wwPDB X-ray Structure Validation Summary Report (i)

Nov 2, 2026 – 06:09 AM EST

PDB ID	:	9Z1G / pdb_00009z1g
Title	:	Crystal structure of NJ receptor binding domain in complex with antibody CC25.4
Authors	:	Feng, Z.; Wilson, I.A.
Deposited on	:	2025-11-04
Resolution	:	2.82 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:

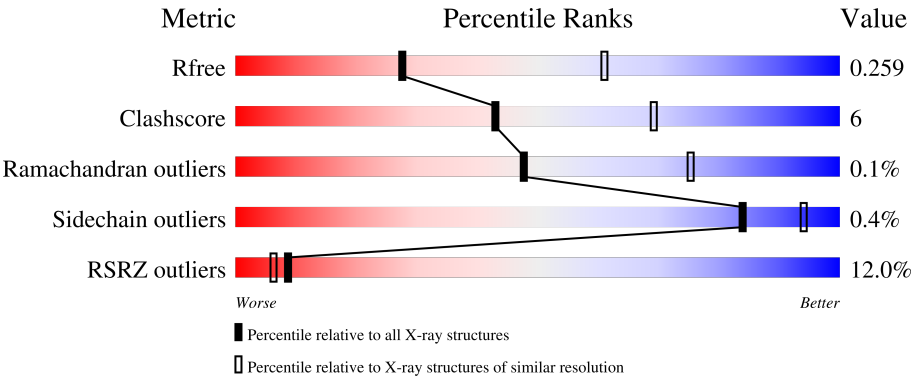
MolProbity	:	4-5-2 with Phenix2.2
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.2
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

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 2.82 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.



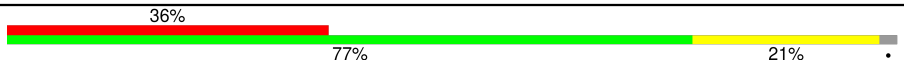
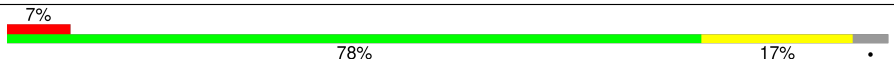
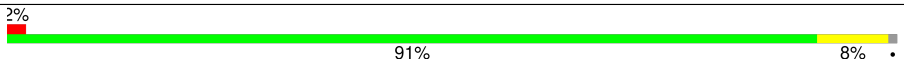
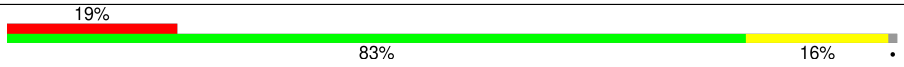
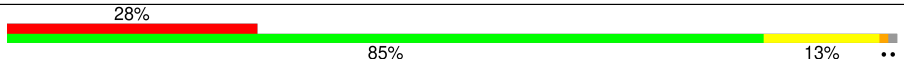
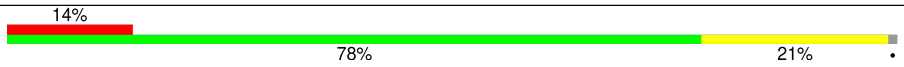
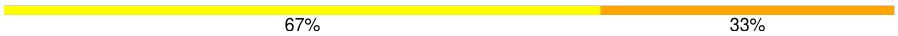
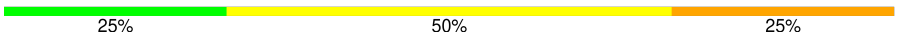
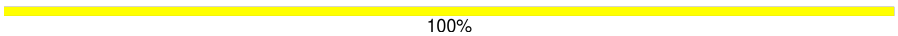
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4591 (2.84-2.80)
Clashscore	190562	5010 (2.84-2.80)
Ramachandran outliers	187476	4916 (2.84-2.80)
Sidechain outliers	187428	4918 (2.84-2.80)
RSRZ outliers	180081	4594 (2.84-2.80)

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	N	203	5% 89% 8%
1	O	203	2% 83% 13%
1	Z	203	7% 82% 14%
2	G	229	80% 16%
2	I	229	7% 86% 13%

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Mol	Chain	Length	Quality of chain
2	K	229	
2	X	229	
3	H	217	
3	J	217	
3	L	217	
3	Y	217	
4	M	2	
4	P	2	
4	Q	2	
5	A	3	
6	B	4	
7	C	5	

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 18171 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 NJ spike protein S1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	N	197	Total	C	N	O	S	0	0	0
			1564	995	273	288	8			
1	O	196	Total	C	N	O	S	0	0	0
			1560	993	272	287	8			
1	Z	195	Total	C	N	O	S	0	0	0
			1554	990	271	285	8			

- Molecule 2 is a protein called Neutralizing antibody CC25.4 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	219	Total	C	N	O	S	0	0	0
			1689	1069	291	320	9			
2	I	227	Total	C	N	O	S	0	0	0
			1737	1095	300	333	9			
2	X	219	Total	C	N	O	S	0	0	0
			1689	1069	291	320	9			
2	K	224	Total	C	N	O	S	0	0	0
			1715	1082	296	328	9			

- Molecule 3 is a protein called Neutralizing antibody CC25.4 light chain.

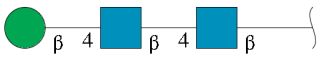
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	215	Total	C	N	O	S	0	0	0
			1566	975	263	324	4			
3	J	214	Total	C	N	O	S	0	0	0
			1557	970	262	321	4			
3	Y	214	Total	C	N	O	S	0	0	0
			1557	970	262	321	4			
3	L	214	Total	C	N	O	S	0	0	0
			1557	970	262	321	4			

- 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	M	2	Total C N O 28 16 2 10	0	0	0
4	P	2	Total C N O 28 16 2 10	0	0	0
4	Q	2	Total C N O 28 16 2 10	0	0	0

- Molecule 5 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.



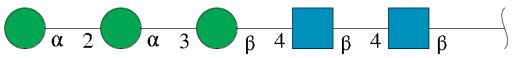
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
5	A	3	Total C N O 39 22 2 15	0	0	0

- Molecule 6 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.



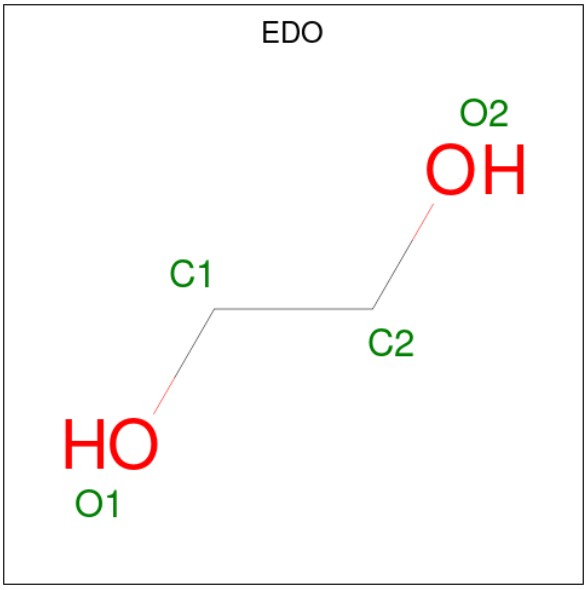
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
6	B	4	Total C N O 50 28 2 20	0	0	0

- Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



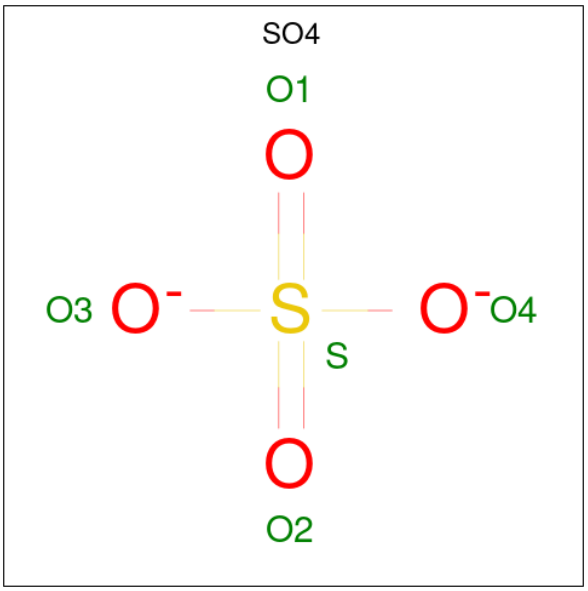
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
7	C	5	Total C N O 61 34 2 25	0	0	0

- Molecule 8 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	N	1	Total C O 4 2 2	0	0
8	I	1	Total C O 4 2 2	0	0

