wwPDB X-ray Structure Validation Summary Report (i)

Dec 17, 2023 – 02:28 PM EST

PDB ID	:	4UBD
Title	:	Crystal structure of a neutralizing human monoclonal antibody with 1968 H3 HA
Authors	:	Shore, D.A.; Yang, H.; Cho, M.; Donis, R.O.; Stevens, J.
Deposited on	:	2014-08-12
Resolution	:	3.50 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 (i)) were used in the production of this report:

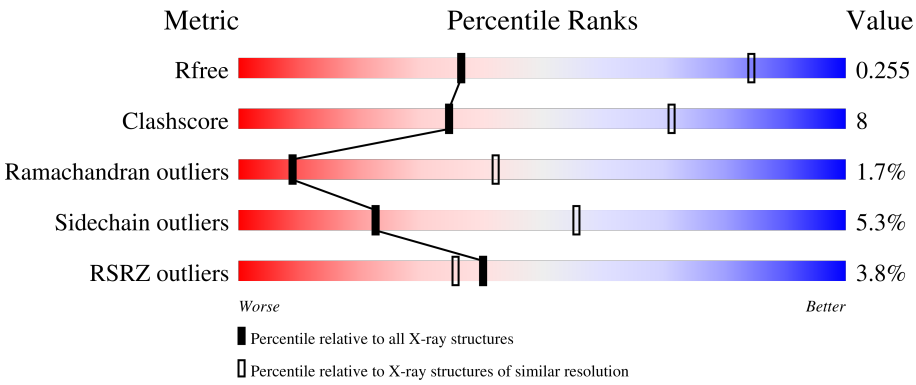
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)

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	321	% 83% 14% • •
1	E	321	81% 17% •
1	I	321	84% 13% • •
1	M	321	83% 15% •
1	Q	321	81% 16% •

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	U	321	.% 83% 16% •
2	B	175	.% 77% 13% 5% 6%
2	F	175	73% 17% • 7%
2	J	175	2% 77% 14% • • 6%
2	N	175	.% 77% 14% • • 7%
2	R	175	.% 75% 15% • • 5%
2	V	175	.% 77% 15% • 6%
3	C	226	73% 18% • • •
3	G	226	2% 74% 18% • • •
3	K	226	19% 75% 18% • • •
3	O	226	24% 73% 19% • • •
3	S	226	2% 74% 19% • • •
3	Y	226	74% 19% • • •
4	D	215	82% 16% • •
4	H	215	81% 16% • •
4	L	215	14% 84% 14% • •
4	P	215	21% 82% 16% •
4	T	215	2% 82% 15% • •
4	X	215	.% 83% 15% • •
5	W	4	100%
5	b	4	100%
5	c	4	100%
5	d	4	100%
5	e	4	100%
5	g	4	100%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
6	Z	2	50% 50%
6	a	2	100%
6	f	2	100%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	MAN	W	4	X	-	-	-
5	MAN	b	4	X	-	-	-
5	MAN	c	4	X	-	-	-
5	MAN	d	4	X	-	-	-
5	MAN	e	4	X	-	-	-
5	MAN	g	4	X	-	-	-

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 43086 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 Hemagglutinin HA1 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	320	2470	1546	434	477	13	0	0	0
1	U	320	2470	1546	434	477	13	0	0	0
1	I	317	2445	1531	429	472	13	0	0	0
1	M	320	2470	1546	434	477	13	0	0	0
1	Q	320	2470	1546	434	477	13	0	0	0
1	E	320	2470	1546	434	477	13	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	329	GLN	-	expression tag	UNP Q91MA7
U	329	GLN	-	expression tag	UNP Q91MA7
I	329	GLN	-	expression tag	UNP Q91MA7
M	329	GLN	-	expression tag	UNP Q91MA7
Q	329	GLN	-	expression tag	UNP Q91MA7
E	329	GLN	-	expression tag	UNP Q91MA7

- Molecule 2 is a protein called Hemagglutinin HA2 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	V	164	1346	831	238	271	6	0	0	0
2	F	163	1338	825	237	270	6	0	0	0
2	B	165	1357	840	239	272	6	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	J	164	1349	834	238	271	6	0	0	0
			Total	C	N	O	S			
2	N	163	1338	825	237	270	6	0	0	0
			Total	C	N	O	S			
2	R	166	1359	839	241	273	6	0	0	0

- Molecule 3 is a protein called monoclonal antibody H chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	219	1637	1036	278	319	4	0	0	0
			Total	C	N	O	S			
3	Y	219	1637	1036	278	319	4	0	0	0
			Total	C	N	O	S			
3	G	219	1637	1036	278	319	4	0	0	0
			Total	C	N	O	S			
3	S	219	1637	1036	278	319	4	0	0	0
			Total	C	N	O	S			
3	O	219	1637	1036	278	319	4	0	0	0
			Total	C	N	O	S			
3	K	219	1637	1036	278	319	4	0	0	0

- Molecule 4 is a protein called monoclonal antibody L chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	213	1650	1029	290	327	4	0	0	0
			Total	C	N	O	S			
4	X	213	1650	1029	290	327	4	0	0	0
			Total	C	N	O	S			
4	H	213	1650	1029	290	327	4	0	0	0
			Total	C	N	O	S			
4	T	213	1650	1029	290	327	4	0	0	0
			Total	C	N	O	S			
4	P	213	1650	1029	290	327	4	0	0	0
			Total	C	N	O	S			
4	L	213	1650	1029	290	327	4	0	0	0

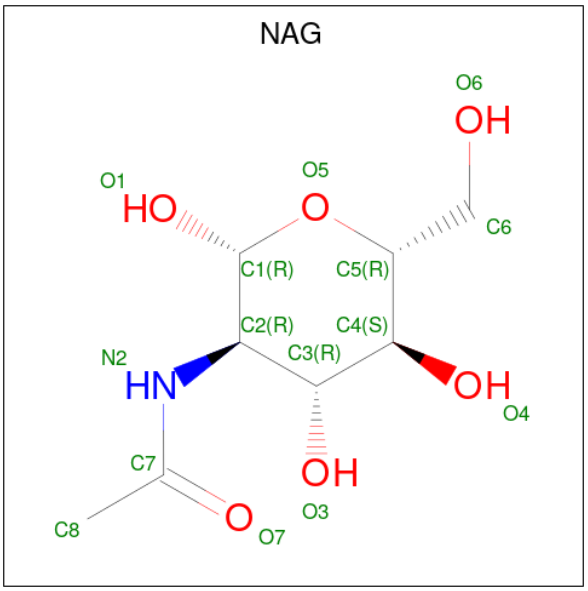
- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
5	W	4	50	28	2	20	0	0	0
5	b	4	50	28	2	20	0	0	0
5	c	4	50	28	2	20	0	0	0
5	d	4	50	28	2	20	0	0	0
5	e	4	50	28	2	20	0	0	0
5	g	4	50	28	2	20	0	0	0

- Molecule 6 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	N	O			
6	Z	2	28	16	2	10	0	0	0
6	a	2	28	16	2	10	0	0	0
6	f	2	28	16	2	10	0	0	0

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



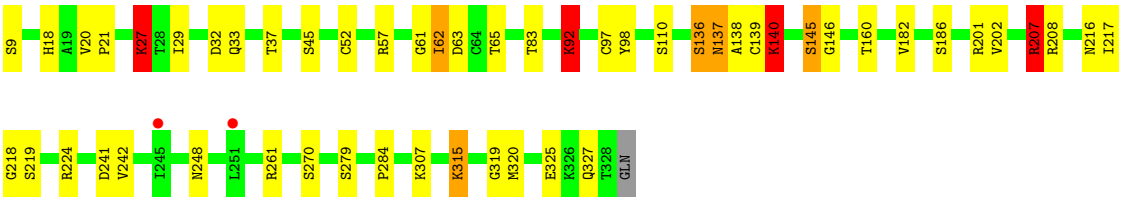
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
7	A	1	14	8	1	5	0	0
			Total	C	N	O		
7	U	1	14	8	1	5	0	0
			Total	C	N	O		
7	V	1	14	8	1	5	0	0
			Total	C	N	O		
7	I	1	14	8	1	5	0	0
			Total	C	N	O		
7	M	1	14	8	1	5	0	0
			Total	C	N	O		
7	Q	1	14	8	1	5	0	0
			Total	C	N	O		
7	F	1	14	8	1	5	0	0

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.

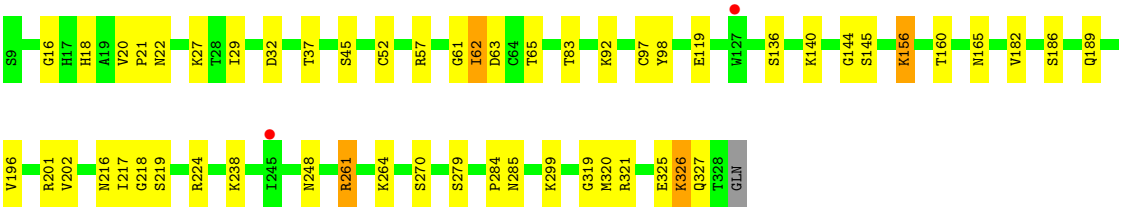
• Molecule 1: Hemagglutinin HA1 chain

Chain A:



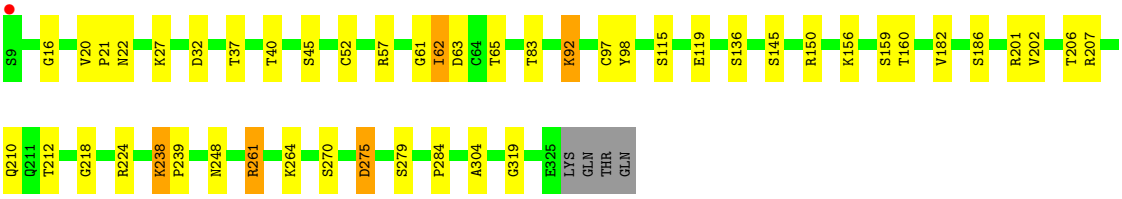
• Molecule 1: Hemagglutinin HA1 chain

Chain U:



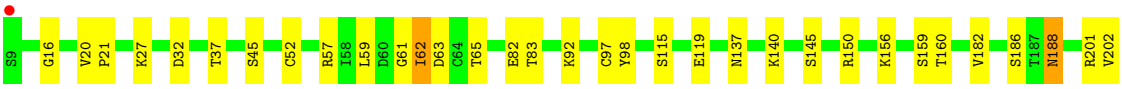
• Molecule 1: Hemagglutinin HA1 chain

Chain I:



• Molecule 1: Hemagglutinin HA1 chain

Chain M:

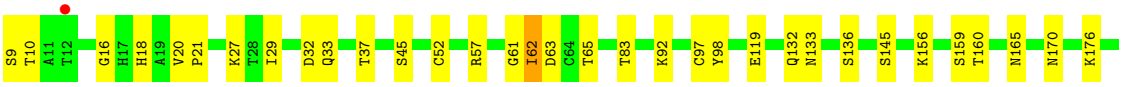


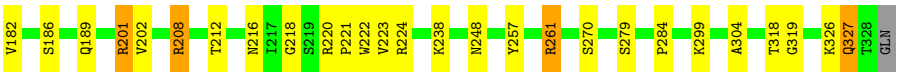
• Molecule 1: Hemagglutinin HA1 chain

Chain Q:

• Molecule 1: Hemagglutinin HA1 chain

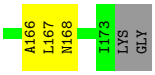
Chain E:





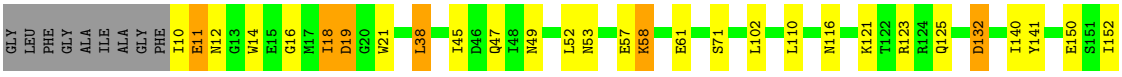
• Molecule 2: Hemagglutinin HA2 chain

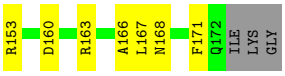
Chain V:



• Molecule 2: Hemagglutinin HA2 chain

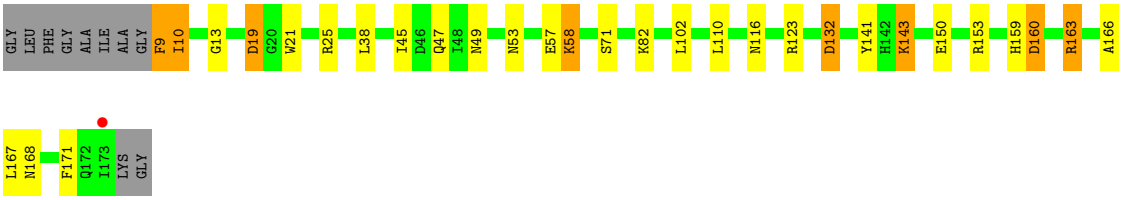
Chain F:





