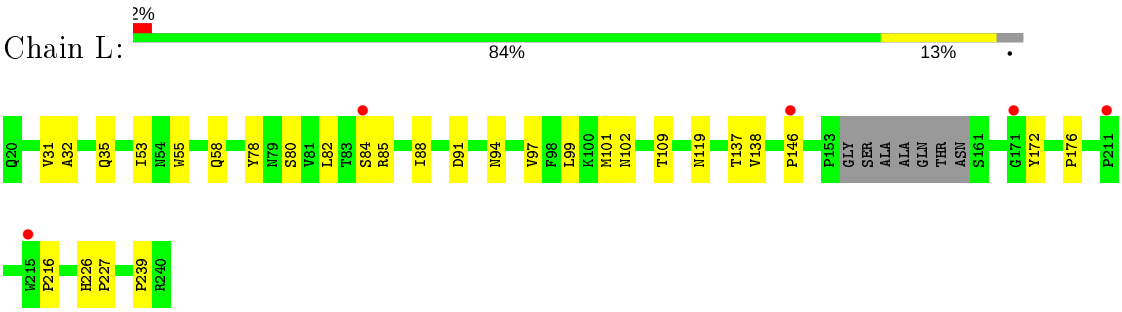
- Molecule 4: MHG-8 Fab light chain

Chain M:



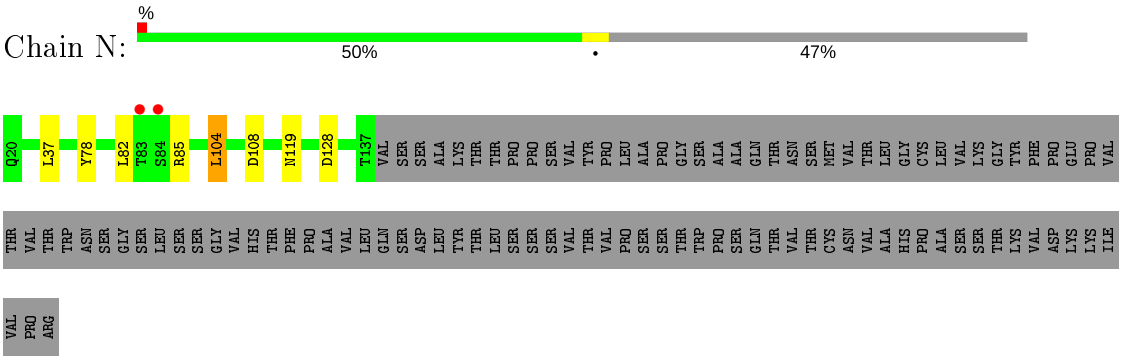
- Molecule 5: MHG-8 Fab heavy chain

Chain L:



- Molecule 5: MHG-8 Fab heavy chain

Chain N:



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

Chain O:

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

Chain P:

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

Chain Q:

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

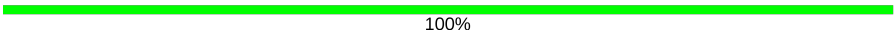
Chain S:

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

Chain T:

• Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R:



• Molecule 8: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain U:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	103.86Å 175.01Å 145.77Å 90.00° 92.23° 90.00°	Depositor
Resolution (Å)	29.92 – 3.10 44.63 – 3.10	Depositor EDS
% Data completeness (in resolution range)	90.1 (29.92-3.10) 90.1 (44.63-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.41 (at 3.12Å)	Xtriage
Refinement program	PHENIX, BUSTER	Depositor
R, R_{free}	0.233 , 0.268 0.235 , 0.271	Depositor DCC
R_{free} test set	4249 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	86.1	Xtriage
Anisotropy	0.236	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 73.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.022 for h,-k,-l	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	21668	wwPDB-VP
Average B, all atoms (Å^2)	96.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.41% 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: BMA, NAG, 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	0.23	0/1086	0.40	0/1494
1	C	0.23	0/1430	0.43	0/1957
1	E	0.24	0/1699	0.42	0/2315
1	G	0.23	0/1676	0.43	0/2281
2	B	0.33	0/877	0.49	0/1204
2	D	0.27	0/873	0.47	0/1195
2	F	0.27	0/877	0.45	0/1201
2	H	0.26	0/876	0.47	0/1196
3	I	0.24	0/4128	0.45	0/5635
3	J	0.24	0/3591	0.44	0/4913
4	K	0.24	0/1543	0.44	0/2119
4	M	0.25	0/734	0.44	0/1010
5	L	0.25	0/1561	0.46	0/2148
5	N	0.23	0/904	0.44	0/1234
All	All	0.25	0/21855	0.44	0/29902

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

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	1070	0	831	12	0
1	C	1410	0	1213	12	0
1	E	1666	0	1575	28	0
1	G	1643	0	1550	18	0
2	B	849	0	758	12	0
2	D	847	0	767	14	0
2	F	850	0	764	12	0
2	H	849	0	796	14	0
3	I	4055	0	3965	43	0
3	J	3533	0	3334	36	0
4	K	1505	0	1267	8	0
4	M	715	0	572	2	0
5	L	1520	0	1299	18	0
5	N	883	0	776	5	0
6	O	39	0	34	0	0
6	P	39	0	34	1	0
6	Q	39	0	34	1	0
6	S	39	0	34	0	0
6	T	39	0	34	1	0
7	R	28	0	25	0	0
8	U	50	0	43	1	0
All	All	21668	0	19705	208	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 5.

The worst 5 of 208 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:G:159:ARG:HH22	1:G:190:SER:HB3	1.51	0.75
1:E:267:ARG:NH2	2:H:377:GLU:OE2	2.20	0.74
1:E:58:ARG:HD2	1:E:267:ARG:HB3	1.68	0.73
2:H:284:TYR:HB2	2:H:295:VAL:HG12	1.69	0.73
1:A:107:GLU:HB2	1:A:264:PRO:HG3	1.71	0.72

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	156/249 (63%)	151 (97%)	5 (3%)	0	100	100
1	C	203/249 (82%)	191 (94%)	12 (6%)	0	100	100
1	E	216/249 (87%)	202 (94%)	14 (6%)	0	100	100
1	G	212/249 (85%)	197 (93%)	15 (7%)	0	100	100
2	B	110/112 (98%)	107 (97%)	3 (3%)	0	100	100
2	D	109/112 (97%)	105 (96%)	4 (4%)	0	100	100
2	F	110/112 (98%)	105 (96%)	5 (4%)	0	100	100
2	H	107/112 (96%)	102 (95%)	5 (5%)	0	100	100
3	I	545/618 (88%)	506 (93%)	39 (7%)	0	100	100
3	J	485/618 (78%)	451 (93%)	34 (7%)	0	100	100
4	K	210/212 (99%)	201 (96%)	9 (4%)	0	100	100
4	M	102/212 (48%)	95 (93%)	7 (7%)	0	100	100
5	L	210/221 (95%)	197 (94%)	13 (6%)	0	100	100
5	N	116/221 (52%)	106 (91%)	10 (9%)	0	100	100
All	All	2891/3546 (82%)	2716 (94%)	175 (6%)	0	100	100

There are no Ramachandran outliers to report.

