Full wwPDB X-ray Structure Validation Report (i)

Jun 22, 2024 – 11:57 AM EDT

PDB ID	:	4Z7Q
Title	:	Integrin alphaIIbbeta3 in complex with AGDV-NH2 peptide
Authors	:	Lin, F.-Y.; Zhu, J.; Springer, T.A.
Deposited on	:	2015-04-07
Resolution	:	2.70 Å(reported)

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

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

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

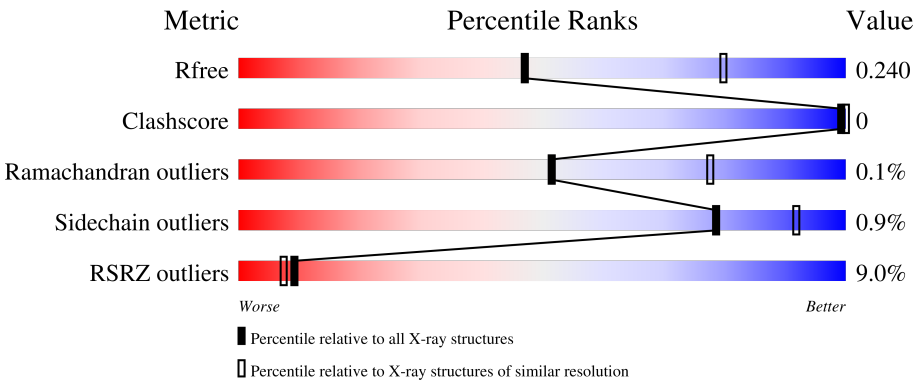
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	454	% 98% .
1	C	454	% 98% .
2	B	471	9% 97% . .
2	D	471	7% 98% .
3	E	219	32% 98% .

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Mol	Chain	Length	Quality of chain
3	H	219	8% 98%
4	F	214	31% 100%
4	L	214	3% 100%
5	G	5	100%
5	I	5	100%
6	J	5	40% 60%
7	K	2	100%
7	N	2	100%
8	M	3	100%

2 Entry composition (i)

There are 16 unique types of molecules in this entry. The entry contains 42446 atoms, of which 20326 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 Integrin alpha-IIb.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	454	6882	2236	3366	606	666	8	0	7	0
1	C	453	6839	2224	3337	604	666	8	0	6	0

- Molecule 2 is a protein called Integrin beta-3.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
2	B	466	7178	2262	3546	620	717	33	6	8	0
2	D	471	7182	2260	3551	620	716	35	10	2	0

- Molecule 3 is a protein called Monoclonal antibody 10E5 heavy chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
3	E	214	3221	1035	1590	264	326	6	0	0	0
3	H	216	3242	1041	1600	266	329	6	0	0	0

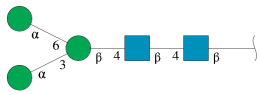
- Molecule 4 is a protein called Monoclonal antibody 10E5 light chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
4	F	214	3190	1019	1553	268	341	9	0	0	0
4	L	214	3190	1019	1553	268	341	9	0	0	0

- Molecule 5 is a protein called Tetrapeptide AGDV-NH2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	H	N	O			
5	G	5	45	14	20	5	6	0	0	1
			Total	C	H	N	O			
5	I	5	45	14	20	5	6	0	0	1

- Molecule 6 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[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.

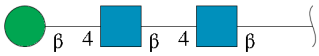


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	H	N	O			
6	J	5	116	34	55	2	25	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	H	N	O			
7	K	2	55	16	27	2	10	0	0	0
			Total	C	H	N	O			
7	N	2	55	16	27	2	10	0	0	0

- Molecule 8 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.

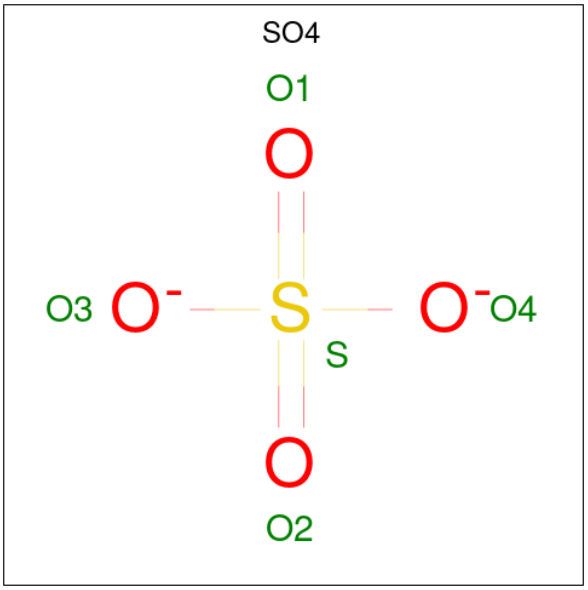


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	H	N	O			
8	M	3	74	22	35	2	15	0	0	0

- Molecule 9 is CALCIUM ION (three-letter code: CA) (formula: Ca).

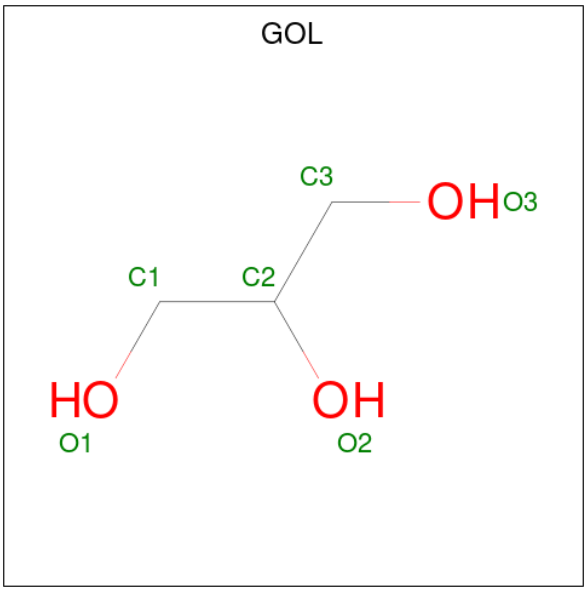
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
9	A	4	4	4	0	0
			Total	Ca		
9	C	4	4	4	0	0

- Molecule 10 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
10	A	1	5	4	1	0	0
			Total	O	S		
10	A	1	5	4	1	0	0
			Total	O	S		
10	A	1	5	4	1	0	0
			Total	O	S		
10	C	1	5	4	1	0	0
			Total	O	S		
10	C	1	5	4	1	0	0
			Total	O	S		
10	C	1	5	4	1	0	0
			Total	O	S		
10	L	1	5	4	1	0	0

- Molecule 11 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

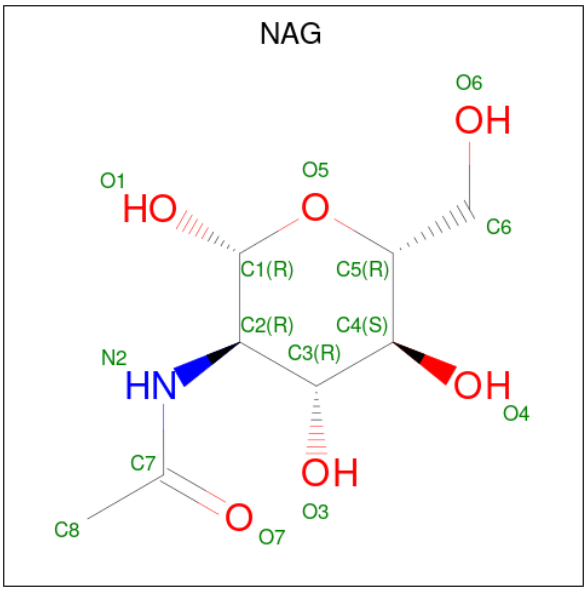


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
11	A	1	14	3	8	3	0	0

- Molecule 12 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

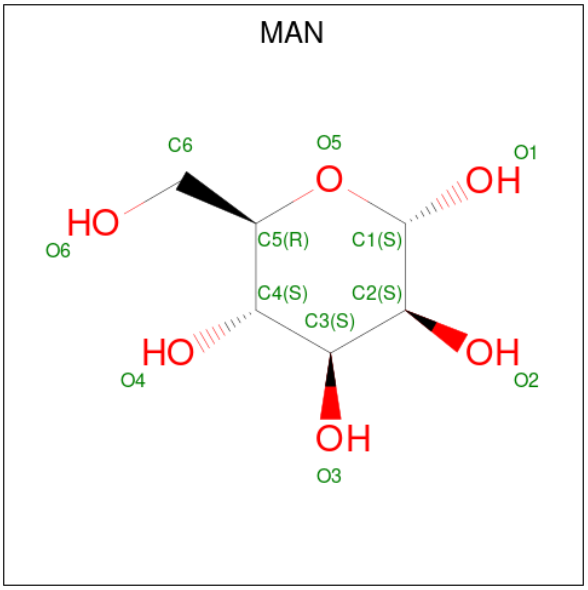
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mn		
12	B	3	3	3	0	0
12	D	3	Total	Mn	0	0
			3	3		