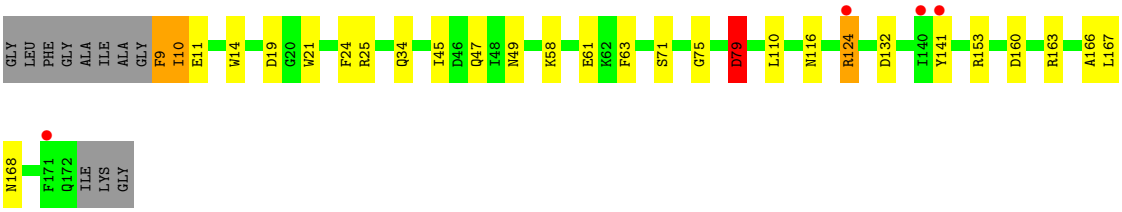
• Molecule 2: Hemagglutinin HA2 chain

Chain B:



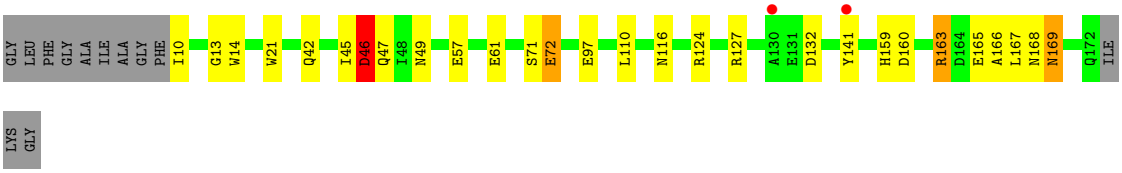
• Molecule 2: Hemagglutinin HA2 chain

Chain J:



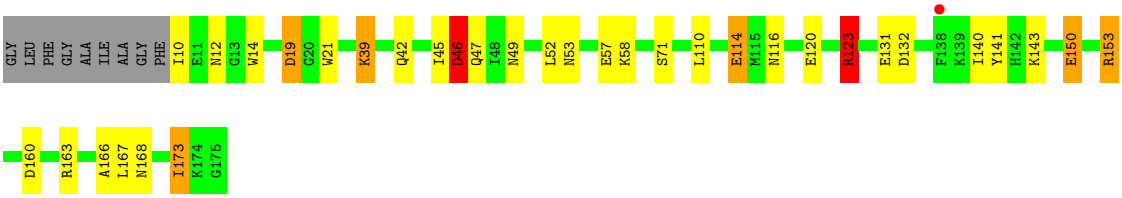
• Molecule 2: Hemagglutinin HA2 chain

Chain N:



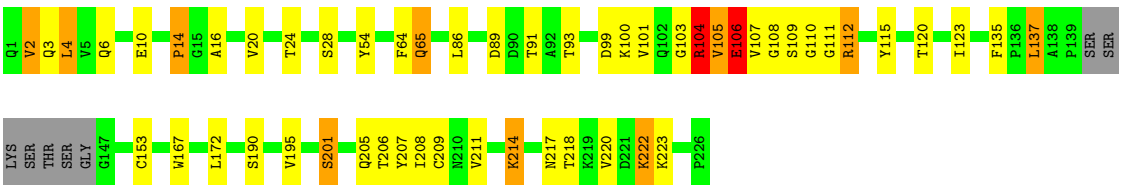
• Molecule 2: Hemagglutinin HA2 chain

Chain R:



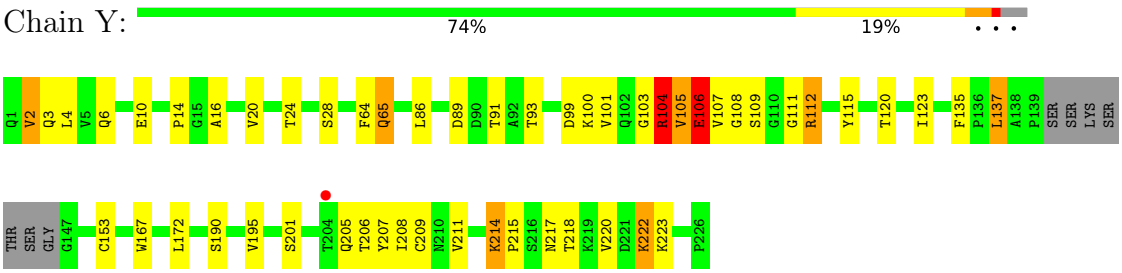
• Molecule 3: monoclonal antibody H chain

Chain C:



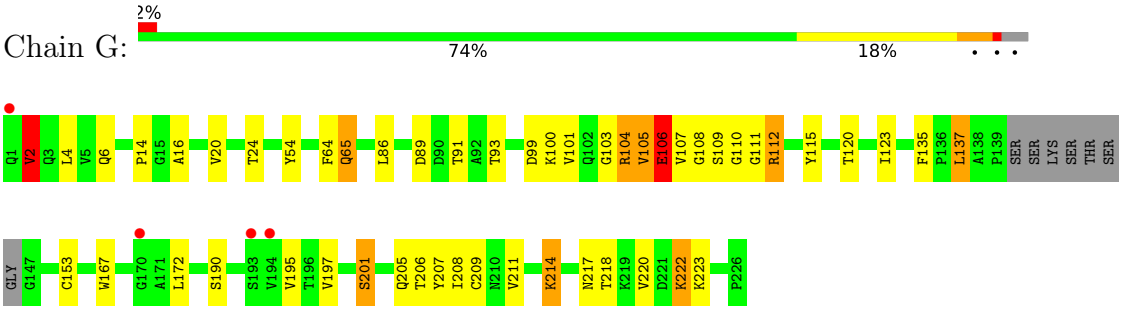
• Molecule 3: monoclonal antibody H chain

Chain Y:



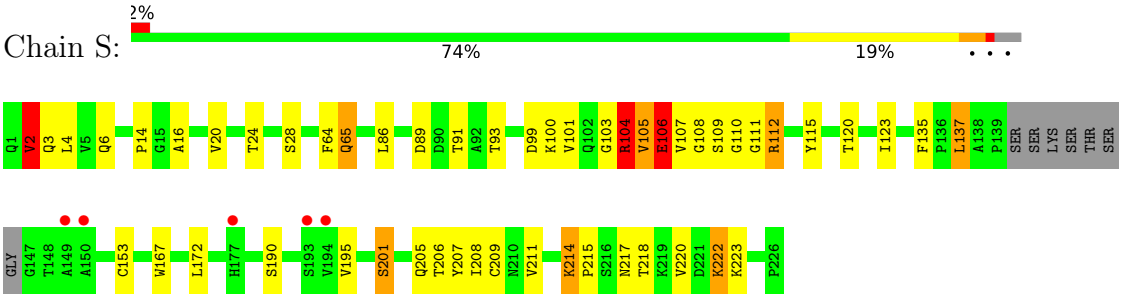
• Molecule 3: monoclonal antibody H chain

Chain G:



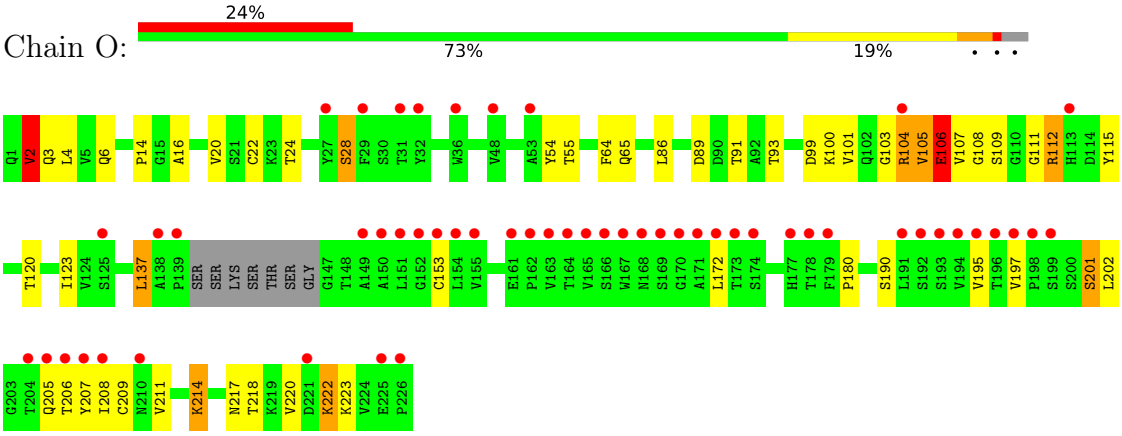
• Molecule 3: monoclonal antibody H chain

Chain S:



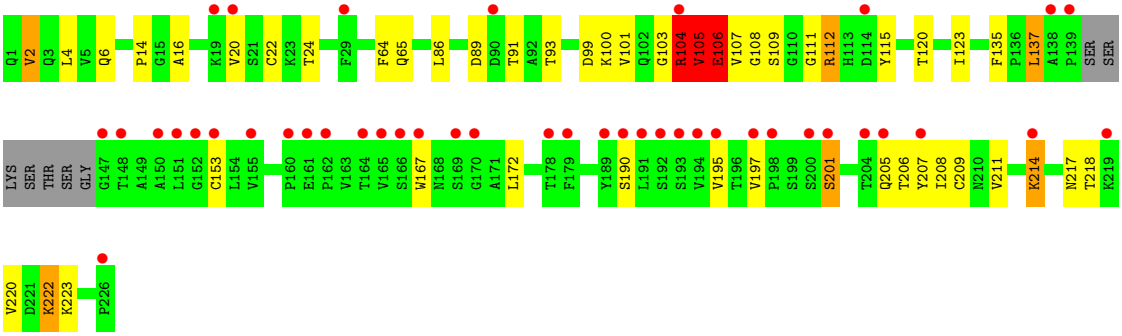
• Molecule 3: monoclonal antibody H chain

Chain O:



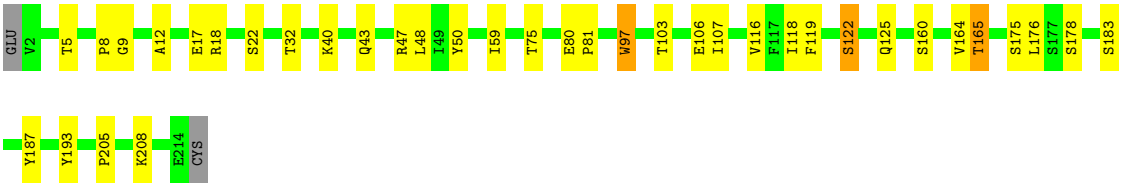
• Molecule 3: monoclonal antibody H chain

Chain K:



• Molecule 4: monoclonal antibody L chain

Chain D:

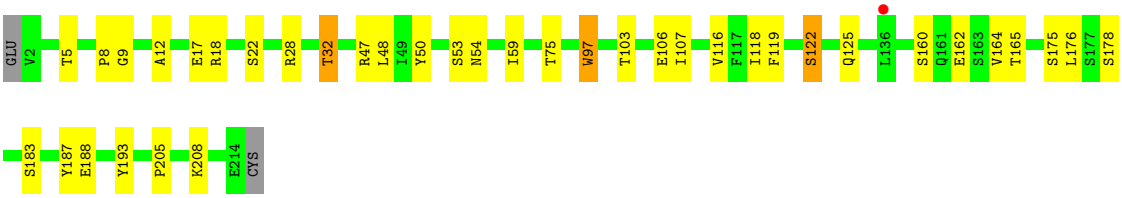


• Molecule 4: monoclonal antibody L chain

Chain X:

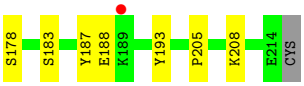
• Molecule 4: monoclonal antibody L chain

Chain H:



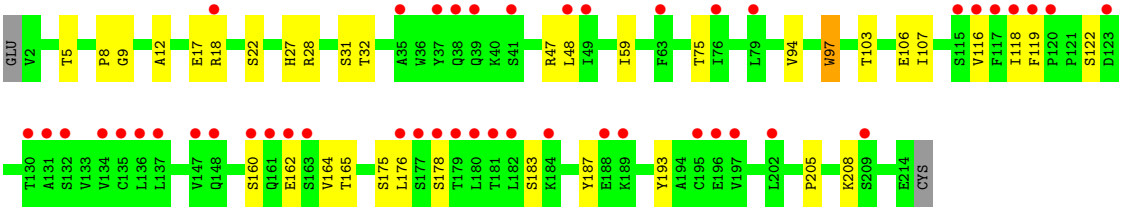
• Molecule 4: monoclonal antibody L chain

Chain T:



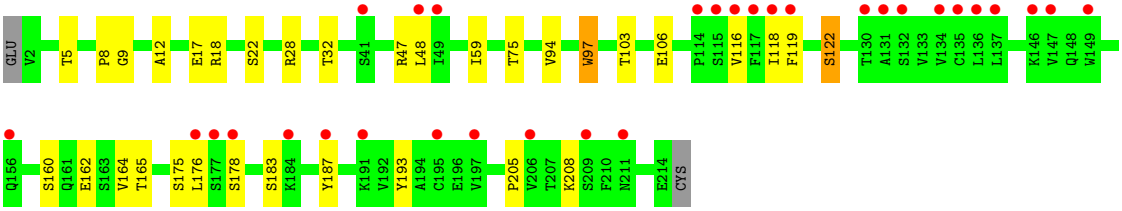
• Molecule 4: monoclonal antibody L chain

Chain P:



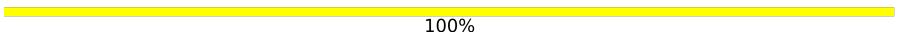
• Molecule 4: monoclonal antibody L chain

Chain L:



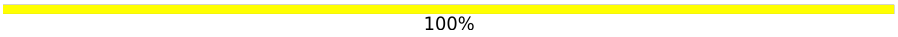
• Molecule 5: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain W:



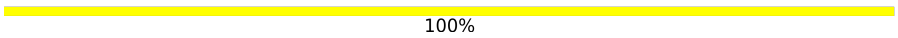
• Molecule 5: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain b:



• Molecule 5: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain c:



• Molecule 5: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain d: 100%

NAG1
NAG2
BMA3
MAN4

• Molecule 5: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain e: 100%

NAG1
NAG2
BMA3
MAN4

• Molecule 5: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain g: 100%

NAG1
NAG2
BMA3
MAN4

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

Chain Z: 50% 50%

NAG1
NAG2

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

Chain a: 100%

NAG1
NAG2

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

Chain f: 100%

NAG1
NAG2

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α, β, γ	128.70Å 128.70Å 428.32Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 3.50 48.26 – 3.50	Depositor EDS
% Data completeness (in resolution range)	99.3 (50.00-3.50) 99.4 (48.26-3.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.06 (at 3.48Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.212 , 0.258 0.216 , 0.255	Depositor DCC
R_{free} test set	4962 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	97.5	Xtriage
Anisotropy	0.212	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 63.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.006 for -h,-k,l 0.410 for h,-h-k,-l 0.018 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	43086	wwPDB-VP
Average B, all atoms (Å^2)	117.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.98% 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: MAN, NAG, BMA

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	0.60	0/2526	0.80	5/3442 (0.1%)
1	E	0.61	0/2526	0.76	1/3442 (0.0%)
1	I	0.64	1/2501 (0.0%)	0.77	2/3409 (0.1%)
1	M	0.62	1/2526 (0.0%)	0.77	2/3442 (0.1%)
1	Q	0.61	0/2526	0.78	2/3442 (0.1%)
1	U	0.61	0/2526	0.78	1/3442 (0.0%)
2	B	0.77	3/1380 (0.2%)	0.92	6/1855 (0.3%)
2	F	0.74	3/1360 (0.2%)	0.92	4/1828 (0.2%)
2	J	0.72	1/1372 (0.1%)	0.89	5/1844 (0.3%)
2	N	0.74	1/1360 (0.1%)	0.95	5/1828 (0.3%)
2	R	0.74	2/1381 (0.1%)	1.05	10/1855 (0.5%)
2	V	0.78	4/1368 (0.3%)	0.92	6/1839 (0.3%)
3	C	0.62	0/1677	0.79	3/2289 (0.1%)
3	G	0.59	0/1677	0.78	1/2289 (0.0%)
3	K	0.53	0/1677	0.75	2/2289 (0.1%)
3	O	0.53	0/1677	0.75	1/2289 (0.0%)
3	S	0.59	0/1677	0.78	2/2289 (0.1%)
3	Y	0.62	0/1677	0.79	3/2289 (0.1%)
4	D	0.61	1/1687 (0.1%)	0.76	1/2292 (0.0%)
4	H	0.62	1/1687 (0.1%)	0.76	1/2292 (0.0%)
4	L	0.49	1/1687 (0.1%)	0.71	1/2292 (0.0%)
4	P	0.50	1/1687 (0.1%)	0.72	1/2292 (0.0%)
4	T	0.62	1/1687 (0.1%)	0.76	1/2292 (0.0%)
4	X	0.62	1/1687 (0.1%)	0.76	1/2292 (0.0%)
All	All	0.63	22/43536 (0.1%)	0.80	67/59154 (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
3	C	0	1
3	G	0	1
3	K	0	1
3	O	0	1
3	S	0	1
3	Y	0	1
All	All	0	6

The worst 5 of 22 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	275	ASP	CB-CG	7.09	1.66	1.51
4	L	97	TRP	CB-CG	6.63	1.62	1.50
1	M	275	ASP	CB-CG	6.58	1.65	1.51
2	V	10	ILE	CA-CB	6.55	1.70	1.54
2	V	19	ASP	CB-CG	6.29	1.65	1.51

The worst 5 of 67 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	R	19	ASP	CB-CG-OD2	16.74	133.37	118.30
1	U	156	LYS	CB-CA-C	-8.49	93.43	110.40
2	V	82	LYS	CD-CE-NZ	8.34	130.89	111.70
2	R	123	ARG	NE-CZ-NH1	8.32	124.46	120.30
2	R	46	ASP	N-CA-CB	8.28	125.51	110.60

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	106	GLU	Peptide
3	G	106	GLU	Peptide
3	O	106	GLU	Peptide
3	S	106	GLU	Peptide
3	Y	106	GLU	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	2470	0	2419	57	0
1	E	2470	0	2422	47	0
1	I	2445	0	2393	29	1
1	M	2470	0	2421	36	1
1	Q	2470	0	2420	45	0
1	U	2470	0	2421	46	0
2	B	1357	0	1275	23	0
2	F	1338	0	1255	26	0
2	J	1349	0	1264	17	0
2	N	1338	0	1255	20	0
2	R	1359	0	1282	23	0
2	V	1346	0	1265	13	0
3	C	1637	0	1610	55	0
3	G	1637	0	1610	52	0
3	K	1637	0	1610	48	0
3	O	1637	0	1610	48	0
3	S	1637	0	1610	52	0
3	Y	1637	0	1610	52	0
4	D	1650	0	1602	20	0
4	H	1650	0	1602	24	1
4	L	1650	0	1602	23	0
4	P	1650	0	1602	23	0
4	T	1650	0	1602	23	1
4	X	1650	0	1602	17	0
5	W	50	0	43	0	0
5	b	50	0	43	0	0
5	c	50	0	43	0	0
5	d	50	0	43	0	0
5	e	50	0	43	0	0
5	g	50	0	43	0	0
6	Z	28	0	25	1	0
6	a	28	0	25	0	0
6	f	28	0	25	0	0
7	A	14	0	13	0	0
7	F	14	0	13	0	0
7	I	14	0	13	2	0
7	M	14	0	13	0	0
7	Q	14	0	13	0	0
7	U	14	0	13	5	0
7	V	14	0	13	0	0
All	All	43086	0	41788	693	2

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 8.

The worst 5 of 693 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:U:285:ASN:ND2	7:U:405:NAG:C1	1.71	1.51
1:U:156:LYS:HE2	1:U:196:VAL:CG2	1.66	1.25
1:A:140:LYS:HD2	1:A:140:LYS:N	1.33	1.22
1:U:156:LYS:CE	1:U:196:VAL:HG23	1.75	1.16
3:G:208:ILE:HA	3:G:223:LYS:HD3	1.21	1.11

All (2) 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:M:275:ASP:OD1	4:T:188:GLU:OE2[1_445]	1.91	0.29
1:I:275:ASP:OD1	4:H:188:GLU:OE2[1_565]	1.92	0.28

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	318/321 (99%)	297 (93%)	18 (6%)	3 (1%)	17	56
1	E	318/321 (99%)	300 (94%)	15 (5%)	3 (1%)	17	56
1	I	315/321 (98%)	297 (94%)	16 (5%)	2 (1%)	25	64
1	M	318/321 (99%)	297 (93%)	18 (6%)	3 (1%)	17	56
1	Q	318/321 (99%)	300 (94%)	15 (5%)	3 (1%)	17	56
1	U	318/321 (99%)	296 (93%)	19 (6%)	3 (1%)	17	56
2	B	163/175 (93%)	150 (92%)	13 (8%)	0	100	100
2	F	161/175 (92%)	151 (94%)	10 (6%)	0	100	100
2	J	162/175 (93%)	149 (92%)	13 (8%)	0	100	100
2	N	161/175 (92%)	150 (93%)	11 (7%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	R	164/175 (94%)	151 (92%)	12 (7%)	1 (1%)	25	64
2	V	162/175 (93%)	149 (92%)	13 (8%)	0	100	100
3	C	215/226 (95%)	188 (87%)	16 (7%)	11 (5%)	2	19
3	G	215/226 (95%)	188 (87%)	16 (7%)	11 (5%)	2	19
3	K	215/226 (95%)	189 (88%)	17 (8%)	9 (4%)	3	23
3	O	215/226 (95%)	189 (88%)	16 (7%)	10 (5%)	2	20
3	S	215/226 (95%)	188 (87%)	16 (7%)	11 (5%)	2	19
3	Y	215/226 (95%)	189 (88%)	17 (8%)	9 (4%)	3	23
4	D	211/215 (98%)	200 (95%)	9 (4%)	2 (1%)	17	56
4	H	211/215 (98%)	201 (95%)	8 (4%)	2 (1%)	17	56
4	L	211/215 (98%)	200 (95%)	9 (4%)	2 (1%)	17	56
4	P	211/215 (98%)	201 (95%)	8 (4%)	2 (1%)	17	56
4	T	211/215 (98%)	201 (95%)	8 (4%)	2 (1%)	17	56
4	X	211/215 (98%)	202 (96%)	7 (3%)	2 (1%)	17	56
All	All	5434/5622 (97%)	5023 (92%)	320 (6%)	91 (2%)	9	42

5 of 91 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	327	GLN
3	C	104	ARG
3	C	105	VAL
3	C	109	SER
3	Y	104	ARG

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	282/283 (100%)	269 (95%)	13 (5%)	27	61
1	E	282/283 (100%)	270 (96%)	12 (4%)	29	62

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	279/283 (99%)	271 (97%)	8 (3%)	42	71
1	M	282/283 (100%)	272 (96%)	10 (4%)	36	67
1	Q	282/283 (100%)	268 (95%)	14 (5%)	24	58
1	U	282/283 (100%)	270 (96%)	12 (4%)	29	62
2	B	145/149 (97%)	135 (93%)	10 (7%)	15	47
2	F	143/149 (96%)	133 (93%)	10 (7%)	15	46
2	J	144/149 (97%)	135 (94%)	9 (6%)	18	51
2	N	143/149 (96%)	135 (94%)	8 (6%)	21	54
2	R	145/149 (97%)	133 (92%)	12 (8%)	11	40
2	V	144/149 (97%)	137 (95%)	7 (5%)	25	59
3	C	181/187 (97%)	171 (94%)	10 (6%)	21	54
3	G	181/187 (97%)	172 (95%)	9 (5%)	24	58
3	K	181/187 (97%)	171 (94%)	10 (6%)	21	54
3	O	181/187 (97%)	171 (94%)	10 (6%)	21	54
3	S	181/187 (97%)	172 (95%)	9 (5%)	24	58
3	Y	181/187 (97%)	172 (95%)	9 (5%)	24	58
4	D	184/186 (99%)	172 (94%)	12 (6%)	17	50
4	H	184/186 (99%)	173 (94%)	11 (6%)	19	52
4	L	184/186 (99%)	173 (94%)	11 (6%)	19	52
4	P	184/186 (99%)	173 (94%)	11 (6%)	19	52
4	T	184/186 (99%)	173 (94%)	11 (6%)	19	52
4	X	184/186 (99%)	172 (94%)	12 (6%)	17	50
All	All	4743/4830 (98%)	4493 (95%)	250 (5%)	22	55

5 of 250 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	R	39	LYS
4	P	32	THR
4	D	160	SER
4	P	17	GLU
3	K	206	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 56 such sidechains are listed below:

Mol	Chain	Res	Type
3	Y	210	ASN
4	L	148	GLN
3	G	210	ASN
4	L	139	ASN
4	P	139	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)

25 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	NAG	a	1	6,1	14,14,15	0.97	1 (7%)	17,19,21	2.29	8 (47%)
5	NAG	b	2	5	14,14,15	0.56	0	17,19,21	2.12	3 (17%)
6	NAG	a	2	6	14,14,15	0.82	1 (7%)	17,19,21	2.26	7 (41%)
5	NAG	e	1	5,1	14,14,15	0.75	1 (7%)	17,19,21	1.74	6 (35%)
5	NAG	g	1	5,1	14,14,15	0.71	0	17,19,21	1.49	3 (17%)
6	NAG	Z	2	6	14,14,15	0.74	0	17,19,21	1.91	3 (17%)
5	NAG	c	2	5	14,14,15	0.81	1 (7%)	17,19,21	3.79	10 (58%)
5	NAG	d	2	5	14,14,15	0.69	0	17,19,21	2.54	7 (41%)
7	NAG	V	201	2	14,14,15	0.99	1 (7%)	17,19,21	2.64	7 (41%)
6	NAG	Z	1	6,1	14,14,15	0.88	1 (7%)	17,19,21	2.68	6 (35%)
7	NAG	A	409	1	14,14,15	1.05	1 (7%)	17,19,21	3.28	8 (47%)
6	NAG	f	1	6,1	14,14,15	1.08	1 (7%)	17,19,21	2.97	7 (41%)
5	NAG	b	1	5,1	14,14,15	0.73	0	17,19,21	1.76	4 (23%)
5	NAG	c	1	5,1	14,14,15	0.79	0	17,19,21	3.93	9 (52%)
7	NAG	U	405	-	14,14,15	1.34	2 (14%)	17,19,21	2.90	9 (52%)
5	NAG	e	2	5	14,14,15	0.56	0	17,19,21	2.44	8 (47%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
7	NAG	M	405	1	14,14,15	1.03	1 (7%)	17,19,21	1.31	2 (11%)
5	NAG	d	1	5,1	14,14,15	0.55	0	17,19,21	2.17	4 (23%)
5	NAG	W	1	5,1	14,14,15	0.68	0	17,19,21	1.66	4 (23%)
6	NAG	f	2	6	14,14,15	0.85	0	17,19,21	1.75	5 (29%)
7	NAG	I	405	1	14,14,15	1.58	2 (14%)	17,19,21	3.21	10 (58%)
7	NAG	Q	407	1	14,14,15	1.42	2 (14%)	17,19,21	3.34	9 (52%)
5	NAG	g	2	5	14,14,15	0.78	0	17,19,21	3.23	10 (58%)
7	NAG	F	201	-	14,14,15	0.96	0	17,19,21	2.29	5 (29%)
5	NAG	W	2	5	14,14,15	0.68	0	17,19,21	2.58	7 (41%)