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	69/222 (31%)	69 (100%)	0	100 100
1	C	112/222 (50%)	112 (100%)	0	100 100
1	E	166/222 (75%)	166 (100%)	0	100 100
1	G	165/222 (74%)	164 (99%)	1 (1%)	86 94
2	B	86/100 (86%)	86 (100%)	0	100 100
2	D	87/100 (87%)	86 (99%)	1 (1%)	73 89
2	F	86/100 (86%)	85 (99%)	1 (1%)	71 88
2	H	91/100 (91%)	90 (99%)	1 (1%)	73 89
3	I	425/530 (80%)	424 (100%)	1 (0%)	93 97
3	J	353/530 (67%)	352 (100%)	1 (0%)	92 96
4	K	134/187 (72%)	133 (99%)	1 (1%)	84 93
4	M	58/187 (31%)	58 (100%)	0	100 100
5	L	145/193 (75%)	145 (100%)	0	100 100
5	N	89/193 (46%)	88 (99%)	1 (1%)	73 89
All	All	2066/3108 (66%)	2058 (100%)	8 (0%)	91 96

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	351	SER
5	N	104	LEU
3	J	463	PHE
1	G	270	HIS
3	I	463	PHE

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

Mol	Chain	Res	Type
5	L	102	ASN

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)

21 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	$\#\|Z\| > 2$
6	NAG	O	1	3,6	14,14,15	0.39	0	17,19,21	0.46	0
6	NAG	O	2	6	14,14,15	0.21	0	17,19,21	0.49	0
6	BMA	O	3	6	11,11,12	0.56	0	15,15,17	0.83	0
6	NAG	P	1	3,6	14,14,15	0.39	0	17,19,21	0.45	0
6	NAG	P	2	6	14,14,15	0.16	0	17,19,21	0.59	1 (5%)
6	BMA	P	3	6	11,11,12	0.54	0	15,15,17	0.78	0
6	NAG	Q	1	3,6	14,14,15	0.18	0	17,19,21	0.47	0
6	NAG	Q	2	6	14,14,15	0.19	0	17,19,21	0.44	0
6	BMA	Q	3	6	11,11,12	0.59	0	15,15,17	0.68	0
7	NAG	R	1	3,7	14,14,15	0.24	0	17,19,21	0.45	0
7	NAG	R	2	7	14,14,15	0.39	0	17,19,21	0.52	0
6	NAG	S	1	3,6	14,14,15	0.43	0	17,19,21	0.49	0
6	NAG	S	2	6	14,14,15	0.20	0	17,19,21	0.48	0
6	BMA	S	3	6	11,11,12	0.61	0	15,15,17	0.86	0
6	NAG	T	1	3,6	14,14,15	0.37	0	17,19,21	0.46	0
6	NAG	T	2	6	14,14,15	0.19	0	17,19,21	0.60	1 (5%)
6	BMA	T	3	6	11,11,12	0.60	0	15,15,17	0.73	0
8	NAG	U	1	8,3	14,14,15	0.21	0	17,19,21	0.49	0
8	NAG	U	2	8	14,14,15	0.28	0	17,19,21	0.73	0
8	BMA	U	3	8	11,11,12	0.54	0	15,15,17	0.79	0
8	MAN	U	4	8	11,11,12	0.70	0	15,15,17	1.21	2 (13%)

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
6	NAG	O	1	3,6	-	0/6/23/26	0/1/1/1
6	NAG	O	2	6	-	0/6/23/26	0/1/1/1
6	BMA	O	3	6	-	0/2/19/22	0/1/1/1
6	NAG	P	1	3,6	-	2/6/23/26	0/1/1/1
6	NAG	P	2	6	-	0/6/23/26	0/1/1/1
6	BMA	P	3	6	-	0/2/19/22	0/1/1/1
6	NAG	Q	1	3,6	-	0/6/23/26	0/1/1/1
6	NAG	Q	2	6	-	0/6/23/26	0/1/1/1
6	BMA	Q	3	6	-	0/2/19/22	0/1/1/1
7	NAG	R	1	3,7	-	0/6/23/26	0/1/1/1
7	NAG	R	2	7	-	1/6/23/26	0/1/1/1
6	NAG	S	1	3,6	-	0/6/23/26	0/1/1/1
6	NAG	S	2	6	-	2/6/23/26	0/1/1/1
6	BMA	S	3	6	-	0/2/19/22	0/1/1/1
6	NAG	T	1	3,6	-	0/6/23/26	0/1/1/1
6	NAG	T	2	6	-	2/6/23/26	0/1/1/1
6	BMA	T	3	6	-	0/2/19/22	0/1/1/1
8	NAG	U	1	8,3	-	0/6/23/26	0/1/1/1
8	NAG	U	2	8	-	0/6/23/26	0/1/1/1
8	BMA	U	3	8	-	0/2/19/22	0/1/1/1
8	MAN	U	4	8	-	1/2/19/22	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	U	4	MAN	C1-O5-C5	2.88	116.09	112.19
8	U	4	MAN	O2-C2-C3	-2.09	105.94	110.14
6	T	2	NAG	C1-O5-C5	2.09	115.02	112.19
6	P	2	NAG	C1-O5-C5	2.07	114.99	112.19

