wwPDB X-ray Structure Validation Summary Report (i)

May 15, 2025 – 04:09 pm BST

PDB ID	:	9F7Z / pdb_00009f7z
Title	:	Crystal structure of human 4-1BB/TNFRSF9 in complex with the anti-4-1BB DARPin protein
Authors	:	Malvezzi, F.; Domke, C.; Hospodarsch, T.; Lammens, A.; Blaesse, M.; Krapp, S.; Reichen, C.
Deposited on	:	2024-05-06
Resolution	:	2.81 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

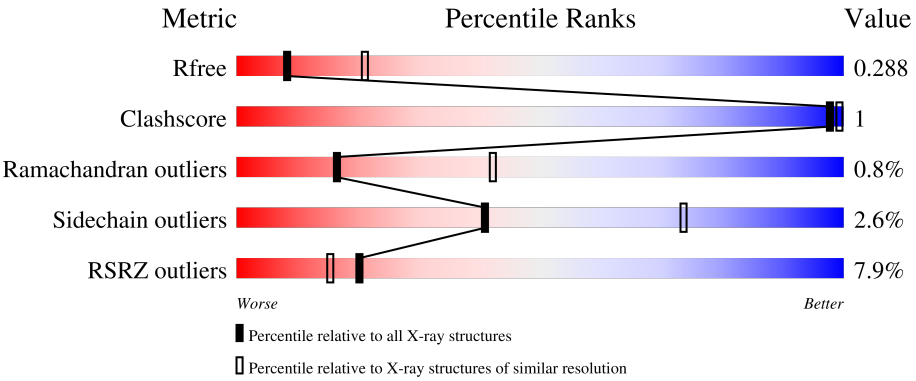
MolProbity	:	4-5-2 with Phenix2.0rc1
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

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 2.81 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}	164625	4293 (2.84-2.80)
Clashscore	180529	4801 (2.84-2.80)
Ramachandran outliers	177936	4739 (2.84-2.80)
Sidechain outliers	177891	4741 (2.84-2.80)
RSRZ outliers	164620	4295 (2.84-2.80)

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	126	6% 95%
1	C	126	3% 95%
1	E	126	2% 96%
1	G	126	5% 95%
1	I	126	6% 94%

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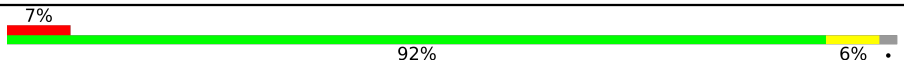
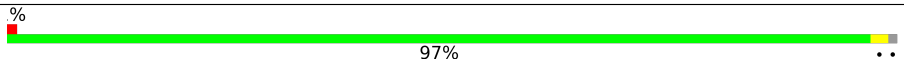
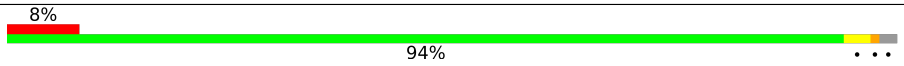
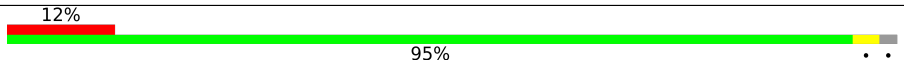
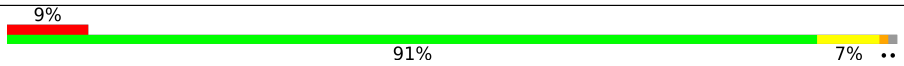
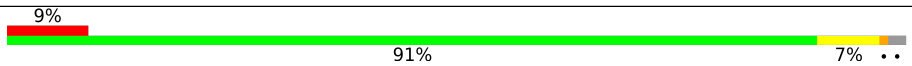
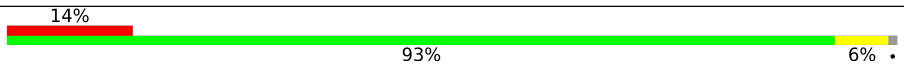
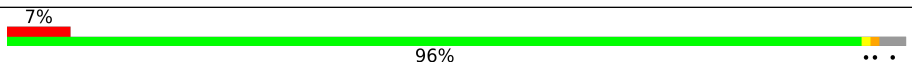
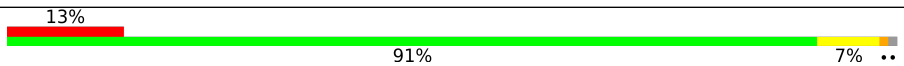
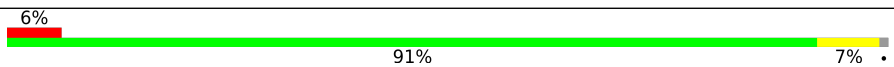
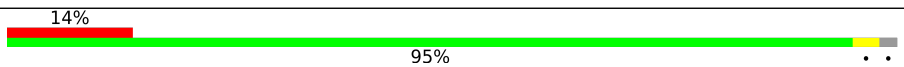
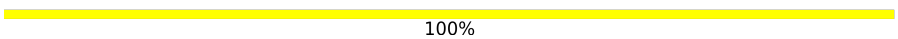
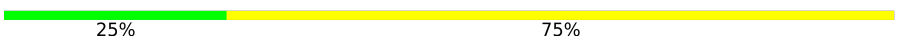
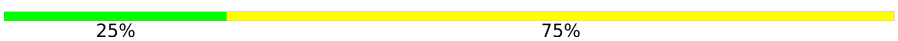
Mol	Chain	Length	Quality of chain
1	K	126	
1	M	126	
1	O	126	
2	B	138	
2	D	138	
2	F	138	
2	H	138	
2	J	138	
2	L	138	
2	N	138	
2	P	138	
3	Q	2	
4	R	4	
4	S	4	
4	T	4	
4	U	4	
4	W	4	
5	V	2	

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 15717 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 anti-4-1BB DARPin.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	124	Total 918	C 574	N 164	O 180	63	0	0
1	C	125	Total 924	C 577	N 165	O 182	49	0	0
1	E	124	Total 918	C 574	N 164	O 180	23	0	0
1	G	126	Total 928	C 579	N 166	O 183	49	0	0
1	I	124	Total 918	C 574	N 164	O 180	63	0	0
1	K	124	Total 918	C 574	N 164	O 180	77	0	0
1	M	125	Total 924	C 577	N 165	O 182	40	0	0
1	O	124	Total 918	C 574	N 164	O 180	74	0	0

- Molecule 2 is a protein called Tumor necrosis factor receptor superfamily member 9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	135	Total 997	C 589	N 187	O 199	S 22	66	0	0
2	D	136	Total 1003	C 592	N 188	O 201	S 22	57	0	0
2	F	135	Total 995	C 588	N 187	O 198	S 22	63	0	0
2	H	136	Total 1006	C 594	N 189	O 201	S 22	95	0	0
2	J	134	Total 987	C 584	N 183	O 198	S 22	53	0	0
2	L	136	Total 1006	C 594	N 189	O 201	S 22	61	0	0

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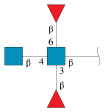
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	N	136	Total	C	N	O	S	48	0	0
			1006	594	189	201	22			
2	P	135	Total	C	N	O	S	59	0	0
			997	589	187	199	22			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	Q	2	Total	C	N	O	0	0	0
			24	14	1	9			

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

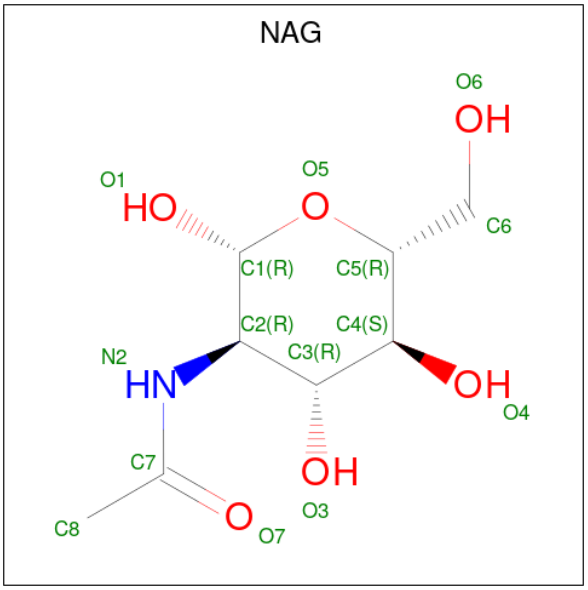


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	R	4	Total	C	N	O	4	0	0
			48	28	2	18			
4	S	4	Total	C	N	O	6	0	0
			48	28	2	18			
4	T	4	Total	C	N	O	1	0	0
			48	28	2	18			
4	U	4	Total	C	N	O	1	0	0
			48	28	2	18			
4	W	4	Total	C	N	O	4	0	0
			48	28	2	18			

- Molecule 5 is an oligosaccharide called beta-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
5	V	2	Total C N O 24 14 1 9	0	0	0

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	N	1	Total C N O 14 8 1 5	3	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	2	Total O 2 2	0	0
7	B	4	Total O 4 4	0	0
7	C	2	Total O 2 2	0	0
7	D	1	Total O 1 1	0	0
7	E	3	Total O 3 3	0	0
7	F	5	Total O 5 5	0	0
7	G	7	Total O 7 7	0	0

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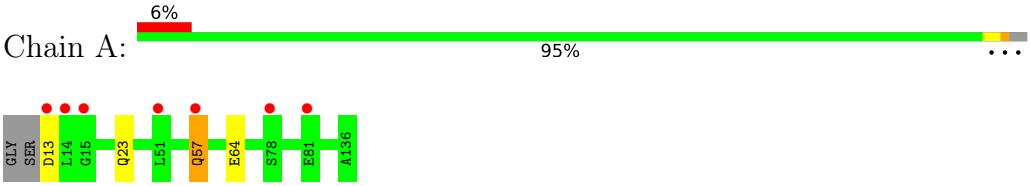
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	H	2	Total O 2 2	0	0
7	I	3	Total O 3 3	0	0
7	J	4	Total O 4 4	0	0
7	K	1	Total O 1 1	0	0
7	L	2	Total O 2 2	0	0
7	M	2	Total O 2 2	0	0
7	N	8	Total O 8 8	0	0
7	O	2	Total O 2 2	0	0
7	P	4	Total O 4 4	0	0

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.