- Molecule 9 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	N	1	Total O S 5 4 1	0	0
9	N	1	Total O S 5 4 1	0	0
9	N	1	Total O S 5 4 1	0	0
9	N	1	Total O S 5 4 1	0	0
9	N	1	Total O S 5 4 1	0	0
9	O	1	Total O S 5 4 1	0	0
9	O	1	Total O S 5 4 1	0	0
9	O	1	Total O S 5 4 1	0	0
9	Z	1	Total O S 5 4 1	0	0
9	Z	1	Total O S 5 4 1	0	0
9	Z	1	Total O S 5 4 1	0	0
9	G	1	Total O S 5 4 1	0	0
9	G	1	Total O S 5 4 1	0	0
9	G	1	Total O S 5 4 1	0	0
9	I	1	Total O S 5 4 1	0	0
9	I	1	Total O S 5 4 1	0	0
9	I	1	Total O S 5 4 1	0	0
9	X	1	Total O S 5 4 1	0	0
9	H	1	Total O S 5 4 1	0	0
9	H	1	Total O S 5 4 1	0	0
9	H	1	Total O S 5 4 1	0	0
9	J	1	Total O S 5 4 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	Y	1	Total O S 5 4 1	0	0

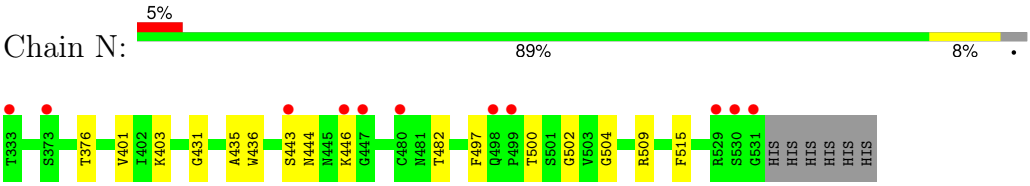
- Molecule 10 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	N	6	Total O 6 6	0	0
10	O	9	Total O 9 9	0	0
10	Z	10	Total O 10 10	0	0
10	G	11	Total O 11 11	0	0
10	I	7	Total O 7 7	0	0
10	X	6	Total O 6 6	0	0
10	H	10	Total O 10 10	0	0
10	J	4	Total O 4 4	0	0
10	Y	2	Total O 2 2	0	0
10	L	4	Total O 4 4	0	0

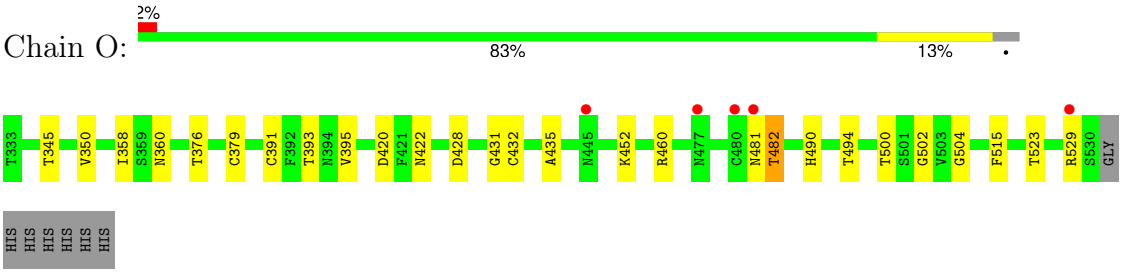
3 Residue-property plots (i)

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.

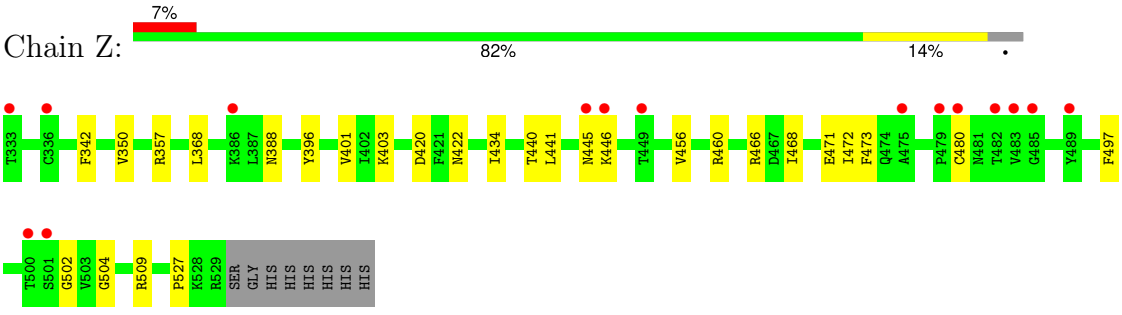
• Molecule 1: NJ spike protein S1



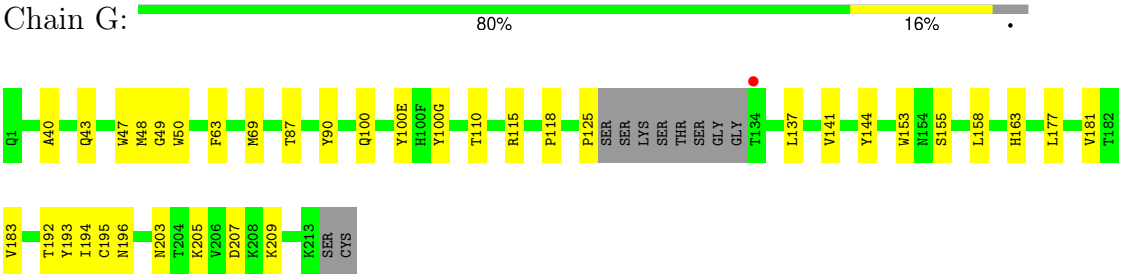
• Molecule 1: NJ spike protein S1



• Molecule 1: NJ spike protein S1

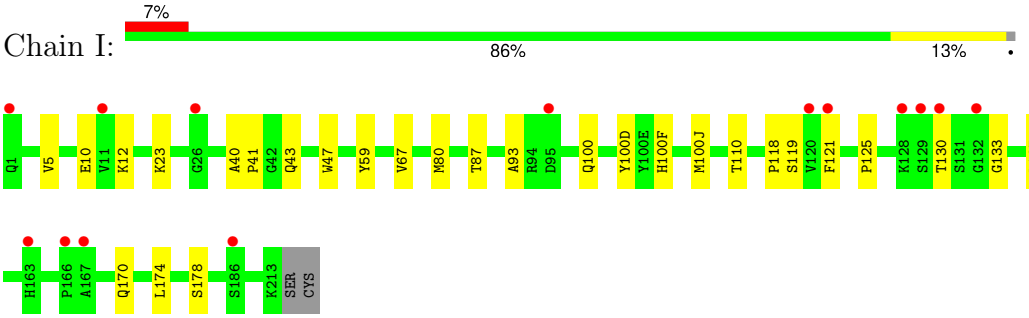


• Molecule 2: Neutralizing antibody CC25.4 heavy chain



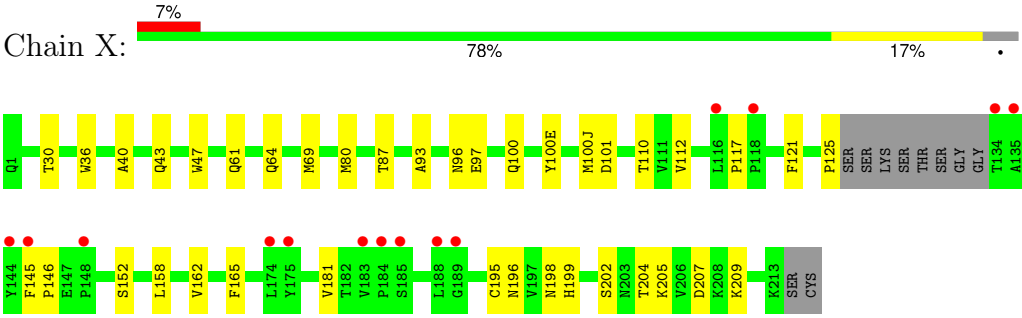
• Molecule 2: Neutralizing antibody CC25.4 heavy chain

Chain I:



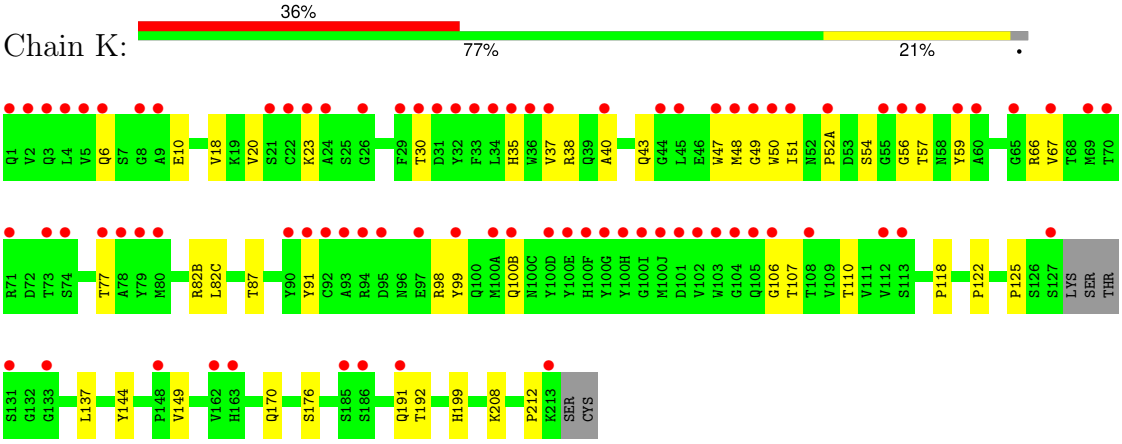
• Molecule 2: Neutralizing antibody CC25.4 heavy chain