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	a	1	6,1	-	0/6/23/26	0/1/1/1
5	NAG	b	2	5	-	2/6/23/26	0/1/1/1
6	NAG	a	2	6	-	2/6/23/26	0/1/1/1
5	NAG	e	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	g	1	5,1	-	2/6/23/26	0/1/1/1
6	NAG	Z	2	6	-	4/6/23/26	0/1/1/1
5	NAG	c	2	5	-	0/6/23/26	0/1/1/1
5	NAG	d	2	5	-	1/6/23/26	0/1/1/1
7	NAG	V	201	2	-	2/6/23/26	0/1/1/1
6	NAG	Z	1	6,1	-	0/6/23/26	0/1/1/1
7	NAG	A	409	1	-	4/6/23/26	0/1/1/1
6	NAG	f	1	6,1	-	2/6/23/26	0/1/1/1
5	NAG	b	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	c	1	5,1	-	2/6/23/26	0/1/1/1
7	NAG	U	405	-	-	2/6/23/26	0/1/1/1
5	NAG	e	2	5	-	0/6/23/26	0/1/1/1
7	NAG	M	405	1	-	3/6/23/26	0/1/1/1
5	NAG	d	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	W	1	5,1	-	0/6/23/26	0/1/1/1
6	NAG	f	2	6	-	4/6/23/26	0/1/1/1
7	NAG	I	405	1	-	0/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	Q	407	1	-	4/6/23/26	0/1/1/1
5	NAG	g	2	5	-	1/6/23/26	0/1/1/1
7	NAG	F	201	-	-	2/6/23/26	0/1/1/1
5	NAG	W	2	5	-	2/6/23/26	0/1/1/1

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	I	405	NAG	C1-C2	4.30	1.58	1.52
6	f	1	NAG	C1-C2	3.45	1.57	1.52
7	Q	407	NAG	C4-C5	3.19	1.59	1.53
7	M	405	NAG	C1-C2	2.92	1.56	1.52
7	U	405	NAG	C3-C2	2.85	1.58	1.52

The worst 5 of 161 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	c	1	NAG	C1-O5-C5	12.12	128.61	112.19
5	c	2	NAG	C1-O5-C5	8.98	124.36	112.19
6	Z	1	NAG	C1-O5-C5	8.09	123.15	112.19
7	I	405	NAG	O5-C1-C2	-7.98	98.68	111.29
7	A	409	NAG	C1-O5-C5	7.85	122.83	112.19

There are no chirality outliers.

5 of 43 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	409	NAG	C3-C2-N2-C7
7	Q	407	NAG	C3-C2-N2-C7
6	Z	2	NAG	O5-C5-C6-O6
7	U	405	NAG	O5-C5-C6-O6
5	b	2	NAG	C4-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	Z	1	NAG	1	0
7	U	405	NAG	5	0
7	I	405	NAG	2	0

5.5 Carbohydrates (i)

30 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	W	1	5,1	14,14,15	0.68	0	17,19,21	1.66	4 (23%)
5	NAG	W	2	5	14,14,15	0.68	0	17,19,21	2.58	7 (41%)
5	BMA	W	3	5	11,11,12	1.10	0	15,15,17	3.35	8 (53%)
5	MAN	W	4	5	11,11,12	0.78	0	15,15,17	2.82	4 (26%)
6	NAG	Z	1	6,1	14,14,15	0.88	1 (7%)	17,19,21	2.68	6 (35%)
6	NAG	Z	2	6	14,14,15	0.74	0	17,19,21	1.91	3 (17%)
6	NAG	a	1	6,1	14,14,15	0.97	1 (7%)	17,19,21	2.29	8 (47%)
6	NAG	a	2	6	14,14,15	0.82	1 (7%)	17,19,21	2.26	7 (41%)
5	NAG	b	1	5,1	14,14,15	0.73	0	17,19,21	1.76	4 (23%)
5	NAG	b	2	5	14,14,15	0.56	0	17,19,21	2.12	3 (17%)
5	BMA	b	3	5	11,11,12	1.02	0	15,15,17	2.95	6 (40%)
5	MAN	b	4	5	11,11,12	0.82	0	15,15,17	2.91	6 (40%)
5	NAG	c	1	5,1	14,14,15	0.79	0	17,19,21	3.93	9 (52%)
5	NAG	c	2	5	14,14,15	0.81	1 (7%)	17,19,21	3.79	10 (58%)
5	BMA	c	3	5	11,11,12	0.98	0	15,15,17	3.76	9 (60%)
5	MAN	c	4	5	11,11,12	1.23	2 (18%)	15,15,17	2.82	5 (33%)
5	NAG	d	1	5,1	14,14,15	0.55	0	17,19,21	2.17	4 (23%)
5	NAG	d	2	5	14,14,15	0.69	0	17,19,21	2.54	7 (41%)
5	BMA	d	3	5	11,11,12	0.54	0	15,15,17	2.78	6 (40%)
5	MAN	d	4	5	11,11,12	0.77	1 (9%)	15,15,17	1.87	6 (40%)
5	NAG	e	1	5,1	14,14,15	0.75	1 (7%)	17,19,21	1.74	6 (35%)
5	NAG	e	2	5	14,14,15	0.56	0	17,19,21	2.44	8 (47%)
5	BMA	e	3	5	11,11,12	1.19	1 (9%)	15,15,17	2.78	6 (40%)
5	MAN	e	4	5	11,11,12	1.05	1 (9%)	15,15,17	2.37	6 (40%)
6	NAG	f	1	6,1	14,14,15	1.08	1 (7%)	17,19,21	2.97	7 (41%)
6	NAG	f	2	6	14,14,15	0.85	0	17,19,21	1.75	5 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	NAG	g	1	5,1	14,14,15	0.71	0	17,19,21	1.49	3 (17%)
5	NAG	g	2	5	14,14,15	0.78	0	17,19,21	3.23	10 (58%)
5	BMA	g	3	5	11,11,12	1.23	1 (9%)	15,15,17	3.25	6 (40%)
5	MAN	g	4	5	11,11,12	0.72	0	15,15,17	2.45	5 (33%)

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	W	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	W	2	5	-	2/6/23/26	0/1/1/1
5	BMA	W	3	5	-	2/2/19/22	0/1/1/1
5	MAN	W	4	5	1/1/4/5	2/2/19/22	0/1/1/1
6	NAG	Z	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	Z	2	6	-	4/6/23/26	0/1/1/1
6	NAG	a	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	a	2	6	-	2/6/23/26	0/1/1/1
5	NAG	b	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	b	2	5	-	2/6/23/26	0/1/1/1
5	BMA	b	3	5	-	2/2/19/22	0/1/1/1
5	MAN	b	4	5	1/1/4/5	2/2/19/22	0/1/1/1
5	NAG	c	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	c	2	5	-	0/6/23/26	0/1/1/1
5	BMA	c	3	5	-	2/2/19/22	0/1/1/1
5	MAN	c	4	5	1/1/4/5	2/2/19/22	0/1/1/1
5	NAG	d	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	d	2	5	-	1/6/23/26	0/1/1/1
5	BMA	d	3	5	-	2/2/19/22	0/1/1/1
5	MAN	d	4	5	1/1/4/5	1/2/19/22	0/1/1/1
5	NAG	e	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	e	2	5	-	0/6/23/26	0/1/1/1
5	BMA	e	3	5	-	2/2/19/22	0/1/1/1
5	MAN	e	4	5	1/1/4/5	2/2/19/22	0/1/1/1
6	NAG	f	1	6,1	-	2/6/23/26	0/1/1/1
6	NAG	f	2	6	-	4/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

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

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	f	1	NAG	C1-C2	3.45	1.57	1.52
5	e	3	BMA	C2-C3	2.57	1.56	1.52
5	e	4	MAN	C1-C2	2.47	1.57	1.52
5	c	4	MAN	C2-C3	2.45	1.56	1.52
5	c	2	NAG	C3-C2	2.37	1.57	1.52

The worst 5 of 184 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	c	1	NAG	C1-O5-C5	12.12	128.61	112.19
5	c	3	BMA	C1-O5-C5	9.86	125.55	112.19
5	c	2	NAG	C1-O5-C5	8.98	124.36	112.19
5	g	3	BMA	C1-C2-C3	8.74	120.41	109.67
5	c	4	MAN	C1-O5-C5	-8.32	100.91	112.19

5 of 6 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	W	4	MAN	C1
5	b	4	MAN	C1
5	c	4	MAN	C1
5	d	4	MAN	C1
5	e	4	MAN	C1

5 of 49 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	W	4	MAN	C4-C5-C6-O6
5	g	4	MAN	O5-C5-C6-O6
6	Z	2	NAG	O5-C5-C6-O6
5	c	3	BMA	O5-C5-C6-O6
5	g	3	BMA	C4-C5-C6-O6

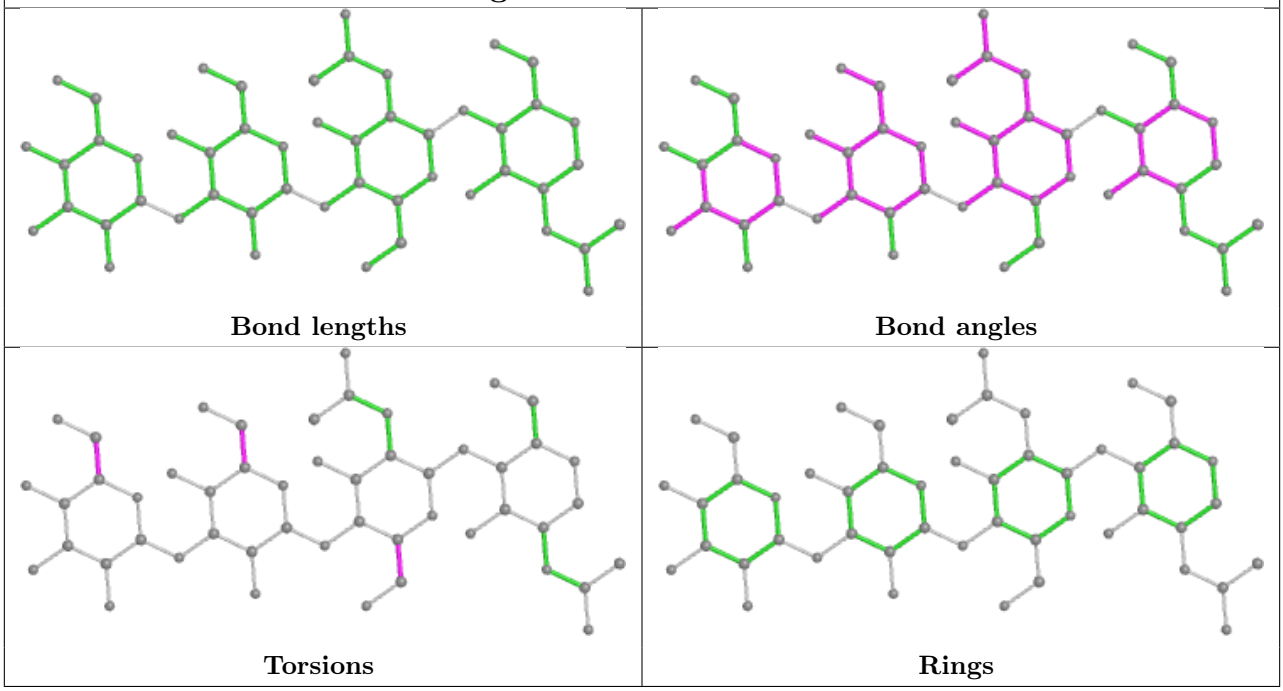
There are no ring outliers.

