wwPDB X-ray Structure Validation Summary Report (i)

Sep 17, 2023 – 11:28 PM EDT

PDB ID	:	4XNZ
Title	:	Crystal structure of broadly and potently neutralizing antibody VRC06B in complex with HIV-1 clade A/E strain 93TH057 gp120
Authors	:	Zhou, T.; Srivatsan, S.; Kwong, P.D.
Deposited on	:	2015-01-16
Resolution	:	3.39 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:

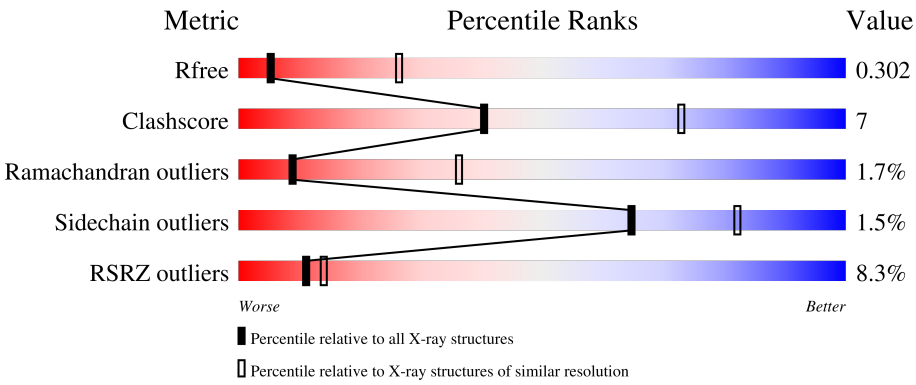
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.39 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	1691 (3.46-3.30)
Clashscore	141614	1762 (3.46-3.30)
Ramachandran outliers	138981	1732 (3.46-3.30)
Sidechain outliers	138945	1731 (3.46-3.30)
RSRZ outliers	127900	1635 (3.46-3.30)

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	353	9% 75% 22% •
1	D	353	7% 74% 19% • 7%
1	G	353	14% 75% 21% •
2	B	234	7% 79% 14% • 5%
2	E	234	9% 75% 18% • 6%

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Mol	Chain	Length	Quality of chain
2	H	234	8% 77% 17% 5%
3	C	209	3% 79% 18%
3	F	209	6% 76% 21%
3	L	209	3% 78% 21%
4	I	3	67% 33%
4	J	3	67% 33%
4	K	3	33% 67%

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
4	NAG	I	2	-	-	-	X
4	FUC	I	3	-	-	-	X
4	FUC	K	3	X	-	-	-
5	NAG	G	504	-	-	-	X
5	NAG	G	506	-	-	-	X

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 18134 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 Envelope glycoprotein gp160,Envelope glycoprotein gp160.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	G	340	2667	1674	463	509	21	0	0	0
1	A	341	2665	1669	463	511	22	0	0	0
1	D	330	2598	1634	452	492	20	0	0	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	124	GLY	-	linker	UNP Q0ED31
G	198	GLY	-	linker	UNP Q0ED31
G	318	GLY	-	linker	UNP Q0ED31
G	319	GLY	-	linker	UNP Q0ED31
G	320	SER	-	linker	UNP Q0ED31
G	321	GLY	-	linker	UNP Q0ED31
G	322	SER	-	linker	UNP Q0ED31
G	323	GLY	-	linker	UNP Q0ED31
A	124	GLY	-	linker	UNP Q0ED31
A	198	GLY	-	linker	UNP Q0ED31
A	318	GLY	-	linker	UNP Q0ED31
A	319	GLY	-	linker	UNP Q0ED31
A	320	SER	-	linker	UNP Q0ED31
A	321	GLY	-	linker	UNP Q0ED31
A	322	SER	-	linker	UNP Q0ED31
A	323	GLY	-	linker	UNP Q0ED31
D	124	GLY	-	linker	UNP Q0ED31
D	198	GLY	-	linker	UNP Q0ED31
D	318	GLY	-	linker	UNP Q0ED31
D	319	GLY	-	linker	UNP Q0ED31
D	320	SER	-	linker	UNP Q0ED31
D	321	GLY	-	linker	UNP Q0ED31
D	322	SER	-	linker	UNP Q0ED31

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Chain	Residue	Modelled	Actual	Comment	Reference
D	323	GLY	-	linker	UNP Q0ED31

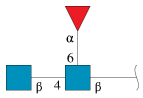
- Molecule 2 is a protein called HEAVY CHAIN OF ANTIBODY VRC06B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	H	222	1686	1070	293	313	10	0	0	0
2	B	222	1687	1071	294	312	10	0	0	0
2	E	220	1670	1062	291	307	10	0	0	0

- Molecule 3 is a protein called LIGHT CHAIN OF ANTIBODY VRC06B.

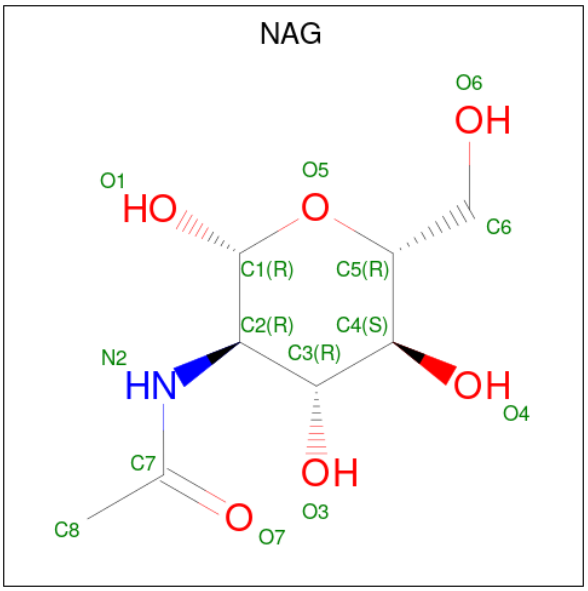
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	L	207	1604	1006	276	318	4	0	0	0
3	C	206	1596	999	275	318	4	0	0	0
3	F	206	1595	1001	275	315	4	0	0	0

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	I	3	38	22	2	14	0	0	0
4	J	3	38	22	2	14	0	0	0
4	K	3	38	22	2	14	0	0	0