- Molecule 13 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	N	O		
13	B	1	28	8	14	1	5	0	0
			Total	C	H	N	O		
13	D	1	28	8	14	1	5	0	0

- Molecule 14 is alpha-D-mannopyranose (three-letter code: MAN) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
14	C	1	21	6	10	5	0	0

- Molecule 15 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
15	C	1	1	1	0	0

- Molecule 16 is water.

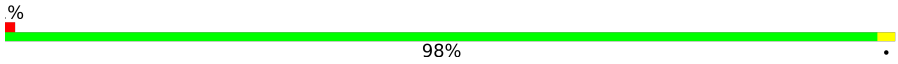
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
16	A	369	369	369	0	0
			Total	O		
16	B	183	183	183	0	0
			Total	O		
16	C	165	165	165	0	0
			Total	O		
16	D	141	141	141	0	0
			Total	O		
16	E	18	18	18	0	0
			Total	O		
16	F	19	19	19	0	0
			Total	O		
16	H	36	36	36	0	0
			Total	O		
16	L	54	54	54	0	0
			Total	O		
16	G	3	3	3	0	0
			Total	O		
16	I	3	3	3	0	0

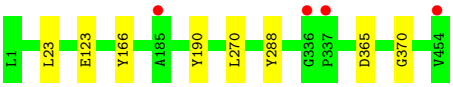
3 Residue-property plots (i)

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: Integrin alpha-IIb

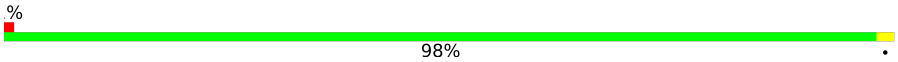
Chain A:

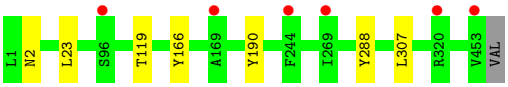




• Molecule 1: Integrin alpha-IIb

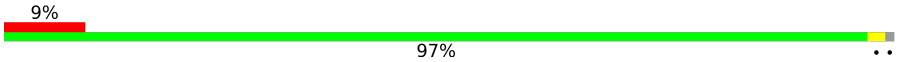
Chain C:

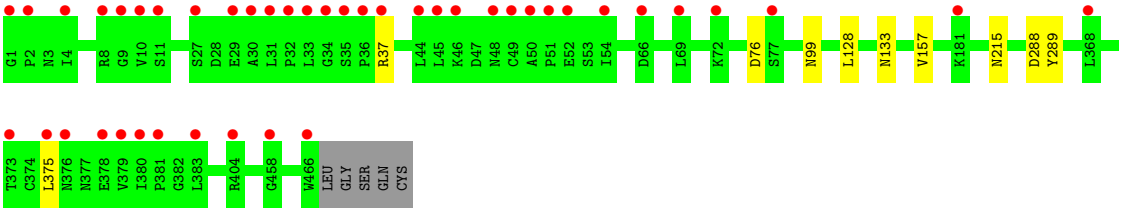




• Molecule 2: Integrin beta-3

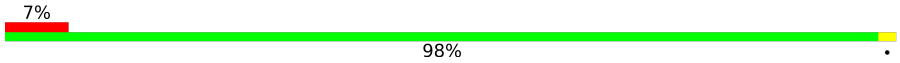
Chain B:

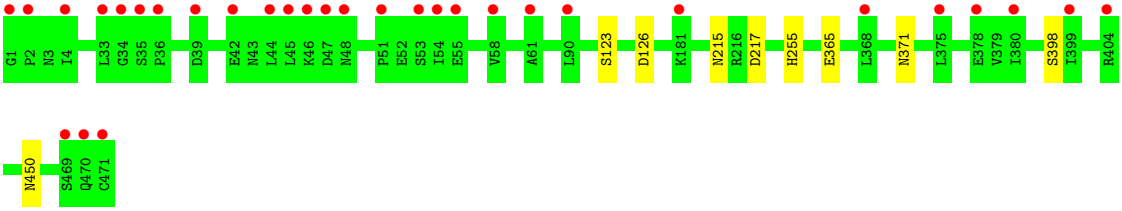




• Molecule 2: Integrin beta-3

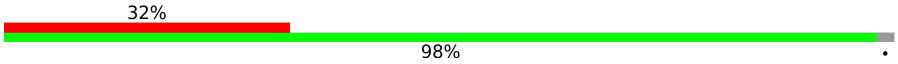
Chain D:

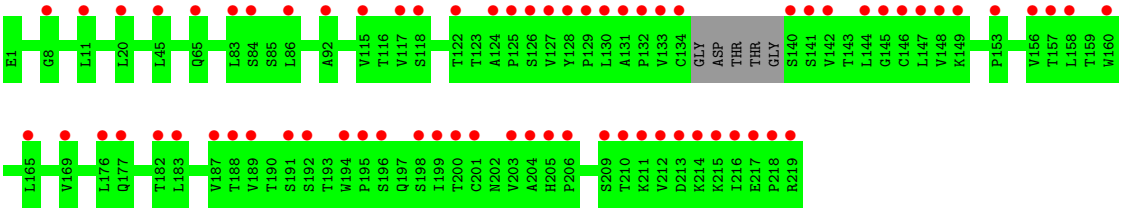




• Molecule 3: Monoclonal antibody 10E5 heavy chain

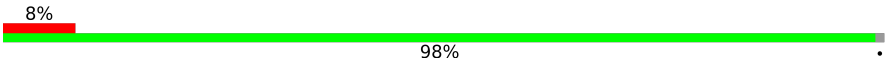
Chain E:

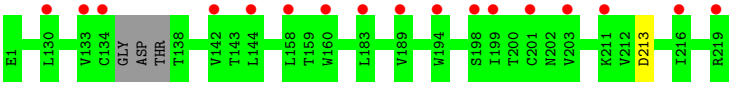




• Molecule 3: Monoclonal antibody 10E5 heavy chain

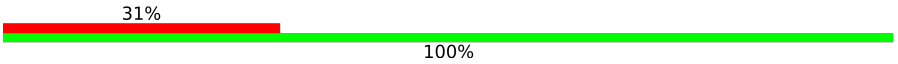
Chain H:

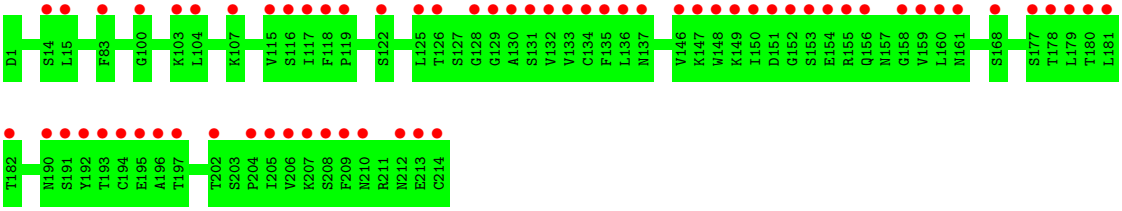




• Molecule 4: Monoclonal antibody 10E5 light chain

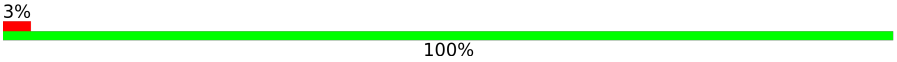
Chain F:

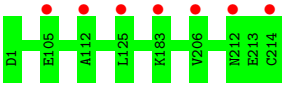




• Molecule 4: Monoclonal antibody 10E5 light chain

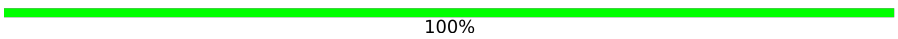
Chain L:





• Molecule 5: Tetrapeptide AGDV-NH2

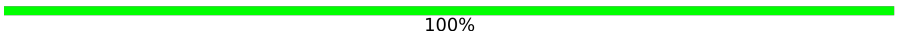
Chain G:



There are no outlier residues recorded for this chain.