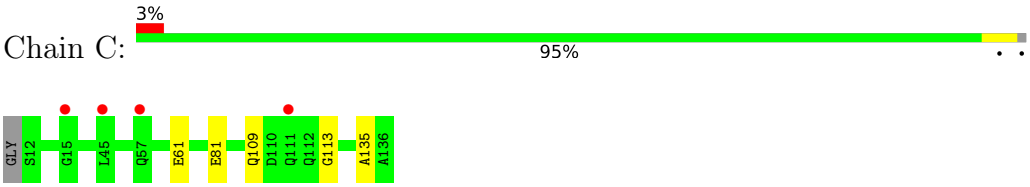
- Molecule 1: anti-4-1BB DARPin

Chain A:



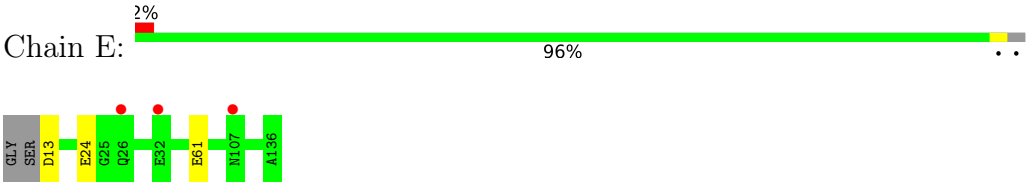
- Molecule 1: anti-4-1BB DARPin

Chain C:



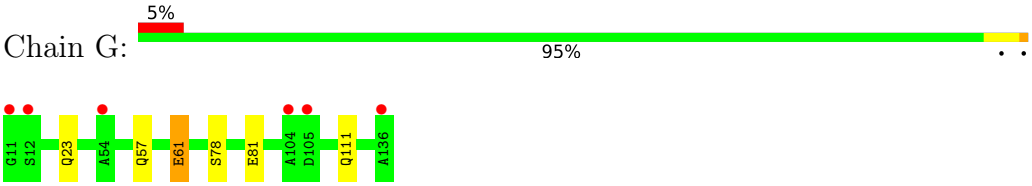
- Molecule 1: anti-4-1BB DARPin

Chain E:



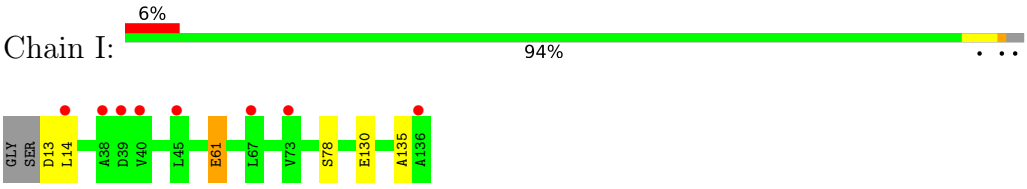
- Molecule 1: anti-4-1BB DARPin

Chain G:



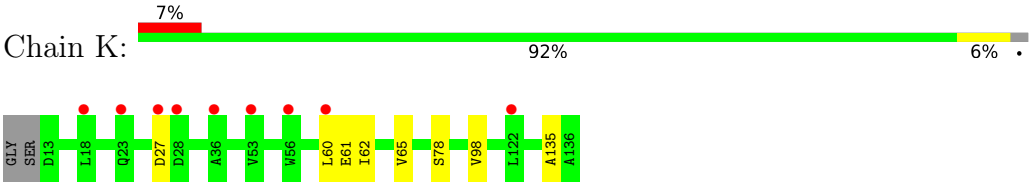
- Molecule 1: anti-4-1BB DARPin

Chain I:



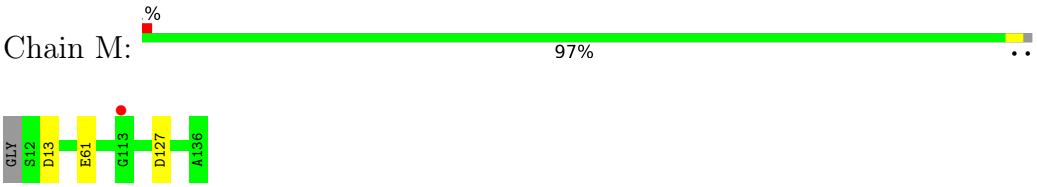
- Molecule 1: anti-4-1BB DARPin

Chain K:



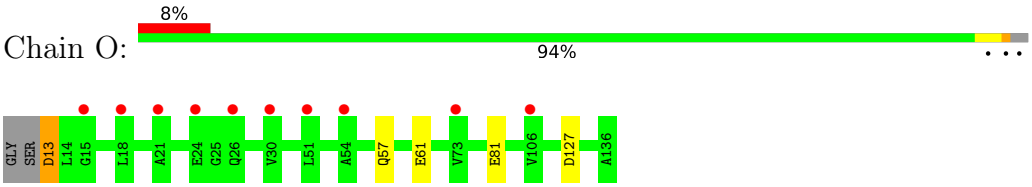
• Molecule 1: anti-4-1BB DARPin

Chain M:



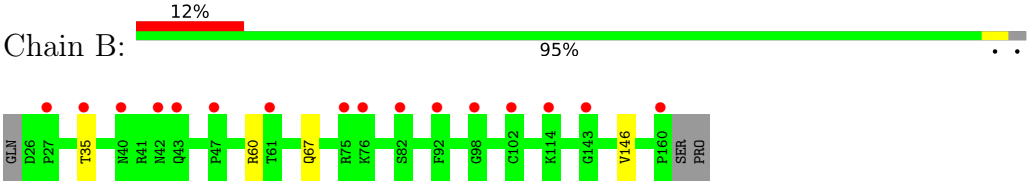
• Molecule 1: anti-4-1BB DARPin

Chain O:



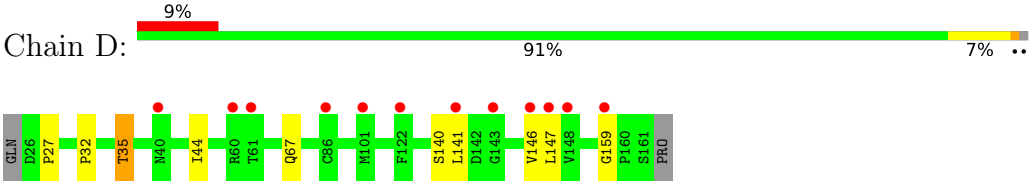
• Molecule 2: Tumor necrosis factor receptor superfamily member 9

Chain B:



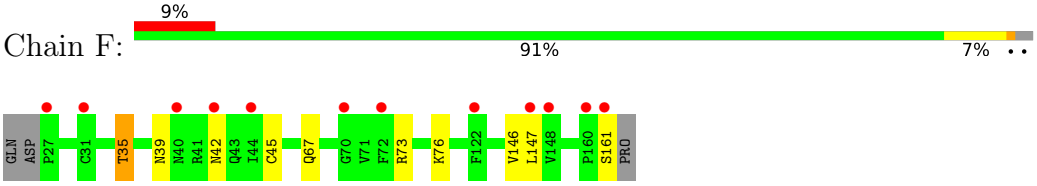
• Molecule 2: Tumor necrosis factor receptor superfamily member 9

Chain D:



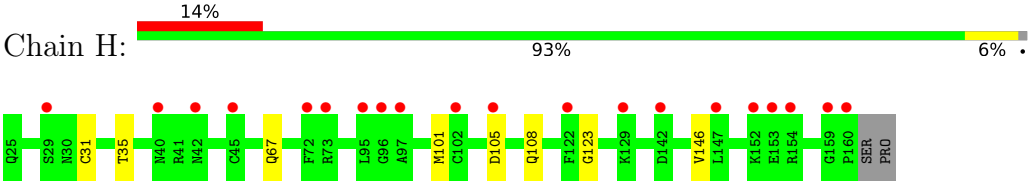
• Molecule 2: Tumor necrosis factor receptor superfamily member 9

Chain F:



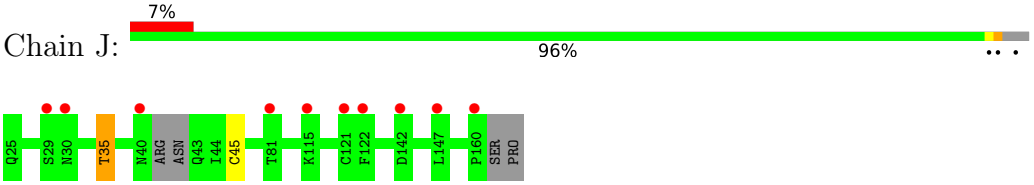
• Molecule 2: Tumor necrosis factor receptor superfamily member 9

Chain H:



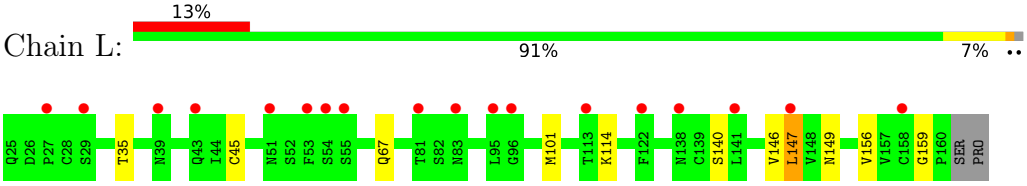
• Molecule 2: Tumor necrosis factor receptor superfamily member 9

Chain J:



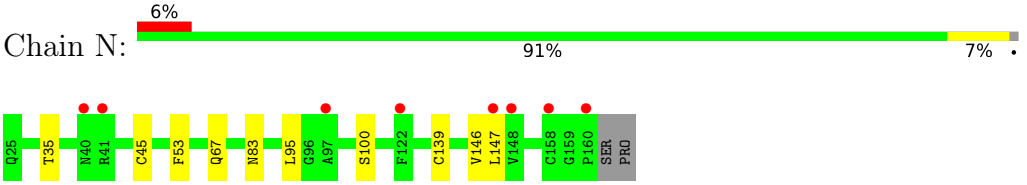
• Molecule 2: Tumor necrosis factor receptor superfamily member 9

Chain L:



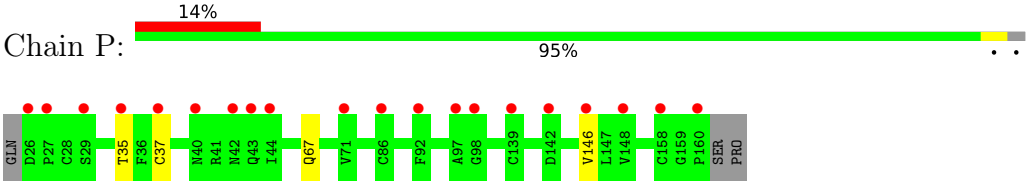
• Molecule 2: Tumor necrosis factor receptor superfamily member 9

Chain N:



• Molecule 2: Tumor necrosis factor receptor superfamily member 9

Chain P:

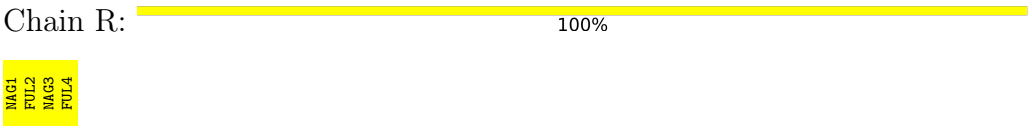


• Molecule 3: beta-L-fucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q:

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

Chain R:



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

Chain S:

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

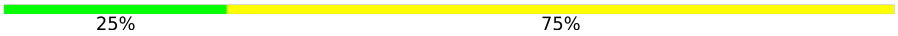
Chain T:

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

Chain U:

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

Chain W:



• Molecule 5: beta-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain V:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	170.33Å 102.47Å 167.37Å 90.00° 91.54° 90.00°	Depositor
Resolution (Å)	167.31 – 2.81 167.31 – 2.81	Depositor EDS
% Data completeness (in resolution range)	67.2 (167.31-2.81) 67.2 (167.31-2.81)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	0.16	Depositor
$< I/\sigma(I) >$ [1]	1.72 (at 2.82Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.241 , 0.291 0.242 , 0.288	Depositor DCC
R_{free} test set	3454 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å^2)	65.8	Xtriage
Anisotropy	0.018	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 60.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.25$	Xtriage
Estimated twinning fraction	0.020 for -1/2*h+3/2*k,1/2*h+1/2*k,-l 0.025 for -1/2*h-3/2*k,-1/2*h+1/2*k,-l 0.025 for 1/2*h+3/2*k,1/2*h-1/2*k,-l 0.037 for 1/2*h-3/2*k,-1/2*h-1/2*k,-l 0.055 for -h,-k,l	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	15717	wwPDB-VP
Average B, all atoms (Å^2)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 23.38 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.7131e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: NAG, FUL

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	1.05	0/928	1.65	1/1256 (0.1%)
1	C	1.06	0/934	1.65	0/1264
1	E	1.03	0/928	1.66	1/1256 (0.1%)
1	G	1.08	0/938	1.68	2/1269 (0.2%)
1	I	1.09	0/928	1.64	3/1256 (0.2%)
1	K	1.07	0/928	1.65	1/1256 (0.1%)
1	M	1.03	0/934	1.65	0/1264
1	O	1.07	0/928	1.64	1/1256 (0.1%)
2	B	1.10	0/1013	1.48	0/1361
2	D	1.08	0/1019	1.46	0/1369
2	F	1.06	0/1011	1.49	0/1357
2	H	1.10	0/1022	1.49	1/1373 (0.1%)
2	J	1.09	0/1002	1.51	0/1345
2	L	1.09	0/1022	1.47	0/1373
2	N	1.05	0/1022	1.47	2/1373 (0.1%)
2	P	1.05	0/1013	1.45	0/1361
All	All	1.07	0/15570	1.56	12/20989 (0.1%)

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
2	F	0	1

There are no bond length outliers.

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	111	GLN	CB-CG-CD	-6.64	101.31	112.60
1	K	27	ASP	CA-CB-CG	6.27	118.87	112.60
2	H	105	ASP	CA-CB-CG	6.23	118.83	112.60
1	A	13	ASP	CA-CB-CG	6.03	118.63	112.60
1	E	13	ASP	CA-CB-CG	5.96	118.56	112.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	F	42	ASN	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	918	0	931	1	1
1	C	924	0	936	1	0
1	E	918	0	931	1	0
1	G	928	0	939	1	0
1	I	918	0	931	1	0
1	K	918	0	931	2	0
1	M	924	0	936	0	0
1	O	918	0	931	0	0
2	B	997	0	918	0	0
2	D	1003	0	923	5	0
2	F	995	0	920	2	0
2	H	1006	0	926	4	0
2	J	987	0	908	2	0
2	L	1006	0	926	3	0
2	N	1006	0	926	2	0
2	P	997	0	918	0	0
3	Q	24	0	22	0	0
4	R	48	0	43	0	0
4	S	48	0	43	0	0
4	T	48	0	43	0	0
4	U	48	0	43	0	0
4	W	48	0	43	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	V	24	0	22	0	0
6	N	14	0	13	0	0
7	A	2	0	0	0	0
7	B	4	0	0	0	0
7	C	2	0	0	0	0
7	D	1	0	0	0	0
7	E	3	0	0	0	0
7	F	5	0	0	0	0
7	G	7	0	0	0	0
7	H	2	0	0	0	0
7	I	3	0	0	0	0
7	J	4	0	0	0	0
7	K	1	0	0	0	0
7	L	2	0	0	0	0
7	M	2	0	0	0	0
7	N	8	0	0	0	0
7	O	2	0	0	0	0
7	P	4	0	0	0	0
All	All	15717	0	15103	21	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 1.

The worst 5 of 21 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:E:24:GLU:HG2	2:F:39:ASN:HB3	1.88	0.56
2:L:149:ASN:O	2:L:156:VAL:HG22	2.05	0.56
2:J:35:THR:CG2	2:J:45:CYS:HB3	2.36	0.55
2:J:35:THR:HG23	2:J:45:CYS:HB3	1.90	0.54
2:D:27:PRO:HB2	2:D:44:ILE:HD11	1.88	0.54

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)
1:A:64:GLU:OE2	1:A:64:GLU:OE2[2_756]	1.96	0.24

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	122/126 (97%)	116 (95%)	6 (5%)	0	100	100
1	C	123/126 (98%)	116 (94%)	5 (4%)	2 (2%)	8	25
1	E	122/126 (97%)	116 (95%)	5 (4%)	1 (1%)	16	42
1	G	124/126 (98%)	117 (94%)	6 (5%)	1 (1%)	16	42
1	I	122/126 (97%)	115 (94%)	5 (4%)	2 (2%)	8	25
1	K	122/126 (97%)	116 (95%)	4 (3%)	2 (2%)	8	25
1	M	123/126 (98%)	117 (95%)	6 (5%)	0	100	100
1	O	122/126 (97%)	115 (94%)	6 (5%)	1 (1%)	16	42
2	B	133/138 (96%)	126 (95%)	6 (4%)	1 (1%)	16	42
2	D	134/138 (97%)	130 (97%)	3 (2%)	1 (1%)	19	46
2	F	133/138 (96%)	129 (97%)	3 (2%)	1 (1%)	16	42
2	H	134/138 (97%)	129 (96%)	4 (3%)	1 (1%)	19	46
2	J	130/138 (94%)	125 (96%)	5 (4%)	0	100	100
2	L	134/138 (97%)	131 (98%)	2 (2%)	1 (1%)	19	46
2	N	134/138 (97%)	129 (96%)	4 (3%)	1 (1%)	19	46
2	P	133/138 (96%)	128 (96%)	4 (3%)	1 (1%)	16	42
All	All	2045/2112 (97%)	1955 (96%)	74 (4%)	16 (1%)	16	42

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	135	ALA
1	E	61	GLU
1	O	61	GLU
1	C	61	GLU
1	G	61	GLU

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	91/92 (99%)	90 (99%)	1 (1%)	70 90
1	C	92/92 (100%)	91 (99%)	1 (1%)	70 90
1	E	91/92 (99%)	91 (100%)	0	100 100
1	G	92/92 (100%)	90 (98%)	2 (2%)	47 78
1	I	91/92 (99%)	89 (98%)	2 (2%)	47 78
1	K	91/92 (99%)	90 (99%)	1 (1%)	70 90
1	M	92/92 (100%)	89 (97%)	3 (3%)	33 65
1	O	91/92 (99%)	87 (96%)	4 (4%)	24 55
2	B	117/120 (98%)	114 (97%)	3 (3%)	41 73
2	D	118/120 (98%)	115 (98%)	3 (2%)	42 74
2	F	117/120 (98%)	111 (95%)	6 (5%)	20 49
2	H	118/120 (98%)	115 (98%)	3 (2%)	42 74
2	J	116/120 (97%)	115 (99%)	1 (1%)	75 92
2	L	118/120 (98%)	112 (95%)	6 (5%)	20 49
2	N	118/120 (98%)	113 (96%)	5 (4%)	25 57
2	P	117/120 (98%)	114 (97%)	3 (3%)	41 73
All	All	1670/1696 (98%)	1626 (97%)	44 (3%)	41 73

5 of 44 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	L	147	LEU
2	N	100	SER
1	M	13	ASP
2	N	35	THR
1	O	13	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 25 such sidechains are listed below:

Mol	Chain	Res	Type
2	H	108	GLN
2	L	67	GLN
2	P	108	GLN
1	K	109	GLN
2	L	104	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)