1 monomer is involved in 1 short contact:

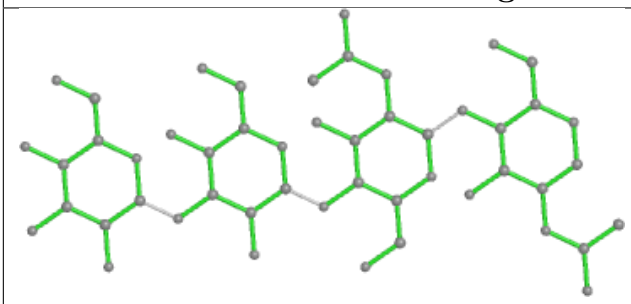
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	Z	1	NAG	1	0

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

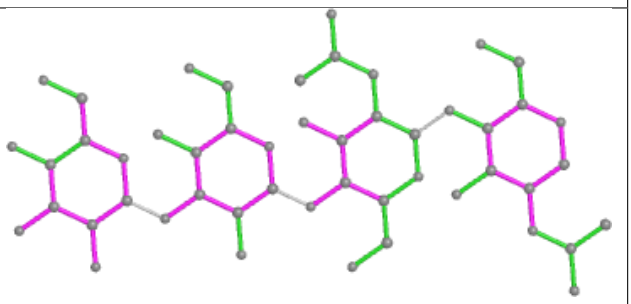
Oligosaccharide Chain W



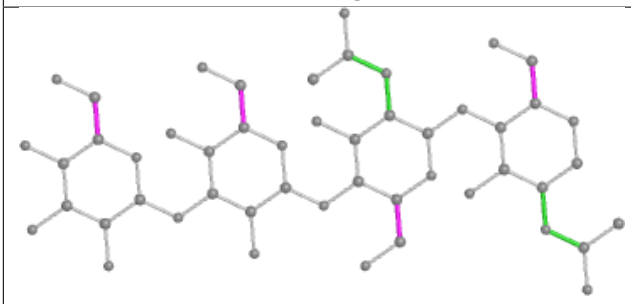
Oligosaccharide Chain b



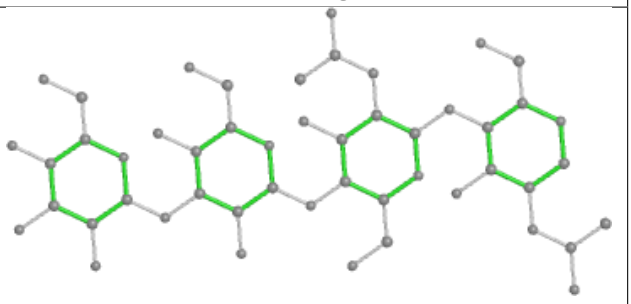
Bond lengths



Bond angles

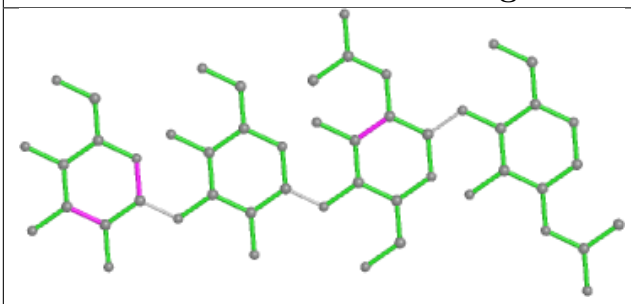


Torsions

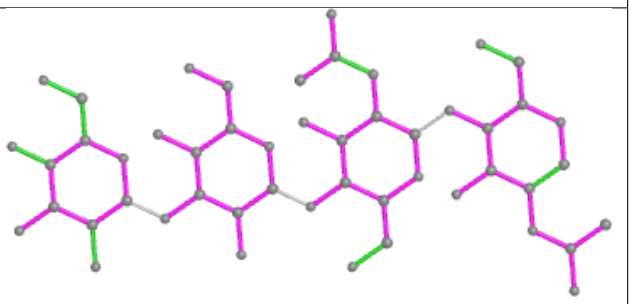


Rings

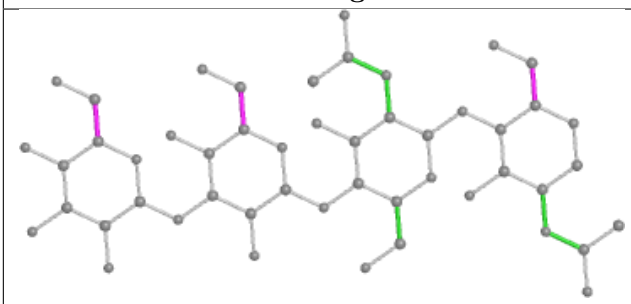
Oligosaccharide Chain c



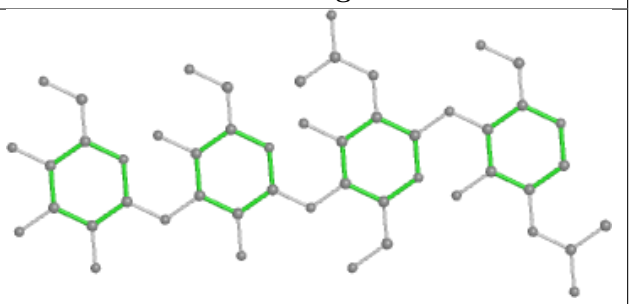
Bond lengths



Bond angles

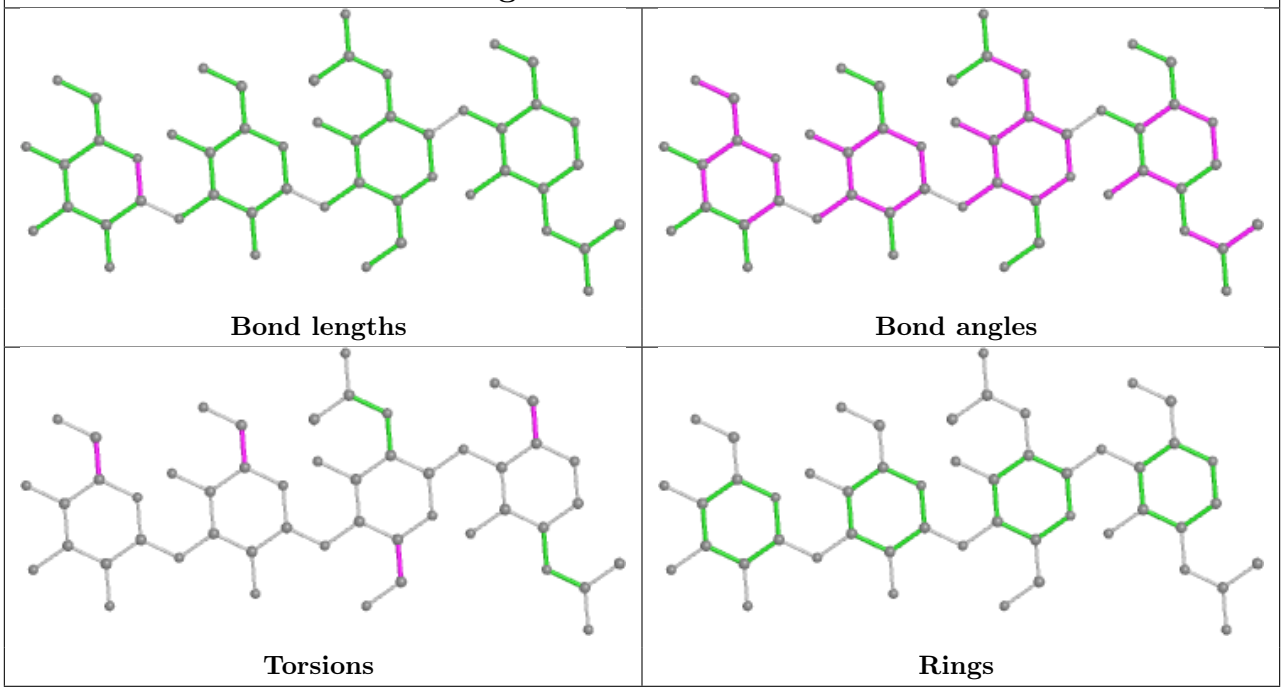


Torsions

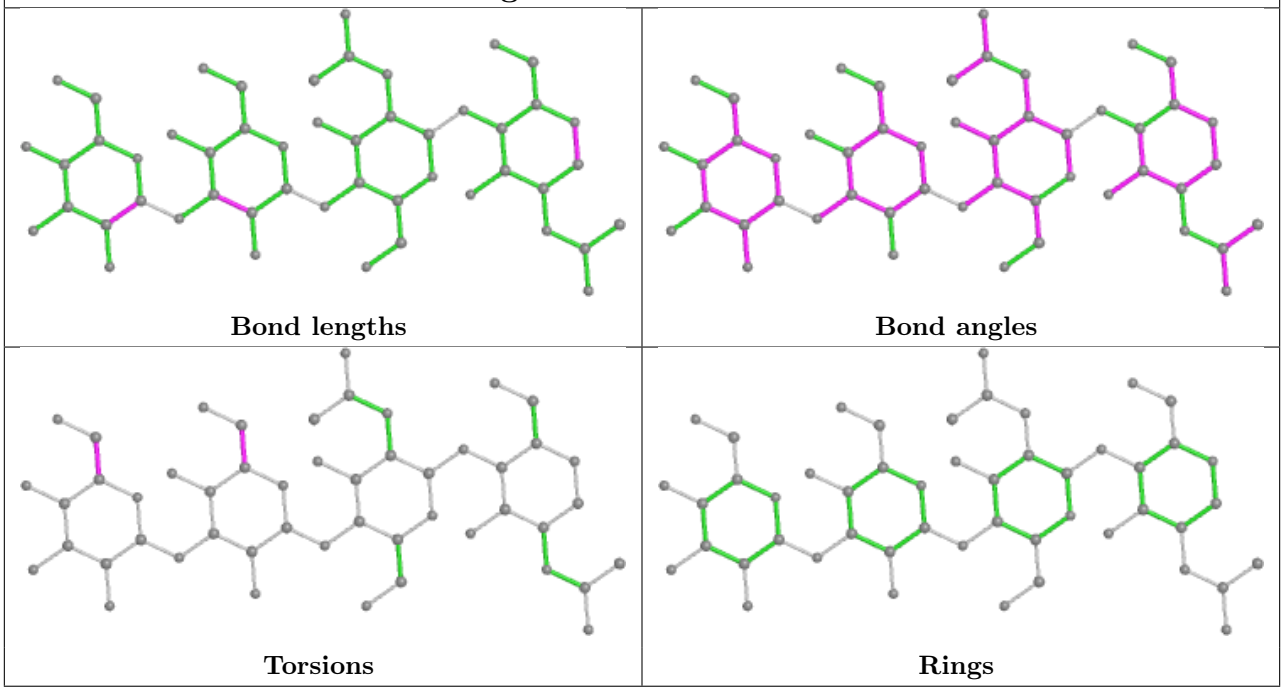


Rings

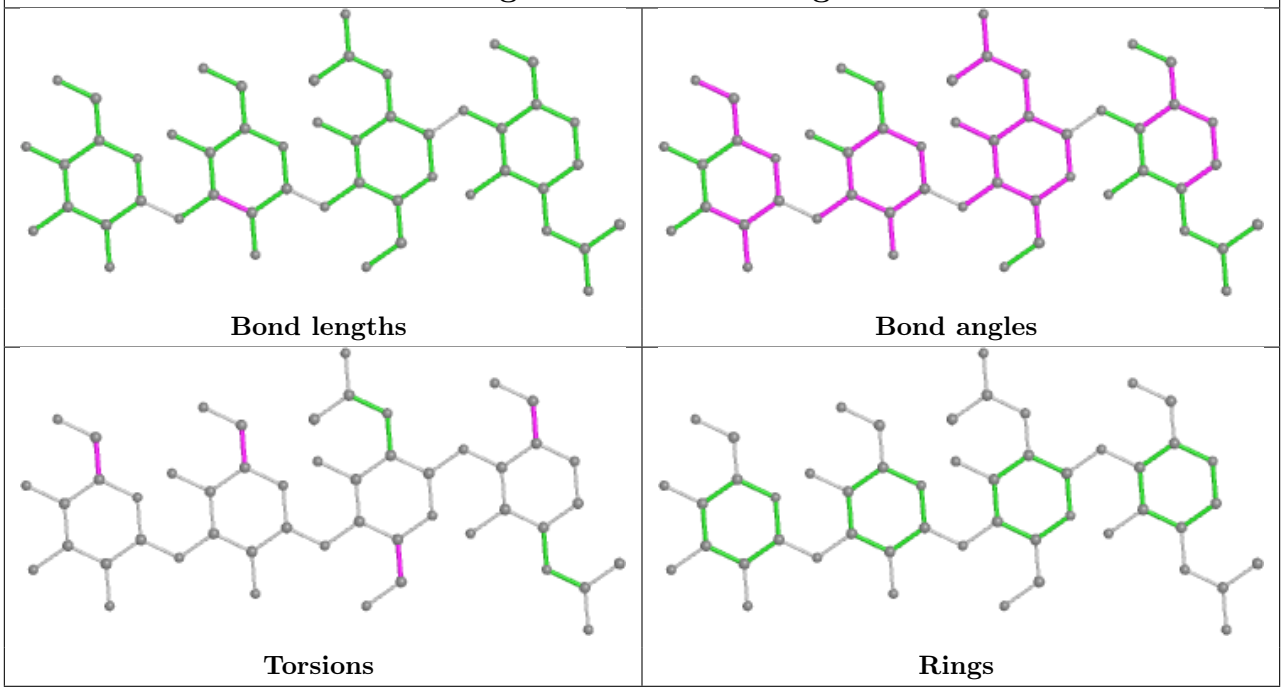
Oligosaccharide Chain d



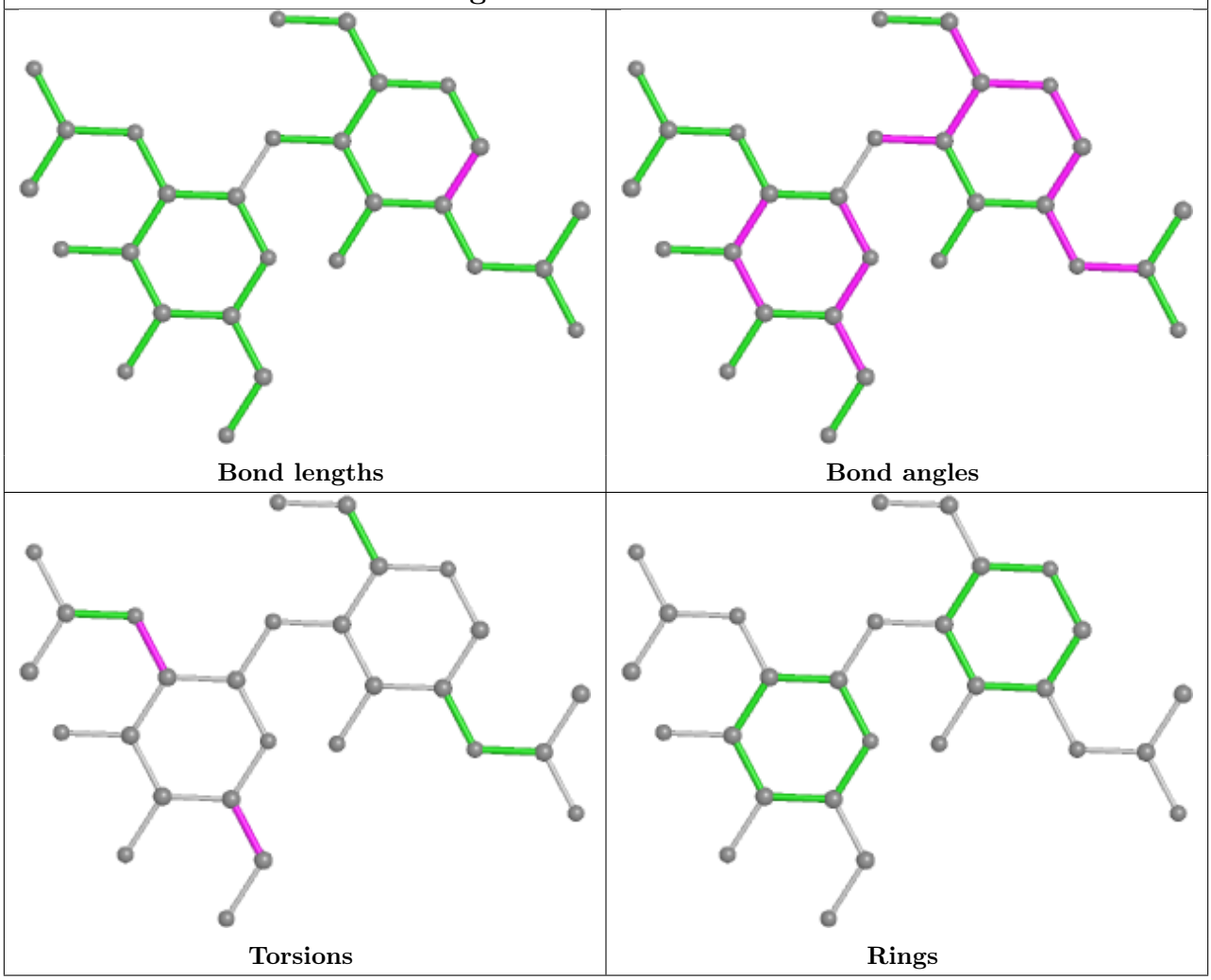
Oligosaccharide Chain e



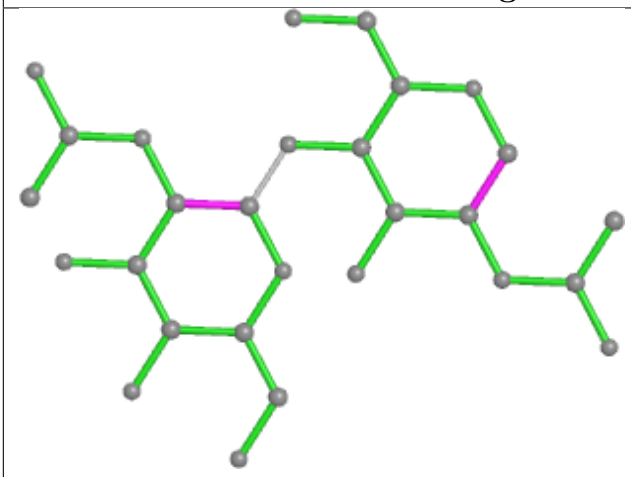
Oligosaccharide Chain g



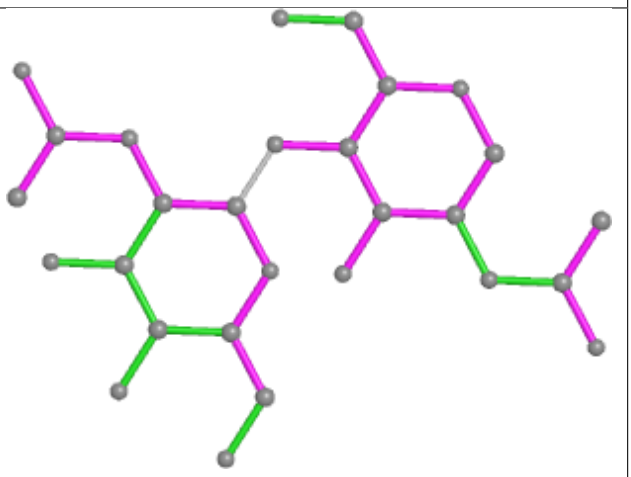
Oligosaccharide Chain Z



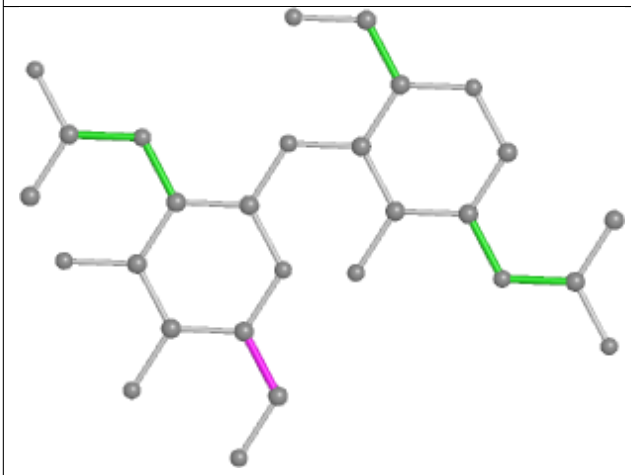
Oligosaccharide Chain a



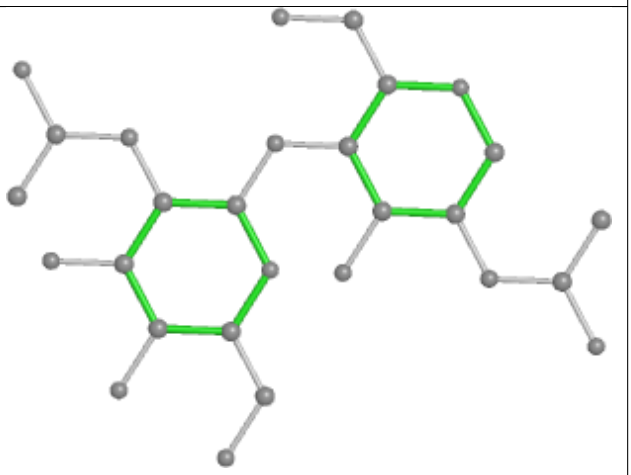
Bond lengths



Bond angles

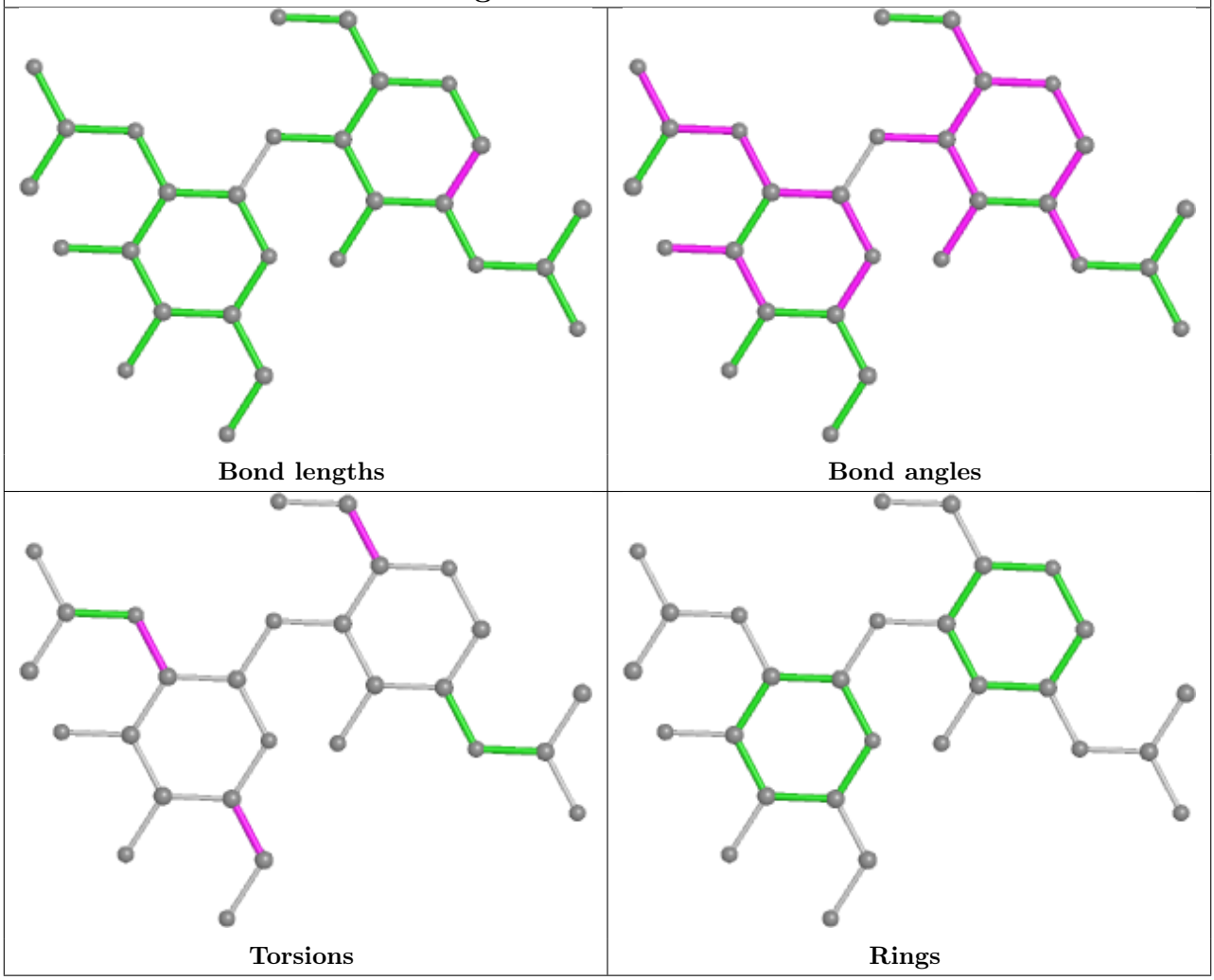


Torsions



Rings

Oligosaccharide Chain f



5.6 Ligand geometry (i)