Chain X:



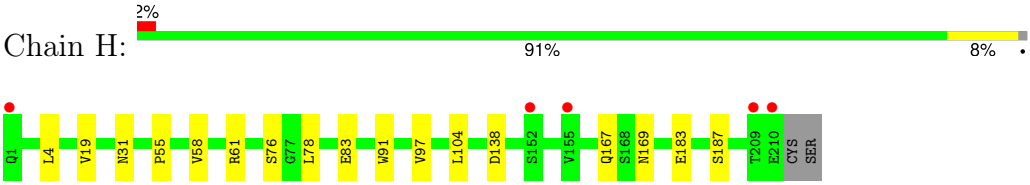
• Molecule 2: Neutralizing antibody CC25.4 heavy chain

Chain K:



• Molecule 3: Neutralizing antibody CC25.4 light chain

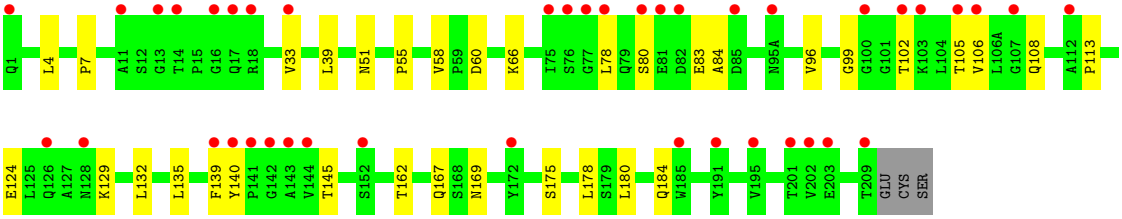
Chain H:



• Molecule 3: Neutralizing antibody CC25.4 light chain

Chain J:

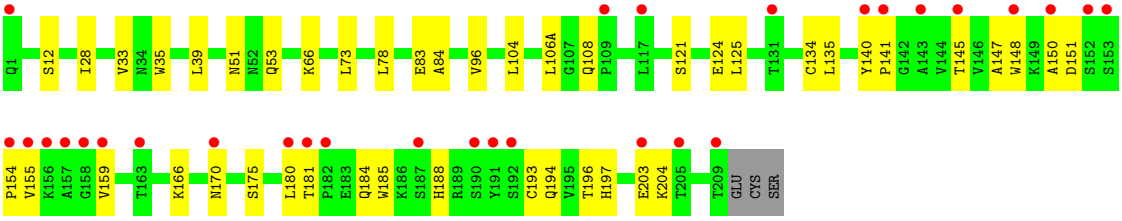




• Molecule 3: Neutralizing antibody CC25.4 light chain

Chain Y:

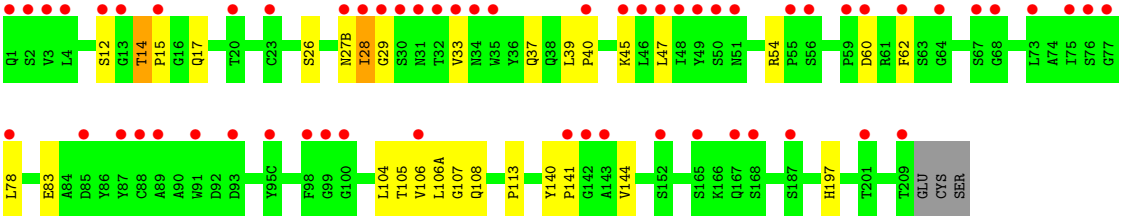




• Molecule 3: Neutralizing antibody CC25.4 light chain

Chain L:





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

Chain M:





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

Chain P:





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

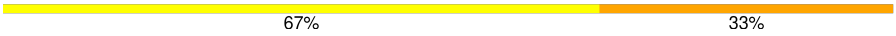
Chain Q:





• Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

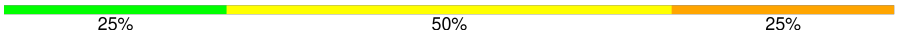
Chain A:





• Molecule 6: 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

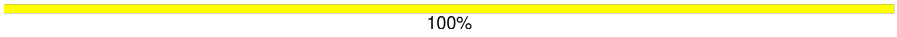
Chain B:





• Molecule 7: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	126.40Å 239.54Å 152.22Å 90.00° 113.91° 90.00°	Depositor
Resolution (Å)	38.71 – 2.82 38.71 – 2.82	Depositor EDS
% Data completeness (in resolution range)	86.4 (38.71-2.82) 86.3 (38.71-2.82)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.83 (at 2.81Å)	Xtriage
Refinement program	PHENIX (1.21.2_5419: ???)	Depositor
R, R_{free}	0.226 , 0.259 0.225 , 0.259	Depositor DCC
R_{free} test set	2000 reflections (2.02%)	wwPDB-VP
Wilson B-factor (Å^2)	52.7	Xtriage
Anisotropy	0.088	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 47.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	18171	wwPDB-VP
Average B, all atoms (Å^2)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.19% 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: MAN, BMA, SO4, NAG, EDO

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	N	0.09	0/1605	0.28	0/2176
1	O	0.08	0/1601	0.25	0/2171
1	Z	0.09	0/1595	0.26	0/2163
2	G	0.09	0/1734	0.26	0/2366
2	I	0.11	0/1783	0.29	0/2432
2	K	0.16	0/1760	0.34	0/2400
2	X	0.12	0/1734	0.31	0/2366
3	H	0.08	0/1604	0.28	0/2200
3	J	0.13	0/1595	0.32	0/2188
3	L	0.12	0/1595	0.36	0/2188
3	Y	0.13	0/1595	0.36	0/2188
All	All	0.11	0/18201	0.30	0/24838

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	N	1564	0	1510	9	0
1	O	1560	0	1507	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Z	1554	0	1502	17	0
2	G	1689	0	1617	26	0
2	I	1737	0	1664	19	0
2	K	1715	0	1638	27	0
2	X	1689	0	1617	28	0
3	H	1566	0	1465	12	0
3	J	1557	0	1459	25	0
3	L	1557	0	1459	29	0
3	Y	1557	0	1459	27	0
4	M	28	0	25	0	0
4	P	28	0	25	0	0
4	Q	28	0	25	1	0
5	A	39	0	34	1	0
6	B	50	0	43	1	0
7	C	61	0	52	0	0
8	I	4	0	6	0	0
8	N	4	0	6	0	0
9	G	15	0	0	1	0
9	H	15	0	0	0	0
9	I	15	0	0	0	0
9	J	5	0	0	0	0
9	N	25	0	0	0	0
9	O	15	0	0	0	0
9	X	5	0	0	0	0
9	Y	5	0	0	0	0
9	Z	15	0	0	0	0
10	G	11	0	0	0	0
10	H	10	0	0	0	0
10	I	7	0	0	0	0
10	J	4	0	0	0	0
10	L	4	0	0	0	0
10	N	6	0	0	0	0
10	O	9	0	0	0	0
10	X	6	0	0	0	0
10	Y	2	0	0	0	0
10	Z	10	0	0	0	0
All	All	18171	0	17113	219	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 6.

The worst 5 of 219 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)
3:L:140:TYR:HD1	3:L:141:PRO:HA	1.45	0.81
2:I:40:ALA:HB3	2:I:43:GLN:HB2	1.72	0.72
2:K:87:THR:HG23	2:K:110:THR:HA	1.73	0.70
2:G:193:TYR:H	2:G:209:LYS:HZ3	1.37	0.70
2:G:155:SER:H	2:G:196:ASN:HD21	1.39	0.67

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	N	195/203 (96%)	183 (94%)	12 (6%)	0	100	100
1	O	194/203 (96%)	187 (96%)	6 (3%)	1 (0%)	24	53
1	Z	193/203 (95%)	187 (97%)	6 (3%)	0	100	100
2	G	215/229 (94%)	214 (100%)	1 (0%)	0	100	100
2	I	225/229 (98%)	221 (98%)	4 (2%)	0	100	100
2	K	220/229 (96%)	211 (96%)	9 (4%)	0	100	100
2	X	215/229 (94%)	210 (98%)	5 (2%)	0	100	100
3	H	213/217 (98%)	210 (99%)	3 (1%)	0	100	100
3	J	212/217 (98%)	205 (97%)	7 (3%)	0	100	100
3	L	212/217 (98%)	195 (92%)	16 (8%)	1 (0%)	24	53
3	Y	212/217 (98%)	196 (92%)	15 (7%)	1 (0%)	24	53
All	All	2306/2393 (96%)	2219 (96%)	84 (4%)	3 (0%)	48	75

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	Y	155	VAL
3	L	28	ILE

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Mol	Chain	Res	Type
1	O	482	THR

