wwPDB X-ray Structure Validation Summary Report (i)

Oct 10, 2021 – 07:40 PM EDT

PDB ID	:	3CSY
Title	:	Crystal structure of the trimeric prefusion Ebola virus glycoprotein in complex with a neutralizing antibody from a human survivor
Authors	:	Lee, J.E.; Fusco, M.L.; Hessell, A.J.; Oswald, W.B.; Burton, D.R.; Saphire, E.O.
Deposited on	:	2008-04-10
Resolution	:	3.40 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 following versions of software and data (see references (i)) were used in the production of this report:

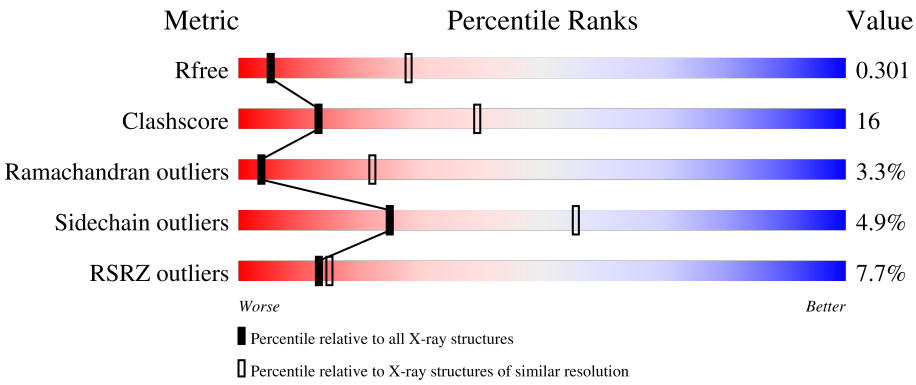
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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 3.40 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	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

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	226	10% 63% 33% ·
1	C	226	4% 67% 30% ·
1	E	226	4% 70% 26% ·
1	G	226	10% 69% 27% ·
2	B	217	16% 69% 27% ·

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Mol	Chain	Length	Quality of chain
2	D	217	10% 76% 21%
2	F	217	7% 71% 27%
2	H	217	21% 69% 28%
3	I	334	2% 43% 25% 29%
3	K	334	3% 44% 22% 31%
3	M	334	2% 42% 22% 31%
3	O	334	5% 40% 23% 33%
4	J	131	2% 47% 25% 25%
4	L	131	3% 42% 27% 29%
4	N	131	4% 47% 24% 27%
4	P	131	3% 52% 18% 29%
5	Q	3	67% 33%
5	U	3	100%
5	W	3	33% 67%
6	R	5	40% 60%
6	V	5	60% 40%
7	S	2	50% 50%
8	T	6	83% 17%
8	X	6	83% 17%

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
6	MAN	R	5	-	-	-	X
8	NAG	T	5	-	-	-	X

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 23539 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 Fab KZ52 heavy chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	226	1687	1059	286	334	4	4	0	0	0
1	C	226	1687	1059	286	334	4	4	0	0	0
1	E	226	1687	1059	286	334	4	4	0	0	0
1	G	226	1687	1059	286	334	4	4	0	0	0

- Molecule 2 is a protein called Fab KZ52 light chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
2	B	217	1682	1056	281	340	4	1	0	0	0
2	D	217	1682	1056	281	340	4	1	0	0	0
2	F	217	1682	1056	281	340	4	1	0	0	0
2	H	217	1682	1056	281	340	4	1	0	0	0

- Molecule 3 is a protein called Envelope glycoprotein GP1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	I	236	1707	1085	293	325	4	0	0	0
3	K	232	1687	1073	289	321	4	0	0	0
3	M	230	1677	1067	287	319	4	0	0	0
3	O	225	1651	1052	282	313	4	0	0	0

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	16	TYR	-	expression tag	UNP Q05320
I	17	PRO	-	expression tag	UNP Q05320
I	18	TYR	-	expression tag	UNP Q05320
I	19	ASP	-	expression tag	UNP Q05320
I	20	VAL	-	expression tag	UNP Q05320
I	21	PRO	-	expression tag	UNP Q05320
I	22	ASP	-	expression tag	UNP Q05320
I	23	TYR	-	expression tag	UNP Q05320
I	24	ALA	-	expression tag	UNP Q05320
I	25	ILE	-	expression tag	UNP Q05320
I	26	GLU	-	expression tag	UNP Q05320
I	27	GLY	-	expression tag	UNP Q05320
I	28	ARG	-	expression tag	UNP Q05320
I	29	GLY	-	expression tag	UNP Q05320
I	30	ALA	-	expression tag	UNP Q05320
I	31	ARG	-	expression tag	UNP Q05320
I	42	VAL	THR	engineered mutation	UNP Q05320
I	230	VAL	THR	engineered mutation	UNP Q05320
K	16	TYR	-	expression tag	UNP Q05320
K	17	PRO	-	expression tag	UNP Q05320
K	18	TYR	-	expression tag	UNP Q05320
K	19	ASP	-	expression tag	UNP Q05320
K	20	VAL	-	expression tag	UNP Q05320
K	21	PRO	-	expression tag	UNP Q05320
K	22	ASP	-	expression tag	UNP Q05320
K	23	TYR	-	expression tag	UNP Q05320
K	24	ALA	-	expression tag	UNP Q05320
K	25	ILE	-	expression tag	UNP Q05320
K	26	GLU	-	expression tag	UNP Q05320
K	27	GLY	-	expression tag	UNP Q05320
K	28	ARG	-	expression tag	UNP Q05320
K	29	GLY	-	expression tag	UNP Q05320
K	30	ALA	-	expression tag	UNP Q05320
K	31	ARG	-	expression tag	UNP Q05320
K	42	VAL	THR	engineered mutation	UNP Q05320
K	230	VAL	THR	engineered mutation	UNP Q05320
M	16	TYR	-	expression tag	UNP Q05320
M	17	PRO	-	expression tag	UNP Q05320
M	18	TYR	-	expression tag	UNP Q05320
M	19	ASP	-	expression tag	UNP Q05320
M	20	VAL	-	expression tag	UNP Q05320
M	21	PRO	-	expression tag	UNP Q05320

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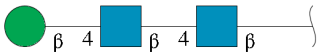
Chain	Residue	Modelled	Actual	Comment	Reference
M	22	ASP	-	expression tag	UNP Q05320
M	23	TYR	-	expression tag	UNP Q05320
M	24	ALA	-	expression tag	UNP Q05320
M	25	ILE	-	expression tag	UNP Q05320
M	26	GLU	-	expression tag	UNP Q05320
M	27	GLY	-	expression tag	UNP Q05320
M	28	ARG	-	expression tag	UNP Q05320
M	29	GLY	-	expression tag	UNP Q05320
M	30	ALA	-	expression tag	UNP Q05320
M	31	ARG	-	expression tag	UNP Q05320
M	42	VAL	THR	engineered mutation	UNP Q05320
M	230	VAL	THR	engineered mutation	UNP Q05320
O	16	TYR	-	expression tag	UNP Q05320
O	17	PRO	-	expression tag	UNP Q05320
O	18	TYR	-	expression tag	UNP Q05320
O	19	ASP	-	expression tag	UNP Q05320
O	20	VAL	-	expression tag	UNP Q05320
O	21	PRO	-	expression tag	UNP Q05320
O	22	ASP	-	expression tag	UNP Q05320
O	23	TYR	-	expression tag	UNP Q05320
O	24	ALA	-	expression tag	UNP Q05320
O	25	ILE	-	expression tag	UNP Q05320
O	26	GLU	-	expression tag	UNP Q05320
O	27	GLY	-	expression tag	UNP Q05320
O	28	ARG	-	expression tag	UNP Q05320
O	29	GLY	-	expression tag	UNP Q05320
O	30	ALA	-	expression tag	UNP Q05320
O	31	ARG	-	expression tag	UNP Q05320
O	42	VAL	THR	engineered mutation	UNP Q05320
O	230	VAL	THR	engineered mutation	UNP Q05320

- Molecule 4 is a protein called Envelope glycoprotein GP2.

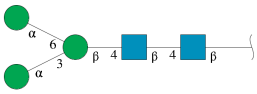
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	J	98	746	477	130	136	3	0	0	0
			Total	C	N	O	S			
4	L	93	727	466	126	132	3	0	0	0
			Total	C	N	O	S			
4	N	95	732	469	128	132	3	0	0	0
			Total	C	N	O	S			
4	P	93	719	462	125	129	3	0	0	0

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



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

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

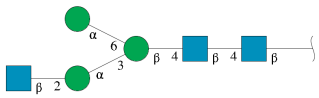


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
6	R	5	61	34	2	25	0	0	0
6	V	5	61	34	2	25	0	0	0

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
7	S	2	28	16	2	10	0	0	0

- Molecule 8 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



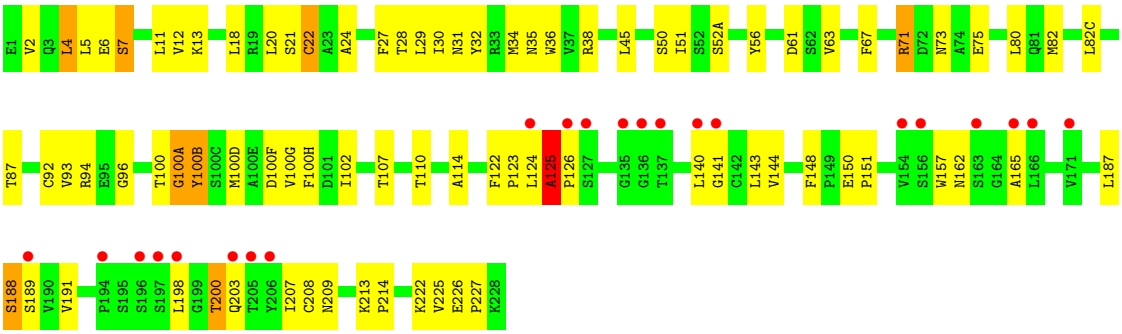
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
8	T	6	75	42	3	30	0	0	0
			Total	C	N	O			
8	X	6	75	42	3	30	0	0	0

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.

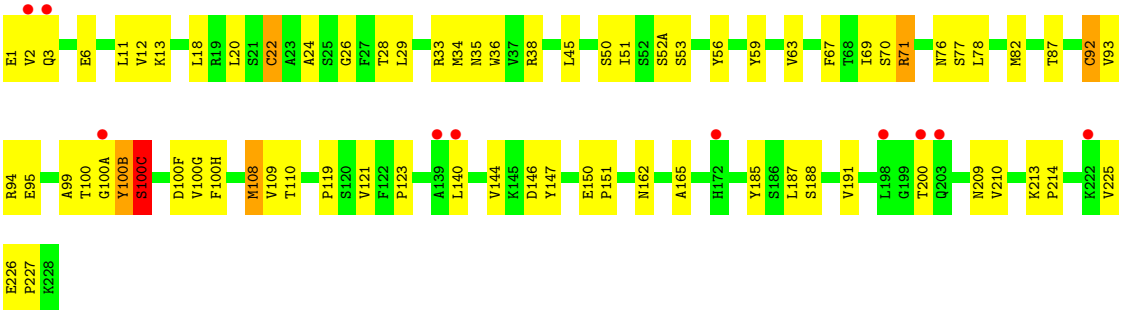
- Molecule 1: Fab KZ52 heavy chain

Chain A:



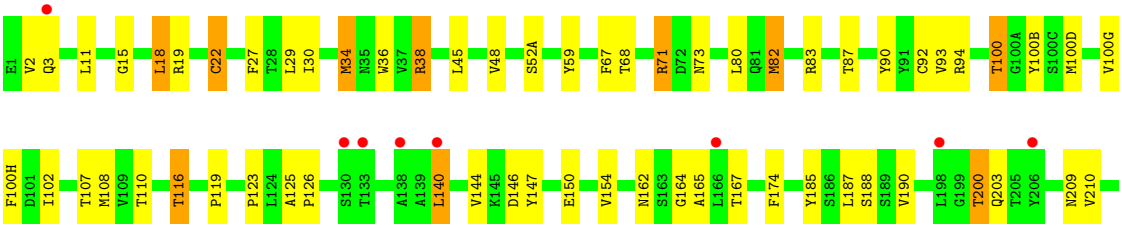
- Molecule 1: Fab KZ52 heavy chain

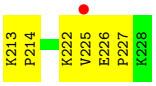
Chain C:



- Molecule 1: Fab KZ52 heavy chain

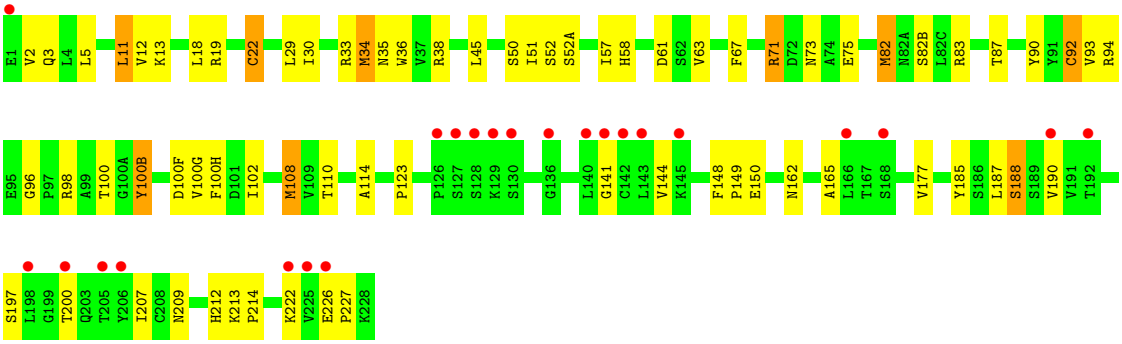
Chain E:





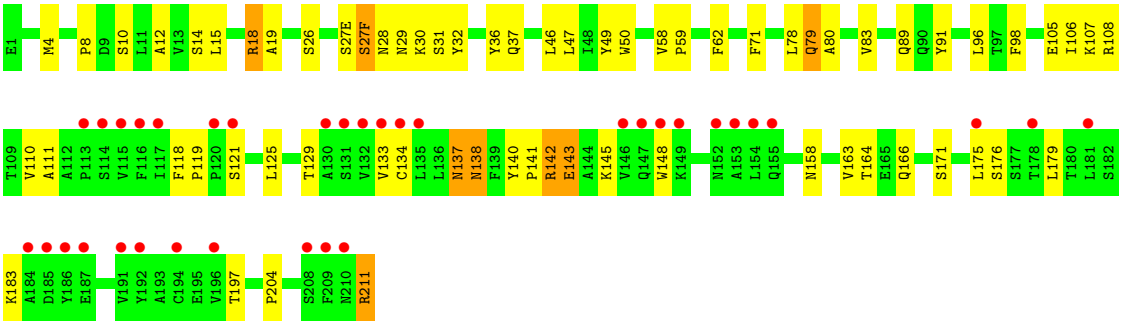
• Molecule 1: Fab KZ52 heavy chain

Chain G:



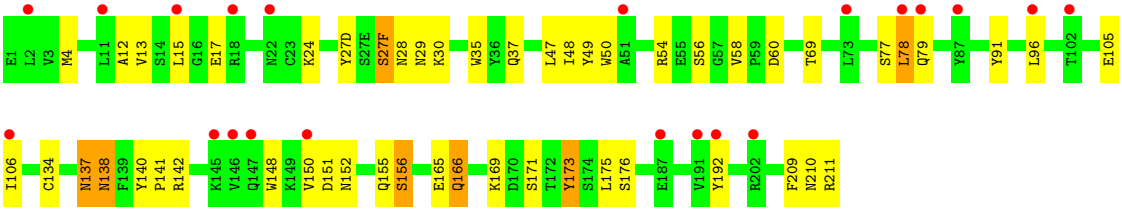
• Molecule 2: Fab KZ52 light chain

Chain B:



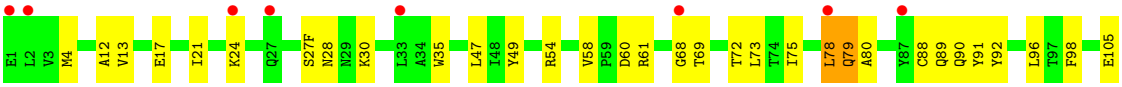
• Molecule 2: Fab KZ52 light chain

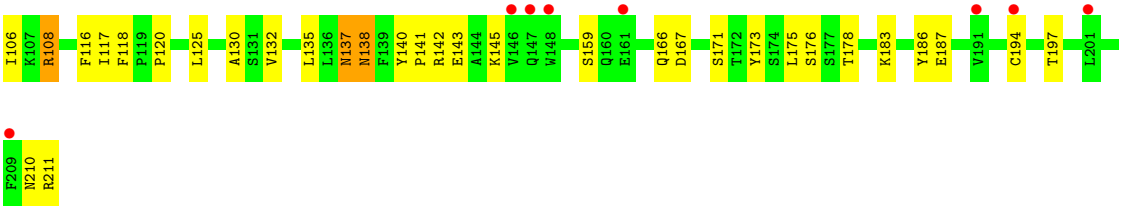
Chain D:



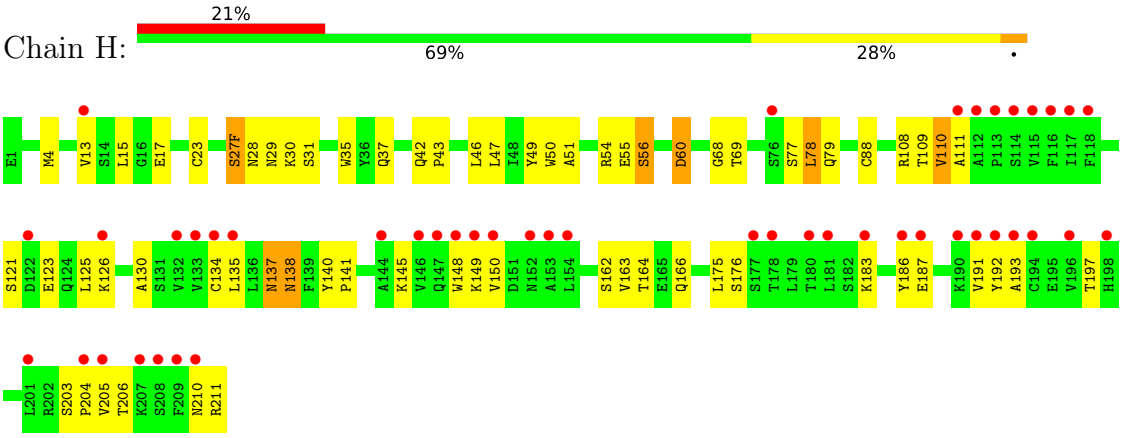
• Molecule 2: Fab KZ52 light chain

Chain F:

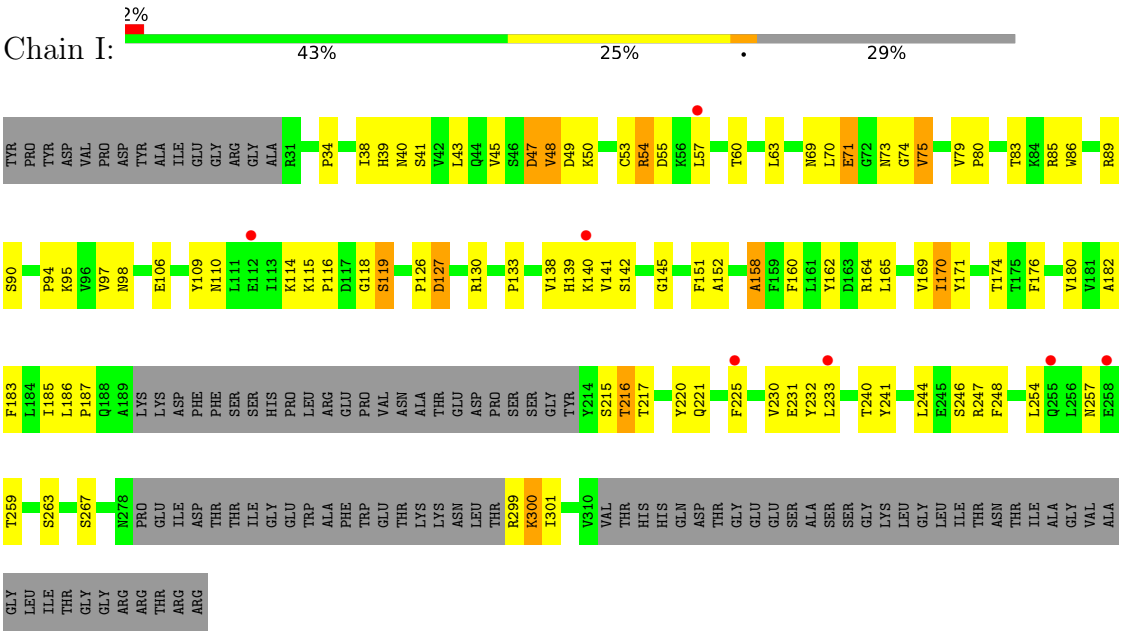




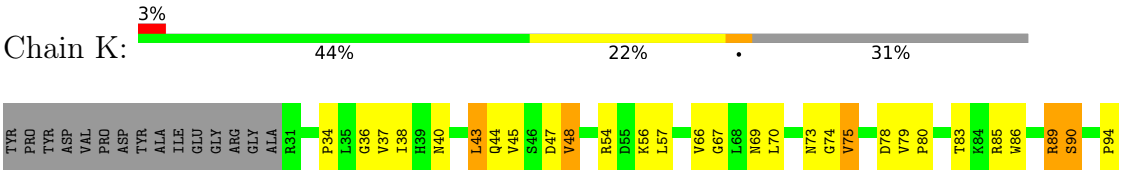
• Molecule 2: Fab KZ52 light chain

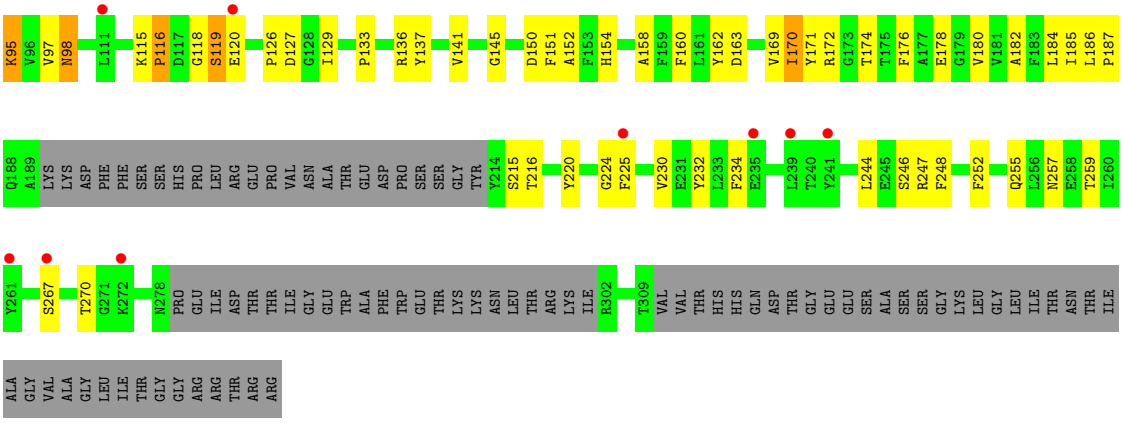


• Molecule 3: Envelope glycoprotein GP1



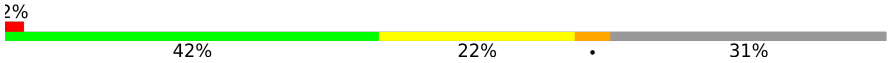
• Molecule 3: Envelope glycoprotein GP1

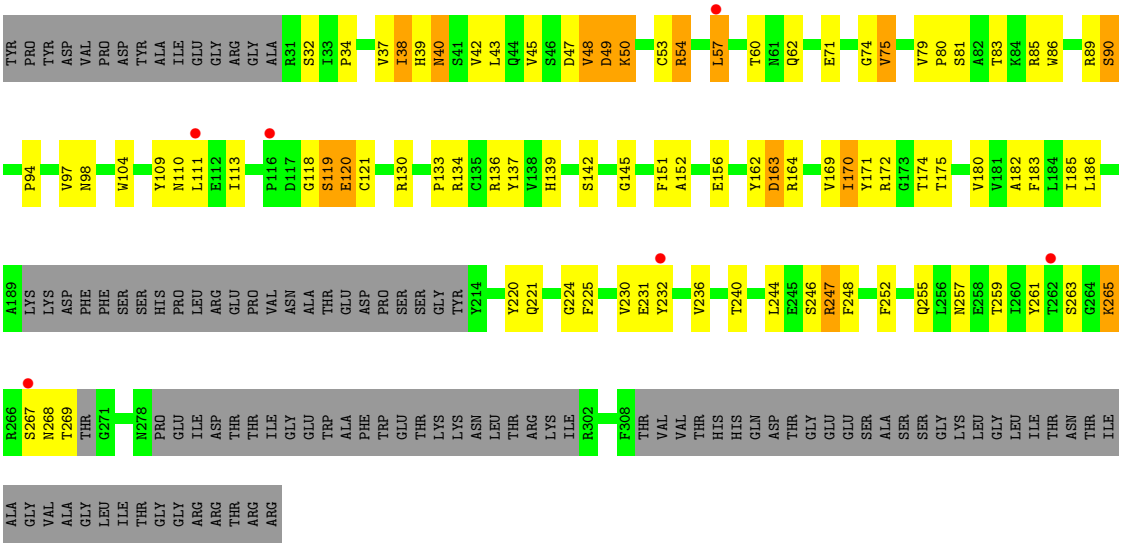




• Molecule 3: Envelope glycoprotein GP1

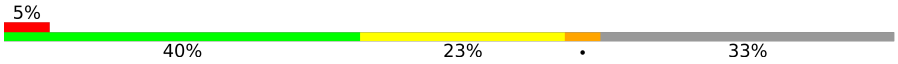
Chain M:

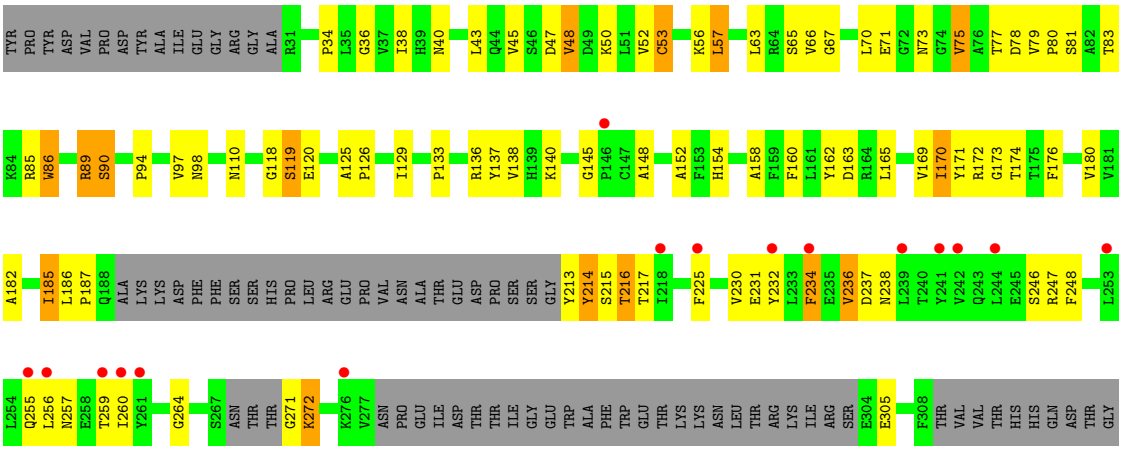


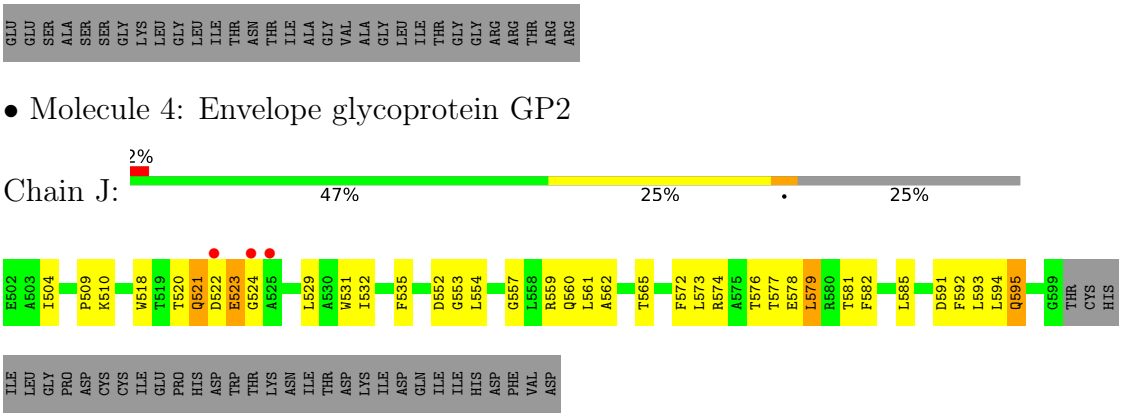


• Molecule 3: Envelope glycoprotein GP1

Chain O:






GLU GLU SER ALA SER SER GLY LYS LEU GLY LEU ILE THR ASN THR ILE ALA GLY VAL ALA GLY LEU ILE THR GLY GLY ARG ARG THR ARG ARG
• Molecule 4: Envelope glycoprotein GP2
Chain J:
2%
47%
25%
25%
E502 A503 I504 P509 K510 W518 T519 T520 Q521 D522 E523 G524 A525 L529 A530 W531 I532 F535 D552 G553 L554 G557 L558 R559 Q560 L561 A562 T565 F572 L573 R574 A575 T576 T577 E578 L579 R580 T581 F582 L585 D591 F592 L593 L594 Q595 G599 THR CYS HIS
ILE LEU GLY PRO ASP CYS CYS ILE GLU PRO HIS ASP TRP THR LYS ASN ILE THR ASP LYS ILE ASP GLN ILE ILE HIS ASP PHE VAL ASP
• Molecule 4: Envelope glycoprotein GP2
Chain L:
3%
42%
27%
29%
GLU A503 I504 N512 H516 Y517 W518 T519 T520 Q521 D522 GLU GLY A525 A526 I527 G528 L529 I532 P537 I542 G546 Q551 D552 G553 L554 L558 R559 Q560 L561 A562 N563 E564 T565 Q570 L573 R574 A575 T576 T577 E578 L579 F582 S583 I590 D591 F592 L593
L594 Q595 R596 W597 GLY GLY GLY THR CYS HIS ILE LEU GLY PRO ASP CYS CYS ILE GLU PRO HIS ASP TRP THR LYS ASN ILE THR ASP LYS ILE ASP GLN ILE ILE HIS ASP PHE VAL ASP
• Molecule 4: Envelope glycoprotein GP2
Chain N:
4%
47%
24%
27%
E502 A503 I504 N512 Y517 W518 Q521 ASP GLU G524 A525 A526 I527 I532 P533 Y534 F535 G536 I542 E545 G546 H549 D552 I555 Q560 L561 A562 N563 E564 T565 T566 Q567 L573 T576 T577 E578 L579 F582 S583 I584 L585 N586 R587 D591 F592 L593
L594 G598 GLY THR CYS HIS ILE LEU GLY PRO ASP CYS CYS ILE GLU PRO HIS ASP TRP THR LYS ASN ILE THR ASP LYS ILE ASP GLN ILE ILE HIS ASP PHE VAL ASP
• Molecule 4: Envelope glycoprotein GP2
Chain P:
3%
52%
18%
29%
GLU A503 I504 V505 N506 P509 K510 W518 Q521 ASP GLU GLY A525 A530 W531 I532 F535 L547 Q560 L561 A562 N563 E564 T565 T566 Q567 L573 T576 T577 E578 L579 S583 I584 L585 N586 R587 F592 Q595 G598 GLY THR CYS HIS ILE LEU GLY PRO
ASP CYS CYS ILE GLU PRO HIS ASP TRP THR LYS ASN ILE THR ASP LYS ILE ASP GLN ILE ILE HIS ASP PHE VAL ASP
• Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose
Chain Q:
67%
33%
NAG1 NAG2 BMA3

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

Chain U: 100%

NAG1 NAG2 BMA3

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

Chain W: 33% 67%

NAG1 NAG2 BMA3

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

Chain R: 40% 60%

NAG1 NAG2 BMA3 MAN4 MAN5

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

Chain V: 60% 40%

NAG1 NAG2 BMA3 MAN4 MAN5

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

Chain S: 50% 50%

NAG1 NAG2

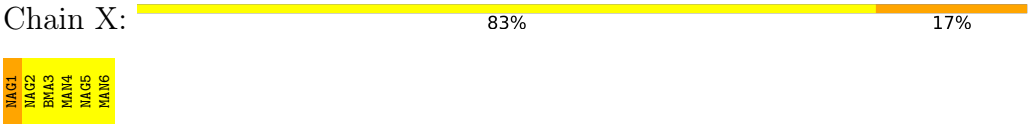
• Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain T: 83% 17%

NAG1 NAG2 BMA3 MAN4 NAG5 MAN6

• Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain X:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α, β, γ	273.71Å 273.71Å 409.43Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.37 – 3.40 48.37 – 3.40	Depositor EDS
% Data completeness (in resolution range)	93.4 (48.37-3.40) 96.9 (48.37-3.40)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.67 (at 3.40Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.261 , 0.302 0.267 , 0.301	Depositor DCC
R_{free} test set	4559 reflections (3.01%)	wwPDB-VP
Wilson B-factor (Å^2)	95.5	Xtriage
Anisotropy	0.075	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 68.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	23539	wwPDB-VP
Average B, all atoms (Å^2)	121.0	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, BMA, NAG

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	0.53	0/1721	0.56	0/2333
1	C	0.49	1/1721 (0.1%)	0.50	0/2333
1	E	0.49	1/1721 (0.1%)	0.52	0/2333
1	G	0.48	0/1721	0.52	0/2333
2	B	0.41	0/1718	0.50	0/2331
2	D	0.37	0/1718	0.49	0/2331
2	F	0.42	0/1718	0.49	0/2331
2	H	0.37	0/1718	0.48	0/2331
3	I	0.49	0/1743	0.57	0/2379
3	K	0.44	0/1723	0.54	0/2351
3	M	0.47	0/1712	0.57	1/2334 (0.0%)
3	O	0.41	0/1686	0.53	0/2298
4	J	0.54	0/762	0.60	0/1038
4	L	0.47	0/742	0.56	0/1010
4	N	0.50	0/747	0.61	0/1016
4	P	0.49	0/734	0.61	0/999
All	All	0.46	2/23605 (0.0%)	0.53	1/32081 (0.0%)

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
1	A	0	1
3	I	0	1
3	K	0	1
4	N	0	1
All	All	0	4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	108	MSE	CG-SE	-5.33	1.77	1.95
1	E	34	MSE	CG-SE	-5.19	1.77	1.95

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	M	265	LYS	N-CA-C	5.20	125.03	111.00

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	125	ALA	Peptide
3	I	55	ASP	Peptide
3	K	54	ARG	Peptide
4	N	536	GLY	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	1687	0	1660	78	0
1	C	1687	0	1660	51	0
1	E	1687	0	1660	59	0
1	G	1687	0	1660	53	0
2	B	1682	0	1638	48	0
2	D	1682	0	1638	39	0
2	F	1682	0	1638	38	0
2	H	1682	0	1638	44	0
3	I	1707	0	1548	81	0
3	K	1687	0	1540	73	0
3	M	1677	0	1535	68	0
3	O	1651	0	1520	73	0
4	J	746	0	722	41	0
4	L	727	0	712	44	0
4	N	732	0	716	39	0
4	P	719	0	706	26	0
5	Q	39	0	34	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	U	39	0	34	0	0
5	W	39	0	34	6	0
6	R	61	0	52	2	0
6	V	61	0	52	3	0
7	S	28	0	25	2	0
8	T	75	0	64	3	0
8	X	75	0	64	4	0
All	All	23539	0	22550	750	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 16.