7 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	$\#\|Z\| > 2$
7	NAG	I	405	1	14,14,15	1.58	2 (14%)	17,19,21	3.21	10 (58%)
7	NAG	Q	407	1	14,14,15	1.42	2 (14%)	17,19,21	3.34	9 (52%)
7	NAG	U	405	-	14,14,15	1.34	2 (14%)	17,19,21	2.90	9 (52%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
7	NAG	V	201	2	14,14,15	0.99	1 (7%)	17,19,21	2.64	7 (41%)
7	NAG	A	409	1	14,14,15	1.05	1 (7%)	17,19,21	3.28	8 (47%)
7	NAG	F	201	-	14,14,15	0.96	0	17,19,21	2.29	5 (29%)
7	NAG	M	405	1	14,14,15	1.03	1 (7%)	17,19,21	1.31	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
7	NAG	I	405	1	-	0/6/23/26	0/1/1/1
7	NAG	Q	407	1	-	4/6/23/26	0/1/1/1
7	NAG	U	405	-	-	2/6/23/26	0/1/1/1
7	NAG	V	201	2	-	2/6/23/26	0/1/1/1
7	NAG	A	409	1	-	4/6/23/26	0/1/1/1
7	NAG	F	201	-	-	2/6/23/26	0/1/1/1
7	NAG	M	405	1	-	3/6/23/26	0/1/1/1

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	I	405	NAG	C1-C2	4.30	1.58	1.52
7	Q	407	NAG	C4-C5	3.19	1.59	1.53
7	M	405	NAG	C1-C2	2.92	1.56	1.52
7	U	405	NAG	C3-C2	2.85	1.58	1.52
7	V	201	NAG	C1-C2	2.66	1.56	1.52

The worst 5 of 50 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	I	405	NAG	O5-C1-C2	-7.98	98.68	111.29
7	A	409	NAG	C1-O5-C5	7.85	122.83	112.19
7	Q	407	NAG	C1-O5-C5	6.90	121.54	112.19
7	V	201	NAG	C1-O5-C5	6.85	121.47	112.19
7	Q	407	NAG	O4-C4-C5	5.63	123.28	109.30

There are no chirality outliers.