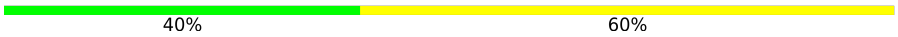
• Molecule 5: Tetrapeptide AGDV-NH2

Chain I:

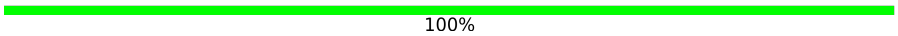


There are no outlier residues recorded for this chain.

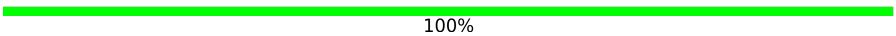
• Molecule 6: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J: 

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

Chain K: 

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

Chain N: 

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

Chain M:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	259.44Å 144.24Å 104.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.94 – 2.70 48.94 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.5 (48.94-2.70) 99.6 (48.94-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.46 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.188 , 0.236 0.191 , 0.240	Depositor DCC
R_{free} test set	1078 reflections (1.00%)	wwPDB-VP
Wilson B-factor (Å^2)	64.7	Xtriage
Anisotropy	0.215	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 64.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	42446	wwPDB-VP
Average B, all atoms (Å^2)	106.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.15% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MN, NH2, BMA, NAG, CL, CA, MAN, GOL, SO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| >5$	RMSZ	$\#\|Z\| >5$
1	A	0.22	0/3633	0.40	0/4951
1	C	0.22	0/3618	0.38	0/4930
2	B	0.22	0/3728	0.39	0/5057
2	D	0.22	0/3710	0.38	0/5029
3	E	0.21	0/1673	0.37	0/2290
3	H	0.21	0/1684	0.38	0/2305
4	F	0.21	0/1673	0.36	0/2269
4	L	0.22	0/1673	0.37	0/2269
5	G	0.16	0/23	0.32	0/30
5	I	0.31	0/23	0.53	0/30
All	All	0.22	0/21438	0.38	0/29160

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 (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	3516	3366	3361	1	0
1	C	3502	3337	3320	1	0
2	B	3632	3546	3516	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	3631	3551	3539	4	0
3	E	1631	1590	1590	0	0
3	H	1642	1600	1600	0	0
4	F	1637	1553	1553	0	0
4	L	1637	1553	1553	0	0
5	G	25	20	20	0	0
5	I	25	20	20	0	0
6	J	61	55	52	0	0
7	K	28	27	25	0	0
7	N	28	27	24	0	0
8	M	39	35	33	0	0
9	A	4	0	0	0	0
9	C	4	0	0	0	0
10	A	15	0	0	0	0
10	C	15	0	0	0	0
10	L	5	0	0	0	0
11	A	6	8	8	0	0
12	B	3	0	0	0	0
12	D	3	0	0	0	0
13	B	14	14	13	0	0
13	D	14	14	13	0	0
14	C	11	10	10	0	0
15	C	1	0	0	0	0
16	A	369	0	0	0	0
16	B	183	0	0	0	0
16	C	165	0	0	0	0
16	D	141	0	0	0	0
16	E	18	0	0	0	0
16	F	19	0	0	0	0
16	G	3	0	0	0	0
16	H	36	0	0	0	0
16	I	3	0	0	0	0
16	L	54	0	0	0	0
All	All	22120	20326	20250	7	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 0.

All (7) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:288:ASP:OD1	2:B:289:TYR:N	2.43	0.52
2:D:371:ASN:HB2	2:D:398:SER:HB3	2.00	0.43
2:D:126:ASP:OD1	2:D:126:ASP:N	2.53	0.42
2:D:217:ASP:OD2	2:D:255:HIS:NE2	2.53	0.41
1:A:365:ASP:OD2	1:A:370:GLY:N	2.47	0.41
2:D:450:ASN:O	2:D:450:ASN:ND2	2.53	0.40
1:C:2:ASN:N	1:C:2:ASN:OD1	2.53	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	459/454 (101%)	439 (96%)	19 (4%)	1 (0%)	47	73
1	C	457/454 (101%)	437 (96%)	20 (4%)	0	100	100
2	B	472/471 (100%)	449 (95%)	21 (4%)	2 (0%)	34	60
2	D	471/471 (100%)	454 (96%)	17 (4%)	0	100	100
3	E	210/219 (96%)	197 (94%)	13 (6%)	0	100	100
3	H	212/219 (97%)	196 (92%)	16 (8%)	0	100	100
4	F	212/214 (99%)	199 (94%)	13 (6%)	0	100	100
4	L	212/214 (99%)	200 (94%)	12 (6%)	0	100	100
5	G	3/5 (60%)	2 (67%)	1 (33%)	0	100	100
5	I	3/5 (60%)	2 (67%)	1 (33%)	0	100	100
All	All	2711/2726 (99%)	2575 (95%)	133 (5%)	3 (0%)	51	78

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	123	GLU

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Mol	Chain	Res	Type
2	B	375	LEU
2	B	157	VAL

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	368/362 (102%)	363 (99%)	5 (1%)	67	86
1	C	366/362 (101%)	360 (98%)	6 (2%)	62	85
2	B	420/416 (101%)	413 (98%)	7 (2%)	60	84
2	D	418/416 (100%)	415 (99%)	3 (1%)	84	94
3	E	186/189 (98%)	186 (100%)	0	100	100
3	H	187/189 (99%)	186 (100%)	1 (0%)	88	96
4	F	188/188 (100%)	188 (100%)	0	100	100
4	L	188/188 (100%)	188 (100%)	0	100	100
5	G	2/2 (100%)	2 (100%)	0	100	100
5	I	2/2 (100%)	2 (100%)	0	100	100
All	All	2325/2314 (100%)	2303 (99%)	22 (1%)	78	92

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	LEU
1	A	166	TYR
1	A	190	TYR
1	A	270	LEU
1	A	288	TYR
2	B	37	ARG
2	B	76	ASP
2	B	99	ASN
2	B	128	LEU
2	B	133[A]	ASN
2	B	133[B]	ASN

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Mol	Chain	Res	Type
2	B	215	ASN
1	C	23	LEU
1	C	119	THR
1	C	166	TYR
1	C	190	TYR
1	C	288	TYR
1	C	307	LEU
2	D	123	SER
2	D	215	ASN
2	D	365	GLU
3	H	213	ASP

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

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)