The worst 5 of 750 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)
4:N:563:ASN:ND2	6:V:1:NAG:C1	1.67	1.54
3:O:257:ASN:HD21	5:W:1:NAG:C1	0.89	1.53
3:I:257:ASN:ND2	5:Q:1:NAG:C1	1.68	1.51
3:K:257:ASN:ND2	7:S:1:NAG:C1	1.68	1.50
4:L:563:ASN:ND2	8:T:1:NAG:C1	1.70	1.49

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	224/226 (99%)	192 (86%)	29 (13%)	3 (1%)	12	39
1	C	224/226 (99%)	194 (87%)	27 (12%)	3 (1%)	12	39
1	E	224/226 (99%)	196 (88%)	26 (12%)	2 (1%)	17	49
1	G	224/226 (99%)	202 (90%)	21 (9%)	1 (0%)	34	67

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	215/217 (99%)	181 (84%)	25 (12%)	9 (4%)	3	18
2	D	215/217 (99%)	183 (85%)	25 (12%)	7 (3%)	4	22
2	F	215/217 (99%)	183 (85%)	26 (12%)	6 (3%)	5	24
2	H	215/217 (99%)	179 (83%)	27 (13%)	9 (4%)	3	18
3	I	230/334 (69%)	184 (80%)	33 (14%)	13 (6%)	1	12
3	K	226/334 (68%)	184 (81%)	33 (15%)	9 (4%)	3	18
3	M	222/334 (66%)	181 (82%)	29 (13%)	12 (5%)	2	13
3	O	217/334 (65%)	171 (79%)	26 (12%)	20 (9%)	1	4
4	J	96/131 (73%)	80 (83%)	14 (15%)	2 (2%)	7	30
4	L	89/131 (68%)	79 (89%)	8 (9%)	2 (2%)	6	29
4	N	91/131 (70%)	80 (88%)	10 (11%)	1 (1%)	14	44
4	P	89/131 (68%)	74 (83%)	13 (15%)	2 (2%)	6	29
All	All	3016/3632 (83%)	2543 (84%)	372 (12%)	101 (3%)	4	22

5 of 101 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	100(B)	TYR
2	B	110	VAL
2	D	27(F)	SER
2	D	78	LEU
2	D	169	LYS

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	190/186 (102%)	175 (92%)	15 (8%)	12	39
1	C	190/186 (102%)	177 (93%)	13 (7%)	16	45
1	E	190/186 (102%)	179 (94%)	11 (6%)	20	50
1	G	190/186 (102%)	175 (92%)	15 (8%)	12	39

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	191/190 (100%)	185 (97%)	6 (3%)	40	68
2	D	191/190 (100%)	188 (98%)	3 (2%)	62	81
2	F	191/190 (100%)	187 (98%)	4 (2%)	53	76
2	H	191/190 (100%)	186 (97%)	5 (3%)	46	72
3	I	163/282 (58%)	156 (96%)	7 (4%)	29	59
3	K	163/282 (58%)	154 (94%)	9 (6%)	21	51
3	M	163/282 (58%)	153 (94%)	10 (6%)	18	48
3	O	162/282 (57%)	152 (94%)	10 (6%)	18	48
4	J	73/110 (66%)	69 (94%)	4 (6%)	21	51
4	L	74/110 (67%)	71 (96%)	3 (4%)	30	59
4	N	73/110 (66%)	70 (96%)	3 (4%)	30	59
4	P	72/110 (66%)	69 (96%)	3 (4%)	30	59
All	All	2467/3072 (80%)	2346 (95%)	121 (5%)	25	55

5 of 121 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	38	ARG
3	O	78	ASP
2	H	211	ARG
3	O	77	THR
4	P	579	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	155	GLN
3	I	110	ASN
4	J	595	GLN
3	O	257	ASN
4	P	563	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

33 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	Q	1	5	14,14,15	0.76	0	17,19,21	2.16	2 (11%)
5	NAG	Q	2	5	14,14,15	0.84	0	17,19,21	1.20	2 (11%)
5	BMA	Q	3	5	11,11,12	1.41	1 (9%)	15,15,17	2.03	4 (26%)
6	NAG	R	1	6	14,14,15	0.96	1 (7%)	17,19,21	1.13	1 (5%)
6	NAG	R	2	6	14,14,15	0.74	0	17,19,21	1.91	5 (29%)
6	BMA	R	3	6	11,11,12	1.17	1 (9%)	15,15,17	2.17	4 (26%)
6	MAN	R	4	6	11,11,12	0.80	1 (9%)	15,15,17	1.63	3 (20%)
6	MAN	R	5	6	11,11,12	0.68	0	15,15,17	1.63	2 (13%)
7	NAG	S	1	7	14,14,15	0.79	0	17,19,21	1.78	2 (11%)
7	NAG	S	2	7	14,14,15	0.68	0	17,19,21	1.34	1 (5%)
8	NAG	T	1	8	14,14,15	1.04	1 (7%)	17,19,21	2.31	5 (29%)
8	NAG	T	2	8	14,14,15	0.55	0	17,19,21	1.60	4 (23%)
8	BMA	T	3	8	11,11,12	1.38	2 (18%)	15,15,17	1.85	3 (20%)
8	MAN	T	4	8	11,11,12	1.00	1 (9%)	15,15,17	1.42	2 (13%)
8	NAG	T	5	8	14,14,15	0.71	0	17,19,21	1.57	3 (17%)
8	MAN	T	6	8	11,11,12	0.81	1 (9%)	15,15,17	1.68	4 (26%)
5	NAG	U	1	5	14,14,15	0.90	0	17,19,21	2.29	3 (17%)
5	NAG	U	2	5	14,14,15	0.57	0	17,19,21	1.47	2 (11%)
5	BMA	U	3	5	11,11,12	1.16	0	15,15,17	1.41	2 (13%)
6	NAG	V	1	6	14,14,15	0.92	1 (7%)	17,19,21	1.83	3 (17%)
6	NAG	V	2	6	14,14,15	1.00	1 (7%)	17,19,21	1.32	3 (17%)
6	BMA	V	3	6	11,11,12	1.22	2 (18%)	15,15,17	1.89	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	MAN	V	4	6	11,11,12	0.90	1 (9%)	15,15,17	1.54	3 (20%)
6	MAN	V	5	6	11,11,12	0.52	0	15,15,17	1.29	2 (13%)
5	NAG	W	1	5	14,14,15	0.75	0	17,19,21	2.03	2 (11%)
5	NAG	W	2	5	14,14,15	0.90	0	17,19,21	1.40	2 (11%)
5	BMA	W	3	5	11,11,12	1.65	2 (18%)	15,15,17	1.75	2 (13%)
8	NAG	X	1	8	14,14,15	0.93	1 (7%)	17,19,21	1.80	5 (29%)
8	NAG	X	2	8	14,14,15	0.73	0	17,19,21	1.52	3 (17%)
8	BMA	X	3	8	11,11,12	1.22	1 (9%)	15,15,17	1.58	3 (20%)
8	MAN	X	4	8	11,11,12	1.18	2 (18%)	15,15,17	1.21	2 (13%)
8	NAG	X	5	8	14,14,15	0.62	0	17,19,21	1.79	1 (5%)
8	MAN	X	6	8	11,11,12	0.65	0	15,15,17	1.33	2 (13%)

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	Q	1	5	-	2/6/23/26	0/1/1/1
5	NAG	Q	2	5	-	3/6/23/26	0/1/1/1
5	BMA	Q	3	5	-	2/2/19/22	0/1/1/1
6	NAG	R	1	6	-	0/6/23/26	0/1/1/1
6	NAG	R	2	6	-	4/6/23/26	0/1/1/1
6	BMA	R	3	6	-	2/2/19/22	0/1/1/1
6	MAN	R	4	6	-	0/2/19/22	0/1/1/1
6	MAN	R	5	6	-	2/2/19/22	0/1/1/1
7	NAG	S	1	7	-	0/6/23/26	0/1/1/1
7	NAG	S	2	7	-	2/6/23/26	0/1/1/1
8	NAG	T	1	8	-	2/6/23/26	0/1/1/1
8	NAG	T	2	8	-	4/6/23/26	0/1/1/1
8	BMA	T	3	8	-	2/2/19/22	0/1/1/1
8	MAN	T	4	8	-	1/2/19/22	0/1/1/1
8	NAG	T	5	8	-	0/6/23/26	0/1/1/1
8	MAN	T	6	8	-	2/2/19/22	0/1/1/1
5	NAG	U	1	5	-	0/6/23/26	0/1/1/1
5	NAG	U	2	5	-	3/6/23/26	0/1/1/1
5	BMA	U	3	5	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	V	1	6	-	0/6/23/26	0/1/1/1
6	NAG	V	2	6	-	3/6/23/26	0/1/1/1
6	BMA	V	3	6	-	2/2/19/22	0/1/1/1
6	MAN	V	4	6	-	0/2/19/22	0/1/1/1
6	MAN	V	5	6	-	2/2/19/22	0/1/1/1
5	NAG	W	1	5	-	2/6/23/26	0/1/1/1
5	NAG	W	2	5	-	5/6/23/26	0/1/1/1
5	BMA	W	3	5	-	2/2/19/22	0/1/1/1
8	NAG	X	1	8	-	1/6/23/26	0/1/1/1
8	NAG	X	2	8	-	4/6/23/26	0/1/1/1
8	BMA	X	3	8	-	2/2/19/22	0/1/1/1
8	MAN	X	4	8	-	2/2/19/22	0/1/1/1
8	NAG	X	5	8	-	0/6/23/26	0/1/1/1
8	MAN	X	6	8	-	2/2/19/22	0/1/1/1

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	W	3	BMA	C2-C3	3.60	1.57	1.52
5	Q	3	BMA	C2-C3	3.02	1.57	1.52
8	T	3	BMA	C2-C3	2.95	1.56	1.52
8	T	1	NAG	O5-C1	-2.84	1.39	1.43
6	V	1	NAG	O5-C1	-2.71	1.39	1.43

The worst 5 of 88 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	U	1	NAG	C1-O5-C5	7.17	121.91	112.19
8	X	5	NAG	C1-O5-C5	6.80	121.41	112.19
5	W	1	NAG	C1-O5-C5	6.61	121.15	112.19
5	Q	1	NAG	C1-O5-C5	6.28	120.69	112.19
6	V	3	BMA	C1-O5-C5	6.13	120.50	112.19

There are no chirality outliers.