- Molecule 5 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		
5	G	1	14	8	1	5	0	0
			Total	C	N	O		
5	G	1	14	8	1	5	0	0
			Total	C	N	O		
5	G	1	14	8	1	5	0	0
			Total	C	N	O		
5	G	1	14	8	1	5	0	0
			Total	C	N	O		
5	G	1	14	8	1	5	0	0
			Total	C	N	O		
5	G	1	14	8	1	5	0	0
			Total	C	N	O		
5	A	1	14	8	1	5	0	0
			Total	C	N	O		
5	A	1	14	8	1	5	0	0
			Total	C	N	O		
5	A	1	14	8	1	5	0	0
			Total	C	N	O		
5	A	1	14	8	1	5	0	0
			Total	C	N	O		
5	A	1	14	8	1	5	0	0
			Total	C	N	O		
5	A	1	14	8	1	5	0	0
			Total	C	N	O		
5	A	1	14	8	1	5	0	0
			Total	C	N	O		
5	D	1	14	8	1	5	0	0

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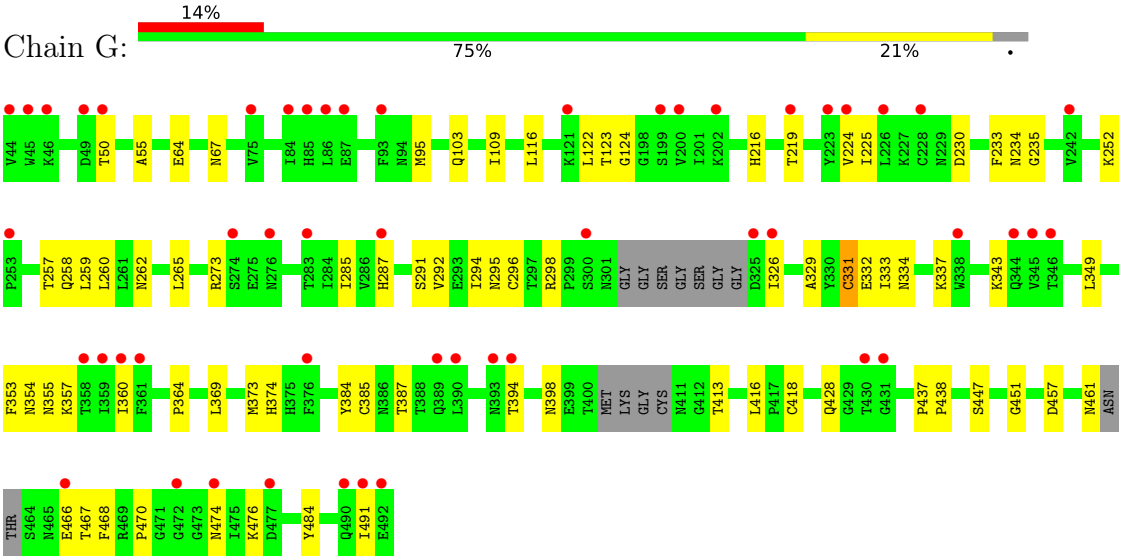
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	D	1	14	8	1	5	0	0
			Total	C	N	O		
5	D	1	14	8	1	5	0	0
			Total	C	N	O		
5	D	1	14	8	1	5	0	0
			Total	C	N	O		
5	D	1	14	8	1	5	0	0

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.

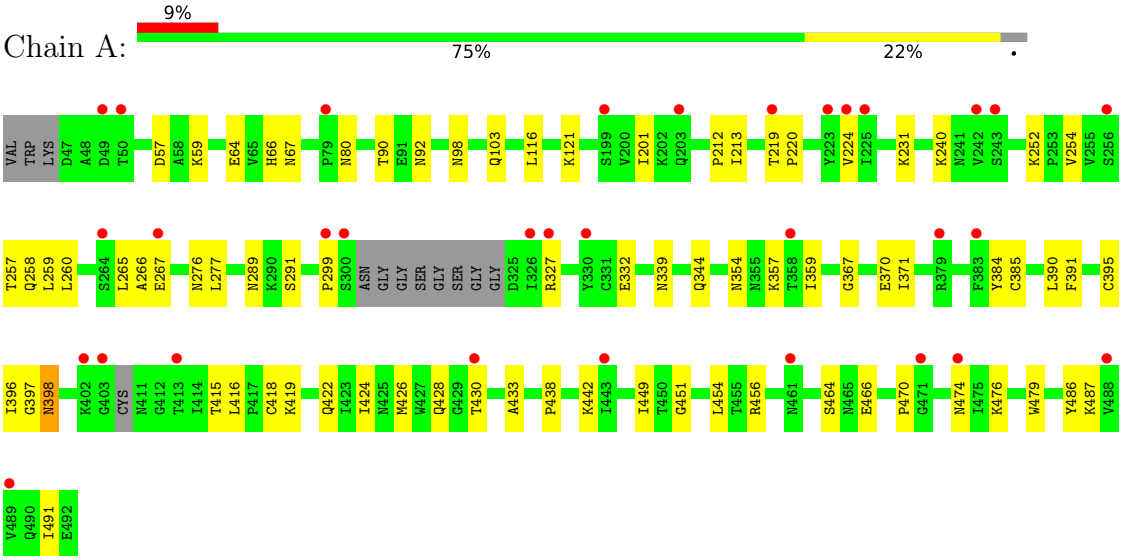
• Molecule 1: Envelope glycoprotein gp160,Envelope glycoprotein gp160

Chain G:



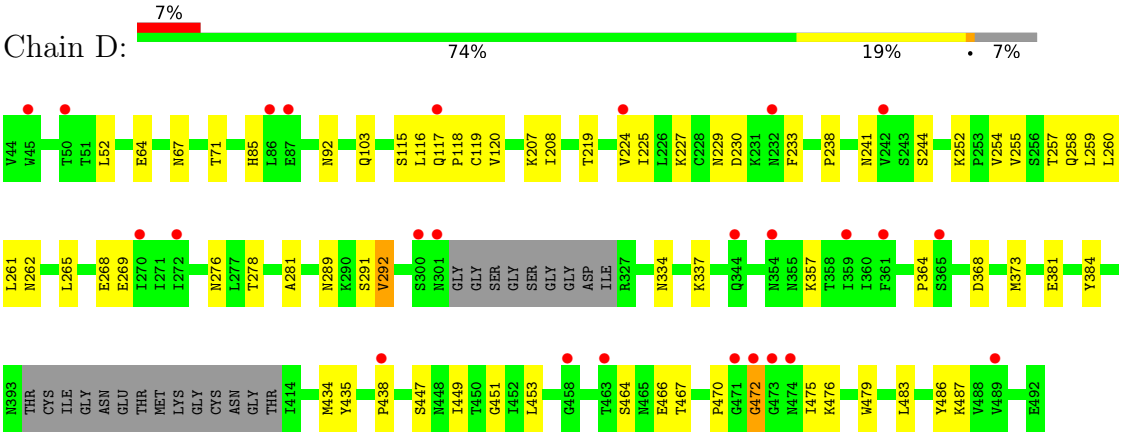
• Molecule 1: Envelope glycoprotein gp160,Envelope glycoprotein gp160

Chain A:



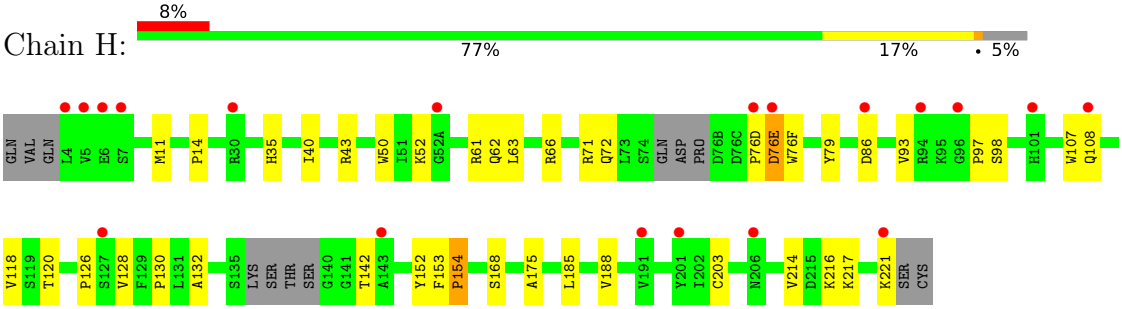
• Molecule 1: Envelope glycoprotein gp160,Envelope glycoprotein gp160

Chain D:



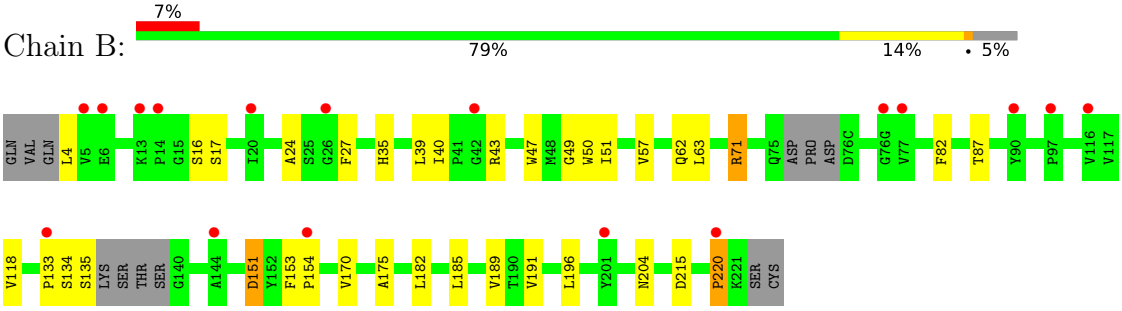
• Molecule 2: HEAVY CHAIN OF ANTIBODY VRC06B

Chain H:



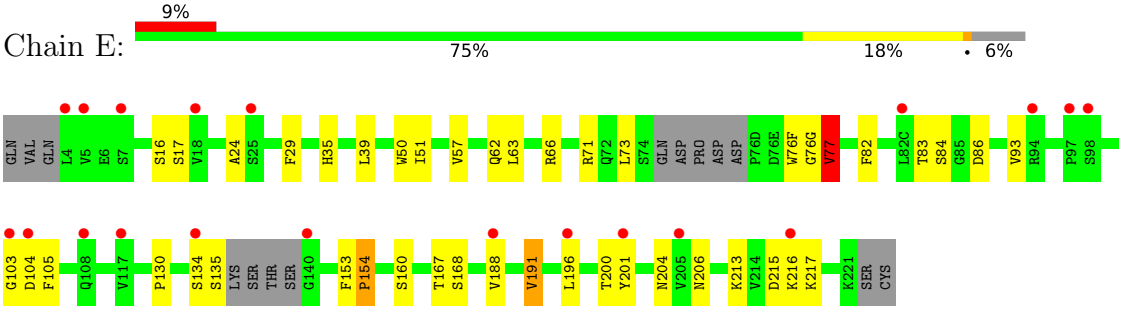
• Molecule 2: HEAVY CHAIN OF ANTIBODY VRC06B

Chain B:



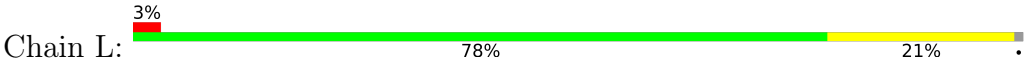
• Molecule 2: HEAVY CHAIN OF ANTIBODY VRC06B

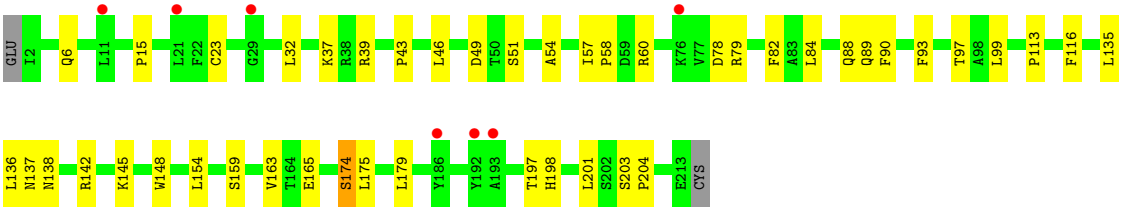
Chain E:



• Molecule 3: LIGHT CHAIN OF ANTIBODY VRC06B

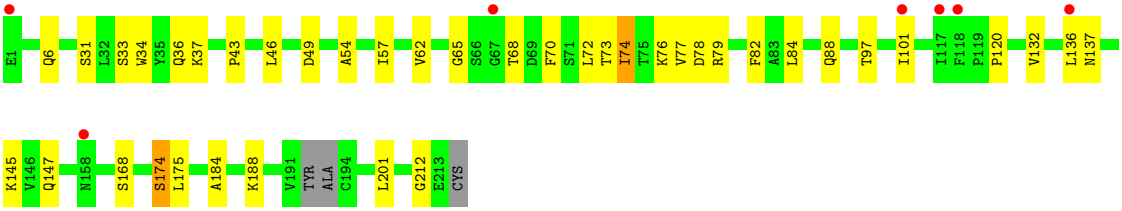
Chain L:





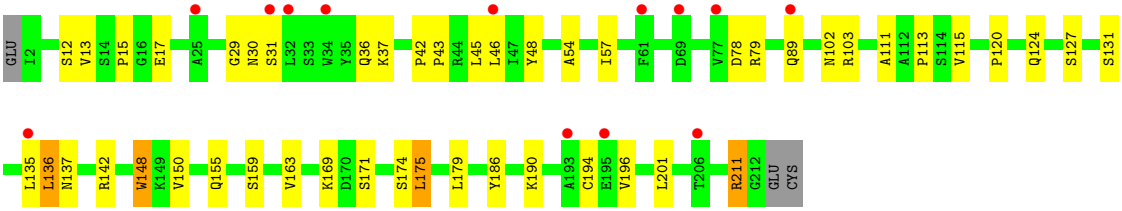
• Molecule 3: LIGHT CHAIN OF ANTIBODY VRC06B