24 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	Q	1	2,3	14,14,15	0.50	0	17,19,21	2.15	3 (17%)
3	FUL	Q	2	3	10,10,11	0.64	0	14,14,16	0.82	0
4	NAG	R	1	2,4	14,14,15	0.47	0	17,19,21	1.23	2 (11%)
4	FUL	R	2	4	10,10,11	0.49	0	14,14,16	1.35	1 (7%)
4	NAG	R	3	4	14,14,15	0.45	0	17,19,21	0.84	1 (5%)
4	FUL	R	4	4	10,10,11	0.73	1 (10%)	14,14,16	1.15	2 (14%)
4	NAG	S	1	2,4	14,14,15	0.62	0	17,19,21	1.59	7 (41%)
4	FUL	S	2	4	10,10,11	0.48	0	14,14,16	0.62	0
4	NAG	S	3	4	14,14,15	0.38	0	17,19,21	1.68	2 (11%)
4	FUL	S	4	4	10,10,11	0.50	0	14,14,16	0.77	0
4	NAG	T	1	2,4	14,14,15	0.34	0	17,19,21	0.98	0
4	FUL	T	2	4	10,10,11	0.46	0	14,14,16	0.92	1 (7%)
4	NAG	T	3	4	14,14,15	0.50	0	17,19,21	1.04	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	FUL	T	4	4	10,10,11	0.35	0	14,14,16	0.69	0
4	NAG	U	1	2,4	14,14,15	0.57	0	17,19,21	2.66	6 (35%)
4	FUL	U	2	4	10,10,11	0.56	0	14,14,16	2.42	3 (21%)
4	NAG	U	3	4	14,14,15	0.62	0	17,19,21	1.03	0
4	FUL	U	4	4	10,10,11	0.52	0	14,14,16	1.12	1 (7%)
5	NAG	V	1	5,2	14,14,15	0.52	0	17,19,21	1.35	2 (11%)
5	FUL	V	2	5	10,10,11	0.52	0	14,14,16	0.82	0
4	NAG	W	1	2,4	14,14,15	0.51	0	17,19,21	1.20	1 (5%)
4	FUL	W	2	4	10,10,11	0.54	0	14,14,16	1.37	2 (14%)
4	NAG	W	3	4	14,14,15	0.62	0	17,19,21	0.85	1 (5%)
4	FUL	W	4	4	10,10,11	0.38	0	14,14,16	0.60	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	Q	1	2,3	-	1/6/23/26	0/1/1/1
3	FUL	Q	2	3	-	-	0/1/1/1
4	NAG	R	1	2,4	-	2/6/23/26	0/1/1/1
4	FUL	R	2	4	-	-	0/1/1/1
4	NAG	R	3	4	-	0/6/23/26	0/1/1/1
4	FUL	R	4	4	-	-	0/1/1/1
4	NAG	S	1	2,4	-	0/6/23/26	0/1/1/1
4	FUL	S	2	4	-	-	0/1/1/1
4	NAG	S	3	4	-	3/6/23/26	0/1/1/1
4	FUL	S	4	4	-	-	0/1/1/1
4	NAG	T	1	2,4	-	2/6/23/26	0/1/1/1
4	FUL	T	2	4	-	-	0/1/1/1
4	NAG	T	3	4	-	2/6/23/26	0/1/1/1
4	FUL	T	4	4	-	-	0/1/1/1
4	NAG	U	1	2,4	-	1/6/23/26	0/1/1/1
4	FUL	U	2	4	-	-	0/1/1/1
4	NAG	U	3	4	-	0/6/23/26	0/1/1/1
4	FUL	U	4	4	-	-	0/1/1/1
5	NAG	V	1	5,2	-	0/6/23/26	0/1/1/1
5	FUL	V	2	5	-	-	0/1/1/1
4	NAG	W	1	2,4	-	0/6/23/26	0/1/1/1
4	FUL	W	2	4	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	W	3	4	-	1/6/23/26	0/1/1/1
4	FUL	W	4	4	-	-	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	R	4	FUL	O4-C4	2.12	1.48	1.43

The worst 5 of 35 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	U	1	NAG	C1-O5-C5	7.60	122.50	112.19
3	Q	1	NAG	C1-O5-C5	6.75	121.33	112.19
4	U	2	FUL	C1-C2-C3	5.83	116.84	109.67
4	S	3	NAG	C2-N2-C7	5.40	130.60	122.90
4	U	2	FUL	C1-O5-C5	4.23	122.36	112.78

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

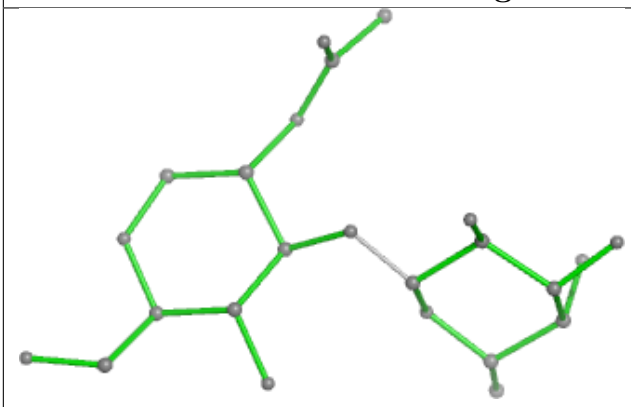
Mol	Chain	Res	Type	Atoms
4	T	1	NAG	C4-C5-C6-O6
4	T	1	NAG	O5-C5-C6-O6
4	T	3	NAG	C4-C5-C6-O6
4	T	3	NAG	O5-C5-C6-O6
4	R	1	NAG	C4-C5-C6-O6

There are no ring outliers.

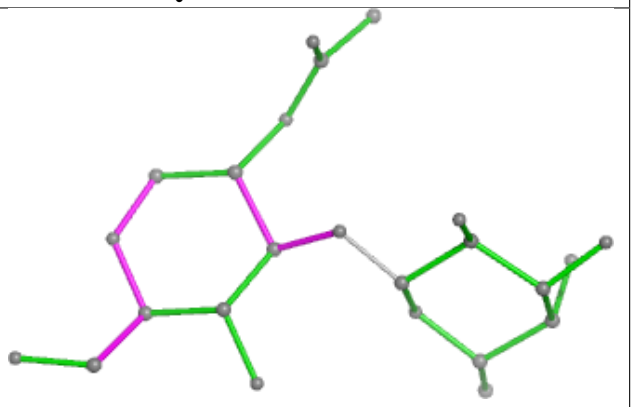
No monomer is involved in short contacts.