5 of 60 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	Q	2	NAG	C8-C7-N2-C2
5	Q	2	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
5	W	2	NAG	C8-C7-N2-C2
5	W	2	NAG	O7-C7-N2-C2
6	R	2	NAG	C8-C7-N2-C2

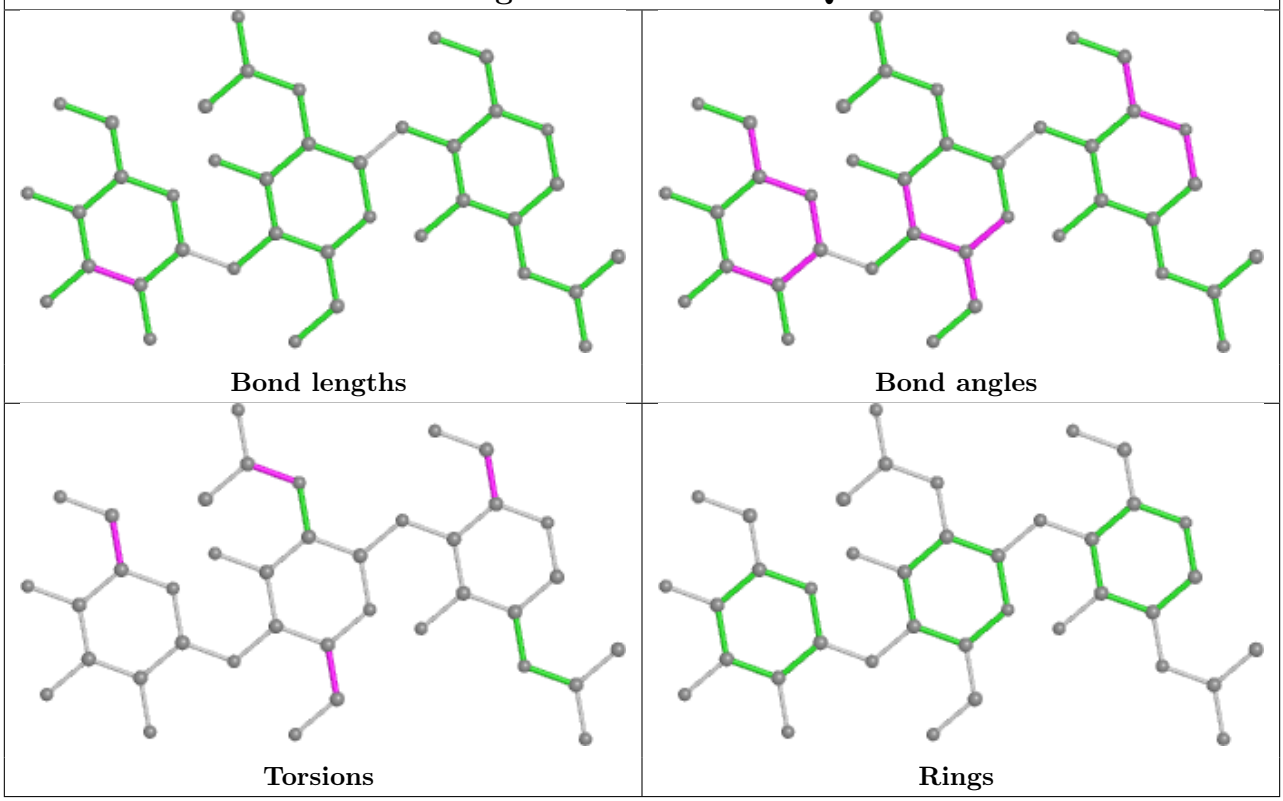
There are no ring outliers.

11 monomers are involved in 24 short contacts:

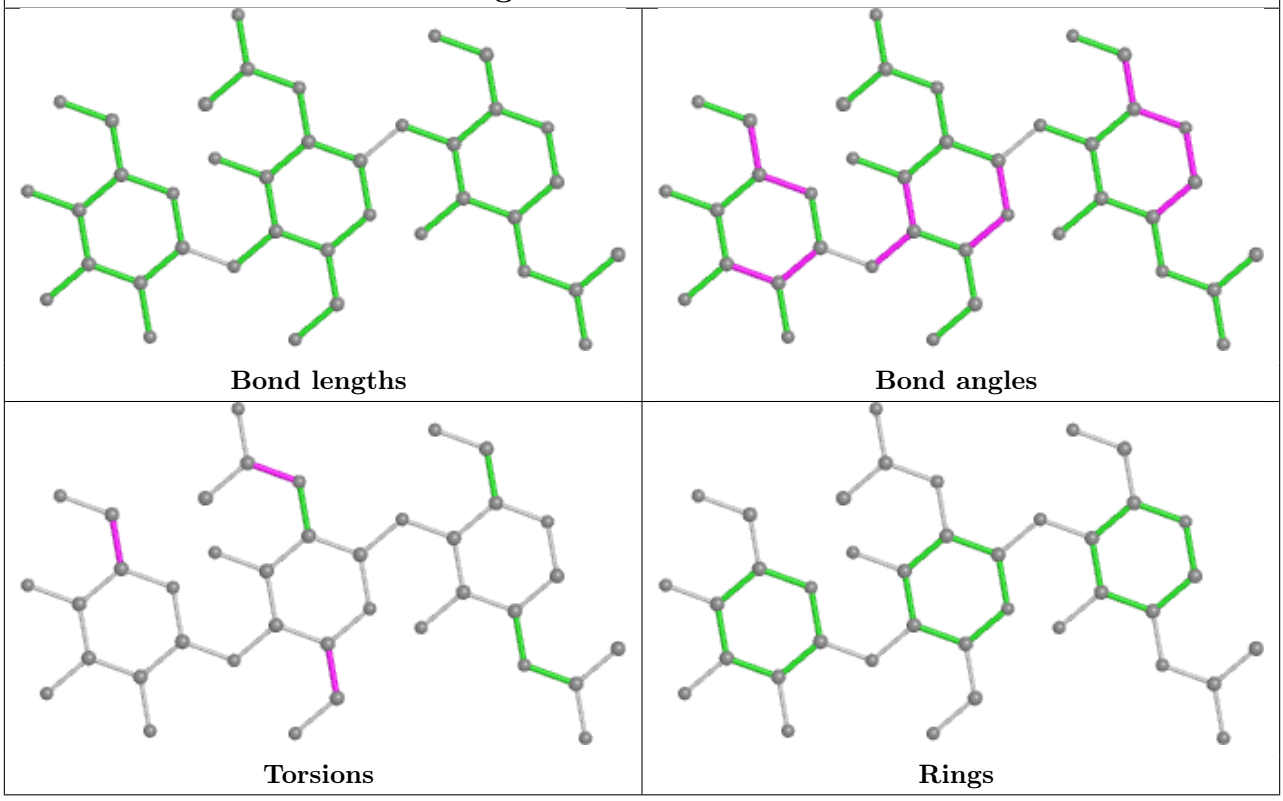
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	Q	1	NAG	4	0
6	R	3	BMA	1	0
6	V	1	NAG	2	0
8	X	1	NAG	4	0
8	T	1	NAG	3	0
5	W	2	NAG	1	0
6	R	5	MAN	1	0
7	S	1	NAG	2	0
6	R	1	NAG	1	0
5	W	1	NAG	6	0
6	V	2	NAG	1	0