Chain C:



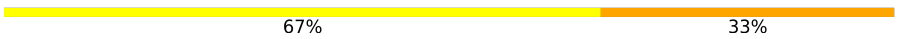
• Molecule 3: LIGHT CHAIN OF ANTIBODY VRC06B

Chain F:



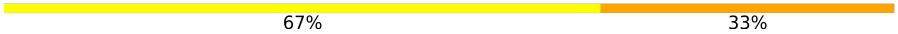
• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:



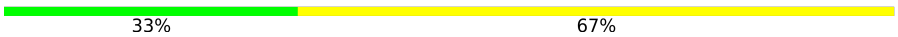
• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:



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

Chain K:



NAG1
NAG2
FUC3

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	68.31Å 189.44Å 219.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.90 – 3.39 39.90 – 3.39	Depositor EDS
% Data completeness (in resolution range)	86.0 (39.90-3.39) 82.0 (39.90-3.39)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.91 (at 3.40Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.244 , 0.301 0.247 , 0.302	Depositor DCC
R_{free} test set	1736 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å^2)	100.3	Xtriage
Anisotropy	0.527	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.25 , 63.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	18134	wwPDB-VP
Average B, all atoms (Å^2)	144.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.46% 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: NAG, FUC

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	0.21	0/2719	0.39	0/3689
1	D	0.20	0/2654	0.37	0/3603
1	G	0.20	0/2722	0.38	0/3694
2	B	0.20	0/1735	0.37	0/2358
2	E	0.21	0/1718	0.41	0/2334
2	H	0.21	0/1734	0.38	0/2357
3	C	0.21	0/1628	0.37	0/2203
3	F	0.21	0/1629	0.38	0/2207
3	L	0.21	0/1638	0.38	0/2219
All	All	0.21	0/18177	0.38	0/24664

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	2665	0	2601	44	0
1	D	2598	0	2540	37	0
1	G	2667	0	2601	42	0
2	B	1687	0	1638	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	1670	0	1627	23	0
2	H	1686	0	1634	22	0
3	C	1596	0	1553	19	1
3	F	1595	0	1553	29	0
3	L	1604	0	1559	23	0
4	I	38	0	34	0	1
4	J	38	0	34	1	0
4	K	38	0	34	1	0
5	A	98	0	91	1	0
5	D	70	0	65	2	0
5	G	84	0	78	0	0
All	All	18134	0	17642	256	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

The worst 5 of 256 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:E:76(G):GLY:HA2	2:E:77:VAL:HB	1.70	0.72
2:E:62:GLN:HG2	2:E:63:LEU:HD12	1.76	0.67
2:H:132:ALA:HB1	2:H:221:LYS:H	1.60	0.66
3:C:74:ILE:HD11	3:C:77:VAL:HG22	1.78	0.66
1:G:374:HIS:HB3	1:G:385:CYS:HB2	1.79	0.65

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:68:THR:OG1	4:I:3:FUC:O4[3_545]	1.86	0.34

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	335/353 (95%)	311 (93%)	18 (5%)	6 (2%)	8	35
1	D	324/353 (92%)	309 (95%)	12 (4%)	3 (1%)	17	51
1	G	332/353 (94%)	306 (92%)	23 (7%)	3 (1%)	17	51
2	B	216/234 (92%)	195 (90%)	19 (9%)	2 (1%)	17	51
2	E	214/234 (92%)	193 (90%)	16 (8%)	5 (2%)	6	31
2	H	216/234 (92%)	194 (90%)	17 (8%)	5 (2%)	6	31
3	C	202/209 (97%)	178 (88%)	19 (9%)	5 (2%)	5	29
3	F	204/209 (98%)	176 (86%)	24 (12%)	4 (2%)	7	33
3	L	205/209 (98%)	176 (86%)	24 (12%)	5 (2%)	6	30
All	All	2248/2388 (94%)	2038 (91%)	172 (8%)	38 (2%)	9	36

5 of 38 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	354	ASN
2	H	76(E)	ASP
1	A	354	ASN
1	A	396	ILE
2	E	76(F)	TRP

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	304/311 (98%)	302 (99%)	2 (1%)	84	92
1	D	296/311 (95%)	291 (98%)	5 (2%)	60	80
1	G	304/311 (98%)	301 (99%)	3 (1%)	76	87
2	B	186/198 (94%)	183 (98%)	3 (2%)	62	81
2	E	184/198 (93%)	178 (97%)	6 (3%)	38	67
2	H	186/198 (94%)	184 (99%)	2 (1%)	73	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	180/182 (99%)	177 (98%)	3 (2%)	60	80
3	F	179/182 (98%)	176 (98%)	3 (2%)	60	80
3	L	180/182 (99%)	177 (98%)	3 (2%)	60	80
All	All	1999/2073 (96%)	1969 (98%)	30 (2%)	65	82

5 of 30 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	84	LEU
3	F	136	LEU
1	D	208	ILE
3	F	211	ARG
2	E	167	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
3	F	30	ASN
3	F	89	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

9 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	$\#\|Z\| > 2$
4	NAG	I	1	3,4	14,14,15	0.58	0	17,19,21	0.78	1 (5%)
4	NAG	I	2	4	14,14,15	0.34	0	17,19,21	0.67	1 (5%)
4	FUC	I	3	4	10,10,11	0.43	0	14,14,16	1.46	2 (14%)
4	NAG	J	1	3,4	14,14,15	0.27	0	17,19,21	0.70	1 (5%)
4	NAG	J	2	4	14,14,15	0.27	0	17,19,21	0.31	0
4	FUC	J	3	4	10,10,11	0.91	1 (10%)	14,14,16	1.41	2 (14%)
4	NAG	K	1	3,4	14,14,15	0.25	0	17,19,21	0.51	0
4	NAG	K	2	4	14,14,15	0.33	0	17,19,21	0.65	0
4	FUC	K	3	4	10,10,11	0.73	0	14,14,16	0.97	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
4	NAG	I	1	3,4	-	0/6/23/26	0/1/1/1
4	NAG	I	2	4	-	4/6/23/26	0/1/1/1
4	FUC	I	3	4	-	-	0/1/1/1
4	NAG	J	1	3,4	-	0/6/23/26	0/1/1/1
4	NAG	J	2	4	-	2/6/23/26	0/1/1/1
4	FUC	J	3	4	-	-	0/1/1/1
4	NAG	K	1	3,4	-	2/6/23/26	0/1/1/1
4	NAG	K	2	4	-	3/6/23/26	0/1/1/1
4	FUC	K	3	4	1/1/4/5	-	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	J	3	FUC	O5-C1	-2.26	1.40	1.43