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

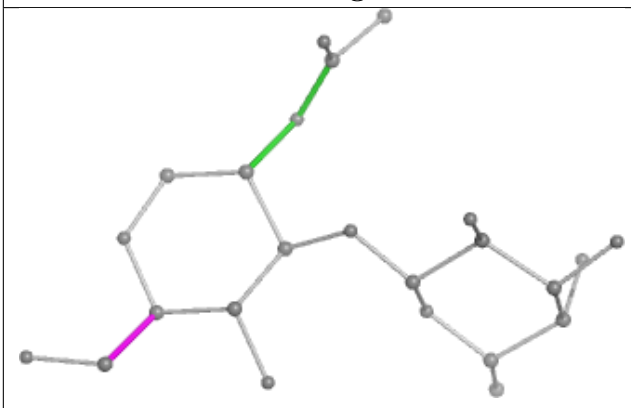
Oligosaccharide Chain Q



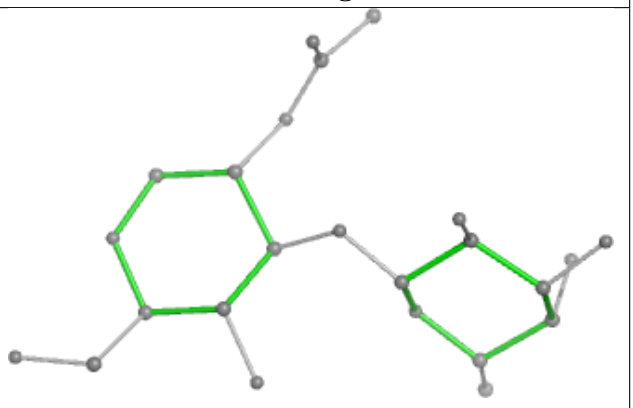
Bond lengths



Bond angles

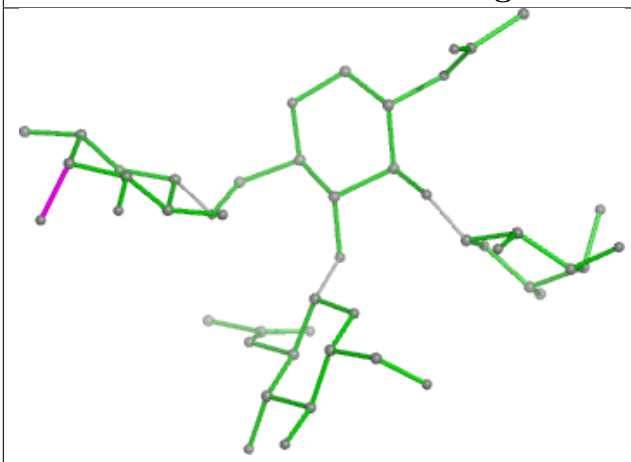


Torsions

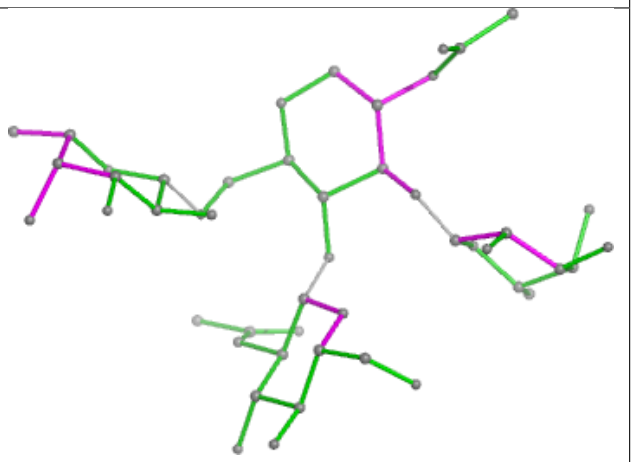


Rings

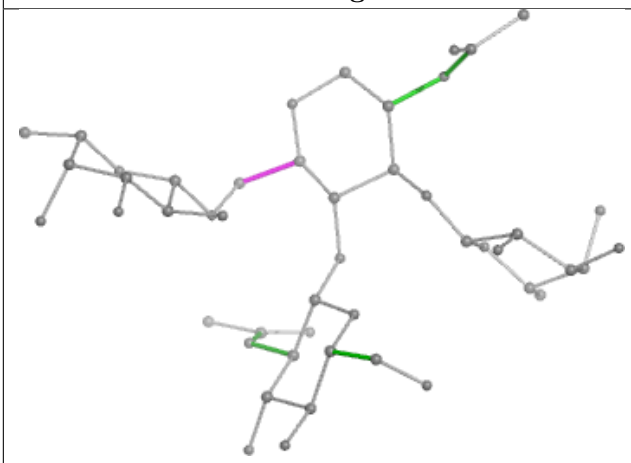
Oligosaccharide Chain R



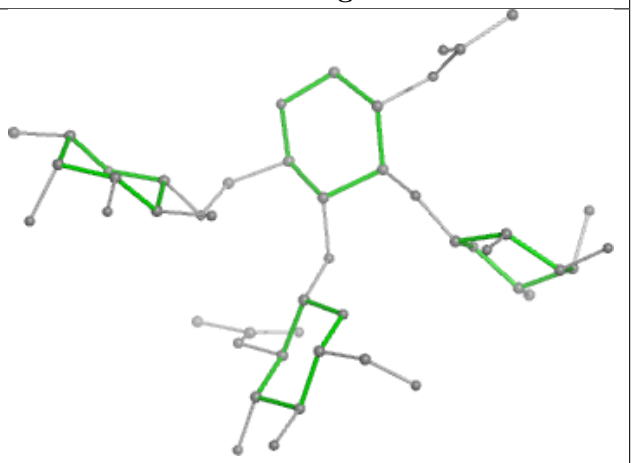
Bond lengths



Bond angles

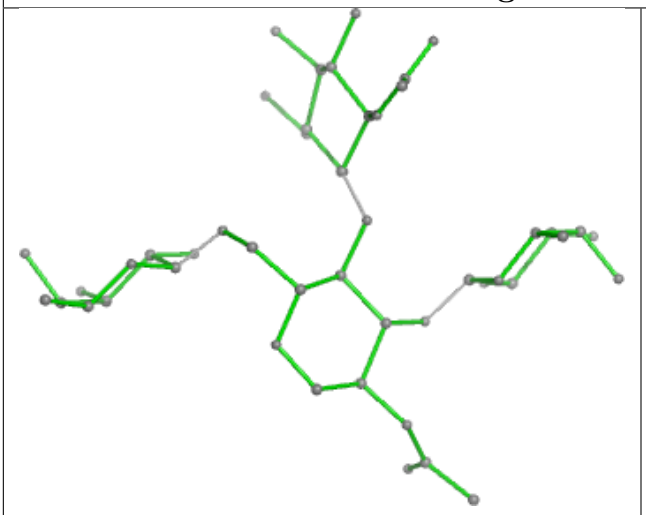


Torsions

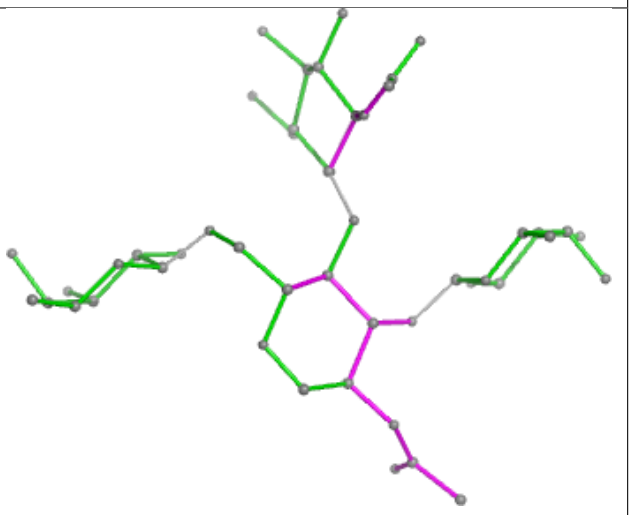


Rings

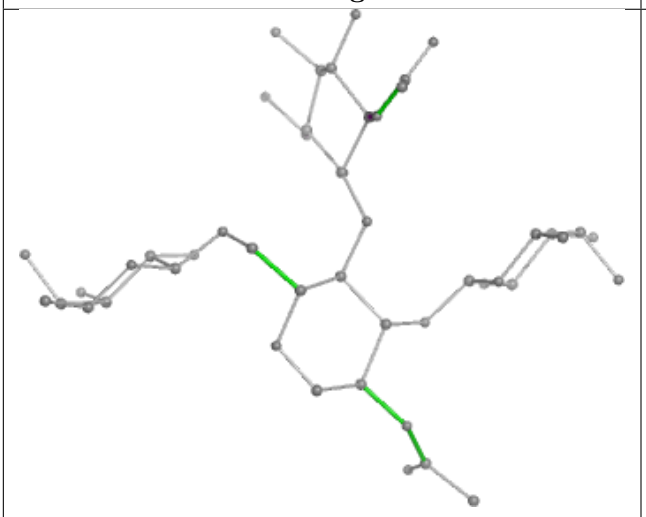
Oligosaccharide Chain S



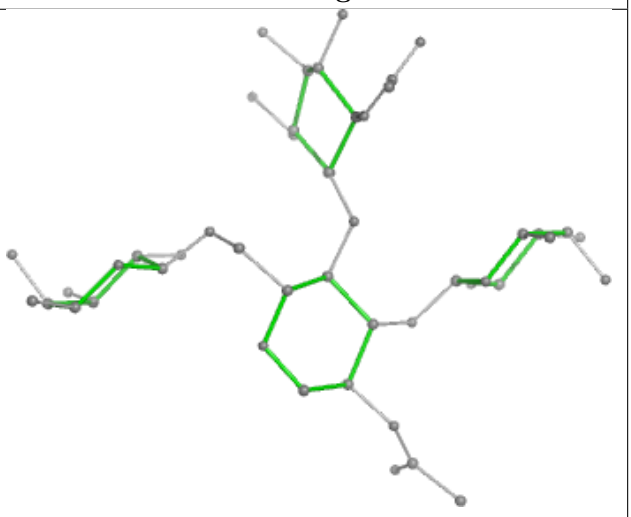
Bond lengths



Bond angles

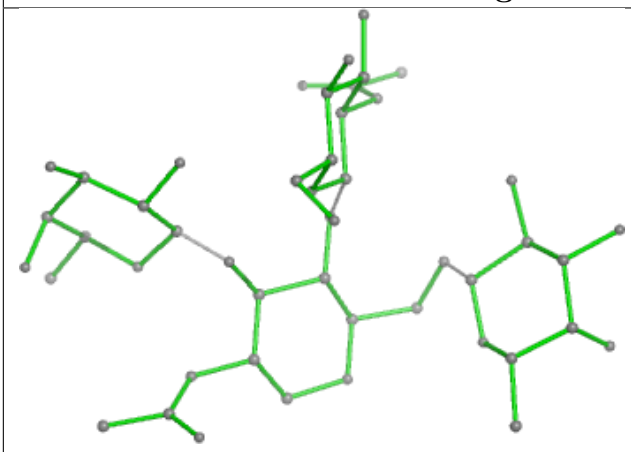


Torsions

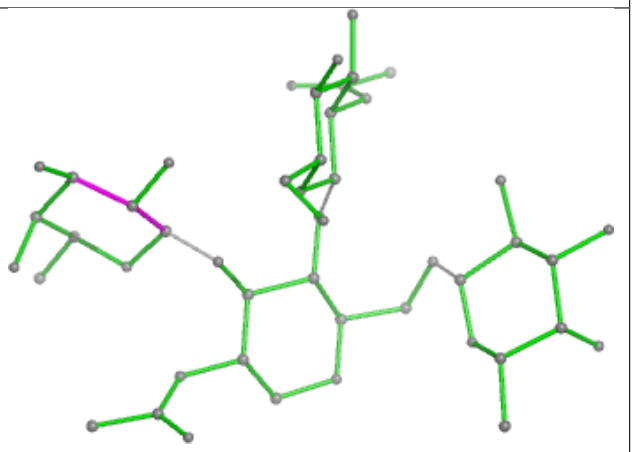


Rings

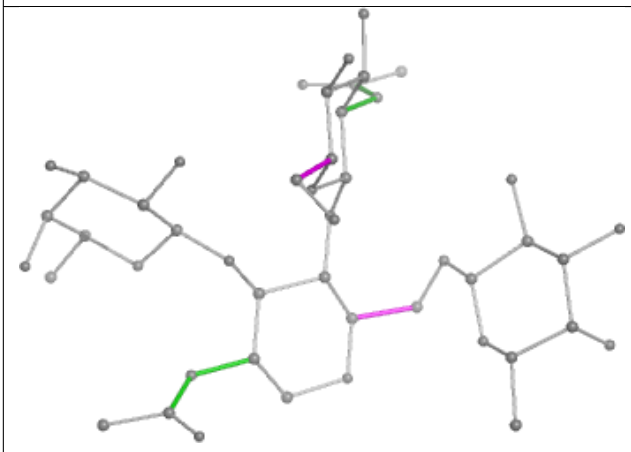
Oligosaccharide Chain T



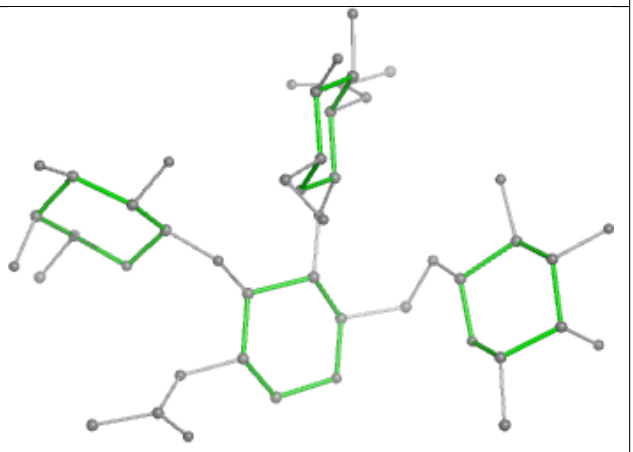
Bond lengths



Bond angles

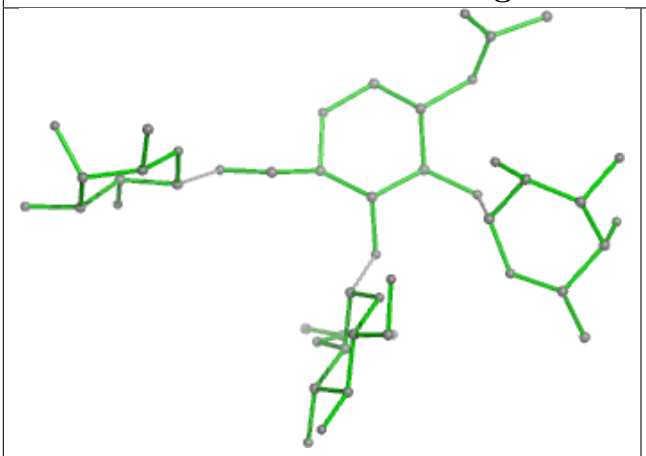