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

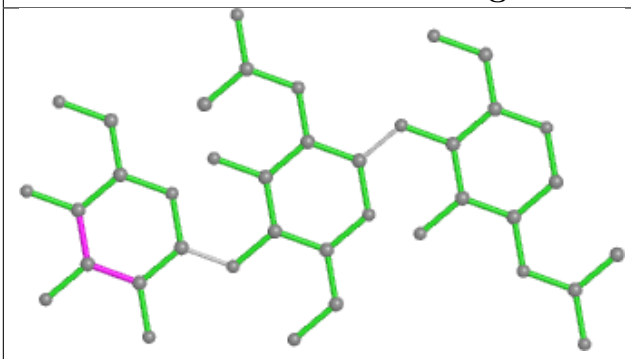
Oligosaccharide Chain Q



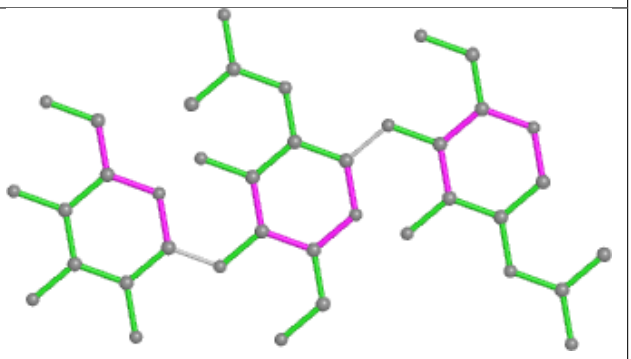
Oligosaccharide Chain U



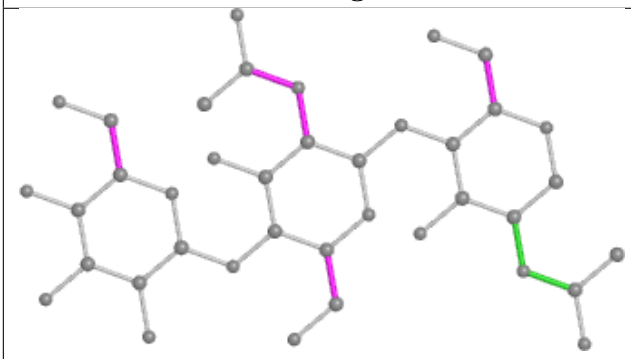
Oligosaccharide Chain W



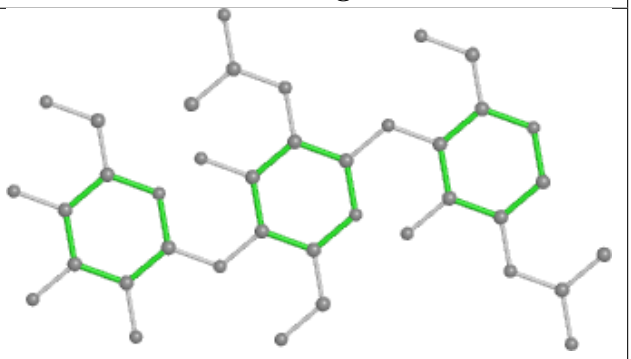
Bond lengths



Bond angles

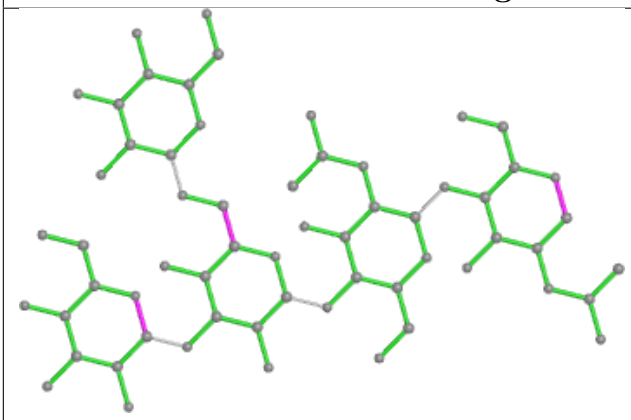


Torsions

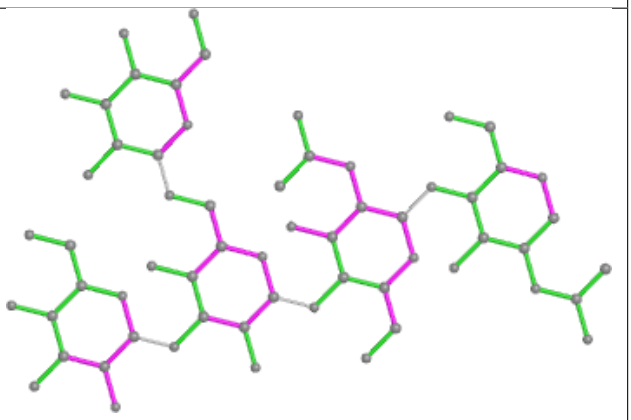


Rings

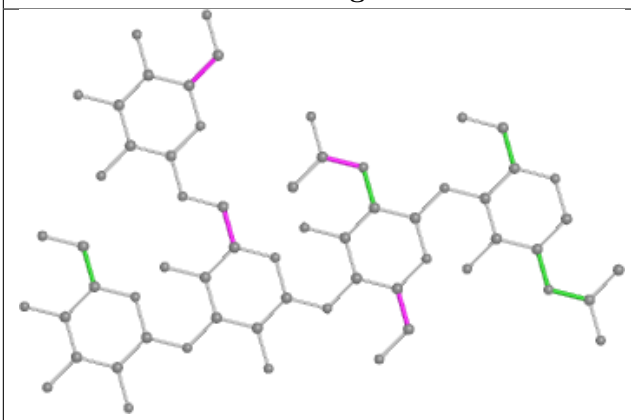
Oligosaccharide Chain R



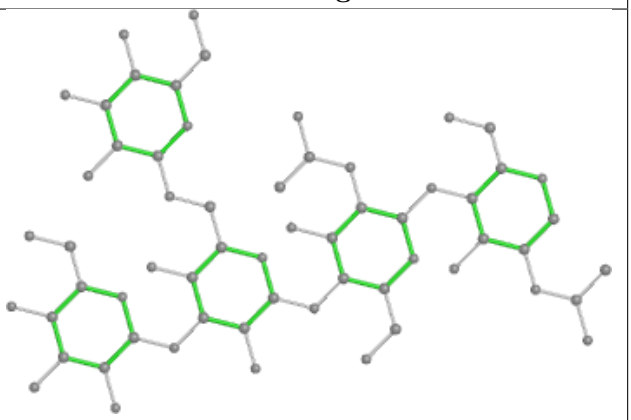
Bond lengths



Bond angles

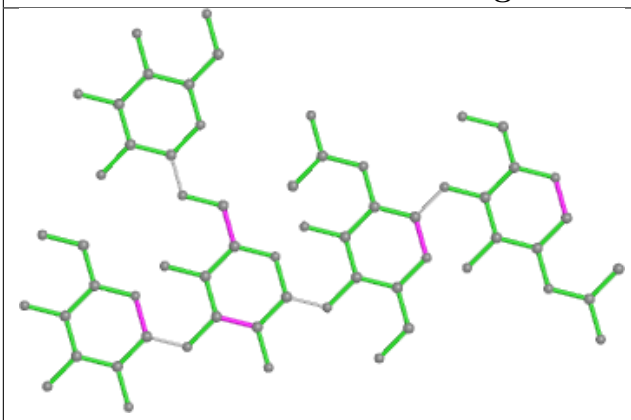


Torsions

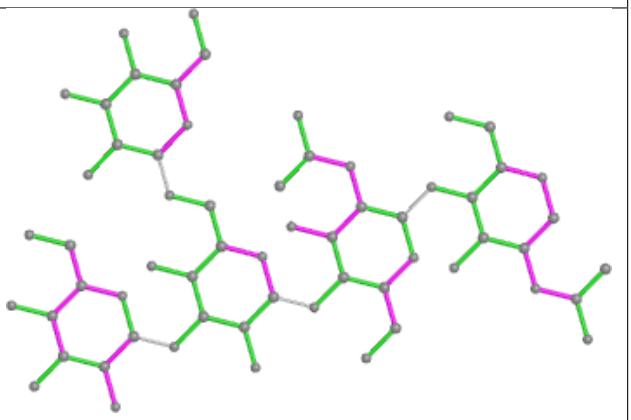


Rings

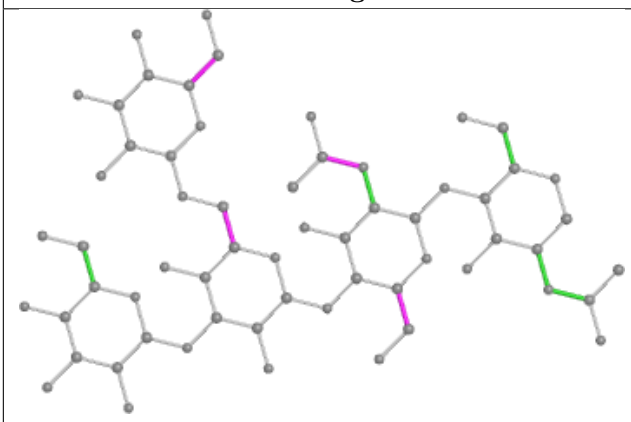
Oligosaccharide Chain V



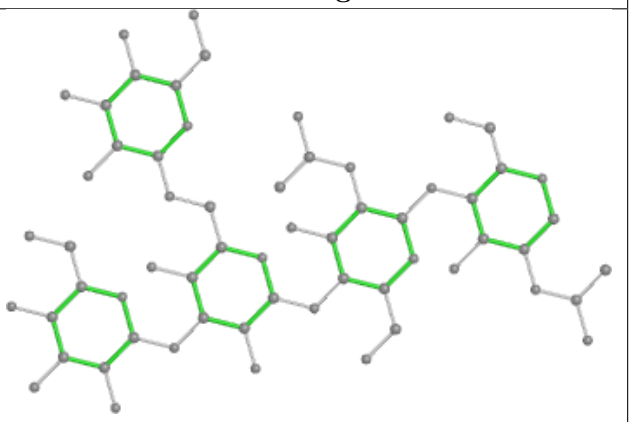
Bond lengths



Bond angles

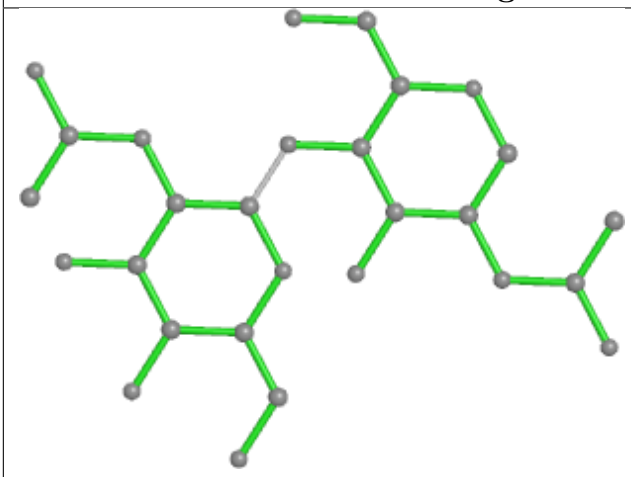


Torsions

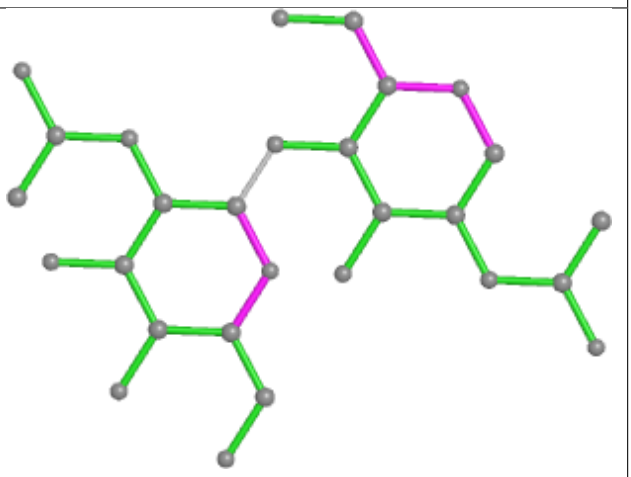


Rings

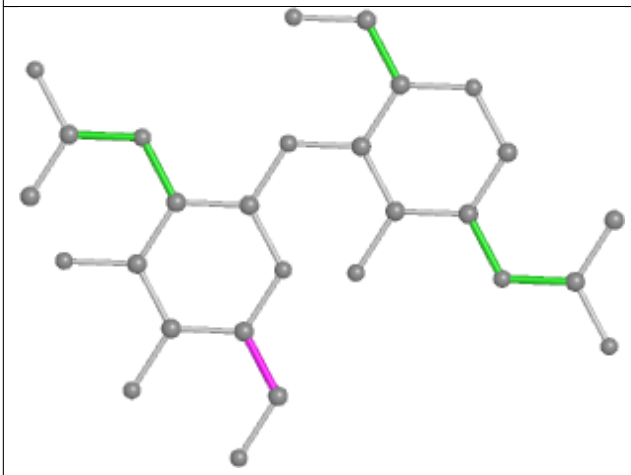
Oligosaccharide Chain S



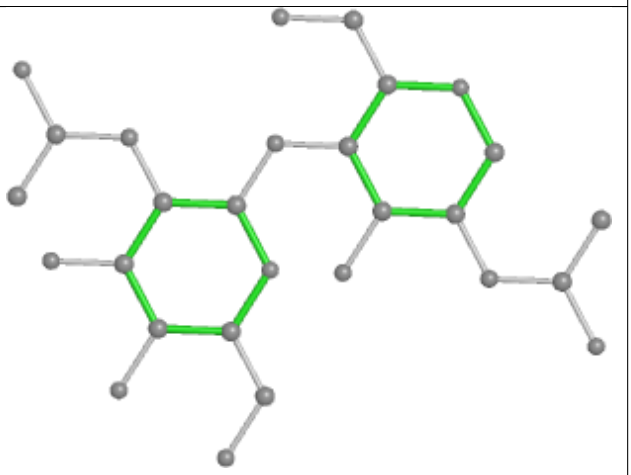
Bond lengths



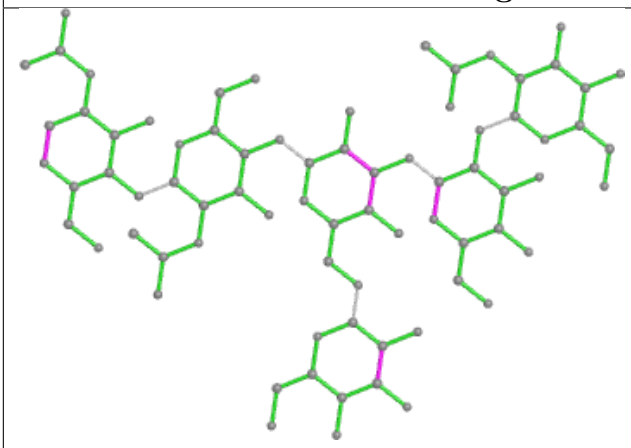
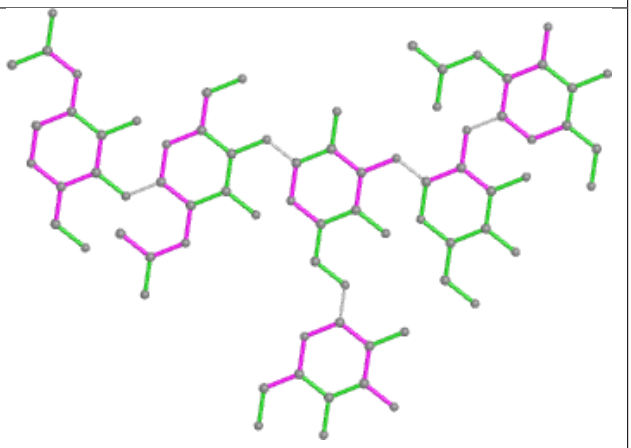
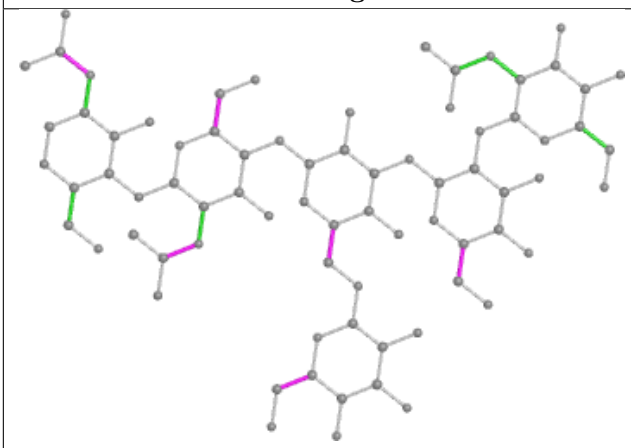
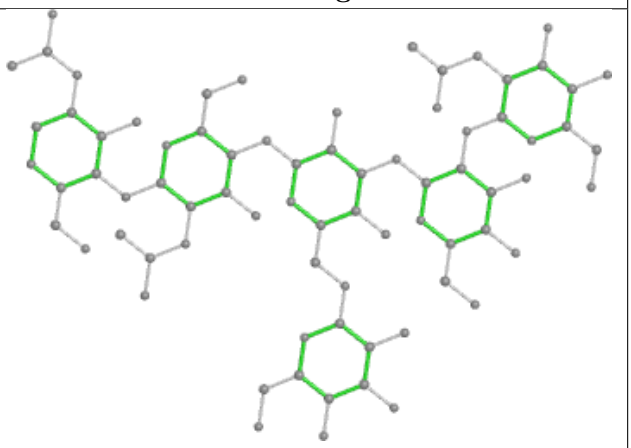
Bond angles