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	J	3	FUC	C1-O5-C5	3.34	120.34	112.78
4	I	3	FUC	C3-C4-C5	2.83	114.18	109.77
4	I	2	NAG	C1-O5-C5	2.33	115.35	112.19
4	J	1	NAG	C1-O5-C5	2.33	115.35	112.19
4	I	3	FUC	O5-C1-C2	-2.20	107.37	110.77

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	K	3	FUC	C1

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	J	2	NAG	O5-C5-C6-O6
4	K	1	NAG	O5-C5-C6-O6
4	J	2	NAG	C4-C5-C6-O6
4	K	2	NAG	O5-C5-C6-O6
4	K	1	NAG	C4-C5-C6-O6

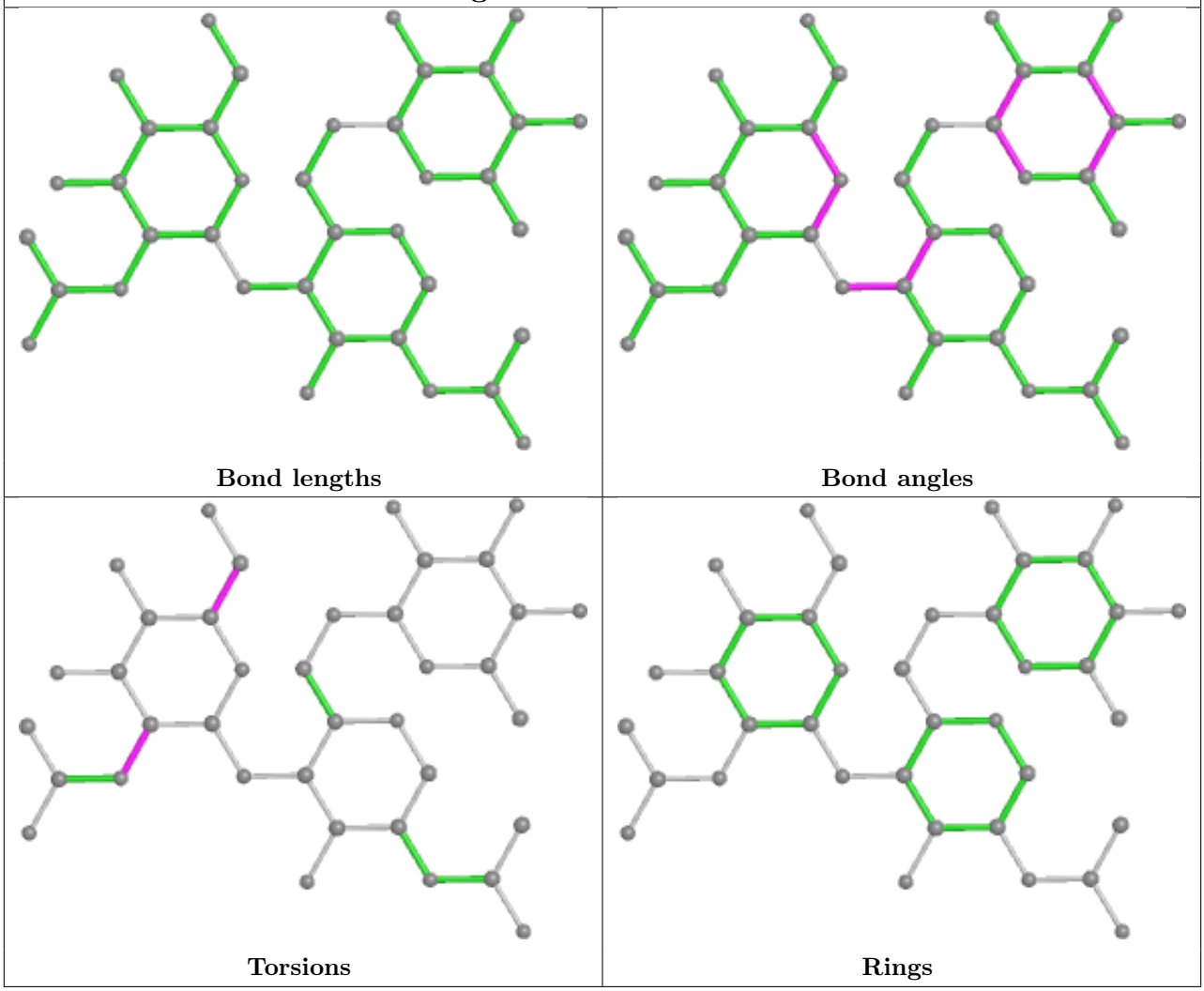
There are no ring outliers.

5 monomers are involved in 3 short contacts:

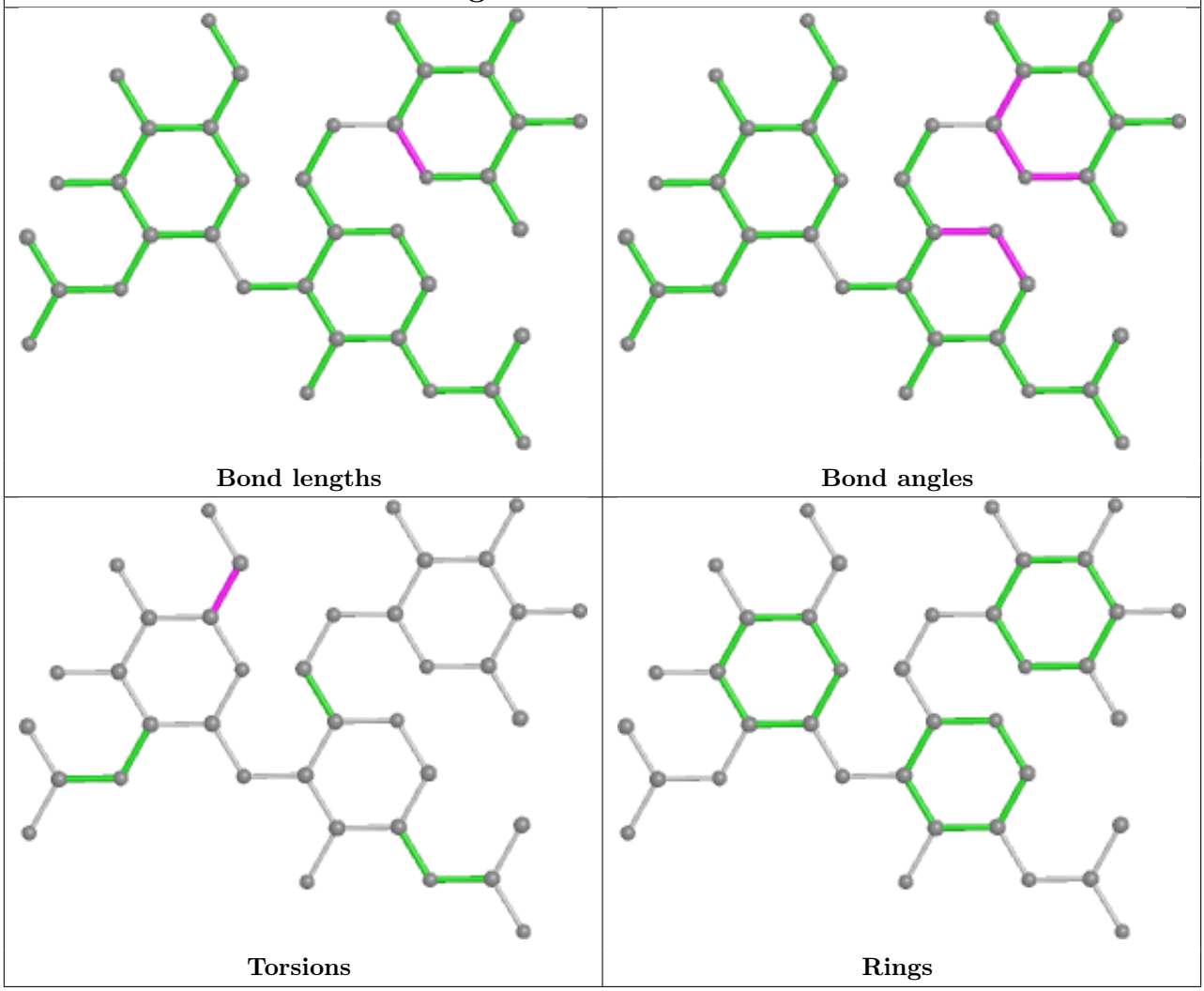
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	K	3	FUC	1	0
4	J	1	NAG	1	0
4	I	3	FUC	0	1
4	K	2	NAG	1	0
4	J	2	NAG	1	0