5 of 17 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	409	NAG	C3-C2-N2-C7
7	Q	407	NAG	C3-C2-N2-C7
7	U	405	NAG	O5-C5-C6-O6
7	A	409	NAG	O5-C5-C6-O6
7	V	201	NAG	O5-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	I	405	NAG	2	0
7	U	405	NAG	5	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 (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	320/321 (99%)	-0.20	2 (0%)	89	86	68, 103, 128, 172	0
1	E	320/321 (99%)	-0.11	1 (0%)	94	91	57, 99, 124, 184	0
1	I	317/321 (98%)	-0.09	1 (0%)	94	91	57, 93, 117, 143	0
1	M	320/321 (99%)	-0.07	1 (0%)	94	91	60, 94, 118, 199	0
1	Q	320/321 (99%)	-0.14	0	100	100	57, 99, 129, 188	0
1	U	320/321 (99%)	-0.19	2 (0%)	89	86	67, 103, 132, 177	0
2	B	165/175 (94%)	-0.07	1 (0%)	89	86	58, 94, 129, 183	0
2	F	163/175 (93%)	-0.07	0	100	100	66, 104, 139, 175	0
2	J	164/175 (93%)	-0.07	4 (2%)	59	53	63, 104, 138, 178	0
2	N	163/175 (93%)	-0.12	2 (1%)	79	73	64, 102, 135, 163	0
2	R	166/175 (94%)	-0.06	1 (0%)	89	86	64, 103, 141, 185	0
2	V	164/175 (93%)	-0.11	1 (0%)	89	86	59, 94, 129, 171	0
3	C	219/226 (96%)	-0.14	0	100	100	70, 96, 142, 202	0
3	G	219/226 (96%)	-0.07	4 (1%)	68	62	77, 117, 170, 219	0
3	K	219/226 (96%)	0.79	43 (19%)	1	1	100, 175, 253, 286	0
3	O	219/226 (96%)	1.25	54 (24%)	0	0	111, 189, 304, 357	0
3	S	219/226 (96%)	0.01	5 (2%)	60	54	83, 117, 169, 217	0
3	Y	219/226 (96%)	-0.11	1 (0%)	91	88	70, 95, 145, 206	0
4	D	213/215 (99%)	-0.03	0	100	100	69, 96, 127, 156	0
4	H	213/215 (99%)	-0.00	1 (0%)	91	88	75, 115, 164, 197	0
4	L	213/215 (99%)	0.63	31 (14%)	2	3	99, 186, 239, 267	0
4	P	213/215 (99%)	0.87	46 (21%)	0	1	96, 205, 273, 317	0
4	T	213/215 (99%)	0.04	5 (2%)	60	54	76, 115, 170, 216	0
4	X	213/215 (99%)	0.01	3 (1%)	75	69	69, 95, 126, 156	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
All	All	5494/5622 (97%)	0.07	209 (3%) 40 36	57, 105, 215, 357	0

The worst 5 of 209 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	O	197	VAL	12.1
3	O	226	PRO	11.3
3	O	167	TRP	10.8
3	O	198	PRO	10.1
4	P	118	ILE	9.1

6.2 Non-standard residues in protein, DNA, RNA chains (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	NAG	f	2	14/15	0.57	0.27	152,179,197,197	0
7	NAG	F	201	14/15	0.58	0.27	155,185,196,198	0
6	NAG	a	1	14/15	0.73	0.20	179,195,202,203	0
7	NAG	V	201	14/15	0.76	0.30	103,112,121,121	0
6	NAG	a	2	14/15	0.83	0.18	151,173,185,190	0
6	NAG	Z	2	14/15	0.83	0.24	147,155,164,165	0
7	NAG	I	405	14/15	0.84	0.21	106,126,133,137	0
5	NAG	W	2	14/15	0.85	0.20	108,122,129,133	0
7	NAG	Q	407	14/15	0.88	0.26	85,101,107,107	0
7	NAG	A	409	14/15	0.88	0.19	89,104,118,124	0
7	NAG	M	405	14/15	0.89	0.24	101,119,136,138	0
7	NAG	U	405	14/15	0.89	0.20	84,97,121,129	0
5	NAG	b	1	14/15	0.90	0.18	120,124,127,128	0
5	NAG	g	1	14/15	0.91	0.19	101,108,117,119	0
5	NAG	g	2	14/15	0.91	0.22	102,121,142,146	0
5	NAG	W	1	14/15	0.91	0.17	105,108,112,113	0
5	NAG	c	1	14/15	0.92	0.16	85,91,92,92	0
6	NAG	Z	1	14/15	0.93	0.20	130,133,144,145	0
5	NAG	e	1	14/15	0.93	0.17	96,104,115,116	0
5	NAG	e	2	14/15	0.93	0.21	107,116,134,136	0
5	NAG	d	1	14/15	0.93	0.16	90,94,96,97	0
5	NAG	b	2	14/15	0.94	0.18	102,125,137,141	0

Continued on next page...

Continued from previous page...

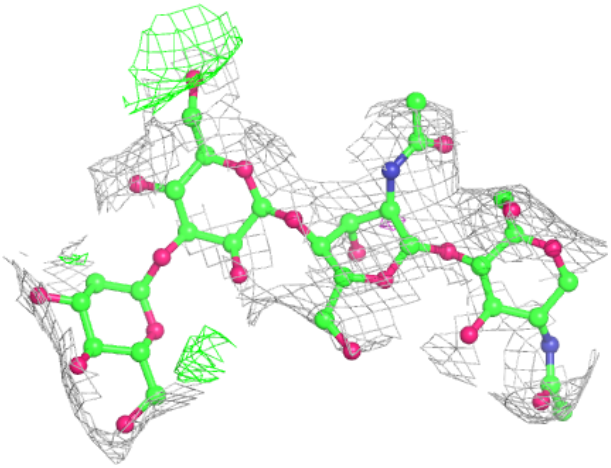
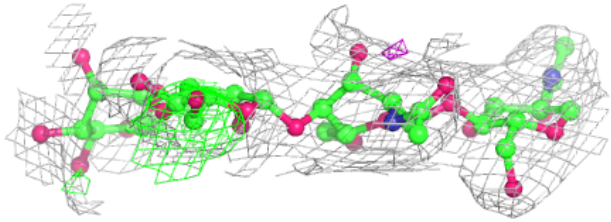
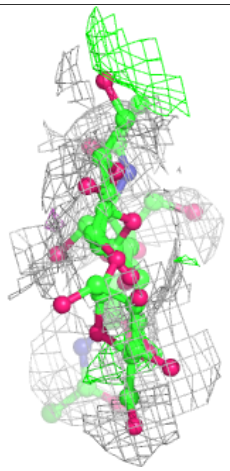
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	NAG	c	2	14/15	0.94	0.25	101,107,116,121	0
6	NAG	f	1	14/15	0.96	0.18	112,128,138,152	0
5	NAG	d	2	14/15	0.96	0.16	94,104,111,111	0

6.3 Carbohydrates (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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.

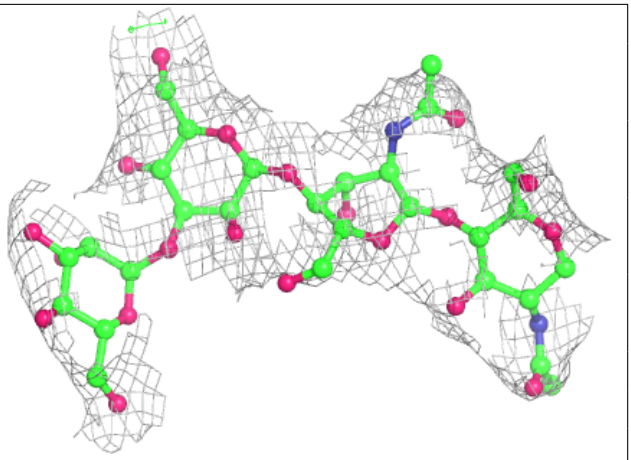
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	NAG	f	2	14/15	0.57	0.27	152,179,197,197	0
5	BMA	g	3	11/12	0.66	0.19	116,129,135,137	0
5	BMA	e	3	11/12	0.70	0.19	107,121,124,132	0
5	BMA	W	3	11/12	0.72	0.21	109,123,131,147	0
6	NAG	a	1	14/15	0.73	0.20	179,195,202,203	0
5	MAN	e	4	11/12	0.77	0.36	129,145,149,150	0
5	MAN	b	4	11/12	0.77	0.19	135,149,150,150	0
5	BMA	b	3	11/12	0.80	0.14	114,124,135,146	0
5	MAN	c	4	11/12	0.81	0.18	134,140,148,169	0
5	BMA	c	3	11/12	0.83	0.17	104,110,118,121	0
6	NAG	a	2	14/15	0.83	0.18	151,173,185,190	0
6	NAG	Z	2	14/15	0.83	0.24	147,155,164,165	0
5	MAN	d	4	11/12	0.84	0.20	141,147,157,173	0
5	NAG	W	2	14/15	0.85	0.20	108,122,129,133	0
5	MAN	W	4	11/12	0.85	0.23	147,149,156,160	0
5	NAG	b	1	14/15	0.90	0.18	120,124,127,128	0
5	NAG	g	1	14/15	0.91	0.19	101,108,117,119	0
5	NAG	g	2	14/15	0.91	0.22	102,121,142,146	0
5	NAG	W	1	14/15	0.91	0.17	105,108,112,113	0
5	MAN	g	4	11/12	0.91	0.14	125,138,145,146	0
5	NAG	c	1	14/15	0.92	0.16	85,91,92,92	0
6	NAG	Z	1	14/15	0.93	0.20	130,133,144,145	0
5	NAG	e	1	14/15	0.93	0.17	96,104,115,116	0
5	NAG	e	2	14/15	0.93	0.21	107,116,134,136	0
5	BMA	d	3	11/12	0.93	0.14	106,111,126,130	0
5	NAG	d	1	14/15	0.93	0.16	90,94,96,97	0
5	NAG	b	2	14/15	0.94	0.18	102,125,137,141	0
5	NAG	c	2	14/15	0.94	0.25	101,107,116,121	0
6	NAG	f	1	14/15	0.96	0.18	112,128,138,152	0
5	NAG	d	2	14/15	0.96	0.16	94,104,111,111	0

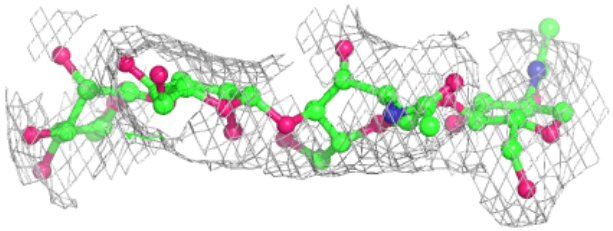
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

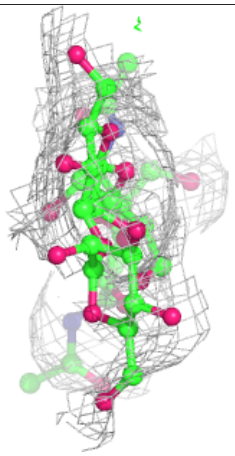
Electron density around Chain W: $2mF_o$-DF_c (at 0.7 rmsd) in gray mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)	
	

Electron density around Chain b:

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

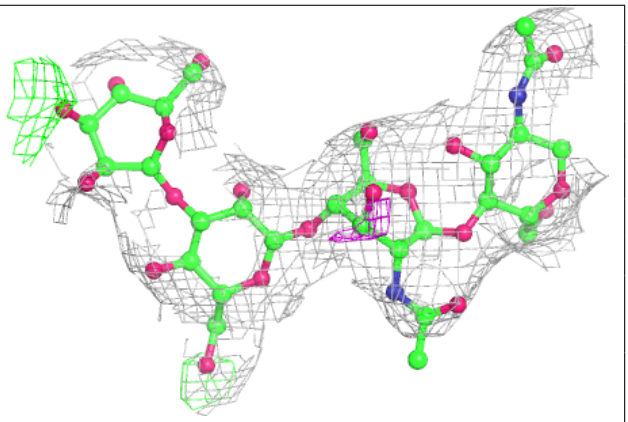


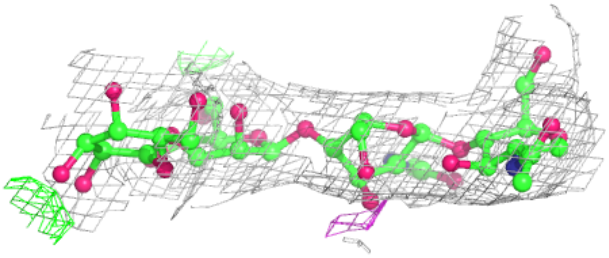


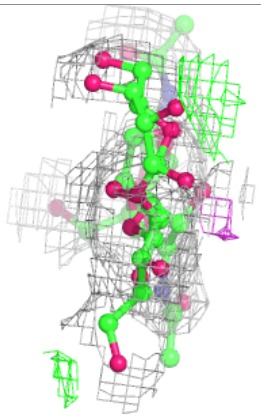


Electron density around Chain c:

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

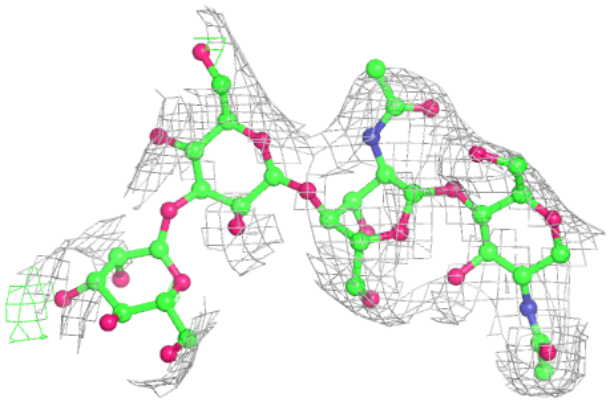


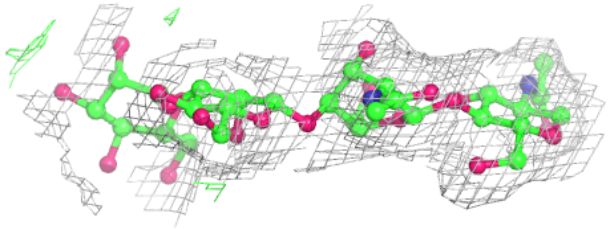


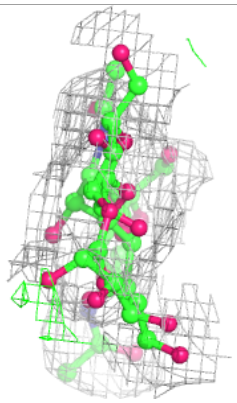


Electron density around Chain d:

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

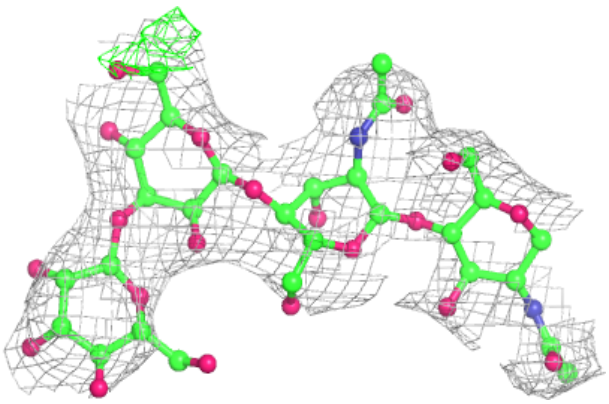


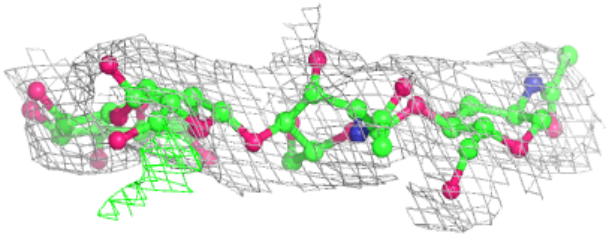


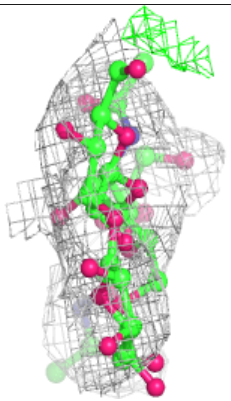


Electron density around Chain e:

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

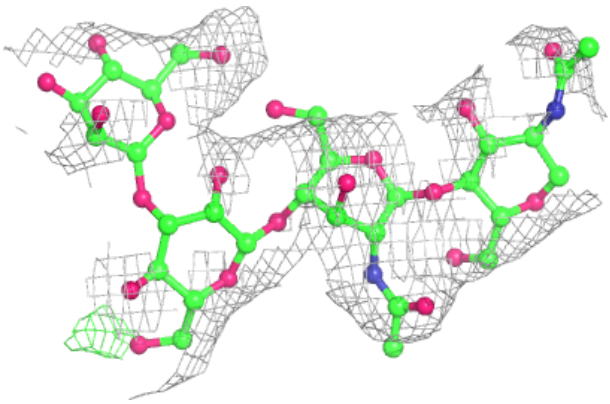


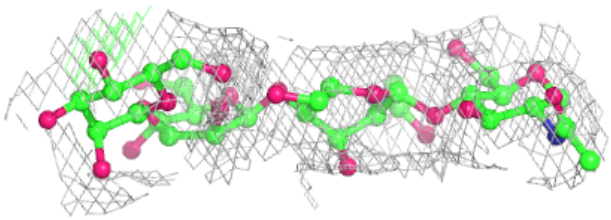


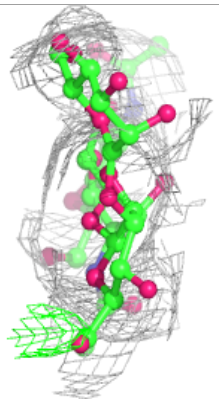


Electron density around Chain g:

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

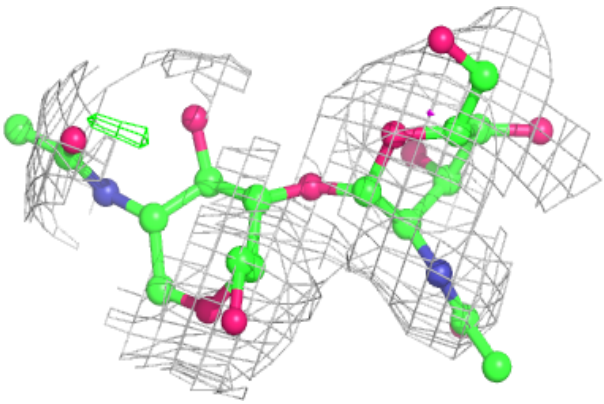


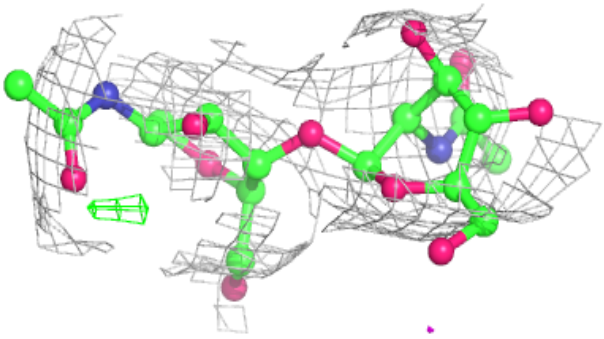


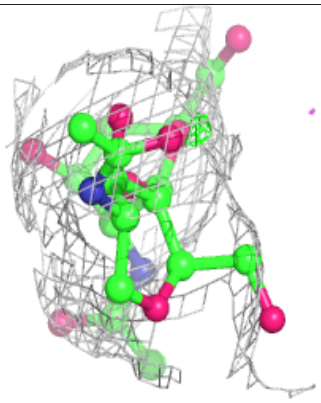


Electron density around Chain Z:

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

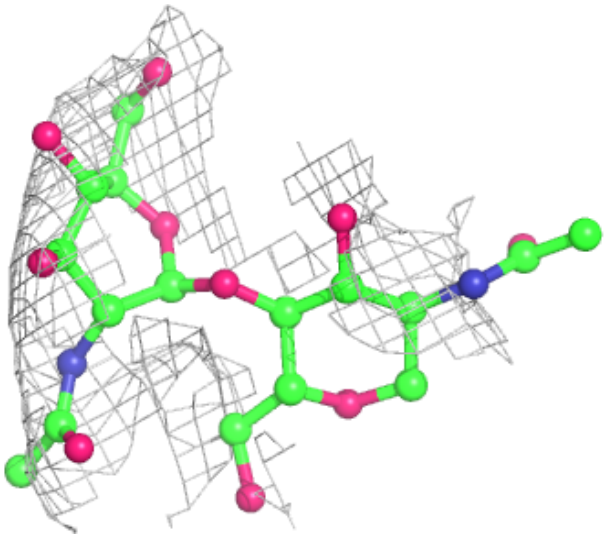


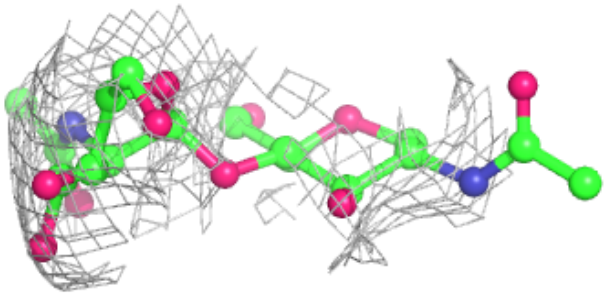


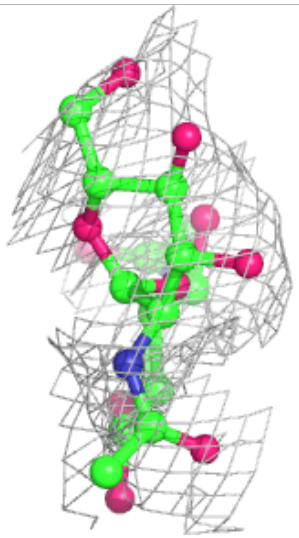


Electron density around Chain a:

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

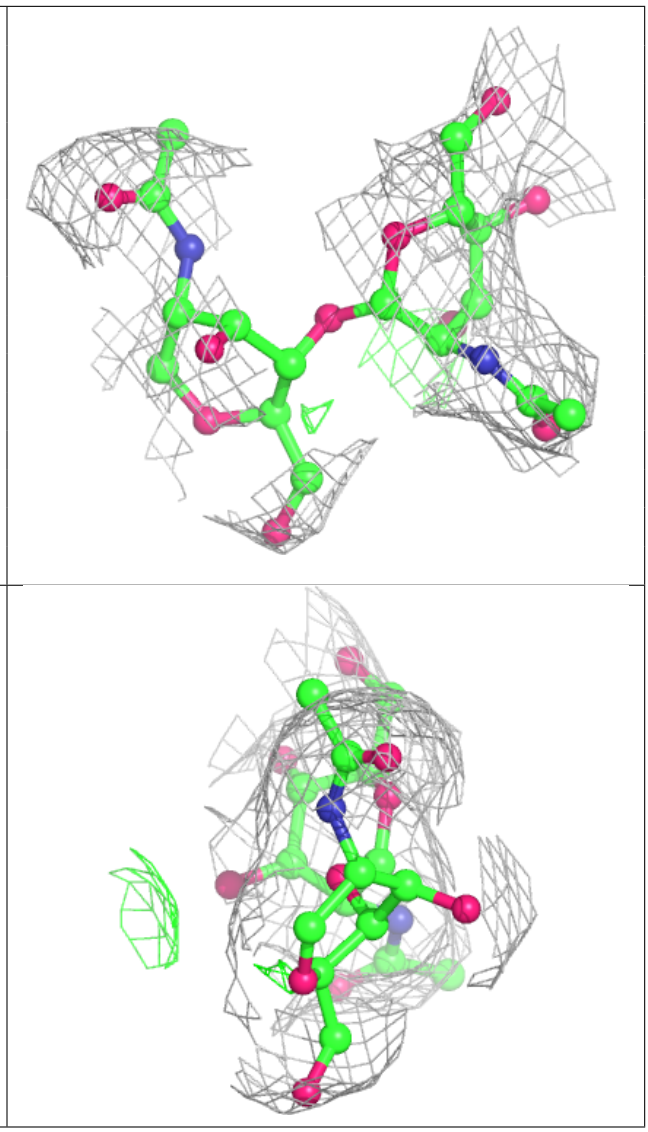






Electron density around Chain f:

$2mF_o$-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
7	NAG	F	201	14/15	0.58	0.27	155,185,196,198	0
7	NAG	V	201	14/15	0.76	0.30	103,112,121,121	0
7	NAG	I	405	14/15	0.84	0.21	106,126,133,137	0
7	NAG	Q	407	14/15	0.88	0.26	85,101,107,107	0
7	NAG	A	409	14/15	0.88	0.19	89,104,118,124	0
7	NAG	U	405	14/15	0.89	0.20	84,97,121,129	0
7	NAG	M	405	14/15	0.89	0.24	101,119,136,138	0

6.5 Other polymers (i)

There are no such residues in this entry.