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

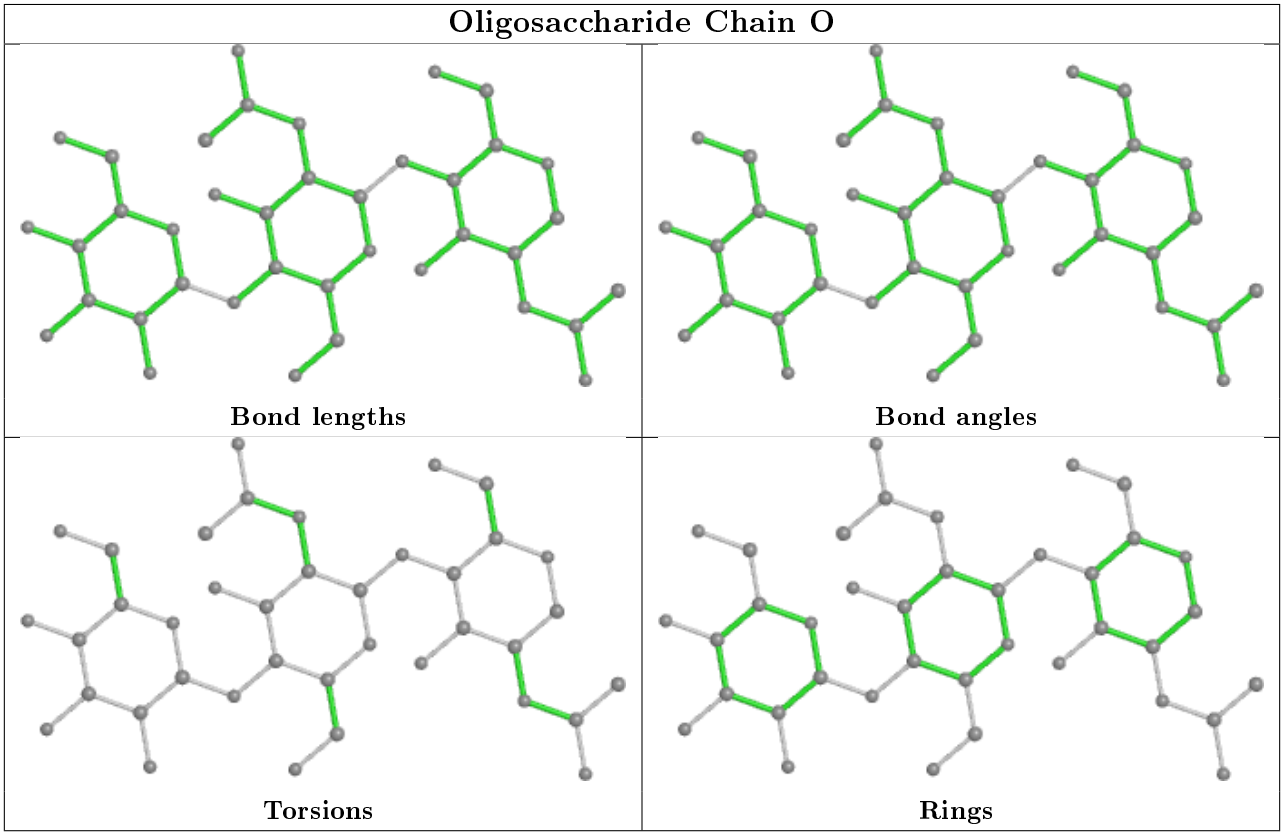
Mol	Chain	Res	Type	Atoms
6	P	1	NAG	C4-C5-C6-O6
6	S	2	NAG	O5-C5-C6-O6
6	P	1	NAG	O5-C5-C6-O6
7	R	2	NAG	C3-C2-N2-C7
6	S	2	NAG	C4-C5-C6-O6

There are no ring outliers.

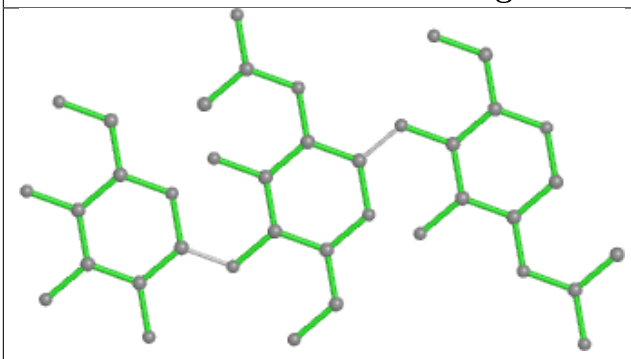
4 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	P	2	NAG	1	0
6	T	2	NAG	1	0
8	U	2	NAG	1	0
6	Q	2	NAG	1	0

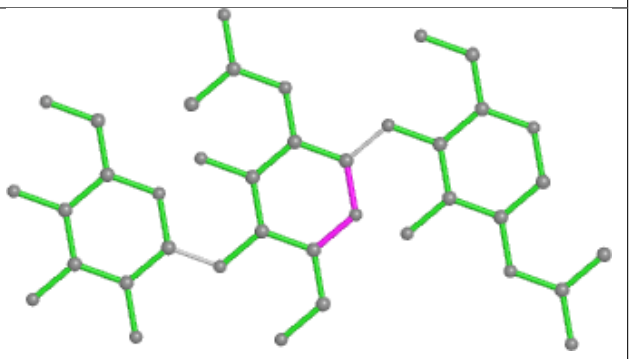
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