12 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	NAG	J	1	6,2	14,14,15	0.34	0	17,19,21	0.50	0
6	NAG	J	2	6	14,14,15	0.33	0	17,19,21	0.47	0
6	BMA	J	3	6	11,11,12	0.94	1 (9%)	15,15,17	0.97	0
6	MAN	J	4	6	11,11,12	0.74	0	15,15,17	1.12	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	MAN	J	5	6	11,11,12	0.94	1 (9%)	15,15,17	1.15	2 (13%)
7	NAG	K	1	7,2	14,14,15	0.28	0	17,19,21	0.39	0
7	NAG	K	2	7	14,14,15	0.21	0	17,19,21	0.47	0
8	NAG	M	1	8,2	14,14,15	0.16	0	17,19,21	0.46	0
8	NAG	M	2	8	14,14,15	0.32	0	17,19,21	0.36	0
8	BMA	M	3	8	11,11,12	0.65	0	15,15,17	0.74	0
7	NAG	N	1	7,2	14,14,15	0.22	0	17,19,21	0.45	0
7	NAG	N	2	7	14,14,15	0.53	0	17,19,21	0.57	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
6	NAG	J	1	6,2	-	0/6/23/26	0/1/1/1
6	NAG	J	2	6	-	2/6/23/26	0/1/1/1
6	BMA	J	3	6	-	0/2/19/22	0/1/1/1
6	MAN	J	4	6	-	0/2/19/22	0/1/1/1
6	MAN	J	5	6	-	1/2/19/22	0/1/1/1
7	NAG	K	1	7,2	-	2/6/23/26	0/1/1/1
7	NAG	K	2	7	-	4/6/23/26	0/1/1/1
8	NAG	M	1	8,2	-	0/6/23/26	0/1/1/1
8	NAG	M	2	8	-	0/6/23/26	0/1/1/1
8	BMA	M	3	8	-	0/2/19/22	0/1/1/1
7	NAG	N	1	7,2	-	0/6/23/26	0/1/1/1
7	NAG	N	2	7	-	2/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	J	3	BMA	O5-C1	-2.16	1.40	1.43
6	J	5	MAN	O5-C1	-2.03	1.40	1.43

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	J	4	MAN	C1-O5-C5	2.97	116.22	112.19
6	J	5	MAN	O2-C2-C3	-2.35	105.42	110.14
6	J	4	MAN	O2-C2-C3	-2.30	105.52	110.14
6	J	5	MAN	O5-C1-C2	2.02	113.90	110.77

There are no chirality outliers.

All (11) torsion outliers are listed below:

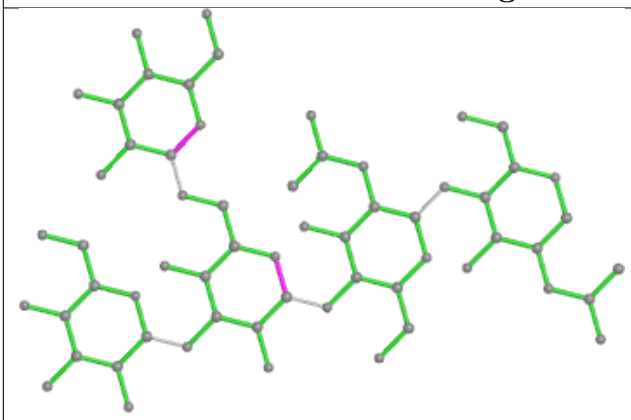
Mol	Chain	Res	Type	Atoms
7	K	1	NAG	C4-C5-C6-O6
7	K	2	NAG	O5-C5-C6-O6
7	K	2	NAG	C4-C5-C6-O6
7	K	1	NAG	O5-C5-C6-O6
7	K	2	NAG	C8-C7-N2-C2
7	K	2	NAG	O7-C7-N2-C2
7	N	2	NAG	C8-C7-N2-C2
7	N	2	NAG	O7-C7-N2-C2
6	J	2	NAG	O5-C5-C6-O6
6	J	2	NAG	C4-C5-C6-O6
6	J	5	MAN	O5-C5-C6-O6

There are no ring outliers.

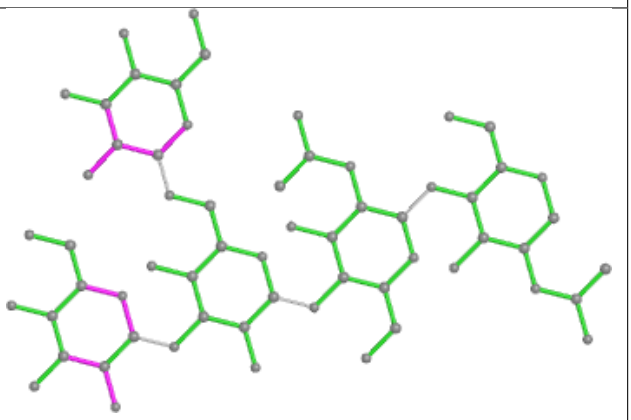
No monomer is involved in short contacts.