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	N	174/180 (97%)	173 (99%)	1 (1%)	78 92
1	O	174/180 (97%)	174 (100%)	0	100 100
1	Z	173/180 (96%)	173 (100%)	0	100 100
2	G	183/197 (93%)	183 (100%)	0	100 100
2	I	189/197 (96%)	188 (100%)	1 (0%)	81 93
2	K	186/197 (94%)	186 (100%)	0	100 100
2	X	183/197 (93%)	182 (100%)	1 (0%)	81 93
3	H	169/182 (93%)	169 (100%)	0	100 100
3	J	168/182 (92%)	167 (99%)	1 (1%)	78 92
3	L	168/182 (92%)	166 (99%)	2 (1%)	63 86
3	Y	168/182 (92%)	167 (99%)	1 (1%)	78 92
All	All	1935/2056 (94%)	1928 (100%)	7 (0%)	84 94

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	J	145	THR
3	Y	175	SER
3	L	144	VAL
3	L	14	THR
2	X	195	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 32 such sidechains are listed below:

Mol	Chain	Res	Type
2	K	43	GLN
2	K	64	GLN
2	I	170	GLN
2	I	3	GLN
3	L	31	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)

18 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	$\#\|Z\| > 2$
5	NAG	A	1	1,5	14,14,15	0.76	0	17,19,21	1.38	2 (11%)
5	NAG	A	2	5	14,14,15	0.70	0	17,19,21	1.43	3 (17%)
5	BMA	A	3	5	11,11,12	0.84	0	15,15,17	2.82	6 (40%)
6	NAG	B	1	1,6	14,14,15	0.77	0	17,19,21	2.39	4 (23%)
6	NAG	B	2	6	14,14,15	0.71	0	17,19,21	0.82	0
6	BMA	B	3	6	11,11,12	0.86	0	15,15,17	2.10	3 (20%)
6	MAN	B	4	6	11,11,12	0.74	0	15,15,17	1.04	1 (6%)
7	NAG	C	1	1,7	14,14,15	0.72	0	17,19,21	1.00	1 (5%)
7	NAG	C	2	7	14,14,15	0.73	0	17,19,21	1.06	2 (11%)
7	BMA	C	3	7	11,11,12	0.81	0	15,15,17	2.34	6 (40%)
7	MAN	C	4	7	11,11,12	0.61	0	15,15,17	1.47	1 (6%)
7	MAN	C	5	7	11,11,12	0.76	0	15,15,17	0.92	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	NAG	M	1	1,4	14,14,15	0.73	0	17,19,21	0.90	1 (5%)
4	NAG	M	2	4	14,14,15	0.69	0	17,19,21	0.89	0
4	NAG	P	1	1,4	14,14,15	0.73	0	17,19,21	0.92	1 (5%)
4	NAG	P	2	4	14,14,15	0.75	0	17,19,21	0.89	0
4	NAG	Q	1	1,4	14,14,15	0.70	0	17,19,21	1.13	2 (11%)
4	NAG	Q	2	4	14,14,15	0.70	0	17,19,21	1.28	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
5	NAG	A	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	A	2	5	-	2/6/23/26	0/1/1/1
5	BMA	A	3	5	-	1/2/19/22	0/1/1/1
6	NAG	B	1	1,6	-	4/6/23/26	0/1/1/1
6	NAG	B	2	6	-	1/6/23/26	0/1/1/1
6	BMA	B	3	6	-	1/2/19/22	0/1/1/1
6	MAN	B	4	6	-	2/2/19/22	0/1/1/1
7	NAG	C	1	1,7	-	0/6/23/26	0/1/1/1
7	NAG	C	2	7	-	3/6/23/26	0/1/1/1
7	BMA	C	3	7	-	2/2/19/22	0/1/1/1
7	MAN	C	4	7	-	0/2/19/22	0/1/1/1
7	MAN	C	5	7	-	0/2/19/22	0/1/1/1
4	NAG	M	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	M	2	4	-	1/6/23/26	0/1/1/1
4	NAG	P	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	P	2	4	-	0/6/23/26	0/1/1/1
4	NAG	Q	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	Q	2	4	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 36 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	3	BMA	C1-O5-C5	8.44	123.49	112.19
6	B	1	NAG	C2-N2-C7	8.41	134.17	122.90
6	B	3	BMA	C1-O5-C5	6.46	120.84	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	C	3	BMA	C1-O5-C5	6.44	120.81	112.19
7	C	4	MAN	C1-O5-C5	4.81	118.64	112.19

There are no chirality outliers.

5 of 21 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	C	3	BMA	O5-C5-C6-O6
5	A	2	NAG	O5-C5-C6-O6
6	B	4	MAN	O5-C5-C6-O6
5	A	2	NAG	C4-C5-C6-O6
6	B	4	MAN	C4-C5-C6-O6

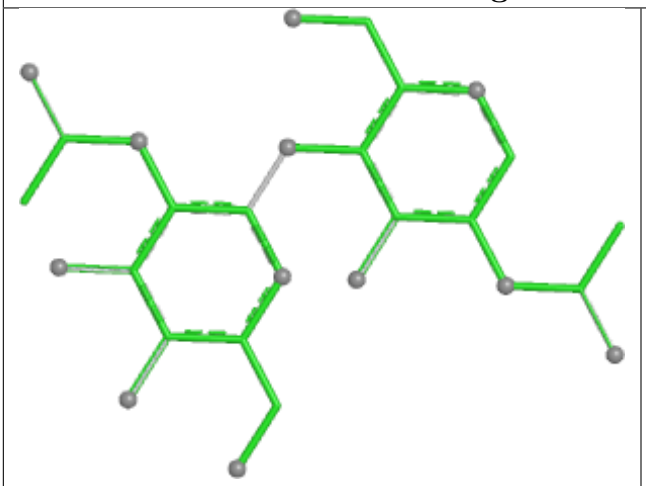
There are no ring outliers.

3 monomers are involved in 3 short contacts:

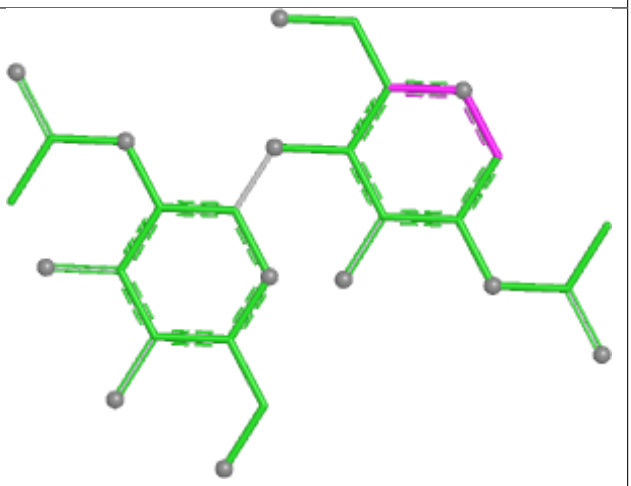
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	2	NAG	1	0
4	Q	1	NAG	1	0
6	B	4	MAN	1	0