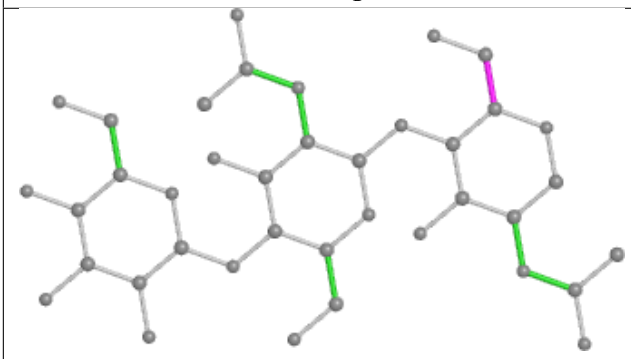
Oligosaccharide Chain P



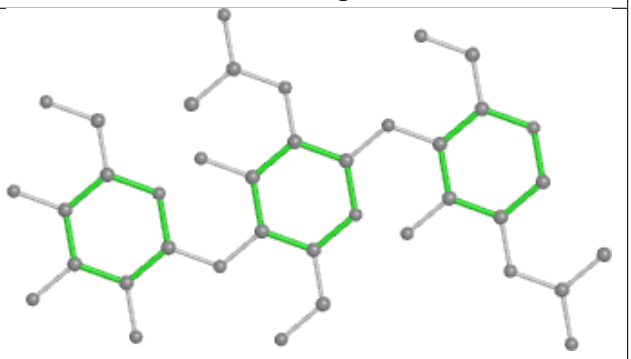
Bond lengths



Bond angles

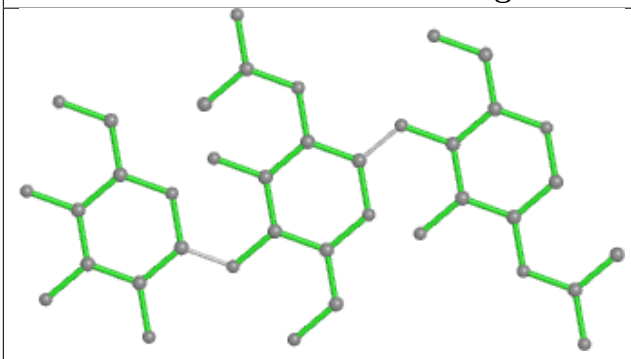


Torsions

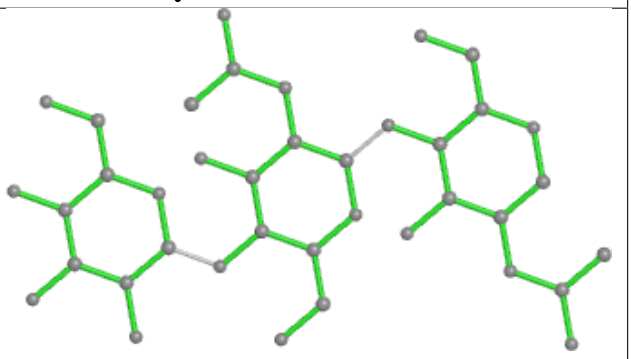


Rings

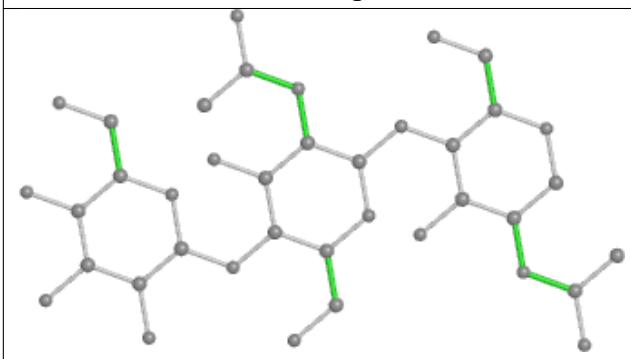
Oligosaccharide Chain Q



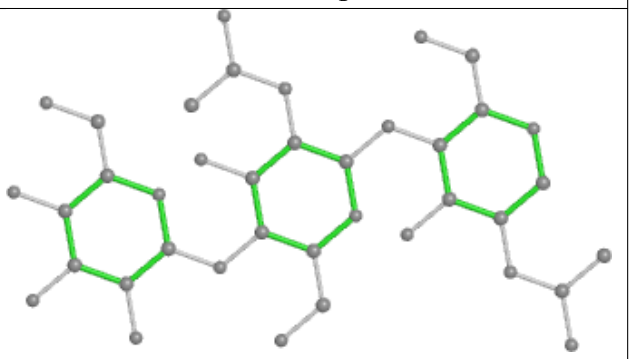
Bond lengths



Bond angles

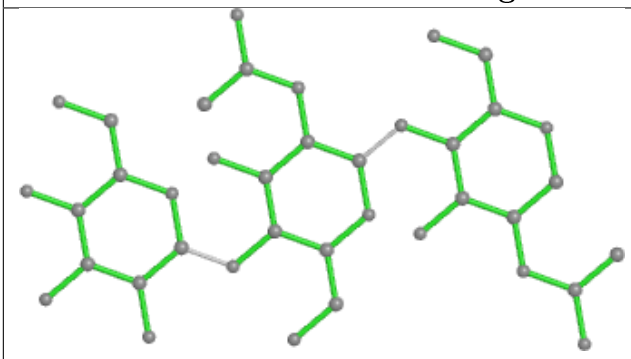


Torsions

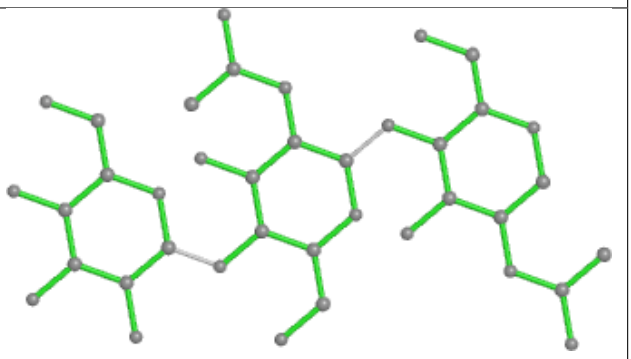


Rings

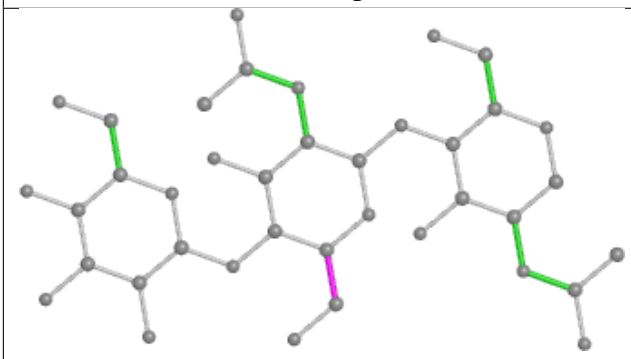
Oligosaccharide Chain S



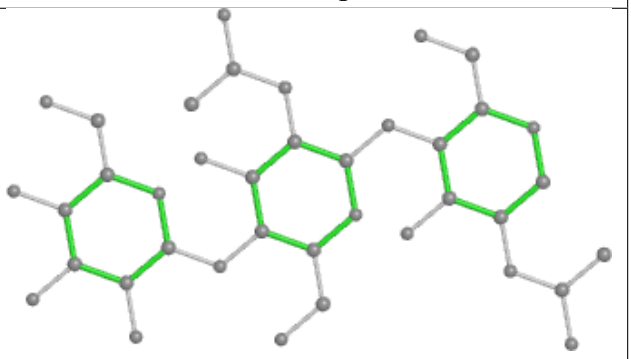
Bond lengths



Bond angles

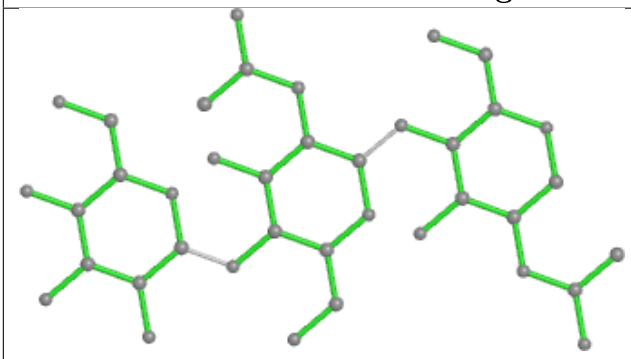


Torsions

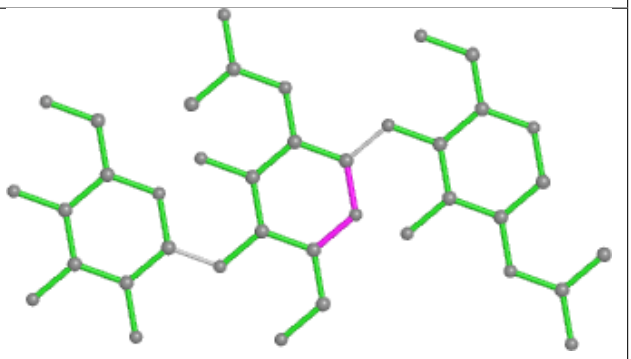


Rings

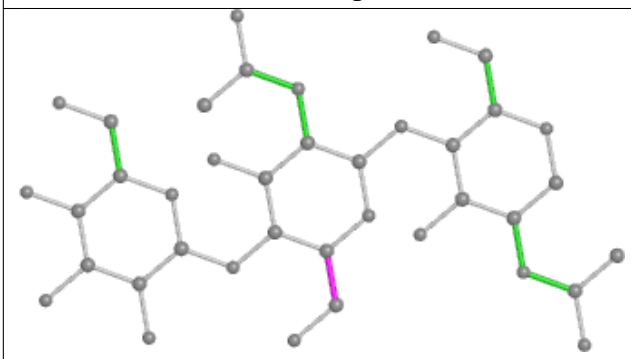
Oligosaccharide Chain T



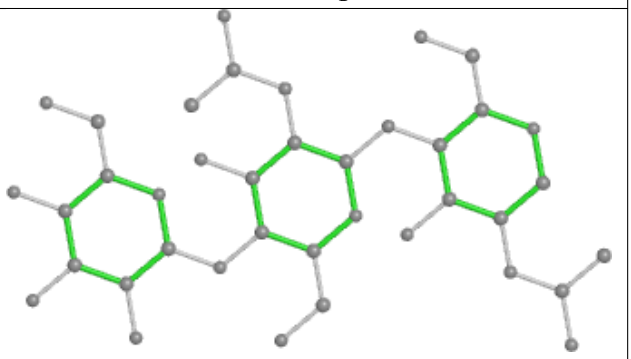
Bond lengths



Bond angles

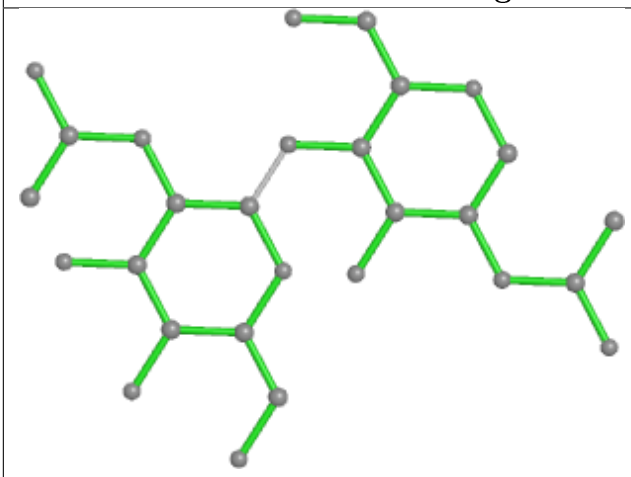


Torsions

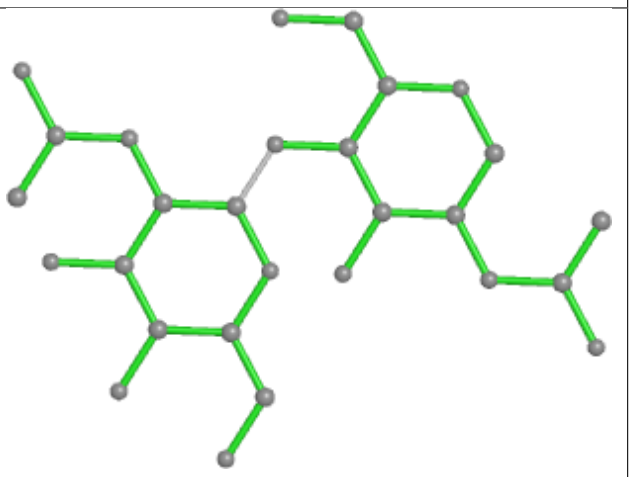


Rings

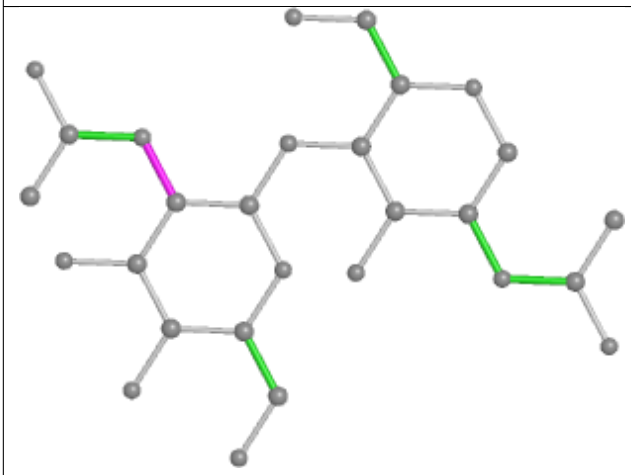
Oligosaccharide Chain R



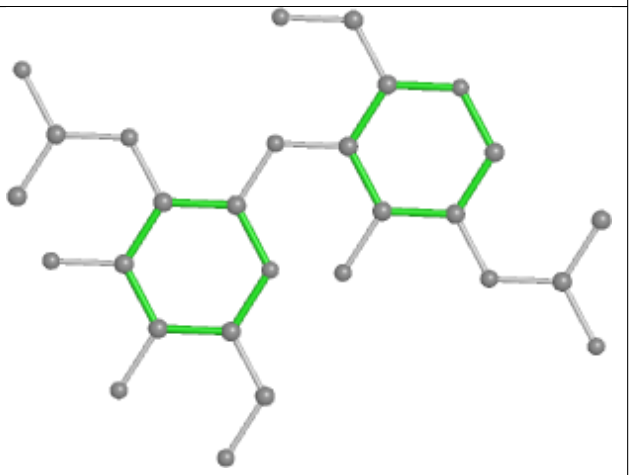
Bond lengths



Bond angles

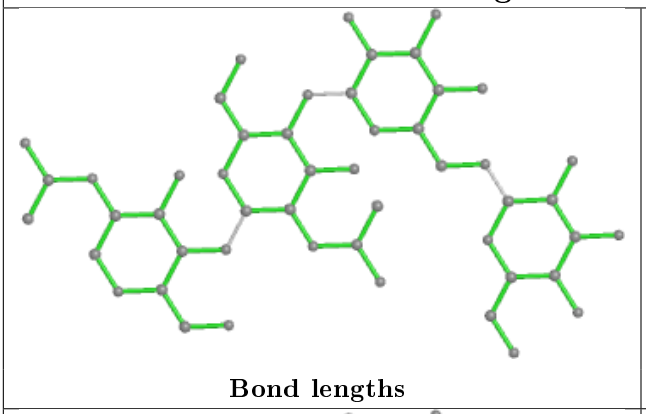


Torsions

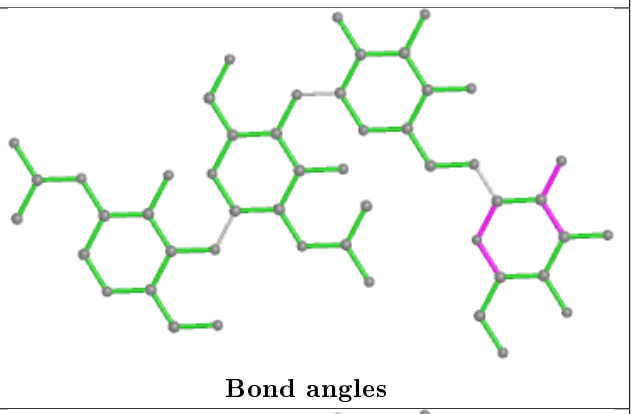