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

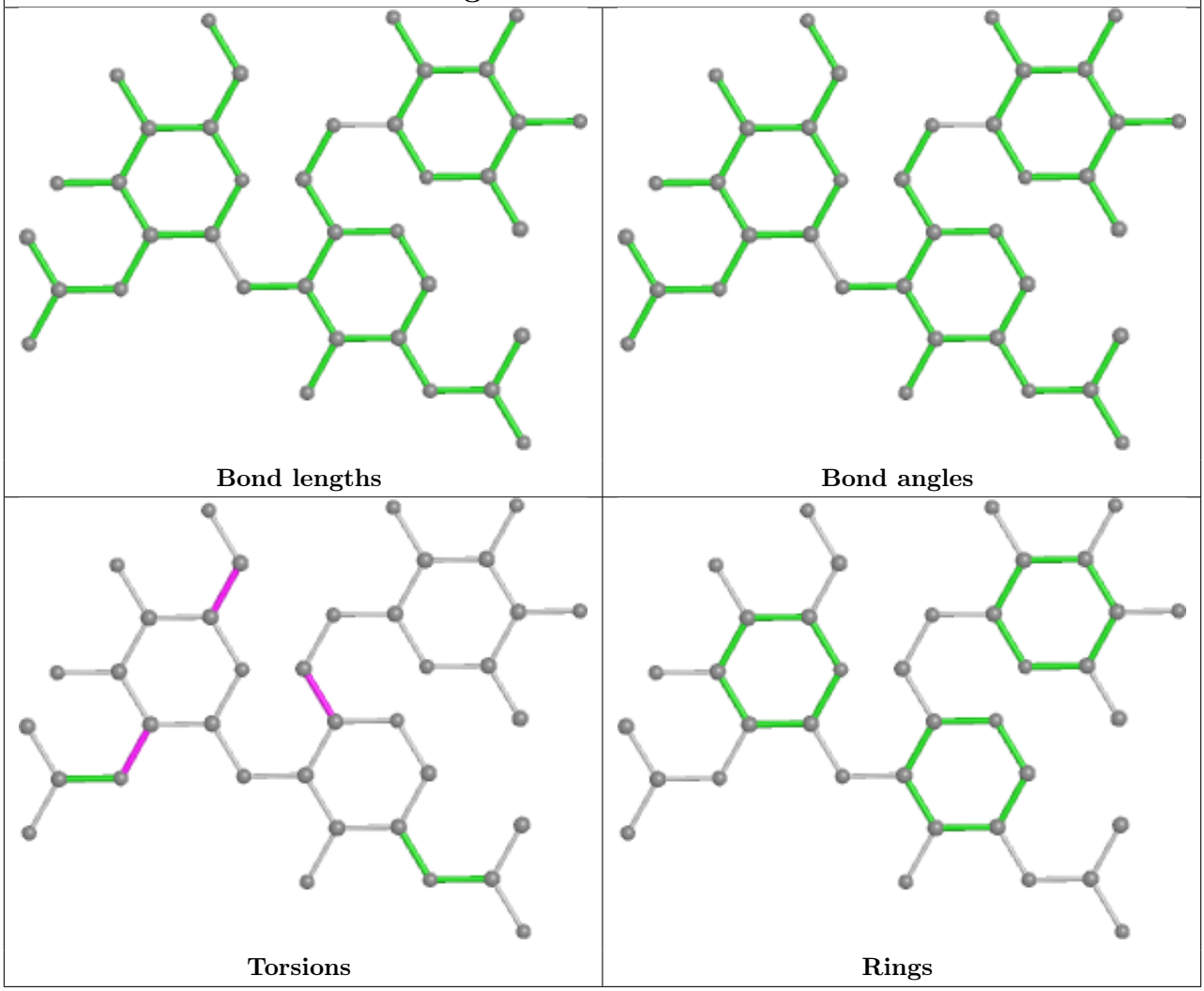
Oligosaccharide Chain I



Oligosaccharide Chain J



Oligosaccharide Chain K



5.6 Ligand geometry (i)

18 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	$\#\|Z\| > 2$
5	NAG	A	502	1	14,14,15	0.31	0	17,19,21	0.45	0
5	NAG	G	502	1	14,14,15	0.23	0	17,19,21	0.46	0
5	NAG	G	501	1	14,14,15	0.20	0	17,19,21	0.38	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	NAG	A	506	1	14,14,15	0.26	0	17,19,21	0.44	0
5	NAG	D	502	1	14,14,15	0.22	0	17,19,21	0.44	0
5	NAG	D	503	1	14,14,15	0.24	0	17,19,21	0.42	0
5	NAG	A	503	1	14,14,15	0.25	0	17,19,21	0.42	0
5	NAG	A	505	1	14,14,15	0.19	0	17,19,21	0.44	0
5	NAG	G	504	1	14,14,15	0.24	0	17,19,21	0.36	0
5	NAG	A	501	1	14,14,15	0.19	0	17,19,21	0.42	0
5	NAG	D	505	1	14,14,15	0.29	0	17,19,21	0.47	0
5	NAG	D	504	1	14,14,15	0.28	0	17,19,21	0.43	0
5	NAG	G	506	1	14,14,15	0.24	0	17,19,21	0.46	0
5	NAG	G	505	1	14,14,15	0.27	0	17,19,21	0.41	0
5	NAG	D	501	1	14,14,15	0.20	0	17,19,21	0.39	0
5	NAG	G	503	1	14,14,15	0.23	0	17,19,21	0.39	0
5	NAG	A	507	1	14,14,15	0.23	0	17,19,21	0.40	0
5	NAG	A	504	1	14,14,15	0.24	0	17,19,21	0.44	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
5	NAG	A	502	1	-	0/6/23/26	0/1/1/1
5	NAG	G	502	1	-	2/6/23/26	0/1/1/1
5	NAG	G	501	1	-	2/6/23/26	0/1/1/1
5	NAG	A	506	1	-	4/6/23/26	0/1/1/1
5	NAG	D	502	1	-	2/6/23/26	0/1/1/1
5	NAG	D	503	1	-	1/6/23/26	0/1/1/1
5	NAG	A	503	1	-	2/6/23/26	0/1/1/1
5	NAG	A	505	1	-	0/6/23/26	0/1/1/1
5	NAG	G	504	1	-	2/6/23/26	0/1/1/1
5	NAG	A	501	1	-	2/6/23/26	0/1/1/1
5	NAG	D	505	1	-	2/6/23/26	0/1/1/1
5	NAG	D	504	1	-	2/6/23/26	0/1/1/1
5	NAG	G	506	1	-	4/6/23/26	0/1/1/1
5	NAG	G	505	1	-	3/6/23/26	0/1/1/1
5	NAG	D	501	1	-	2/6/23/26	0/1/1/1
5	NAG	G	503	1	-	2/6/23/26	0/1/1/1
5	NAG	A	507	1	-	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	A	504	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 38 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	G	502	NAG	O5-C5-C6-O6
5	A	504	NAG	O5-C5-C6-O6
5	A	503	NAG	O5-C5-C6-O6
5	D	505	NAG	O5-C5-C6-O6
5	A	501	NAG	O5-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	502	NAG	1	0
5	D	503	NAG	1	0
5	A	505	NAG	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (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	341/353 (96%)	0.60	32 (9%)	8	11	86, 142, 228, 331	0
1	D	330/353 (93%)	0.45	25 (7%)	13	17	92, 148, 217, 300	0
1	G	340/353 (96%)	0.68	51 (15%)	2	3	93, 151, 224, 305	0
2	B	222/234 (94%)	0.37	17 (7%)	13	16	77, 145, 225, 262	0
2	E	220/234 (94%)	0.40	20 (9%)	9	12	86, 128, 221, 268	0
2	H	222/234 (94%)	0.36	19 (8%)	10	13	82, 133, 224, 285	0
3	C	206/209 (98%)	0.20	7 (3%)	45	48	69, 140, 212, 269	0
3	F	206/209 (98%)	0.45	13 (6%)	20	23	95, 143, 202, 265	0
3	L	207/209 (99%)	0.10	7 (3%)	45	48	67, 114, 173, 230	0
All	All	2294/2388 (96%)	0.43	191 (8%)	11	14	67, 141, 219, 331	0

The worst 5 of 191 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	4	LEU	7.8
1	A	224	VAL	7.0
2	E	134	SER	5.8
1	G	430	THR	5.2
1	A	300	SER	4.7

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,

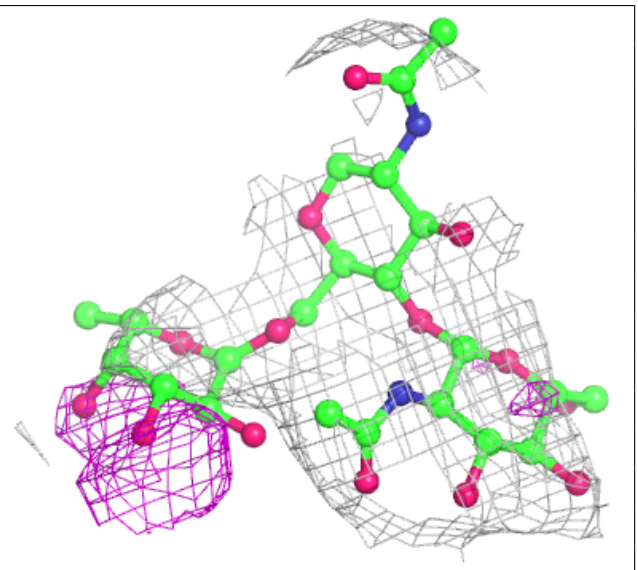
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

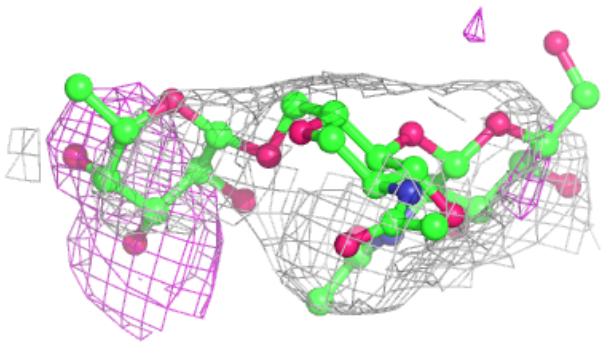
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	FUC	I	3	10/11	0.76	0.82	139,161,170,180	0
4	NAG	I	2	14/15	0.77	0.40	145,151,158,159	0
4	NAG	J	2	14/15	0.78	0.29	164,167,172,174	0
4	NAG	K	1	14/15	0.81	0.26	164,175,184,199	0
4	NAG	I	1	14/15	0.87	0.19	100,114,129,133	0
4	FUC	K	3	10/11	0.87	0.26	159,165,169,173	0
4	NAG	K	2	14/15	0.88	0.42	217,223,230,232	0
4	NAG	J	1	14/15	0.90	0.28	124,140,151,155	0
4	FUC	J	3	10/11	0.94	0.16	156,161,162,162	0