Torsions

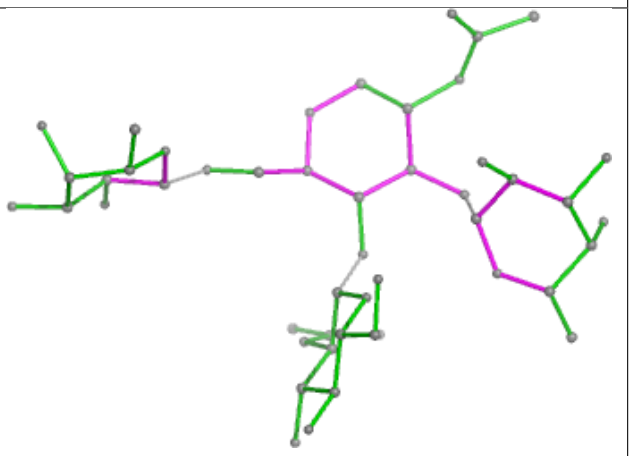


Rings

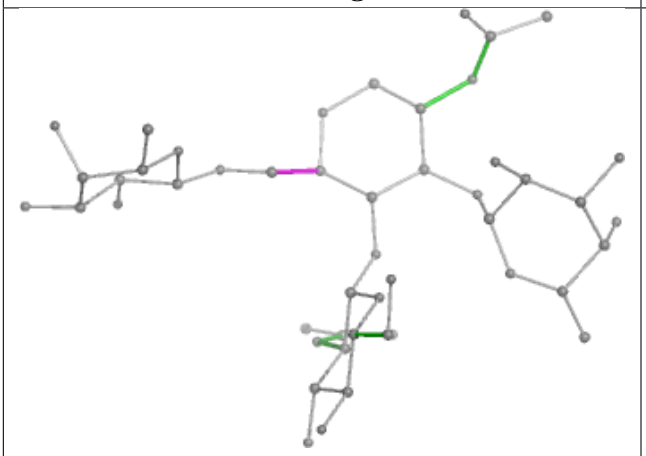
Oligosaccharide Chain U



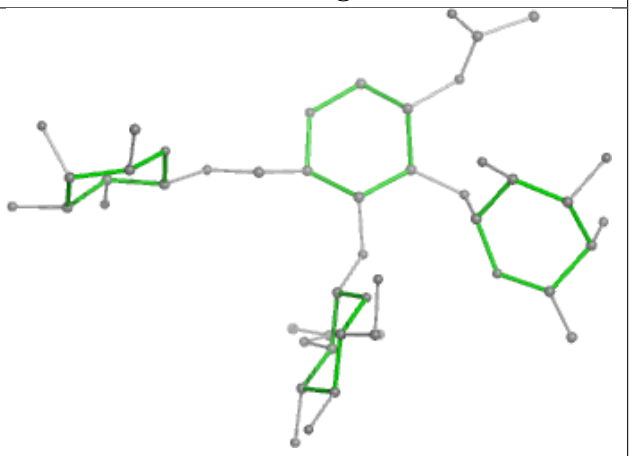
Bond lengths



Bond angles

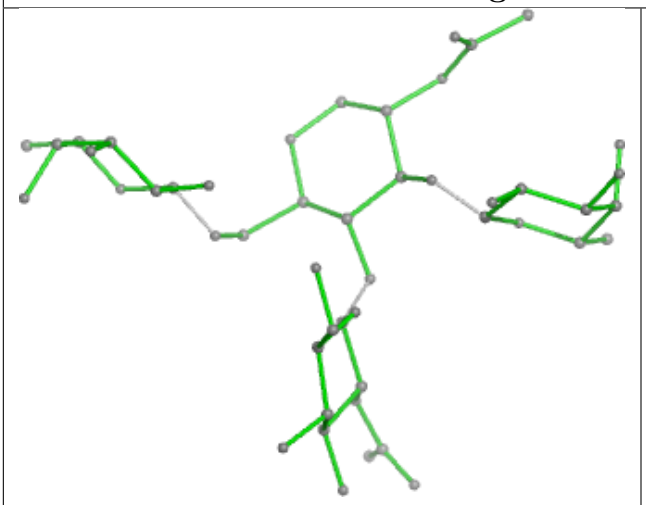


Torsions

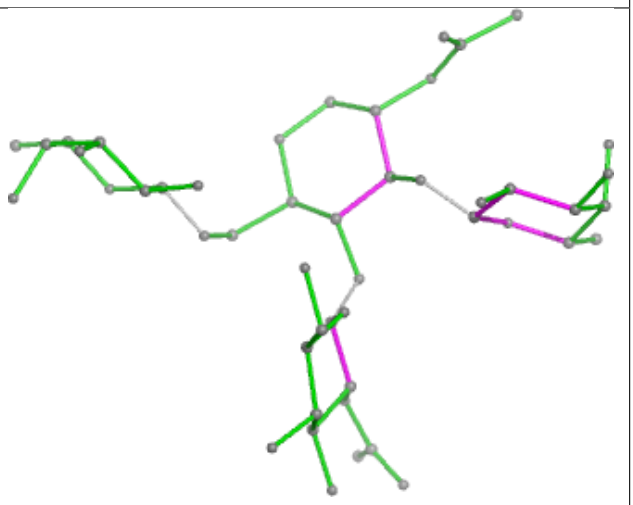


Rings

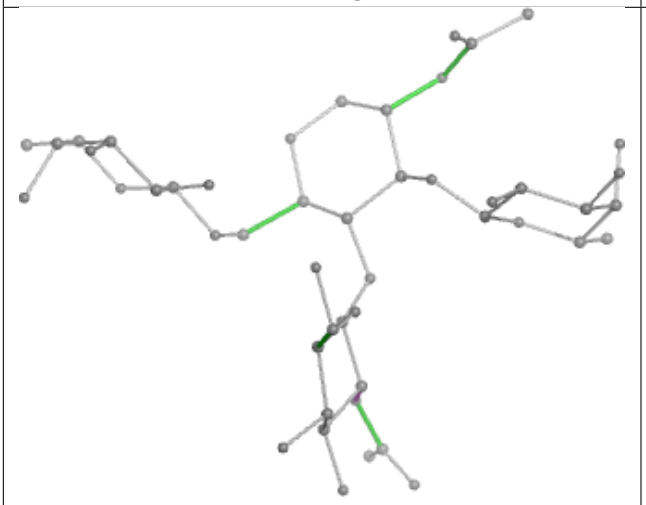
Oligosaccharide Chain W



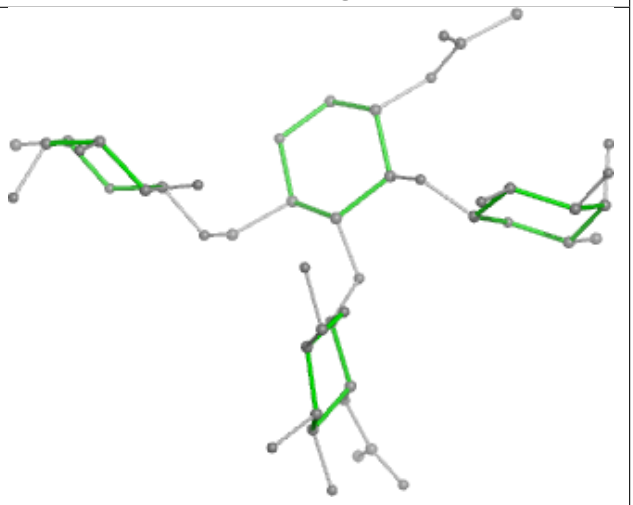
Bond lengths



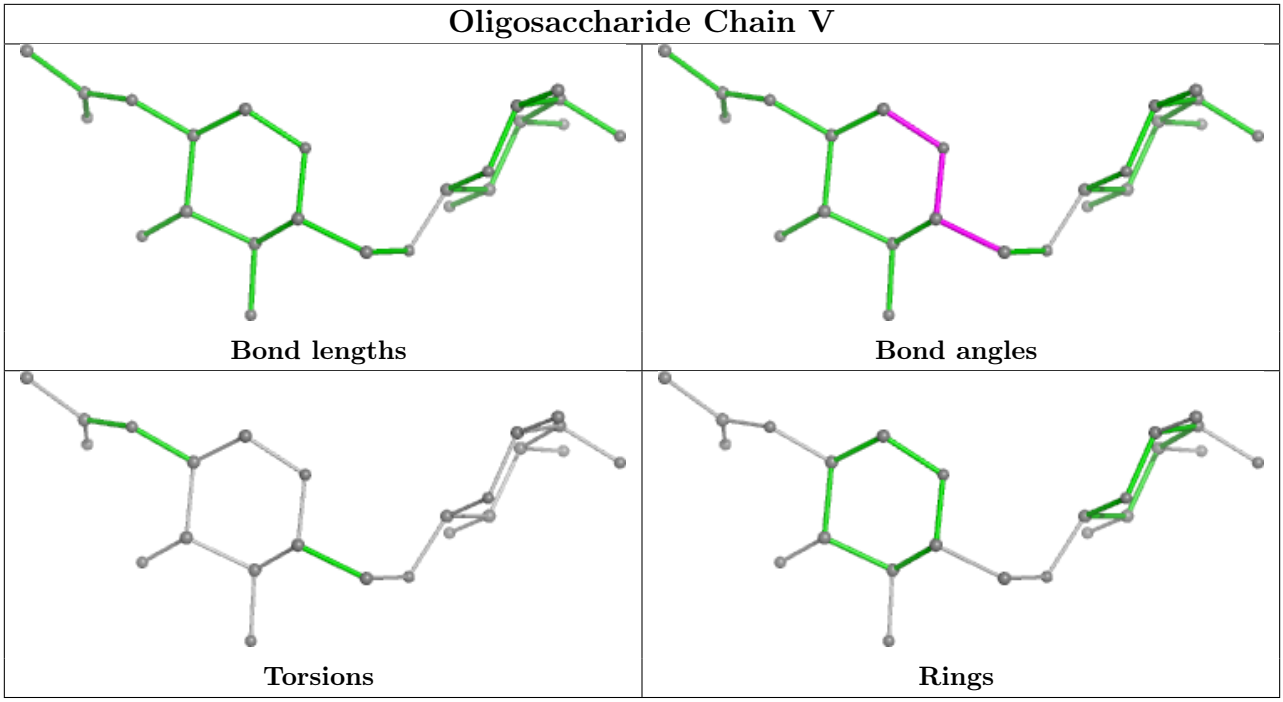
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

1 ligand is 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	N	201	2	14,14,15	0.54	0	17,19,21	1.64	3 (17%)

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	N	201	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	N	201	NAG	C1-O5-C5	4.80	118.70	112.19
6	N	201	NAG	C2-N2-C7	3.64	128.09	122.90
6	N	201	NAG	O5-C5-C6	2.11	110.51	107.20

There are no chirality outliers.

There are no torsion outliers.