Rings

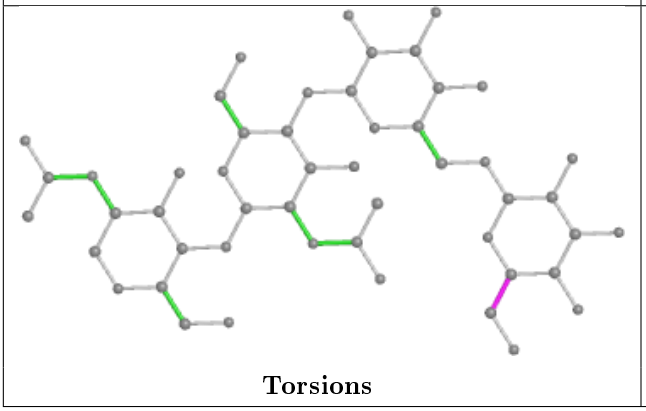
Oligosaccharide Chain U



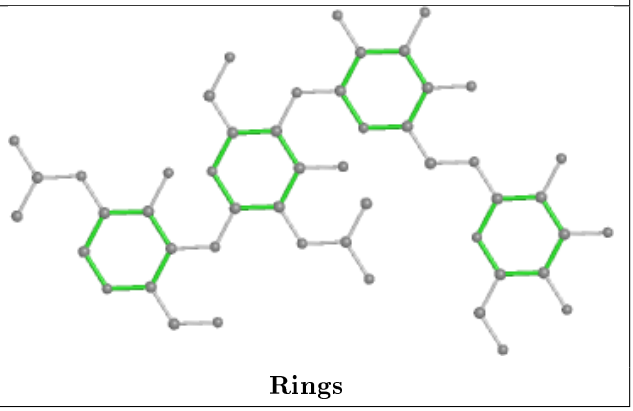
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	168/249 (67%)	-0.18	2 (1%) 79 61	64, 130, 163, 175	0
1	C	209/249 (83%)	0.08	12 (5%) 23 11	46, 114, 177, 206	0
1	E	222/249 (89%)	-0.28	0 100 100	61, 95, 135, 176	0
1	G	218/249 (87%)	-0.36	0 100 100	45, 90, 131, 150	0
2	B	112/112 (100%)	-0.37	1 (0%) 84 69	48, 75, 117, 128	0
2	D	111/112 (99%)	-0.25	0 100 100	47, 83, 135, 216	0
2	F	112/112 (100%)	-0.44	0 100 100	46, 69, 122, 152	0
2	H	109/112 (97%)	-0.32	0 100 100	47, 70, 118, 141	0
3	I	551/618 (89%)	-0.23	5 (0%) 84 69	42, 82, 128, 151	0
3	J	493/618 (79%)	-0.29	4 (0%) 86 72	45, 88, 146, 179	0
4	K	212/212 (100%)	-0.24	0 100 100	63, 119, 149, 159	0
4	M	104/212 (49%)	-0.19	1 (0%) 82 67	71, 125, 171, 195	0
5	L	214/221 (96%)	0.00	5 (2%) 60 39	52, 118, 179, 186	0
5	N	118/221 (53%)	-0.25	2 (1%) 70 49	69, 95, 144, 157	0
All	All	2953/3546 (83%)	-0.23	32 (1%) 80 64	42, 94, 153, 216	0

The worst 5 of 32 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	N	84	SER	6.8
1	C	179	TRP	5.3
5	L	84	SER	4.9
5	L	171	GLY	3.6
1	C	224	SER	3.5