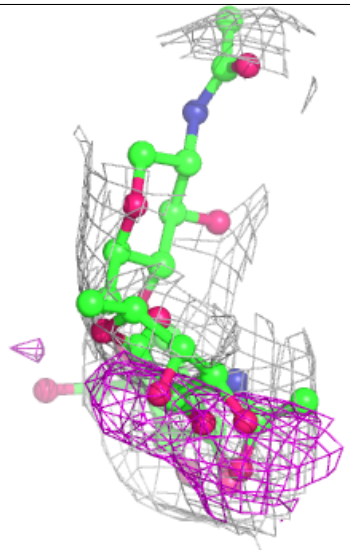
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain I:

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

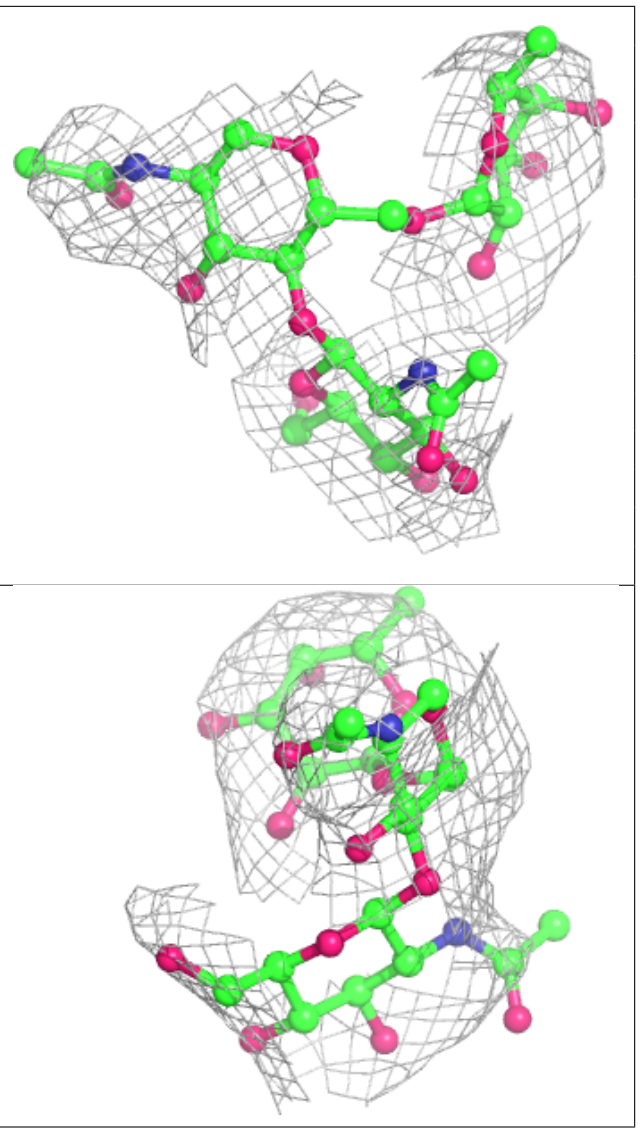






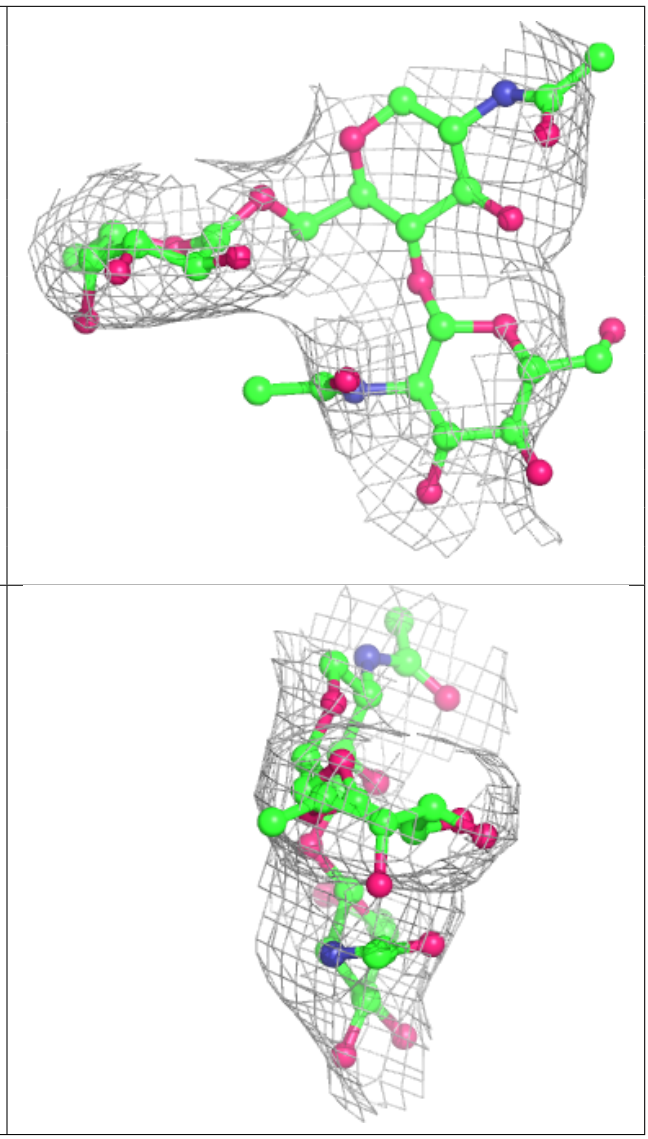
Electron density around Chain J:

$2mF_o$-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)



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
5	NAG	G	506	14/15	0.68	0.49	130,149,155,160	0
5	NAG	G	504	14/15	0.74	0.41	152,171,173,176	0
5	NAG	A	507	14/15	0.74	0.23	121,135,143,145	0
5	NAG	D	505	14/15	0.79	0.32	120,132,135,137	0
5	NAG	G	501	14/15	0.81	0.27	113,121,124,125	0
5	NAG	D	503	14/15	0.82	0.26	137,156,159,161	0
5	NAG	A	504	14/15	0.82	0.24	136,151,170,175	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	NAG	D	504	14/15	0.85	0.24	121,127,131,132	0
5	NAG	D	501	14/15	0.85	0.47	138,144,146,147	0
5	NAG	A	506	14/15	0.86	0.25	100,109,113,114	0
5	NAG	A	502	14/15	0.86	0.37	143,155,165,167	0
5	NAG	A	505	14/15	0.87	0.42	120,133,138,145	0
5	NAG	A	501	14/15	0.88	0.34	123,134,138,138	0
5	NAG	G	502	14/15	0.89	0.34	131,144,150,152	0
5	NAG	D	502	14/15	0.90	0.24	113,119,136,139	0
5	NAG	G	503	14/15	0.90	0.27	112,124,129,131	0
5	NAG	G	505	14/15	0.94	0.20	107,116,125,126	0
5	NAG	A	503	14/15	0.95	0.14	93,98,100,105	0

6.5 Other polymers (i)

There are no such residues in this entry.