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

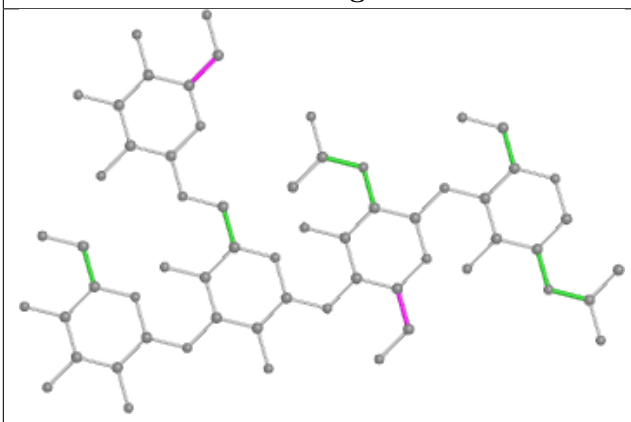
Oligosaccharide Chain J



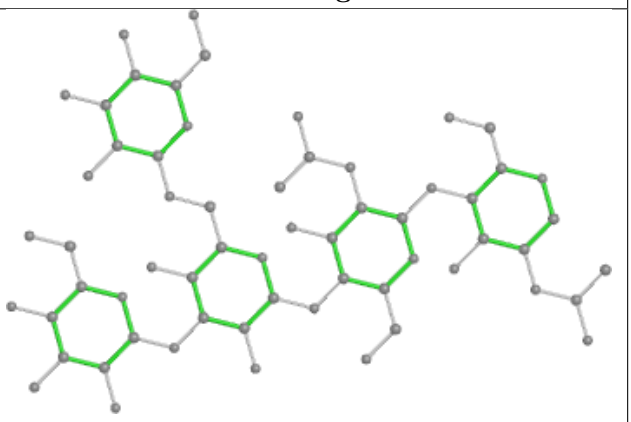
Bond lengths



Bond angles

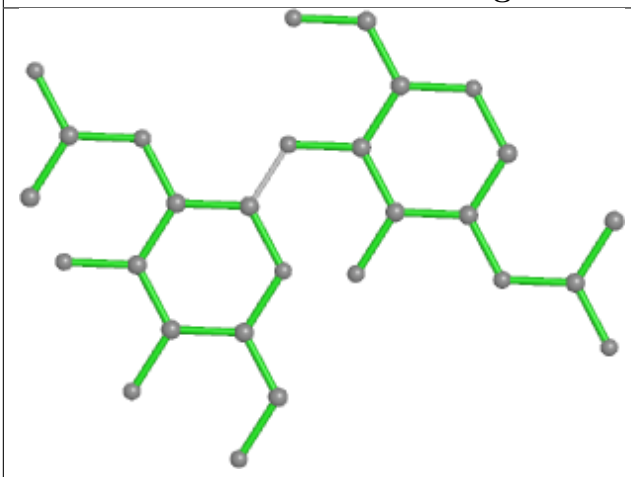


Torsions

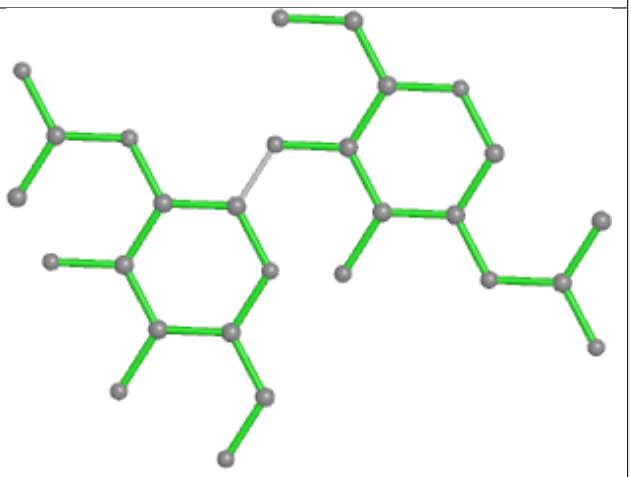


Rings

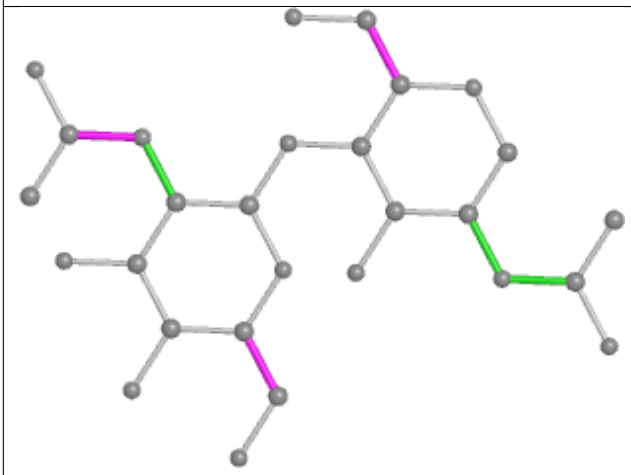
Oligosaccharide Chain K



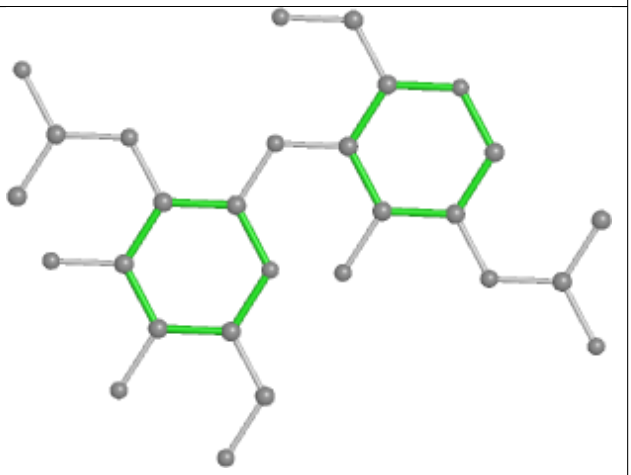
Bond lengths



Bond angles

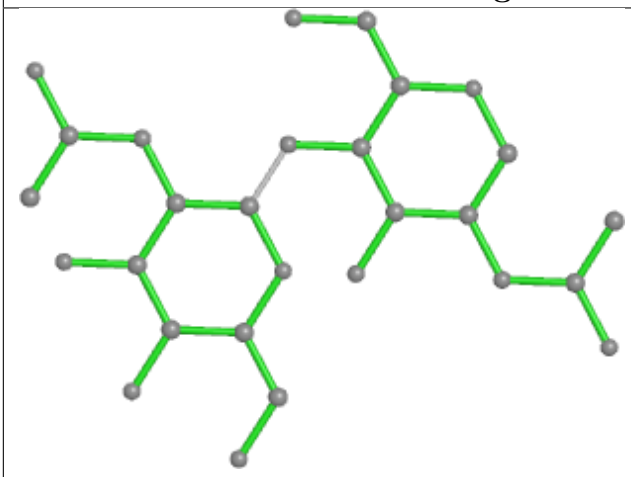


Torsions

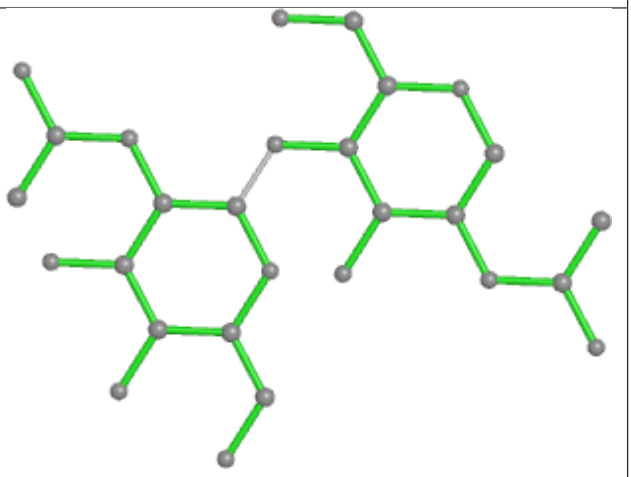


Rings

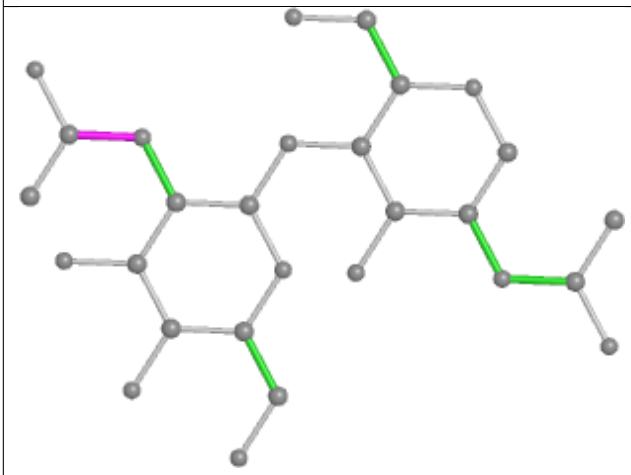
Oligosaccharide Chain N



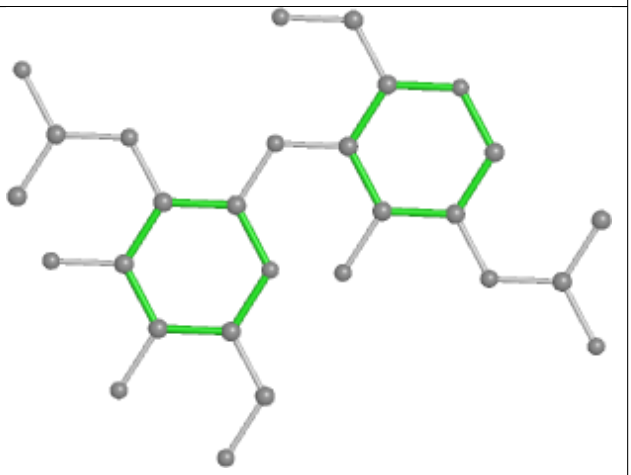
Bond lengths



Bond angles

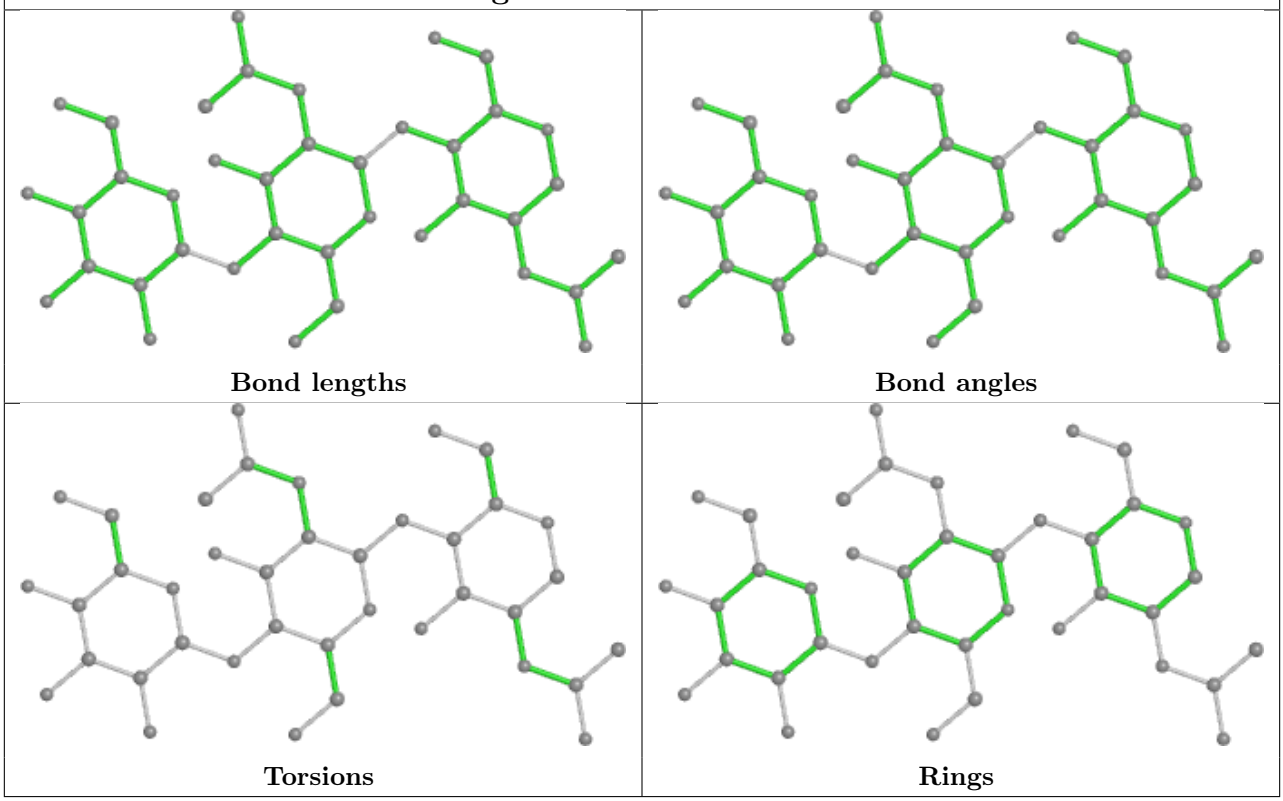


Torsions



Rings

Oligosaccharide Chain M



5.6 Ligand geometry (i)

Of 26 ligands modelled in this entry, 15 are monoatomic - leaving 11 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
10	SO4	C	508	-	4,4,4	0.14	0	6,6,6	0.05	0
10	SO4	C	506	-	4,4,4	0.14	0	6,6,6	0.06	0
10	SO4	A	507	-	4,4,4	0.14	0	6,6,6	0.05	0
10	SO4	C	507	-	4,4,4	0.14	0	6,6,6	0.04	0
10	SO4	L	301	-	4,4,4	0.14	0	6,6,6	0.05	0
10	SO4	A	506	-	4,4,4	0.14	0	6,6,6	0.05	0
14	MAN	C	505	-	11,11,12	0.67	0	15,15,17	1.08	2 (13%)
13	NAG	D	503	2	14,14,15	0.56	0	17,19,21	0.49	0
10	SO4	A	505	-	4,4,4	0.14	0	6,6,6	0.04	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
13	NAG	B	2004	2	14,14,15	0.19	0	17,19,21	0.43	0
11	GOL	A	508	-	5,5,5	0.37	0	5,5,5	0.15	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
14	MAN	C	505	-	-	2/2/19/22	0/1/1/1
11	GOL	A	508	-	-	2/4/4/4	-
13	NAG	D	503	2	-	2/6/23/26	0/1/1/1
13	NAG	B	2004	2	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	C	505	MAN	C1-O5-C5	2.65	115.78	112.19
14	C	505	MAN	O2-C2-C3	-2.44	105.26	110.14

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	B	2004	NAG	O5-C5-C6-O6
13	D	503	NAG	O5-C5-C6-O6
13	D	503	NAG	C4-C5-C6-O6
14	C	505	MAN	O5-C5-C6-O6
13	B	2004	NAG	C4-C5-C6-O6
14	C	505	MAN	C4-C5-C6-O6
11	A	508	GOL	O1-C1-C2-C3
11	A	508	GOL	O1-C1-C2-O2

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 (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	454/454 (100%)	0.42	4 (0%)	84	85	35, 52, 89, 158	0
1	C	453/454 (99%)	0.34	6 (1%)	77	78	44, 73, 117, 171	0