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

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

6.3 Carbohydrates (i)

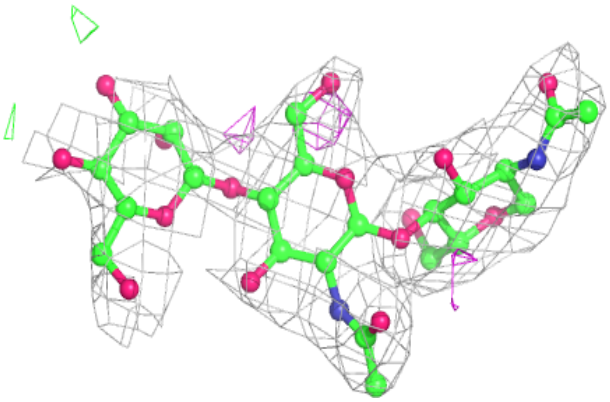
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

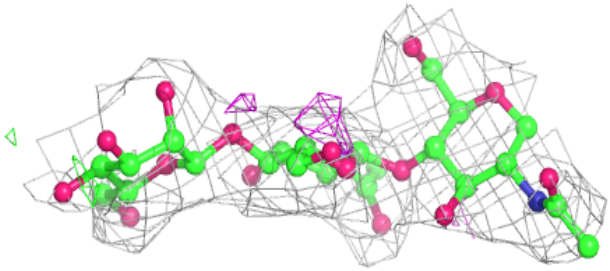
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	BMA	T	3	11/12	0.67	0.34	160,163,165,165	0
6	BMA	O	3	11/12	0.75	0.27	89,112,133,137	0
8	BMA	U	3	11/12	0.78	0.17	118,126,157,203	0
7	NAG	R	2	14/15	0.79	0.37	119,139,148,149	0
6	BMA	S	3	11/12	0.86	0.14	119,126,129,131	0
7	NAG	R	1	14/15	0.87	0.33	101,129,138,143	0
6	BMA	P	3	11/12	0.87	0.12	93,114,140,144	0
6	NAG	T	2	14/15	0.88	0.32	104,126,137,148	0
8	MAN	U	4	11/12	0.88	0.13	101,126,152,167	0
8	NAG	U	2	14/15	0.89	0.20	80,105,110,120	0
6	BMA	Q	3	11/12	0.89	0.18	113,121,124,128	0
8	NAG	U	1	14/15	0.92	0.25	59,77,111,127	0
6	NAG	Q	2	14/15	0.92	0.21	40,94,119,124	0
6	NAG	T	1	14/15	0.94	0.23	54,74,87,90	0
6	NAG	P	2	14/15	0.94	0.21	67,96,116,117	0
6	NAG	O	2	14/15	0.95	0.17	63,69,82,97	0
6	NAG	S	2	14/15	0.95	0.13	63,85,95,113	0
6	NAG	Q	1	14/15	0.95	0.17	46,68,91,94	0
6	NAG	P	1	14/15	0.97	0.14	28,46,66,74	0
6	NAG	O	1	14/15	0.97	0.13	43,49,77,91	0
6	NAG	S	1	14/15	0.98	0.20	46,60,75,76	0