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

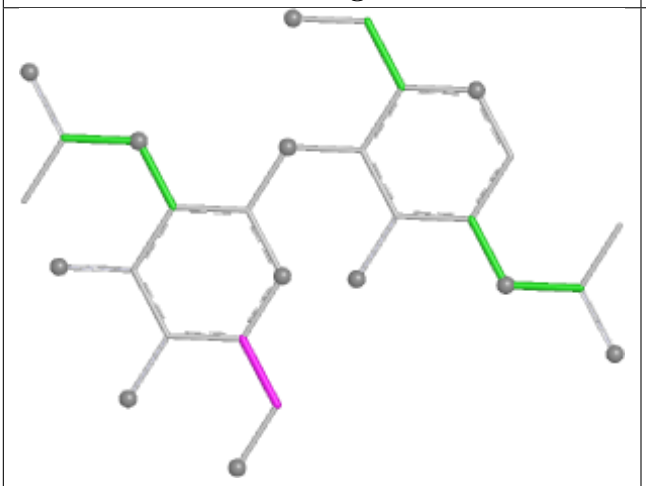
Oligosaccharide Chain M



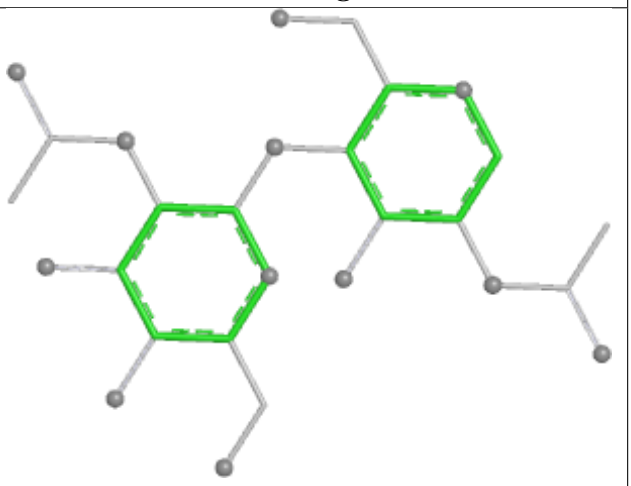
Bond lengths



Bond angles

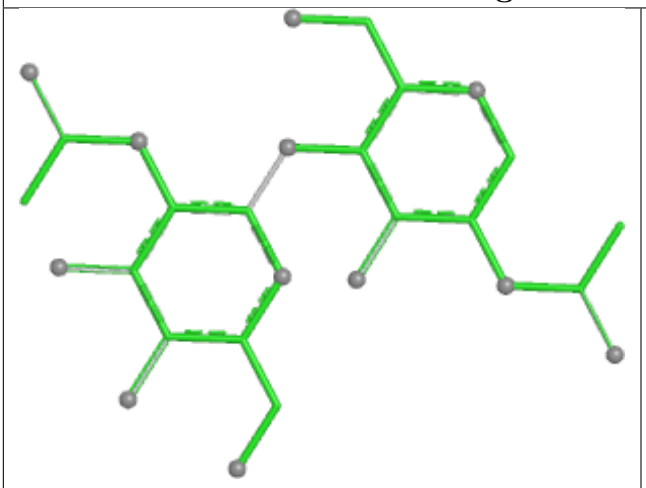


Torsions

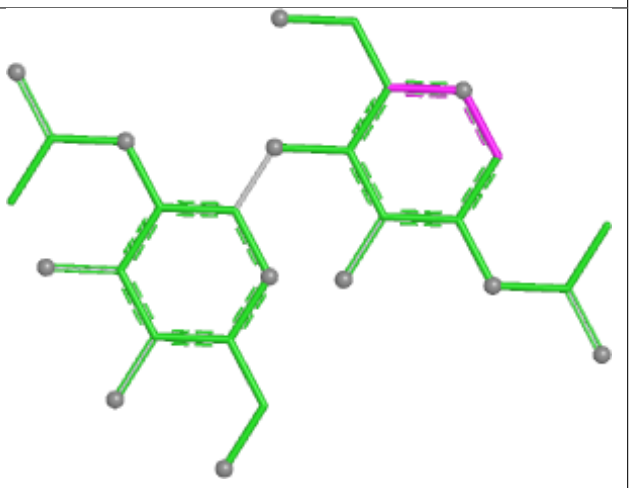


Rings

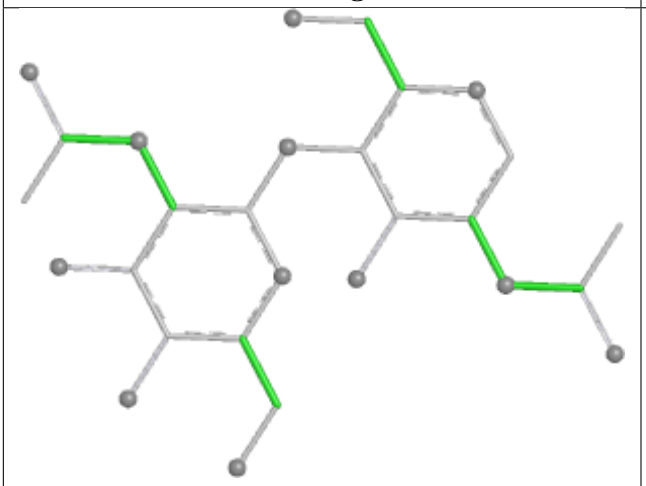
Oligosaccharide Chain P



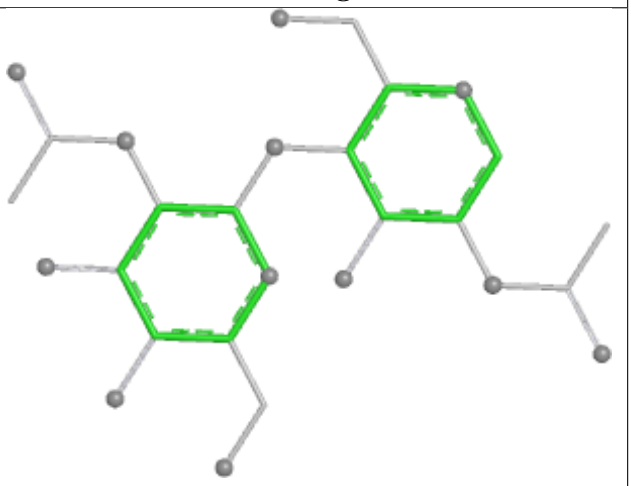
Bond lengths



Bond angles

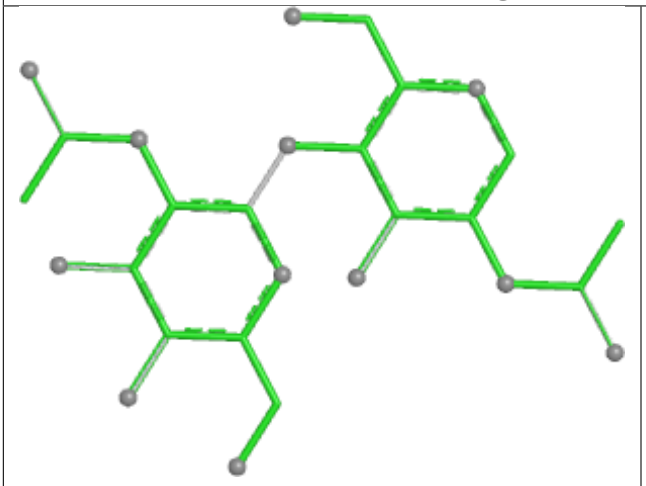


Torsions

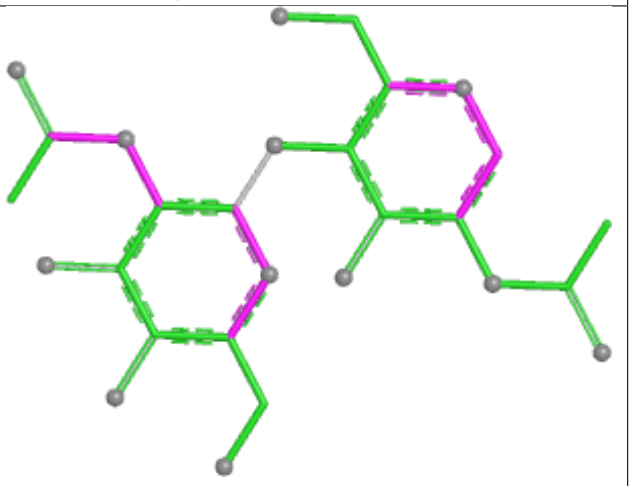


Rings

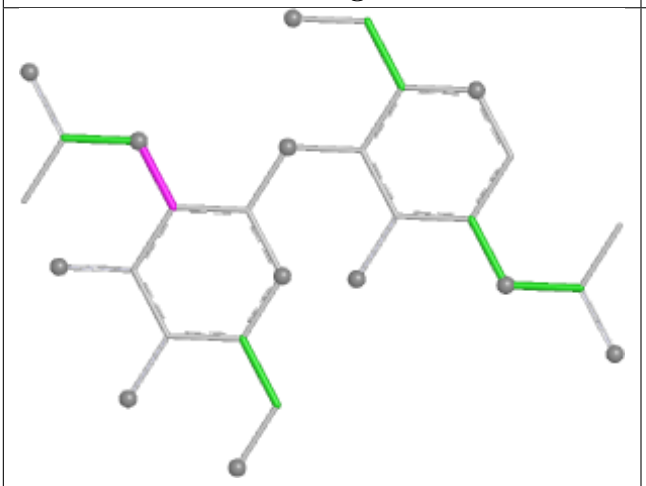
Oligosaccharide Chain Q