2	B	466/471 (98%)	0.64	43 (9%)	9	7	35, 90, 180, 211	1 (0%)
2	D	471/471 (100%)	0.43	31 (6%)	18	16	47, 93, 161, 251	1 (0%)
3	E	214/219 (97%)	1.73	71 (33%)	0	0	80, 153, 227, 280	0
3	H	216/219 (98%)	0.54	17 (7%)	12	10	52, 116, 179, 204	0
4	F	214/214 (100%)	1.48	66 (30%)	0	0	77, 143, 211, 250	0
4	L	214/214 (100%)	0.37	7 (3%)	46	46	57, 102, 141, 204	0
5	G	4/5 (80%)	0.77	0	100	100	59, 64, 67, 76	0
5	I	4/5 (80%)	0.47	0	100	100	81, 87, 92, 102	0
All	All	2710/2726 (99%)	0.64	245 (9%)	9	7	35, 89, 181, 280	2 (0%)

All (245) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	193	THR	11.2
3	E	212	VAL	9.7
3	E	194	TRP	9.5
3	E	147	LEU	9.2
3	E	216	ILE	8.5
3	E	183	LEU	8.0
2	D	469	SER	7.7
3	E	196	SER	7.1
3	E	215	LYS	7.1
4	F	117	ILE	7.0
3	E	201	CYS	6.8
3	E	210	THR	6.8
3	E	148	VAL	6.8

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Mol	Chain	Res	Type	RSRZ
4	F	206	VAL	6.7
3	E	133	VAL	6.6
4	F	181	LEU	6.5
2	B	33	LEU	6.4
4	F	115	VAL	6.4
4	F	214	CYS	6.3
3	E	129	PRO	6.1
2	B	2	PRO	6.1
4	F	180	THR	6.1
3	E	144	LEU	5.9
3	E	134	CYS	5.7
3	E	187	VAL	5.6
3	E	199	ILE	5.5
3	E	195	PRO	5.4
4	F	134	CYS	5.4
3	E	156	VAL	5.4
3	H	203	VAL	5.3
3	E	219	ARG	5.2
4	F	209	PHE	5.2
3	E	198	SER	5.1
3	E	145	GLY	4.8
4	F	130	ALA	4.8
4	F	116	SER	4.7
3	E	205	HIS	4.7
2	B	27	SER	4.7
2	D	44	LEU	4.7
3	E	169	VAL	4.7
4	F	192	TYR	4.7
2	B	1	GLY	4.6
3	E	127	VAL	4.6
3	E	131	ALA	4.6
4	F	154	GLU	4.6
2	B	46	LYS	4.6
2	D	1	GLY	4.5
3	E	142	VAL	4.5
2	B	36	PRO	4.4
3	H	144	LEU	4.4
4	F	135	PHE	4.2
3	H	189	VAL	4.2
3	H	198	SER	4.2
3	E	132	PRO	4.1
4	F	194	CYS	4.1

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Mol	Chain	Res	Type	RSRZ
3	E	200	THR	4.1
4	F	147	LYS	4.1
3	E	160	TRP	4.1
3	E	176	LEU	4.0
3	H	130	LEU	4.0
2	B	375	LEU	4.0
4	F	156	GLN	4.0
4	F	132	VAL	4.0
3	H	199	ILE	3.9
3	E	217	GLU	3.9
2	B	49	CYS	3.9
2	D	54	ILE	3.8
3	H	133	VAL	3.8
4	F	125	LEU	3.8
4	F	148	TRP	3.8
4	F	210	ASN	3.8
3	E	45	LEU	3.7
3	E	130	LEU	3.7
4	F	182	THR	3.7
2	B	34	GLY	3.7
2	D	55	GLU	3.7
3	E	158	LEU	3.7
4	F	104	LEU	3.6
4	F	146	VAL	3.6
3	E	128	TYR	3.6
2	B	72	LYS	3.6
4	F	122	SER	3.6
2	B	32	PRO	3.6
3	E	83	LEU	3.6
2	D	46	LYS	3.6
4	F	159	VAL	3.5
4	F	136	LEU	3.5
4	F	151	ASP	3.5
2	B	35	SER	3.5
4	F	208	SER	3.5
3	E	218	PRO	3.5
2	D	375	LEU	3.5
4	F	103	LYS	3.5
4	F	133	VAL	3.5
4	L	214	CYS	3.5
2	B	44	LEU	3.5
3	H	134	CYS	3.5