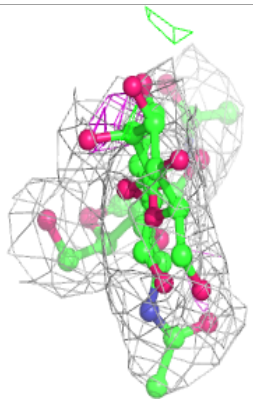
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain O:

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

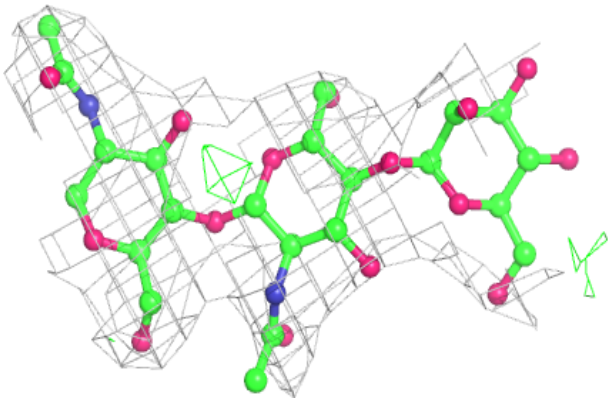


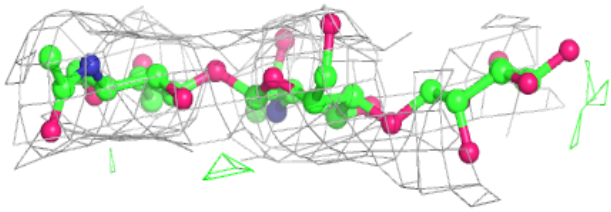


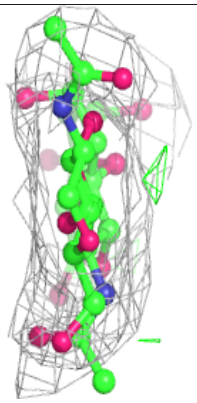


Electron density around Chain P:

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

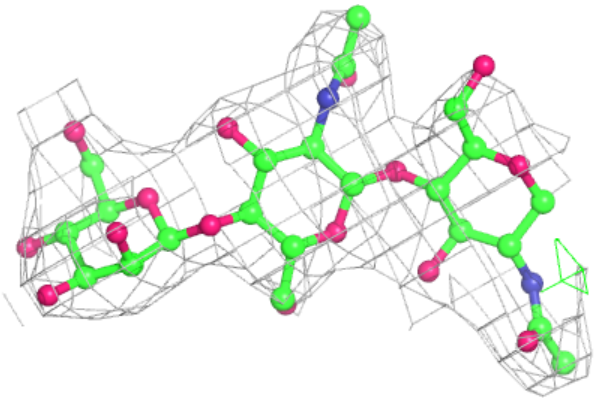


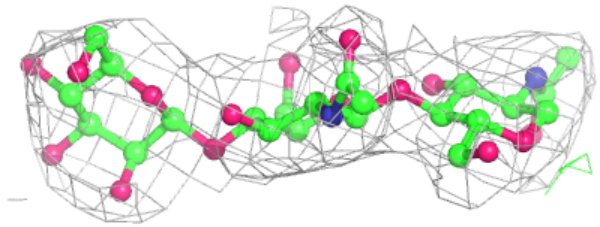


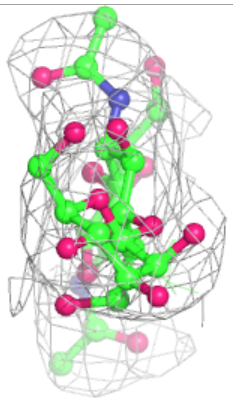


Electron density around Chain Q:

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

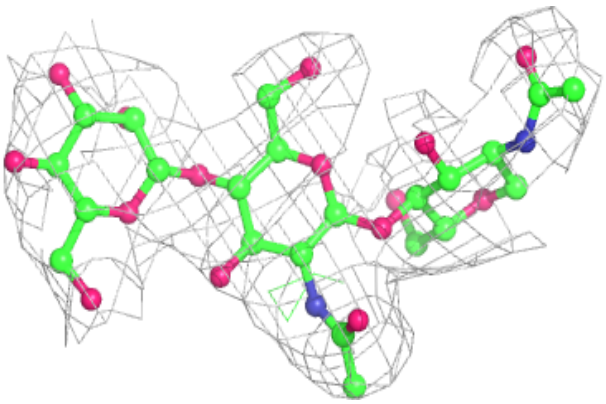


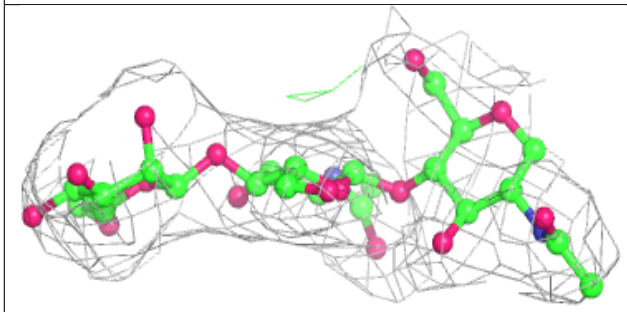


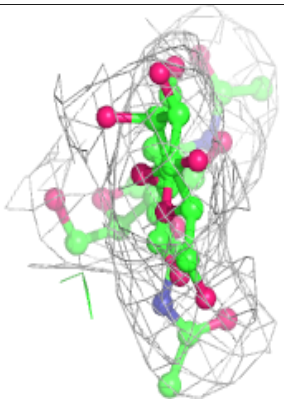


Electron density around Chain S:

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

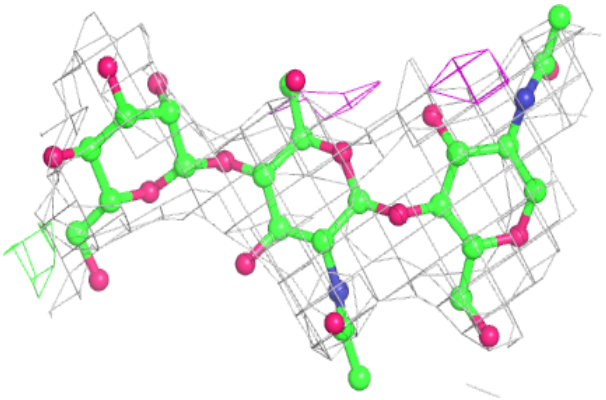


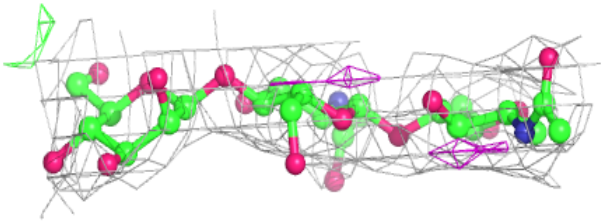


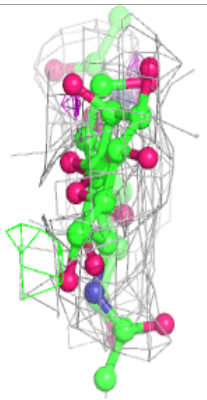


Electron density around Chain T:

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

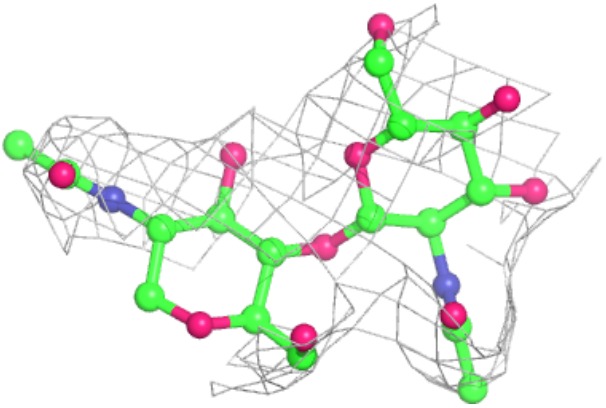


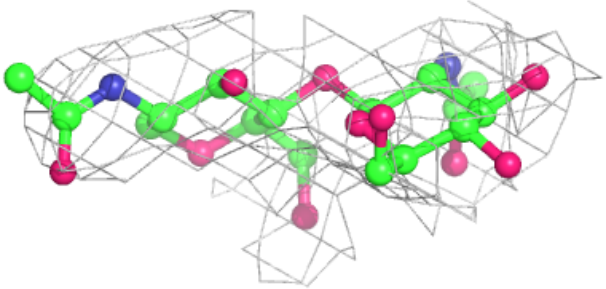


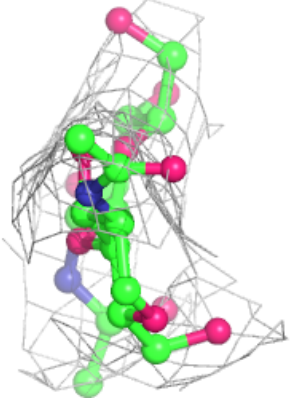


Electron density around Chain R:

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

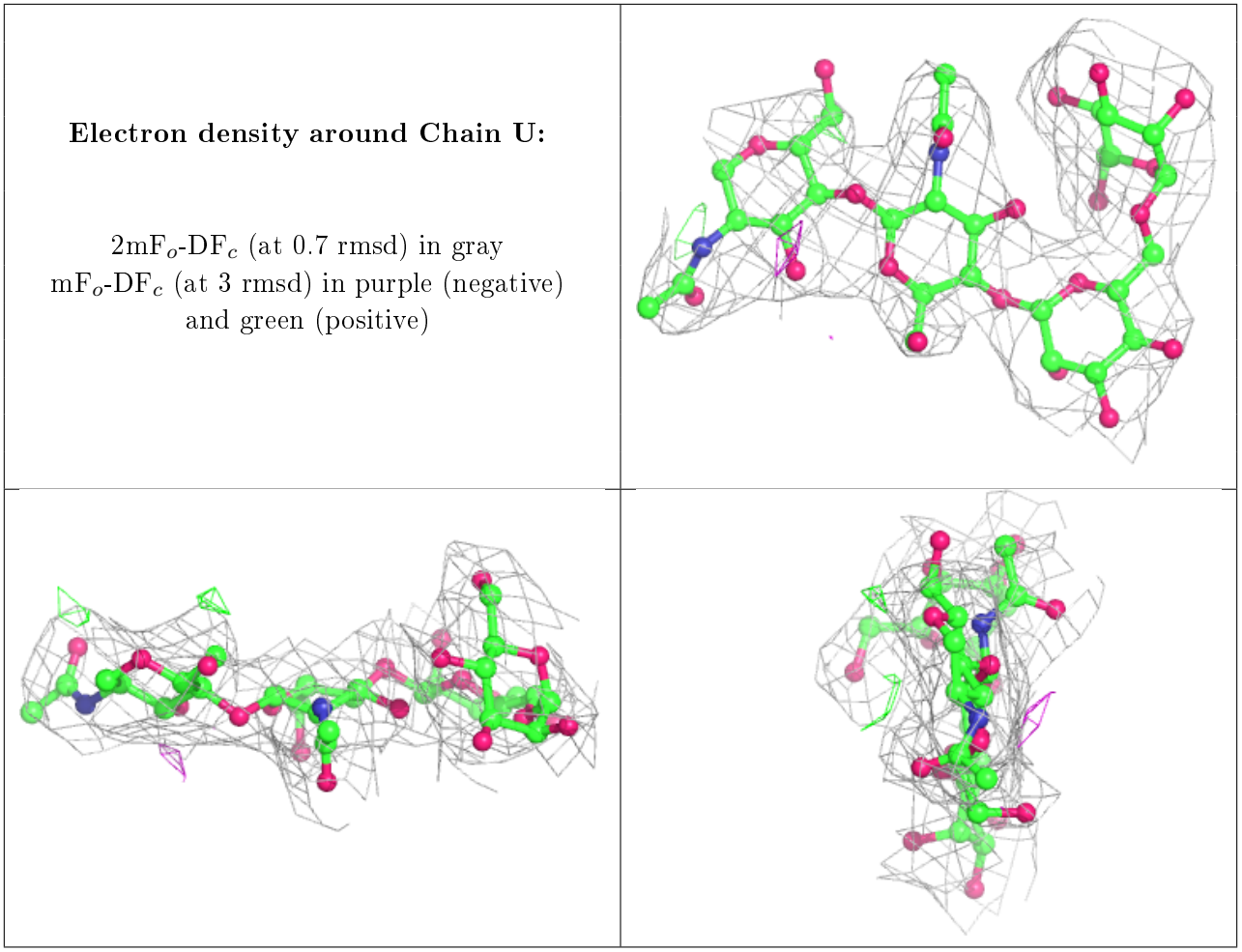






Electron density around Chain U:

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



6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.