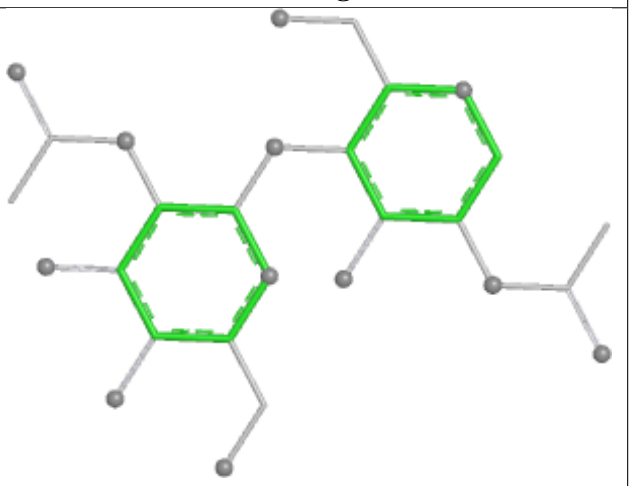
Bond lengths



Bond angles

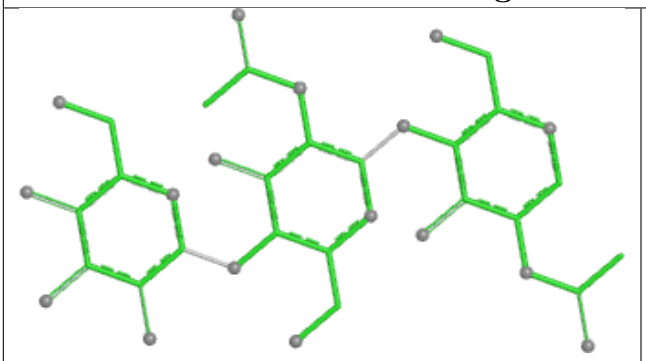


Torsions

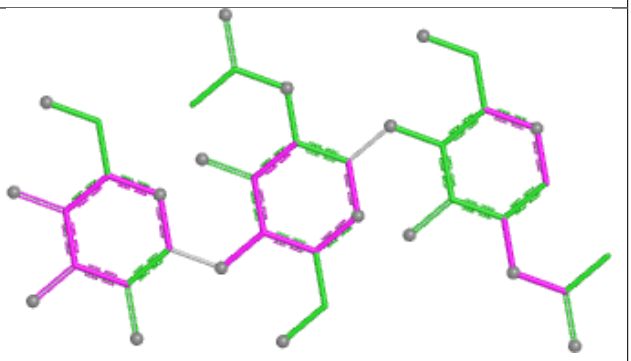


Rings

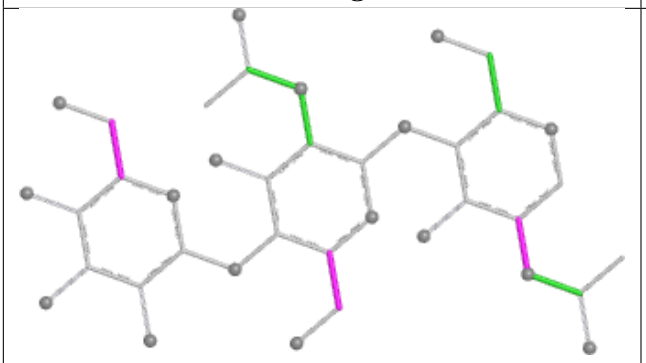
Oligosaccharide Chain A



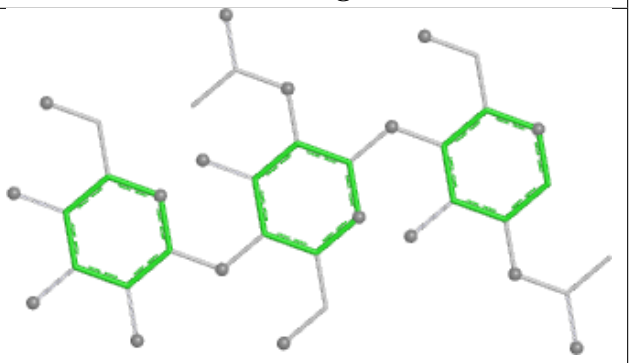
Bond lengths



Bond angles

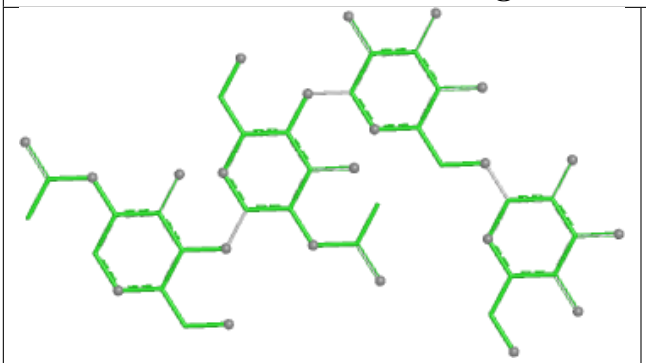


Torsions

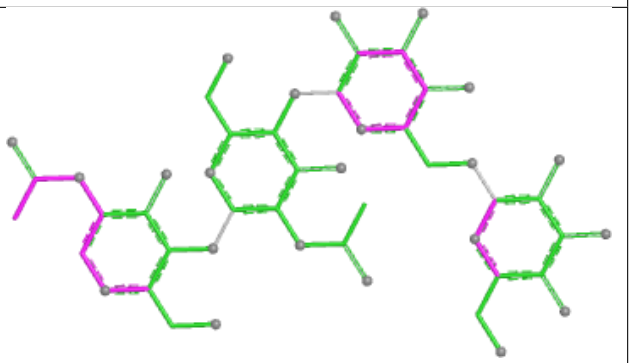


Rings

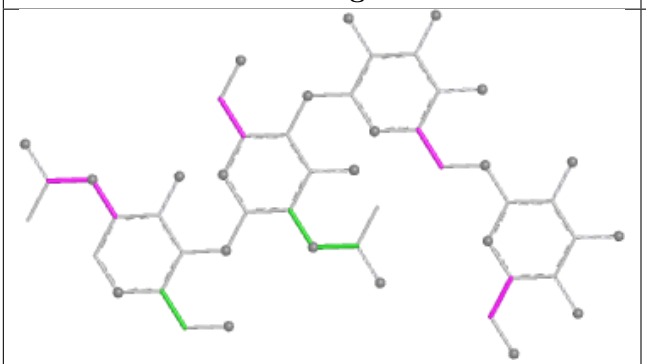
Oligosaccharide Chain B



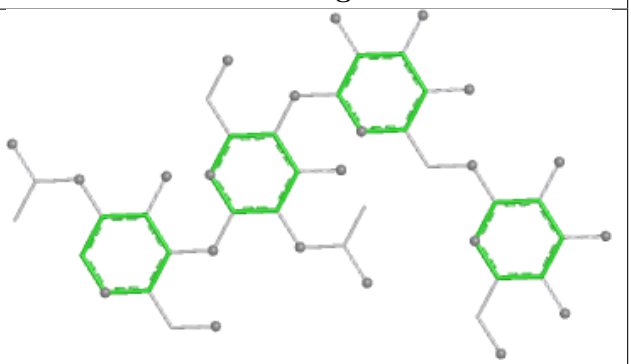
Bond lengths



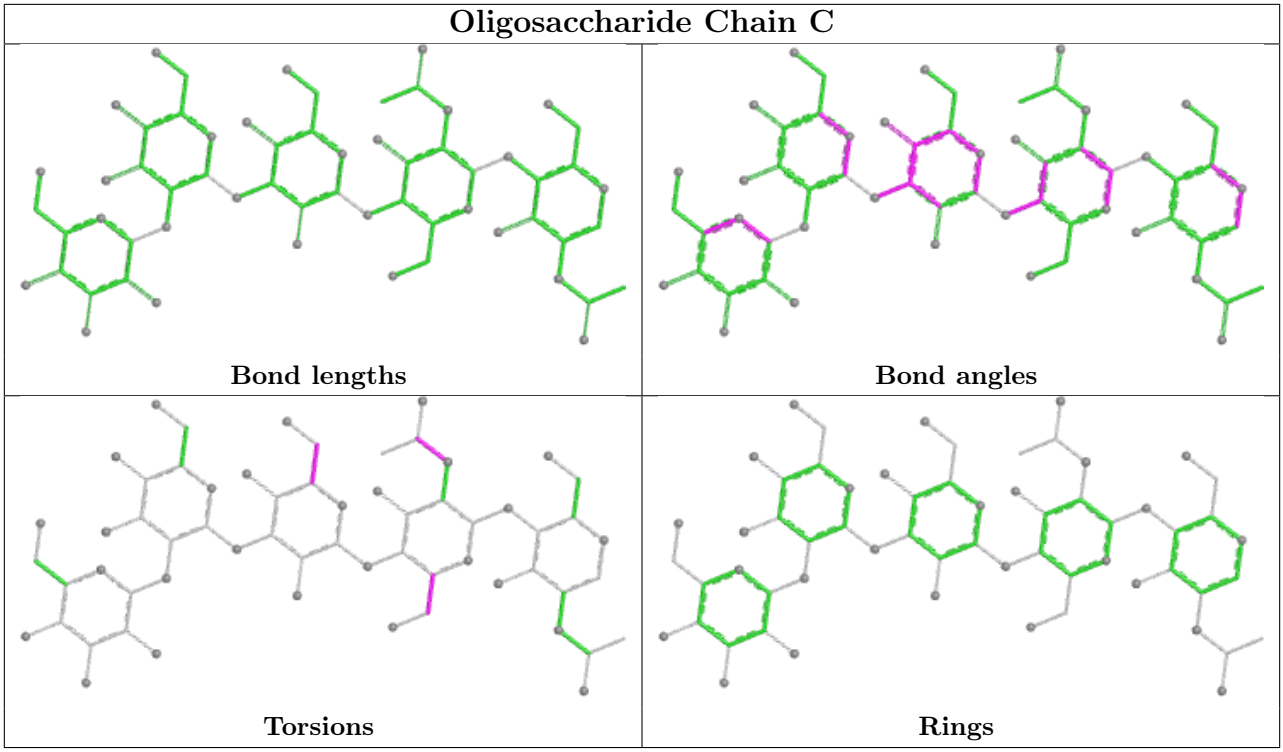
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