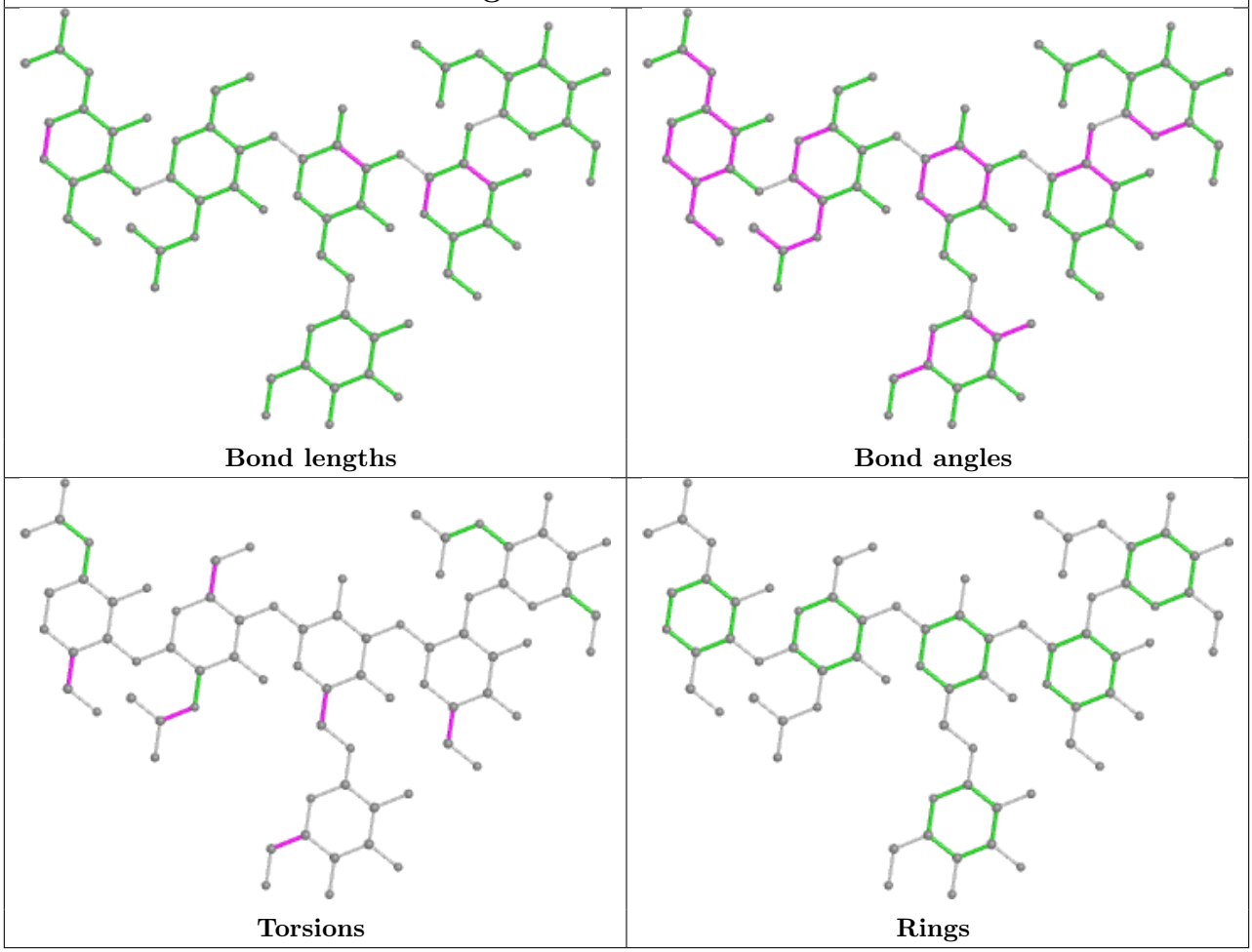
Torsions



Rings

Oligosaccharide Chain T	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Oligosaccharide Chain X



5.6 Ligand geometry (i)

There are no ligands in this entry.

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	222/226 (98%)	0.64	22 (9%)	7	8	73, 105, 211, 230	0
1	C	222/226 (98%)	0.44	10 (4%)	33	33	85, 116, 174, 196	0
1	E	222/226 (98%)	0.41	9 (4%)	37	36	87, 110, 158, 186	0
1	G	222/226 (98%)	0.70	23 (10%)	6	8	90, 116, 186, 207	0
2	B	216/217 (99%)	0.91	35 (16%)	1	2	87, 137, 195, 219	0
2	D	216/217 (99%)	0.63	21 (9%)	7	9	100, 140, 162, 194	0
2	F	216/217 (99%)	0.68	16 (7%)	14	16	104, 123, 156, 176	0
2	H	216/217 (99%)	1.13	46 (21%)	0	1	101, 140, 203, 234	0
3	I	236/334 (70%)	0.34	7 (2%)	50	49	79, 104, 139, 161	0
3	K	232/334 (69%)	0.46	9 (3%)	39	38	85, 118, 157, 184	0
3	M	230/334 (68%)	0.40	6 (2%)	56	54	84, 108, 144, 172	0
3	O	225/334 (67%)	0.55	16 (7%)	16	18	94, 122, 159, 182	0
4	J	98/131 (74%)	0.50	3 (3%)	49	48	70, 98, 155, 186	0
4	L	93/131 (70%)	0.47	4 (4%)	35	35	76, 106, 138, 177	0
4	N	95/131 (72%)	0.56	5 (5%)	26	27	69, 98, 141, 182	0
4	P	93/131 (70%)	0.44	4 (4%)	35	35	80, 105, 135, 163	0
All	All	3054/3632 (84%)	0.59	236 (7%)	13	15	69, 116, 179, 234	0

The worst 5 of 236 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	140	LEU	8.2
2	H	194	CYS	7.7
1	A	206	TYR	7.6
2	H	134	CYS	6.0
2	H	144	ALA	5.7

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
5	BMA	W	3	11/12	0.24	0.39	190,190,190,190	0
8	NAG	T	5	14/15	0.61	0.42	173,173,173,173	0
5	BMA	U	3	11/12	0.62	0.30	168,168,168,168	0
6	MAN	R	5	11/12	0.64	0.44	171,171,171,171	0
8	MAN	X	6	11/12	0.67	0.34	174,174,174,174	0
8	MAN	T	6	11/12	0.70	0.29	162,162,162,162	0
5	BMA	Q	3	11/12	0.70	0.34	172,172,172,172	0
7	NAG	S	2	14/15	0.71	0.36	167,167,167,167	0
6	MAN	V	4	11/12	0.76	0.36	132,132,132,132	0
5	NAG	W	1	14/15	0.80	0.24	140,140,140,140	0
5	NAG	W	2	14/15	0.80	0.30	177,177,177,177	0
8	NAG	X	5	14/15	0.80	0.38	177,177,177,177	0
8	BMA	T	3	11/12	0.80	0.14	118,118,118,118	0
6	BMA	R	3	11/12	0.81	0.18	135,135,135,135	0
8	MAN	T	4	11/12	0.81	0.25	160,160,160,160	0
5	NAG	U	2	14/15	0.81	0.23	162,162,162,162	0
8	BMA	X	3	11/12	0.83	0.17	154,154,154,154	0
5	NAG	Q	1	14/15	0.83	0.24	115,115,115,115	0
6	BMA	V	3	11/12	0.83	0.20	140,140,140,140	0
5	NAG	Q	2	14/15	0.84	0.31	175,175,175,175	0
6	MAN	R	4	11/12	0.85	0.17	148,148,148,148	0
7	NAG	S	1	14/15	0.85	0.25	156,156,156,156	0
5	NAG	U	1	14/15	0.86	0.21	117,117,117,117	0
8	MAN	X	4	11/12	0.86	0.17	144,144,144,144	0
6	MAN	V	5	11/12	0.88	0.20	148,148,148,148	0
8	NAG	T	2	14/15	0.90	0.20	126,126,126,126	0
6	NAG	V	2	14/15	0.92	0.26	115,115,115,115	0
8	NAG	X	2	14/15	0.92	0.18	116,116,116,116	0
8	NAG	X	1	14/15	0.93	0.21	97,97,97,97	0
8	NAG	T	1	14/15	0.93	0.23	98,98,98,98	0
6	NAG	R	2	14/15	0.93	0.16	105,105,105,105	0
6	NAG	R	1	14/15	0.94	0.22	94,94,94,94	0

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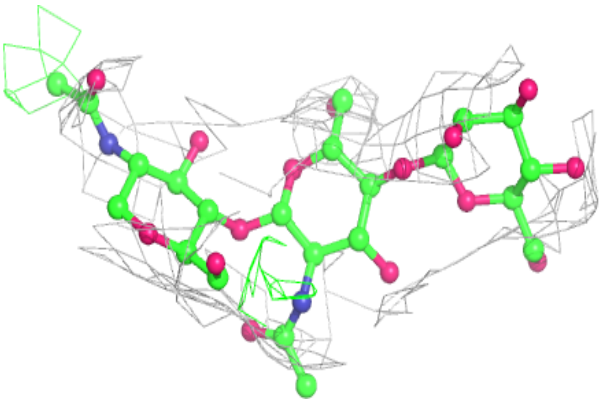
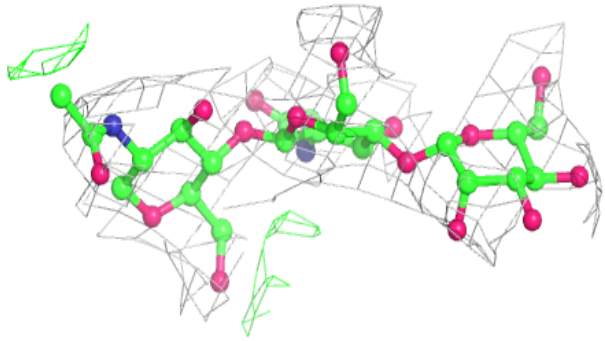
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	NAG	V	1	14/15	0.95	0.25	96,96,96,96	0

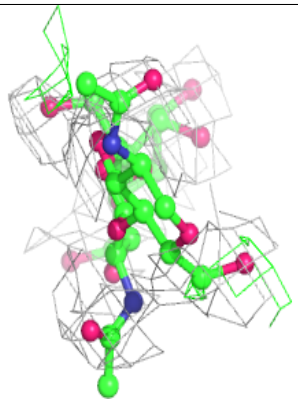
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain Q:

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

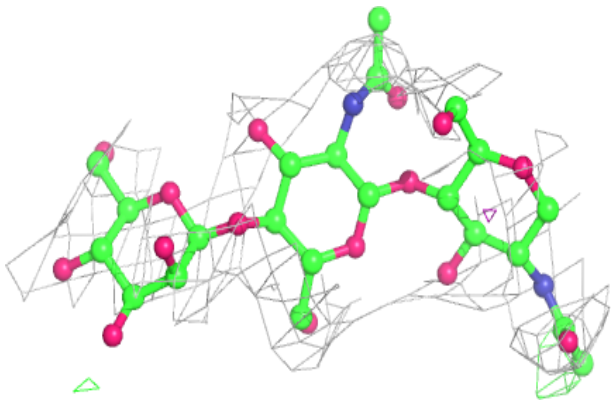


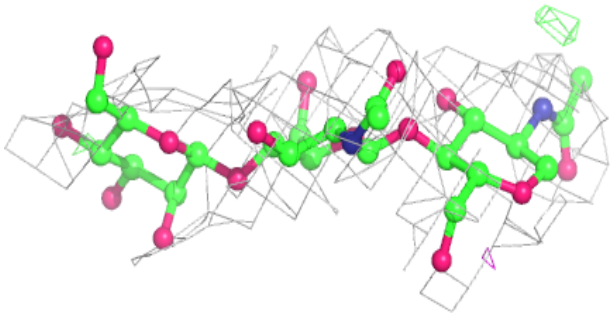


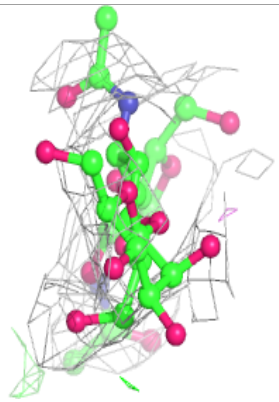


Electron density around Chain U:

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

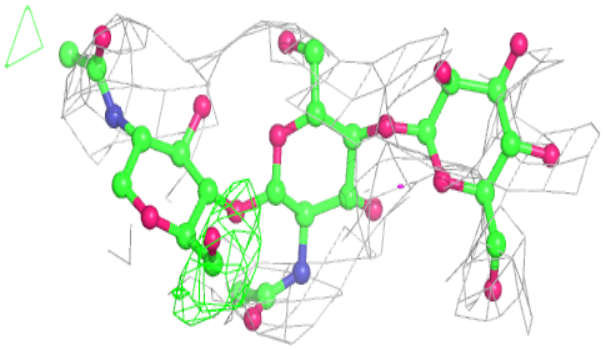


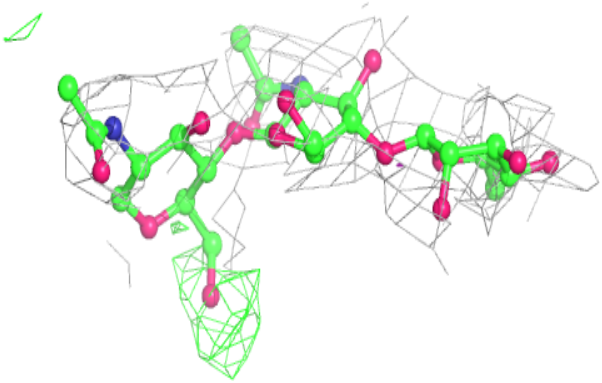


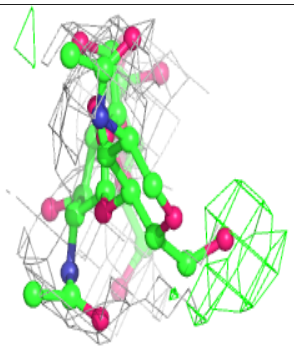


Electron density around Chain W:

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

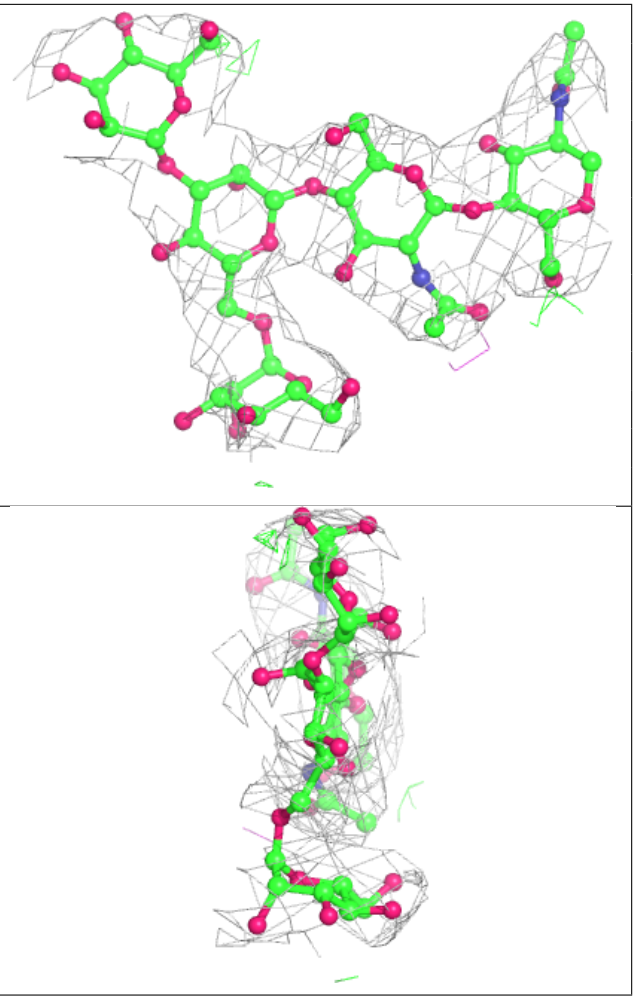


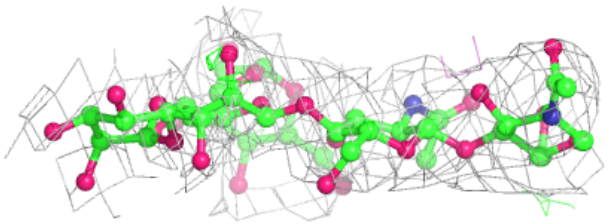




Electron density around Chain R:

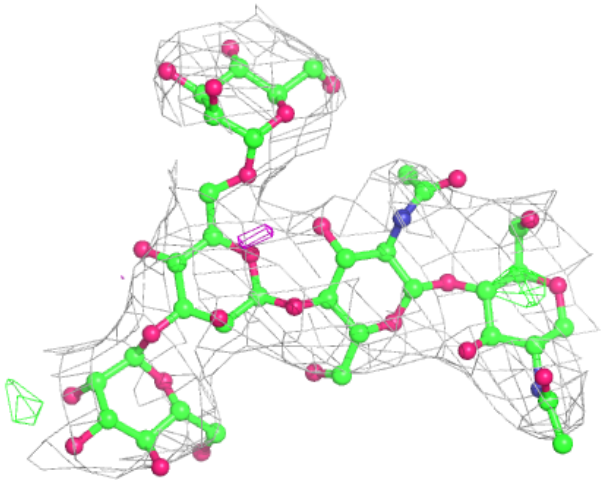
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

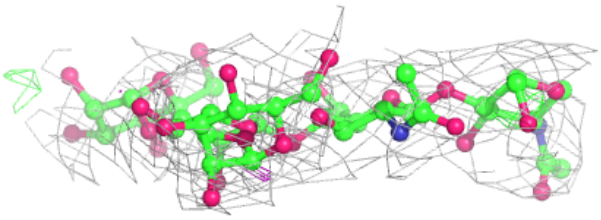


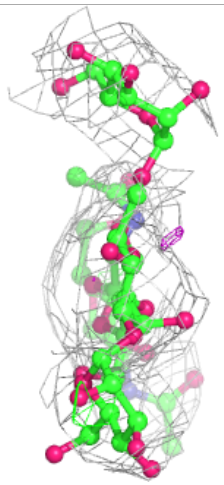


Electron density around Chain V:

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

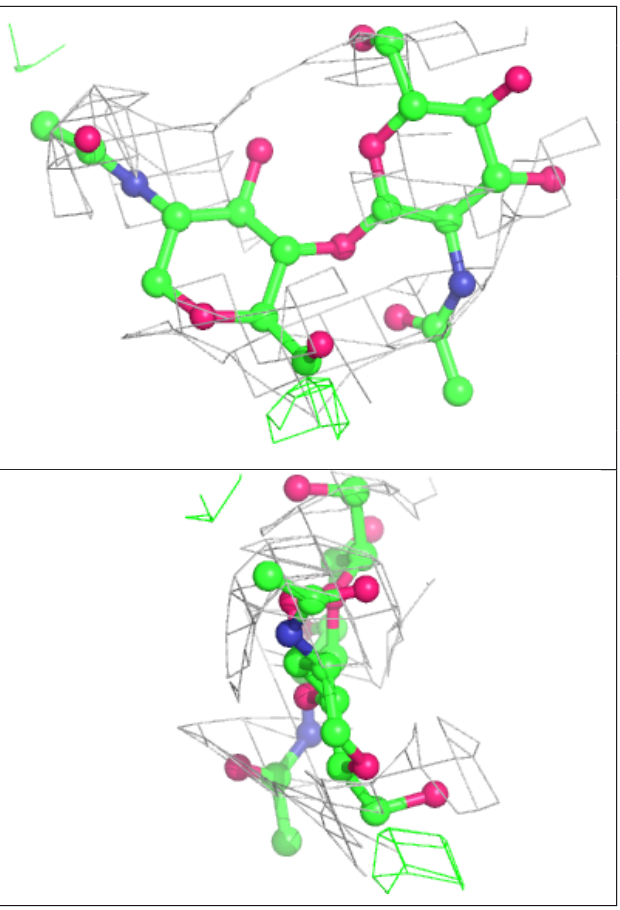


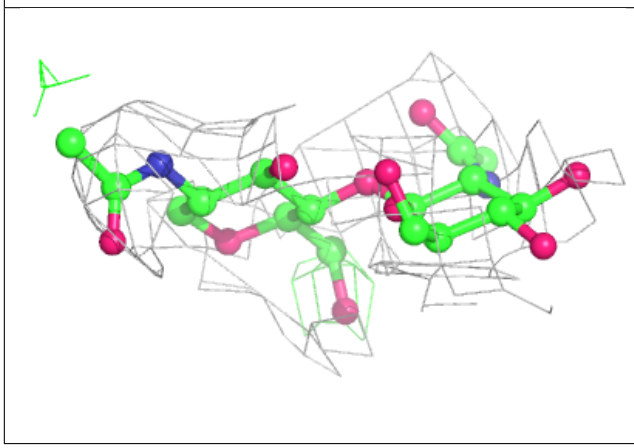




Electron density around Chain S:

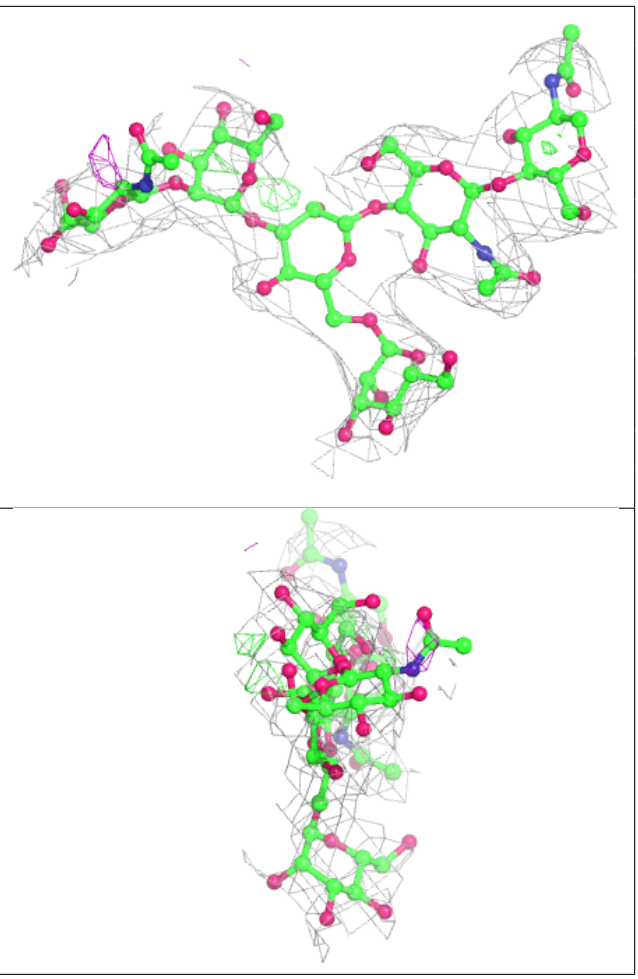
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

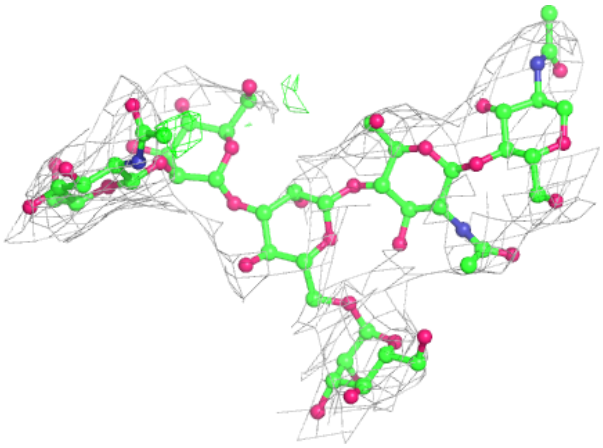
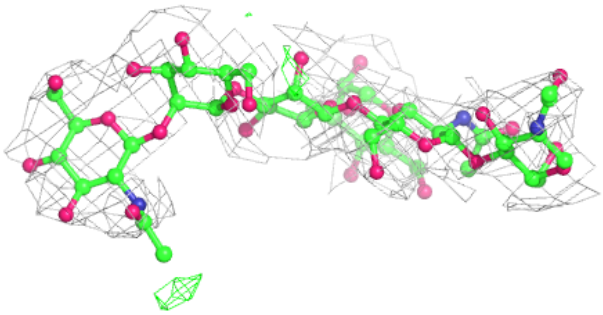
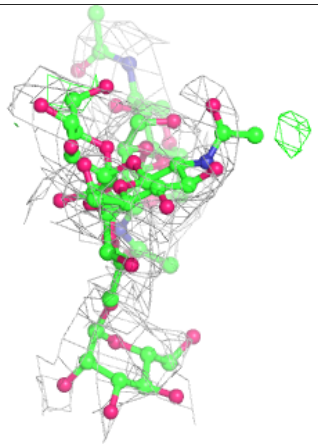




Electron density around Chain T:

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



Electron density around Chain X: 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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.