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Mol	Chain	Res	Type	RSRZ
4	L	212	ASN	3.4
4	F	160	LEU	3.4
2	B	29	GLU	3.4
2	D	36	PRO	3.4
3	E	203	VAL	3.4
2	B	8	ARG	3.4
3	E	204	ALA	3.3
4	F	213	GLU	3.3
3	E	209	SER	3.3
2	B	4	ILE	3.2
1	A	337	PRO	3.2
1	A	454	VAL	3.2
3	H	160	TRP	3.2
4	F	155	ARG	3.2
4	F	207	LYS	3.2
2	B	378	GLU	3.2
2	B	48	ASN	3.2
4	F	212	ASN	3.2
3	H	142	VAL	3.2
4	F	179	LEU	3.2
2	D	51	PRO	3.1
3	H	216	ILE	3.1
4	F	100	GLY	3.1
4	L	125	LEU	3.1
3	E	188	THR	3.0
2	B	181	LYS	3.0
4	F	178	THR	3.0
2	B	10	VAL	3.0
2	D	35	SER	3.0
4	F	118	PHE	3.0
4	F	15	LEU	3.0
2	B	381	PRO	3.0
4	L	105	GLU	3.0
3	E	126	SER	3.0
2	B	30	ALA	3.0
3	E	157	THR	3.0
4	F	131	SER	2.9
4	F	119	PRO	2.9
2	B	52	GLU	2.9
2	D	34	GLY	2.9
3	E	177	GLN	2.9
1	A	336	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
3	E	84	SER	2.9
3	E	149	LYS	2.9
3	E	213	ASP	2.8
3	H	201	CYS	2.8
2	B	458	GLY	2.8
2	D	378	GLU	2.8
2	B	54	ILE	2.8
2	D	33	LEU	2.8
4	F	195	GLU	2.8
3	E	118	SER	2.8
2	B	383	LEU	2.8
2	D	380	ILE	2.8
2	B	466	TRP	2.8
3	E	141	SER	2.8
2	B	45	LEU	2.8
4	F	190	ASN	2.7
3	E	214	LYS	2.7
4	F	152	GLY	2.7
2	B	51	PRO	2.7
3	H	211	LYS	2.7
4	F	205	ILE	2.7
2	D	181	LYS	2.6
1	C	269	ILE	2.6
3	E	140	SER	2.6
2	D	471	CYS	2.6
4	F	149	LYS	2.6
3	E	86	LEU	2.6
3	H	158	LEU	2.6
2	D	368	LEU	2.5
4	F	177	SER	2.5
3	E	65	GLN	2.5
4	F	126	THR	2.5
2	D	42	GLU	2.5
3	E	11	LEU	2.5
3	E	146	CYS	2.5
4	F	83	PHE	2.5
2	B	9	GLY	2.4
4	F	150	ILE	2.4
1	C	244	PHE	2.4
2	B	404	ARG	2.4
4	F	158	GLY	2.4
4	F	204	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
3	H	219	ARG	2.4
2	D	399	ILE	2.4
3	E	117	VAL	2.4
3	E	20	LEU	2.4
4	F	197	THR	2.4
3	E	191	SER	2.4
3	E	92	ALA	2.4
2	B	379	VAL	2.4
3	E	192	SER	2.3
4	F	14	SER	2.3
3	H	194	TRP	2.3
2	D	48	ASN	2.3
2	B	380	ILE	2.3
2	D	45	LEU	2.3
2	B	31	LEU	2.3
2	D	53	SER	2.3
3	E	165	LEU	2.3
2	D	470	GLN	2.3
3	E	124	ALA	2.2
4	L	206	VAL	2.2
2	D	90	LEU	2.2
1	C	320	ARG	2.2
3	E	182	THR	2.2
2	B	77	SER	2.2
2	D	404	ARG	2.2
2	B	50	ALA	2.2
2	D	61	ALA	2.2
4	F	107	LYS	2.2
2	D	58	VAL	2.2
4	F	128	GLY	2.2
3	E	125	PRO	2.2
4	F	196	ALA	2.2
3	E	189	VAL	2.1
1	A	185	ALA	2.1
2	B	11	SER	2.1
4	F	137	ASN	2.1
2	B	376	ASN	2.1
4	F	153	SER	2.1
3	H	183	LEU	2.1
4	L	112	ALA	2.1
4	F	161	ASN	2.1
4	F	191	SER	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	37	ARG	2.1
2	B	66	ASP	2.1
2	D	39	ASP	2.1
3	E	211	LYS	2.1
4	F	129	GLY	2.1
2	D	2	PRO	2.1
1	C	169	ALA	2.1
2	B	69	LEU	2.1
1	C	96	SER	2.1
2	D	47	ASP	2.1
3	E	206	PRO	2.1
2	B	373	THR	2.1
3	E	115	VAL	2.1
3	E	153	PRO	2.1
4	F	168	SER	2.1
2	D	4	ILE	2.0
3	E	122	THR	2.0
4	L	183	LYS	2.0
2	B	368	LEU	2.0
1	C	453	VAL	2.0
4	F	202	THR	2.0
3	E	8	GLY	2.0

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

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

6.3 Carbohydrates (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	MAN	J	5	11/12	0.76	0.17	94,122,147,152	0
6	BMA	J	3	11/12	0.86	0.17	88,134,166,170	0
7	NAG	K	2	14/15	0.88	0.37	117,140,165,168	0
7	NAG	K	1	14/15	0.89	0.25	84,118,145,145	0
7	NAG	N	2	14/15	0.89	0.28	116,135,154,159	0
8	BMA	M	3	11/12	0.89	0.22	97,124,146,149	0

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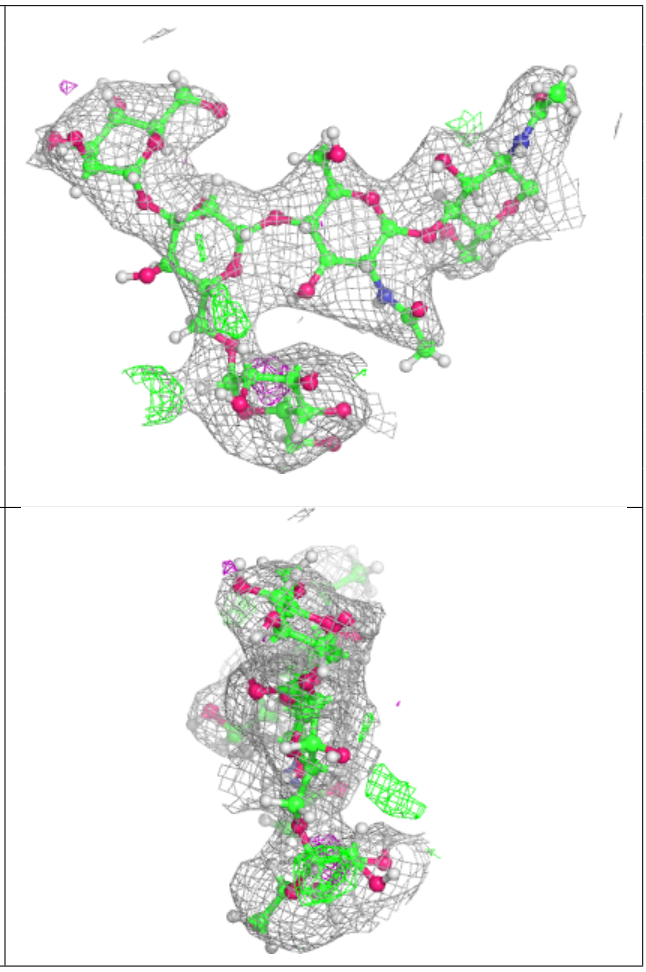
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	NAG	N	1	14/15	0.90	0.29	82,124,151,154	0
8	NAG	M	2	14/15	0.91	0.21	104,125,153,155	0
6	MAN	J	4	11/12	0.93	0.15	92,117,131,143	0
6	NAG	J	2	14/15	0.94	0.18	97,116,143,144	0
8	NAG	M	1	14/15	0.94	0.15	73,96,114,118	0
6	NAG	J	1	14/15	0.97	0.17	55,78,103,103	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.