25 ligands 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	$\#\|Z\| > 2$
8	EDO	I	304	-	3,3,3	0.25	0	2,2,2	0.29	0
9	SO4	N	603	-	4,4,4	0.66	0	6,6,6	0.09	0
9	SO4	O	601	-	4,4,4	0.67	0	6,6,6	0.08	0
9	SO4	H	302	-	4,4,4	0.67	0	6,6,6	0.07	0
9	SO4	Z	601	-	4,4,4	0.67	0	6,6,6	0.07	0
9	SO4	N	606	-	4,4,4	0.67	0	6,6,6	0.08	0
9	SO4	Z	602	-	4,4,4	0.68	0	6,6,6	0.08	0
9	SO4	N	604	-	4,4,4	0.67	0	6,6,6	0.10	0
9	SO4	G	302	-	4,4,4	0.67	0	6,6,6	0.08	0
9	SO4	O	603	-	4,4,4	0.68	0	6,6,6	0.07	0
9	SO4	Y	301	-	4,4,4	0.67	0	6,6,6	0.10	0
8	EDO	N	601	-	3,3,3	0.26	0	2,2,2	0.28	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
9	SO4	H	303	-	4,4,4	0.67	0	6,6,6	0.07	0
9	SO4	X	301	-	4,4,4	0.67	0	6,6,6	0.07	0
9	SO4	G	303	-	4,4,4	0.67	0	6,6,6	0.09	0
9	SO4	I	303	-	4,4,4	0.66	0	6,6,6	0.10	0
9	SO4	N	602	-	4,4,4	0.67	0	6,6,6	0.05	0
9	SO4	G	301	-	4,4,4	0.67	0	6,6,6	0.10	0
9	SO4	H	301	-	4,4,4	0.66	0	6,6,6	0.08	0
9	SO4	O	602	-	4,4,4	0.67	0	6,6,6	0.08	0
9	SO4	I	301	-	4,4,4	0.67	0	6,6,6	0.08	0
9	SO4	I	302	-	4,4,4	0.67	0	6,6,6	0.09	0
9	SO4	Z	603	-	4,4,4	0.67	0	6,6,6	0.09	0
9	SO4	N	605	-	4,4,4	0.67	0	6,6,6	0.05	0
9	SO4	J	301	-	4,4,4	0.67	0	6,6,6	0.10	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
8	EDO	I	304	-	-	0/1/1/1	-
8	EDO	N	601	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	G	301	SO4	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

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	N	197/203 (97%)	0.21	11 (5%) 30 23	19, 40, 87, 105	0
1	O	196/203 (96%)	0.07	5 (2%) 57 47	22, 43, 71, 102	0
1	Z	195/203 (96%)	0.32	15 (7%) 19 14	24, 47, 89, 106	0
2	G	219/229 (95%)	0.05	1 (0%) 87 82	17, 37, 75, 91	0
2	I	227/229 (99%)	0.65	15 (6%) 24 17	23, 50, 71, 100	0
2	K	224/229 (97%)	1.63	83 (37%) 1 0	31, 88, 121, 134	0
2	X	219/229 (95%)	0.62	15 (6%) 23 17	28, 52, 87, 117	0
3	H	215/217 (99%)	0.03	5 (2%) 61 51	15, 39, 67, 98	0
3	J	214/217 (98%)	1.14	41 (19%) 3 2	28, 65, 92, 102	0
3	L	214/217 (98%)	1.39	60 (28%) 1 1	33, 77, 113, 129	0
3	Y	214/217 (98%)	0.96	30 (14%) 6 5	28, 68, 106, 138	0
All	All	2334/2393 (97%)	0.66	281 (12%) 9 6	15, 52, 103, 138	0

The worst 5 of 281 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	K	100(H)	TYR	6.1
2	X	135	ALA	6.1
3	J	76	SER	6.0
3	L	47	LEU	5.9
3	Y	152	SER	5.3

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

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

6.3 Carbohydrates (i)

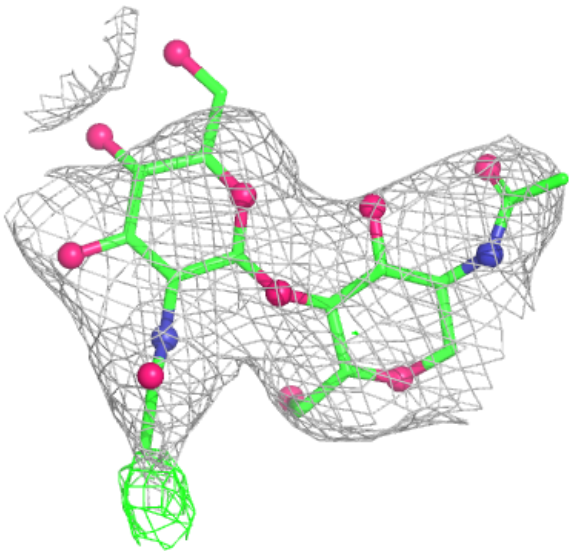
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

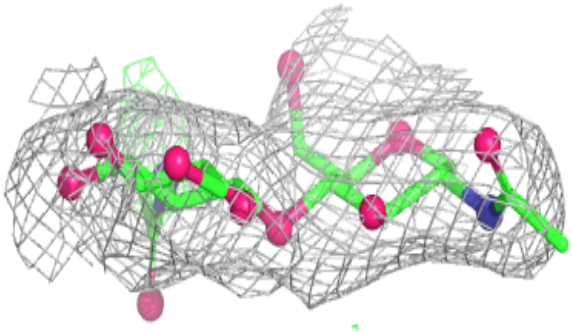
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	NAG	P	2	14/15	0.71	0.17	75,96,118,119	0
4	NAG	M	1	14/15	0.74	0.16	45,67,88,89	0
4	NAG	M	2	14/15	0.76	0.16	72,92,114,116	0
4	NAG	Q	2	14/15	0.80	0.15	83,95,110,112	0
4	NAG	P	1	14/15	0.82	0.14	51,63,78,98	0
4	NAG	Q	1	14/15	0.84	0.12	65,80,93,101	0
5	NAG	A	1	14/15	-	-	62,75,92,95	0
5	NAG	A	2	14/15	-	-	66,95,111,129	0
5	BMA	A	3	11/12	-	-	111,119,129,132	0
6	NAG	B	1	14/15	-	-	45,58,81,82	0
6	NAG	B	2	14/15	-	-	52,72,80,101	0
6	BMA	B	3	11/12	-	-	83,96,108,110	0
6	MAN	B	4	11/12	-	-	74,85,92,99	0
7	NAG	C	1	14/15	-	-	69,77,87,89	0
7	NAG	C	2	14/15	-	-	71,81,93,99	0
7	BMA	C	3	11/12	-	-	75,92,98,104	0
7	MAN	C	4	11/12	-	-	79,93,100,115	0
7	MAN	C	5	11/12	-	-	86,109,120,124	0

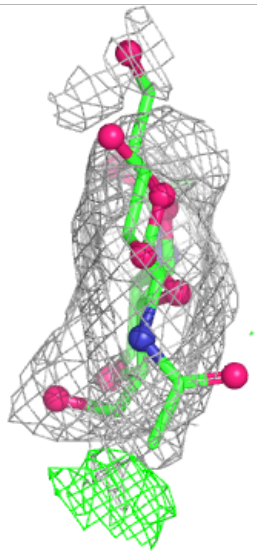
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain M:

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

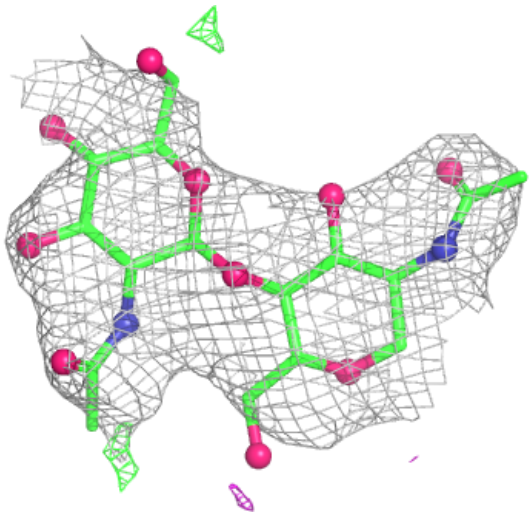


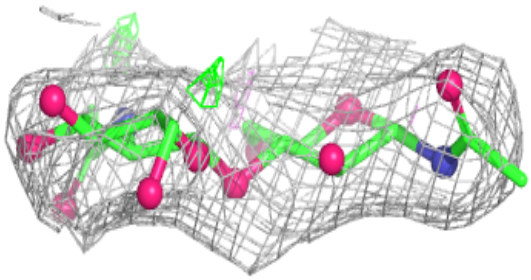


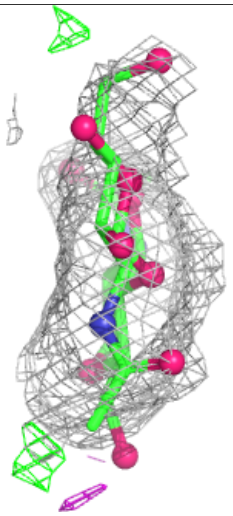


Electron density around Chain P:

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

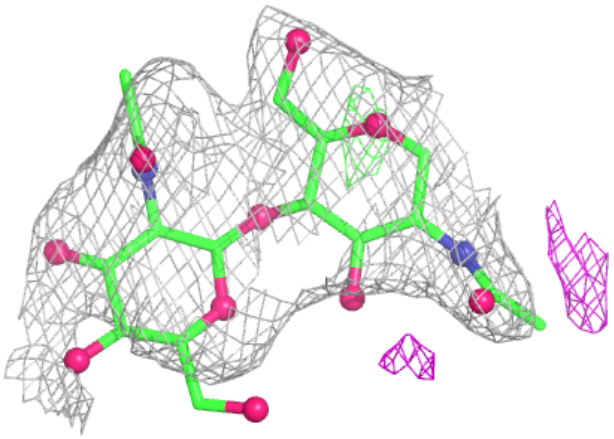


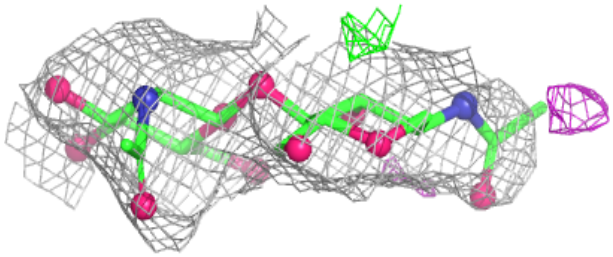


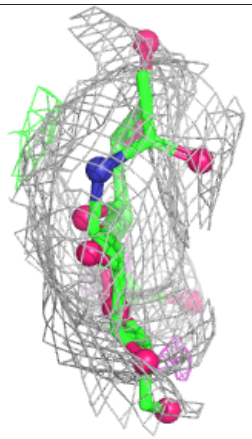


Electron density around Chain Q:

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

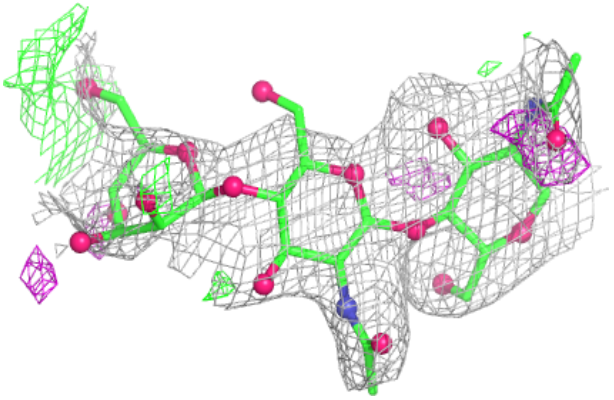


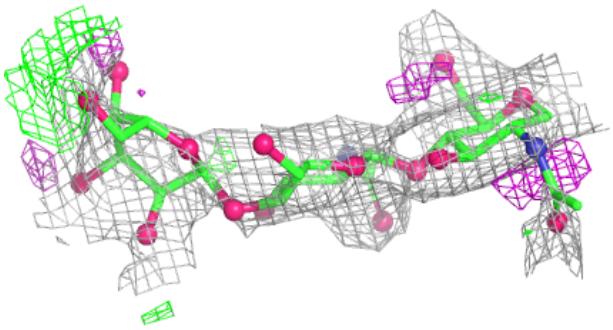


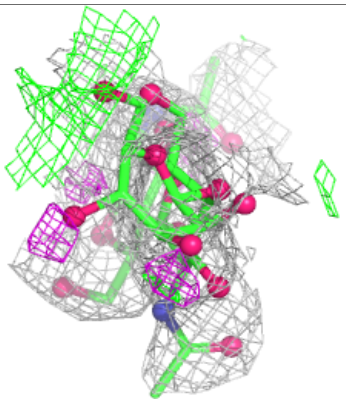


Electron density around Chain A:

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

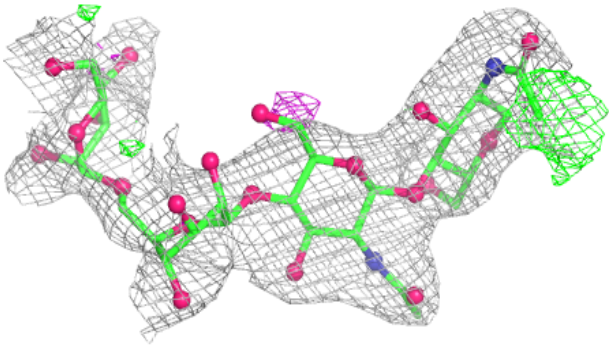


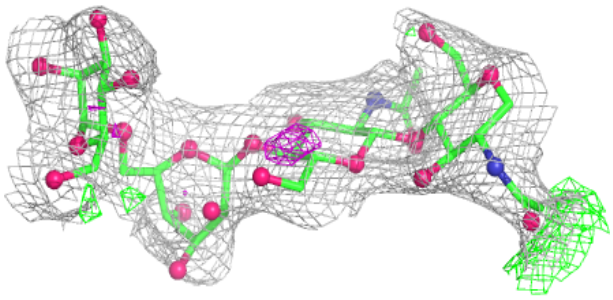


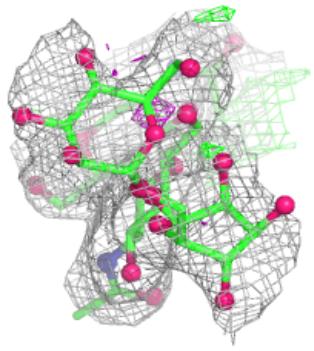


Electron density around Chain B:

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

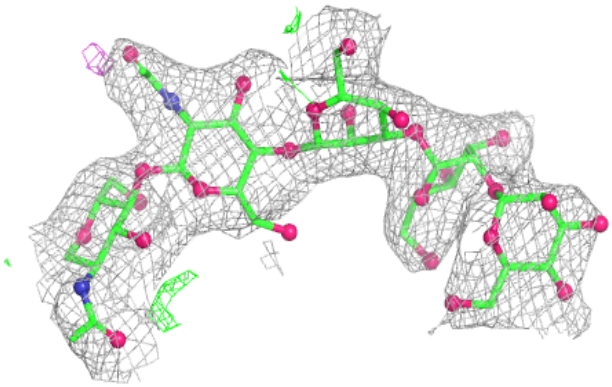


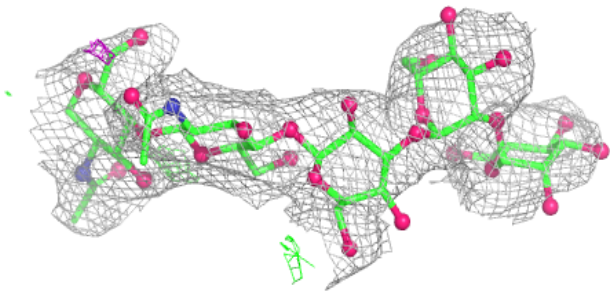


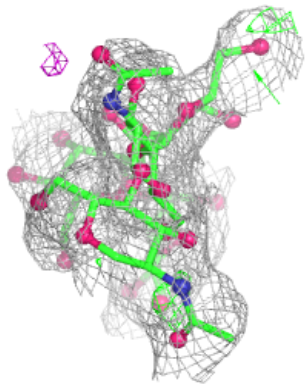


Electron density around Chain C:

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







6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
8	EDO	N	601	4/4	0.72	0.18	52,53,54,54	0
9	SO4	I	303	5/5	0.75	0.24	73,82,110,121	0
9	SO4	I	302	5/5	0.76	0.17	62,72,109,121	0
9	SO4	G	303	5/5	0.77	0.30	89,91,121,134	0
9	SO4	N	605	5/5	0.78	0.16	67,69,86,102	0
9	SO4	G	302	5/5	0.80	0.15	69,82,97,108	0
9	SO4	O	601	5/5	0.81	0.17	55,81,100,117	0
9	SO4	Z	603	5/5	0.81	0.11	95,100,103,116	0
9	SO4	I	301	5/5	0.82	0.14	67,84,99,110	0
9	SO4	X	301	5/5	0.82	0.13	86,87,94,100	0
9	SO4	N	604	5/5	0.84	0.24	71,72,86,88	0
9	SO4	J	301	5/5	0.84	0.17	33,62,83,99	0
9	SO4	Y	301	5/5	0.85	0.17	60,64,75,82	0
9	SO4	G	301	5/5	0.86	0.15	72,89,90,103	0
8	EDO	I	304	4/4	0.88	0.15	35,41,46,54	0
9	SO4	H	303	5/5	0.90	0.11	54,78,99,111	0
9	SO4	Z	601	5/5	0.91	0.11	51,59,72,83	0
9	SO4	N	606	5/5	0.91	0.31	44,68,83,97	0
9	SO4	N	603	5/5	0.92	0.15	59,77,80,90	0
9	SO4	O	602	5/5	0.92	0.15	56,59,78,85	0
9	SO4	Z	602	5/5	0.93	0.13	42,50,68,83	0
9	SO4	H	302	5/5	0.94	0.11	58,59,64,66	0
9	SO4	N	602	5/5	0.95	0.07	46,59,70,74	0
9	SO4	O	603	5/5	0.95	0.14	48,63,75,76	0
9	SO4	H	301	5/5	0.96	0.11	52,53,63,67	0

6.5 Other polymers (i)

There are no such residues in this entry.