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 (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	124/126 (98%)	0.49	7 (5%) 31 24	30, 54, 90, 127	21 (16%)
1	C	125/126 (99%)	0.34	4 (3%) 50 42	27, 51, 88, 133	18 (14%)
1	E	124/126 (98%)	0.33	3 (2%) 59 52	30, 50, 75, 98	9 (7%)
1	G	126/126 (100%)	0.33	6 (4%) 36 29	29, 55, 95, 123	17 (13%)
1	I	124/126 (98%)	0.43	8 (6%) 26 20	31, 57, 100, 140	21 (16%)
1	K	124/126 (98%)	0.69	9 (7%) 22 17	35, 61, 101, 125	25 (20%)
1	M	125/126 (99%)	-0.02	1 (0%) 82 77	26, 43, 66, 87	16 (12%)
1	O	124/126 (98%)	0.77	10 (8%) 19 15	32, 71, 108, 138	25 (20%)
2	B	135/138 (97%)	0.73	16 (11%) 10 8	34, 64, 88, 108	22 (16%)
2	D	136/138 (98%)	0.52	12 (8%) 17 13	29, 52, 95, 108	18 (13%)
2	F	135/138 (97%)	0.48	12 (8%) 17 13	32, 57, 75, 113	20 (14%)
2	H	136/138 (98%)	1.06	20 (14%) 7 6	28, 70, 108, 124	32 (23%)
2	J	134/138 (97%)	0.67	10 (7%) 22 16	24, 62, 93, 114	18 (13%)
2	L	136/138 (98%)	0.84	18 (13%) 8 7	31, 65, 98, 119	21 (15%)
2	N	136/138 (98%)	0.38	8 (5%) 29 23	26, 55, 92, 119	17 (12%)
2	P	135/138 (97%)	0.74	20 (14%) 7 6	27, 61, 96, 117	21 (15%)
All	All	2079/2112 (98%)	0.55	164 (7%) 20 15	24, 58, 97, 140	321 (15%)

The worst 5 of 164 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	O	73	VAL	6.5
1	I	40	VAL	6.1
2	H	154	ARG	5.0
2	F	161	SER	4.8
2	P	42	ASN	4.5

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)

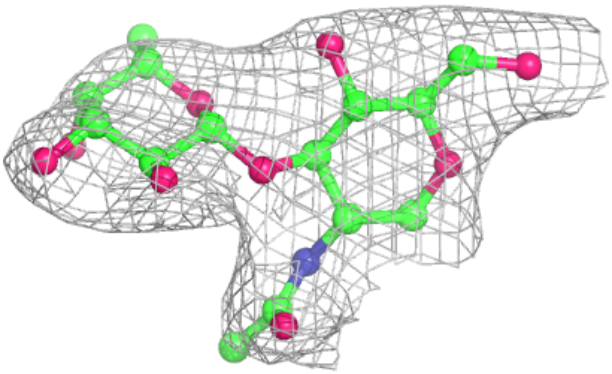
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

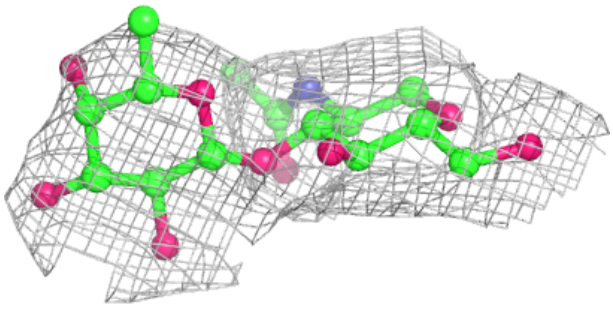
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	FUL	U	4	10/11	0.56	0.16	108,112,118,125	0
4	NAG	W	3	14/15	0.60	0.14	122,133,137,138	4
4	NAG	S	3	14/15	0.62	0.12	106,116,122,122	5
4	NAG	T	3	14/15	0.62	0.17	123,150,160,176	1
4	FUL	R	2	10/11	0.64	0.17	131,138,142,143	0
4	FUL	W	2	10/11	0.66	0.14	122,126,133,134	0
4	FUL	W	4	10/11	0.69	0.15	110,124,128,134	0
4	FUL	S	2	10/11	0.71	0.17	107,116,120,122	0
4	NAG	U	3	14/15	0.74	0.17	89,103,108,109	1
4	FUL	R	4	10/11	0.75	0.18	119,122,126,127	3
4	FUL	T	4	10/11	0.76	0.14	150,156,163,164	0
4	NAG	R	1	14/15	0.77	0.14	102,126,138,142	0
4	NAG	R	3	14/15	0.77	0.15	121,149,155,156	1
5	FUL	V	2	10/11	0.77	0.12	111,113,116,118	0
4	NAG	W	1	14/15	0.79	0.10	104,116,131,135	0
3	FUL	Q	2	10/11	0.80	0.14	94,100,104,109	0
5	NAG	V	1	14/15	0.83	0.11	109,115,122,126	0
4	FUL	T	2	10/11	0.83	0.16	142,147,151,151	0
4	NAG	T	1	14/15	0.84	0.12	114,133,146,148	0
4	NAG	S	1	14/15	0.84	0.09	88,110,122,125	1
4	FUL	S	4	10/11	0.84	0.10	116,119,123,127	0
3	NAG	Q	1	14/15	0.85	0.10	63,78,83,91	0
4	FUL	U	2	10/11	0.86	0.09	99,102,105,110	0
4	NAG	U	1	14/15	0.89	0.09	78,95,99,103	0

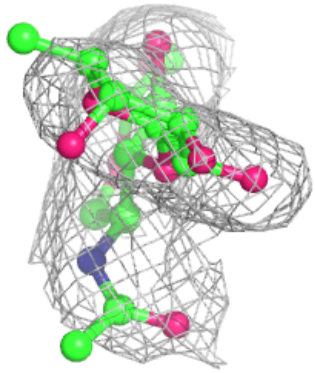
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain Q:

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

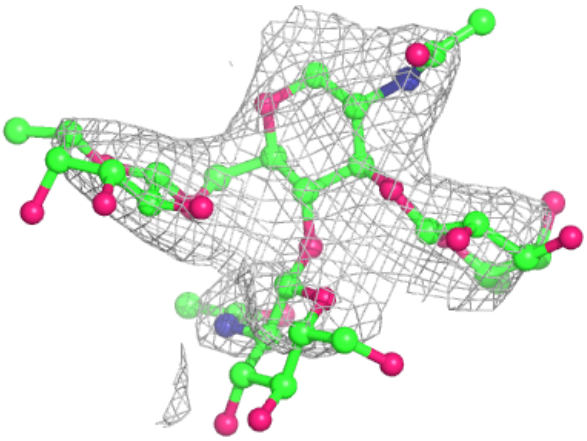


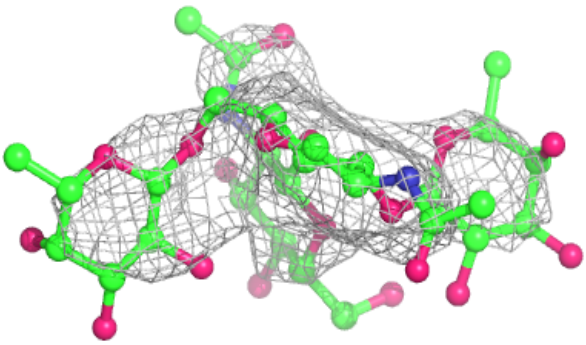


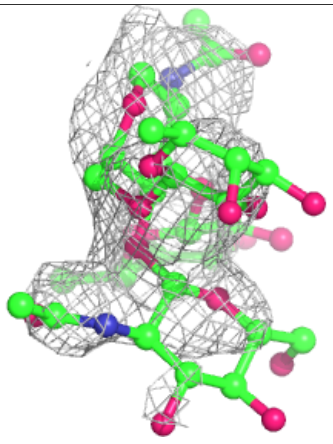


Electron density around Chain R:

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

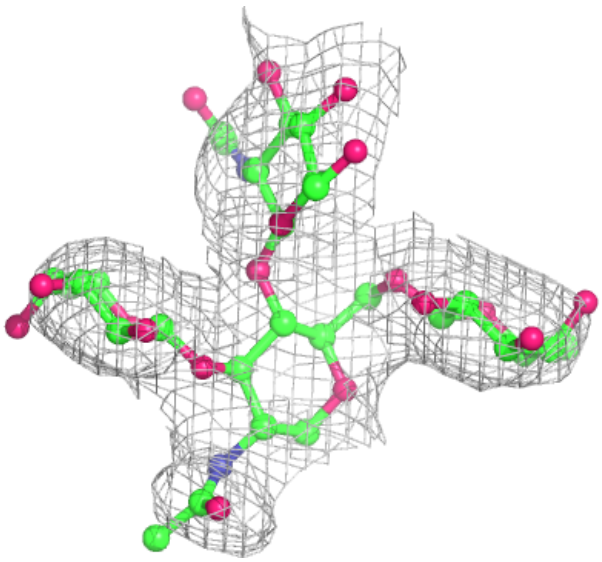


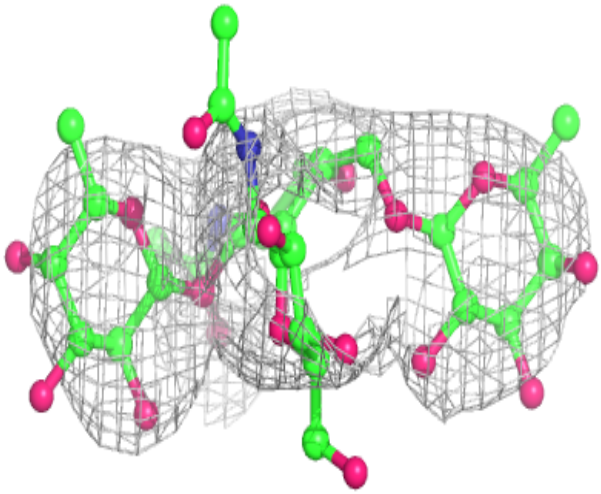


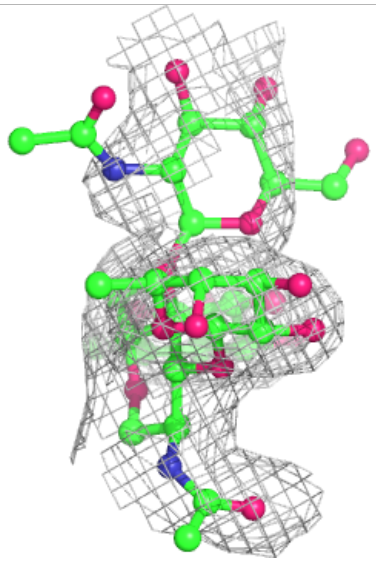


Electron density around Chain S:

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

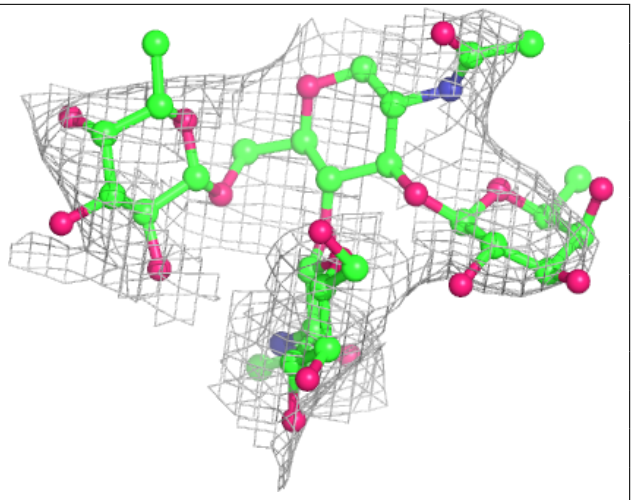


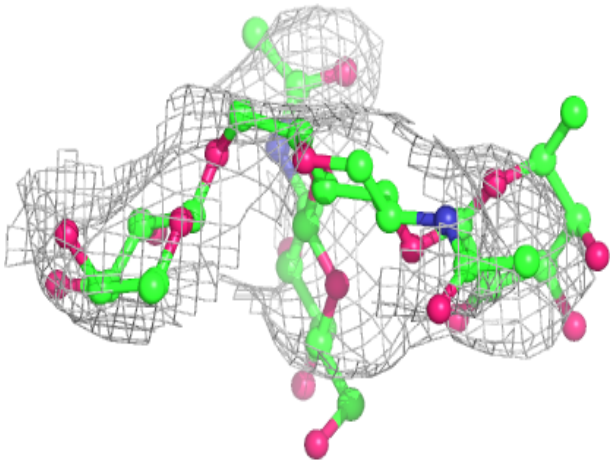


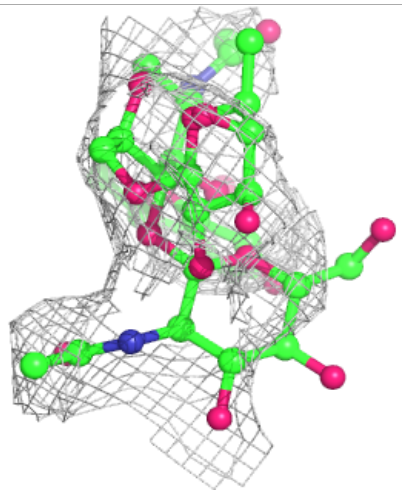


Electron density around Chain T:

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

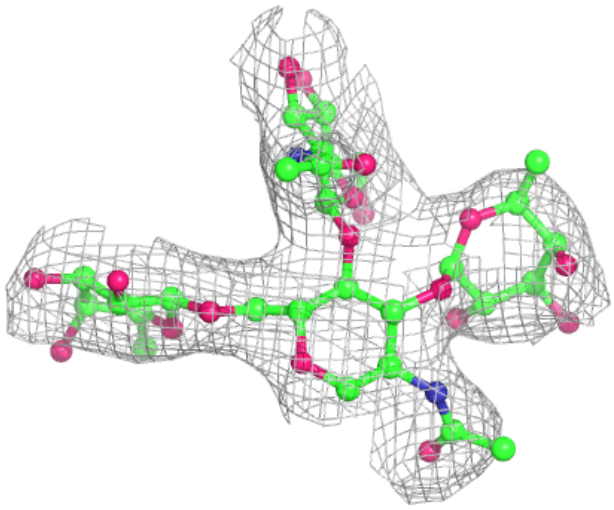


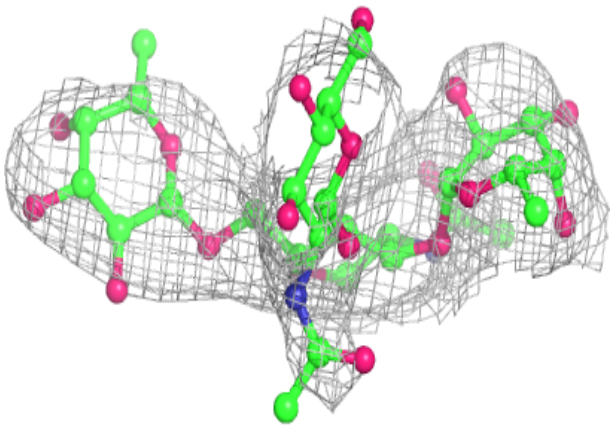


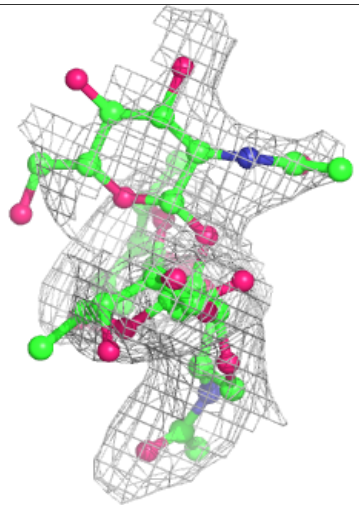


Electron density around Chain U:

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

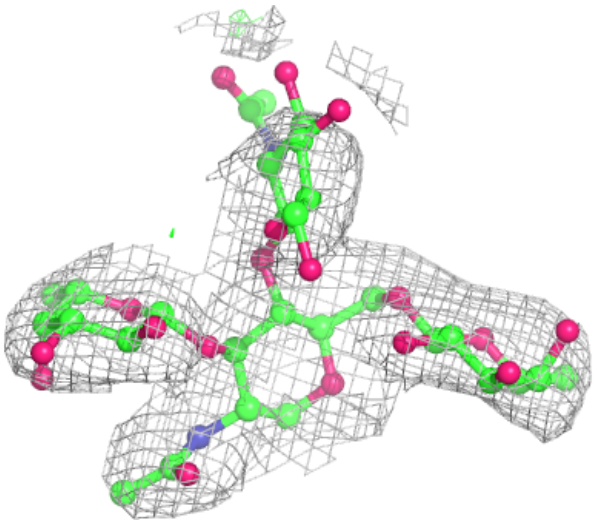


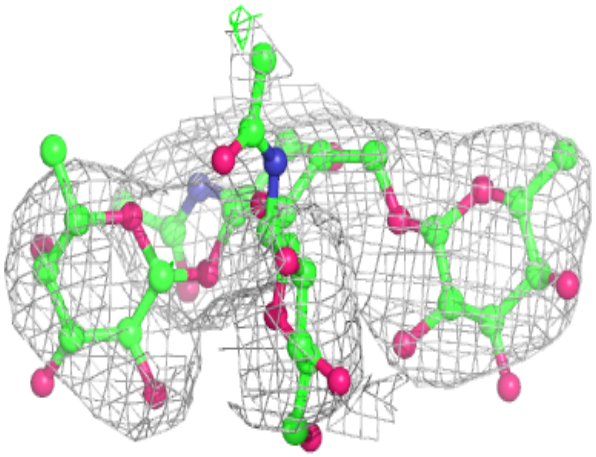


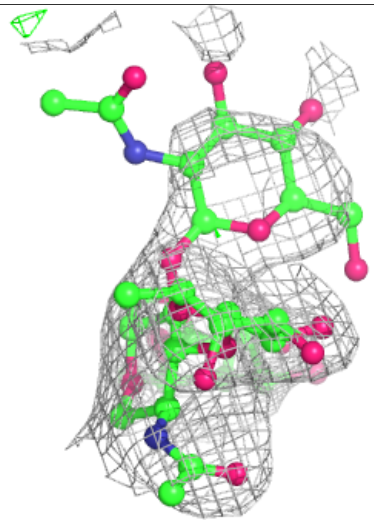


Electron density around Chain W:

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

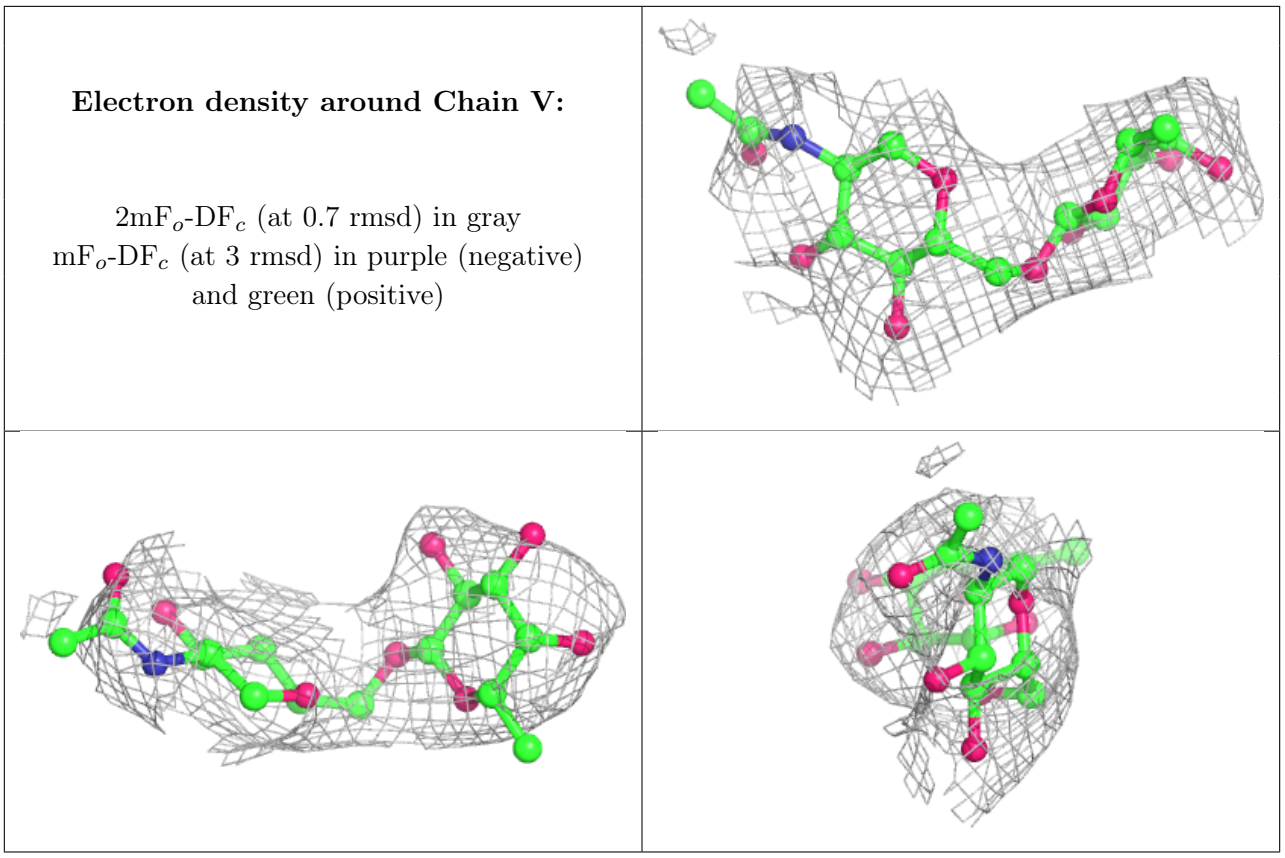






Electron density around Chain V:

$2mF_o$-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
6	NAG	N	201	14/15	0.69	0.13	102,112,123,127	3

6.5 Other polymers

There are no such residues in this entry.