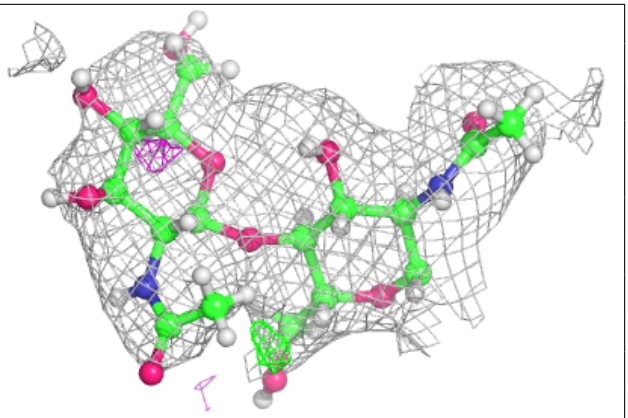
Electron density around Chain J:

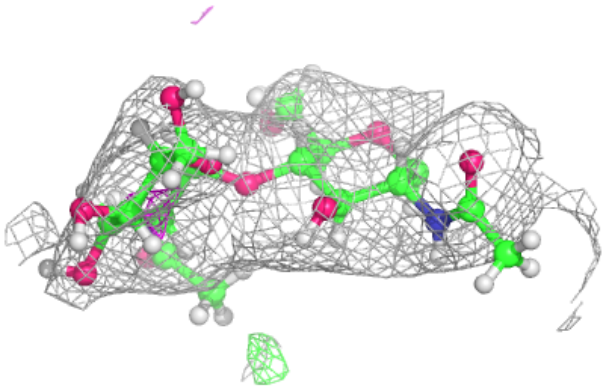
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)

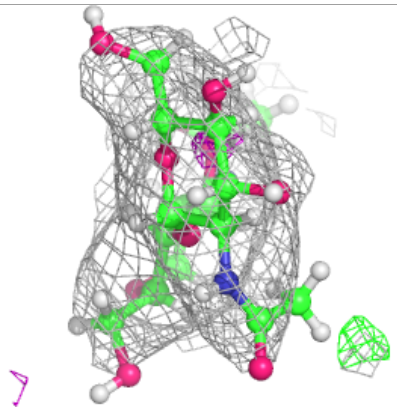


Electron density around Chain K:

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

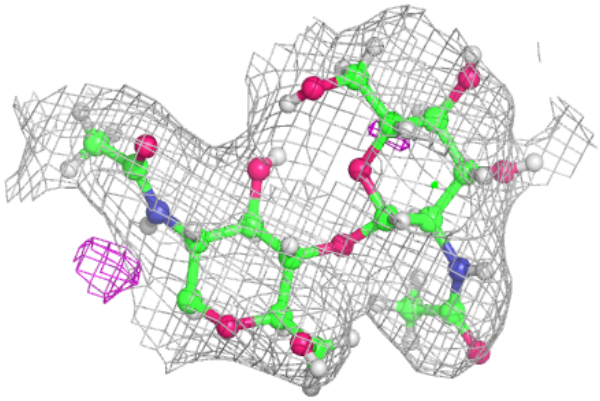


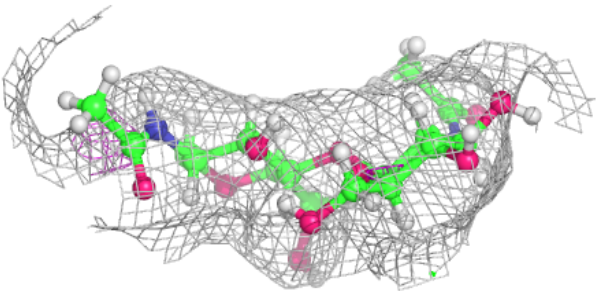


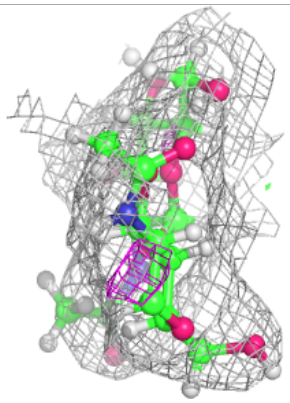


Electron density around Chain N:

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

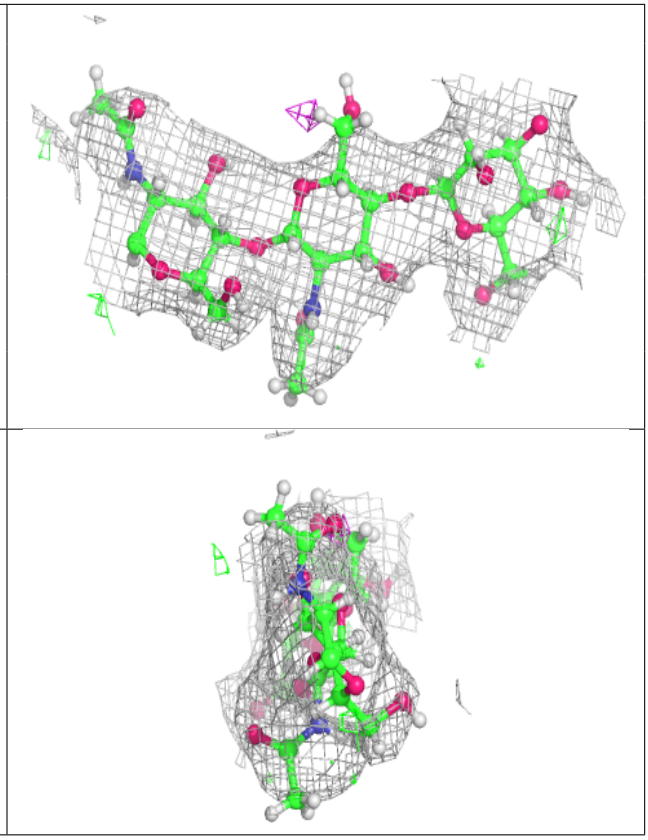






Electron density around Chain M:

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



6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
12	MN	B	2002	1/1	0.71	0.32	341,341,341,341	0
12	MN	D	501	1/1	0.79	0.24	373,373,373,373	0
10	SO4	C	507	5/5	0.86	0.18	142,142,158,159	0
10	SO4	C	506	5/5	0.87	0.29	145,159,162,164	0
13	NAG	B	2004	14/15	0.87	0.37	112,139,164,168	0
13	NAG	D	503	14/15	0.87	0.24	90,120,136,151	0
14	MAN	C	505	11/12	0.90	0.27	105,127,152,153	0
15	CL	C	509	1/1	0.90	0.34	100,100,100,100	0
11	GOL	A	508	6/6	0.91	0.28	69,95,115,117	0
12	MN	B	2003	1/1	0.92	0.19	74,74,74,74	0
10	SO4	A	505	5/5	0.92	0.35	135,139,148,160	0
9	CA	A	502	1/1	0.93	0.17	58,58,58,58	0
9	CA	A	501	1/1	0.93	0.10	65,65,65,65	0
12	MN	D	509	1/1	0.94	0.14	126,126,126,126	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
9	CA	C	504	1/1	0.95	0.19	76,76,76,76	0
9	CA	C	502	1/1	0.95	0.07	77,77,77,77	0
10	SO4	L	301	5/5	0.95	0.12	119,121,128,136	0
10	SO4	A	506	5/5	0.96	0.30	115,126,130,141	0
10	SO4	C	508	5/5	0.96	0.16	128,134,137,137	0
9	CA	C	501	1/1	0.97	0.05	116,116,116,116	0
9	CA	C	503	1/1	0.97	0.16	75,75,75,75	0
12	MN	D	502	1/1	0.98	0.15	81,81,81,81	0
9	CA	A	503	1/1	0.98	0.23	47,47,47,47	0
10	SO4	A	507	5/5	0.98	0.15	88,93,107,118	0
9	CA	A	504	1/1	0.99	0.28	65,65,65,65	0
12	MN	B	2001	1/1	1.00	0.26	49,49,49,49	0

6.5 Other polymers (i)

There are no such residues in this entry.