wwPDB X-ray Structure Validation Summary Report (i)

Oct 9, 2023 – 11:29 PM EDT

PDB ID	:	7RDW
Title	:	Crystal Structure of FH1 Fab bound to HXb2 HIV-1 gp120 core
Authors	:	Weidle, C.; Pancera, M.
Deposited on	:	2021-07-12
Resolution	:	3.55 Å(reported)

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

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

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

The following versions of software and data (see references (1)) were used in the production of this report:

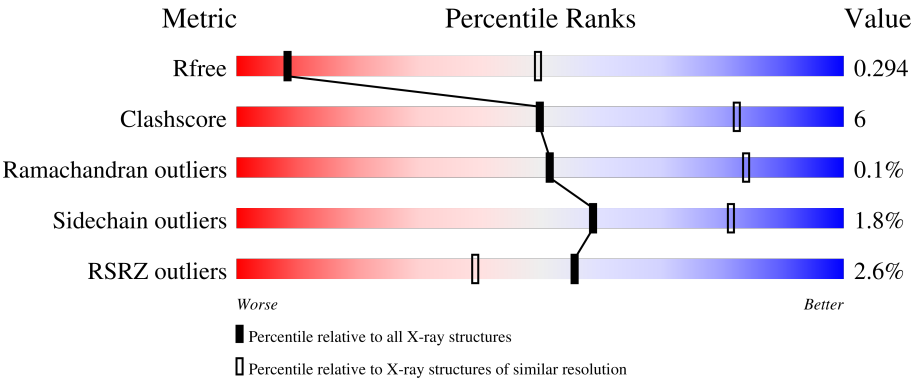
MolProbity	:	4.02b-467
Mogul	:	?.? (???), CSD ??CSD?? (????)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 3.55 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	1020 (3.62-3.50)
Clashscore	141614	1100 (3.62-3.50)
Ramachandran outliers	138981	1065 (3.62-3.50)
Sidechain outliers	138945	1066 (3.62-3.50)
RSRZ outliers	127900	1009 (3.64-3.48)

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	C	373	76% 11% 13%
1	D	373	71% 16% • 12%
1	M	373	72% 15% • 12%
1	N	373	75% 13% • 12%
2	G	225	3% 83% 10% • 7%

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Mol	Chain	Length	Quality of chain
2	U	225	8% 87% 8%
3	H	225	% 84% 9% 7%
3	Q	225	88% 6% 6%
4	I	211	6% 86% 13%
4	L	211	4% 90% 9%
4	R	211	90% 7%
4	V	211	14% 88% 6% 5%
5	O	3	33% 67%
5	c	3	100%
5	m	3	100%
5	y	3	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	NAG	O	2	X	-	-	-
5	NAG	c	2	X	-	-	-
5	BMA	c	3	X	-	-	-
5	NAG	m	2	X	-	-	-
5	NAG	y	2	X	-	-	-
6	NAG	N	608	-	-	-	X

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 21960 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 Glycoprotein 120.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	326	Total	C	N	O	S	0	0	0
			2390	1500	416	451	23			
1	D	329	Total	C	N	O	S	0	0	0
			2440	1524	428	466	22			
1	M	328	Total	C	N	O	S	0	0	0
			2405	1509	417	456	23			
1	N	329	Total	C	N	O	S	0	0	0
			2413	1513	423	454	23			

- Molecule 2 is a protein called FH1 Fab Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	210	Total	C	N	O	S	0	0	0
			1483	932	260	283	8			
2	U	208	Total	C	N	O	S	0	0	0
			1454	915	258	273	8			

- Molecule 3 is a protein called FH1 Fab Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	209	Total	C	N	O	S	0	0	0
			1502	953	262	279	8			
3	Q	212	Total	C	N	O	S	0	0	0
			1595	1010	271	306	8			

- Molecule 4 is a protein called FH1 Fab Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	I	209	Total	C	N	O	S	0	0	0
			1391	861	255	270	5			
4	L	208	Total	C	N	O	S	0	0	0
			1424	901	246	272	5			

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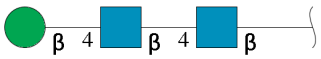
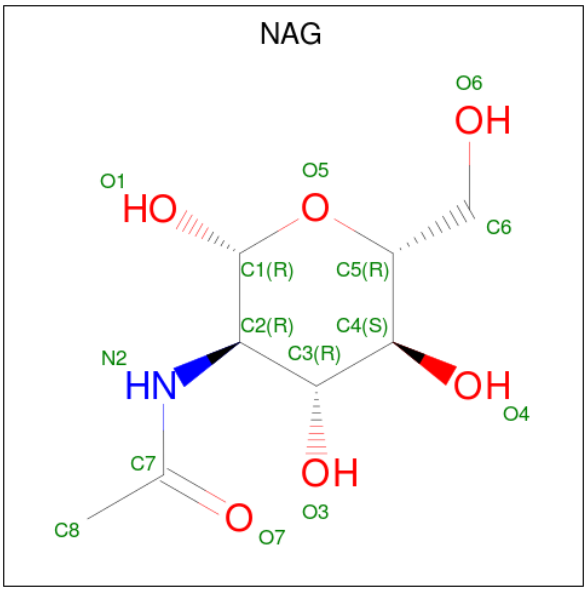
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	R	205	Total	C	N	O	S	0	0	0
			1439	901	244	289	5			
4	V	200	Total	C	N	O	S	0	0	0
			1344	838	240	261	5			

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



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

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

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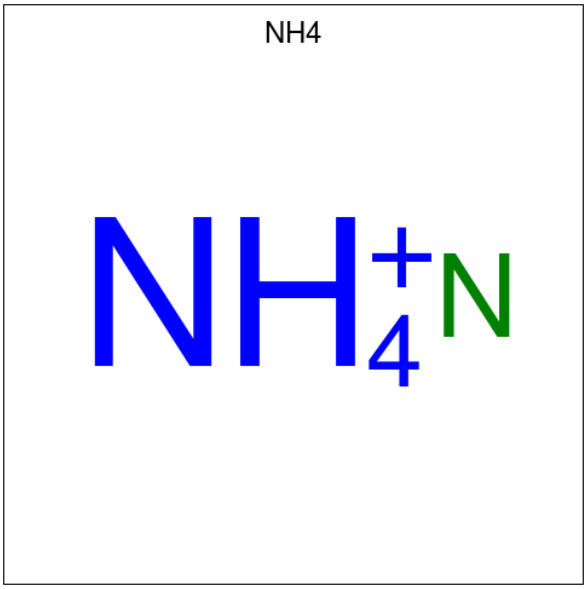
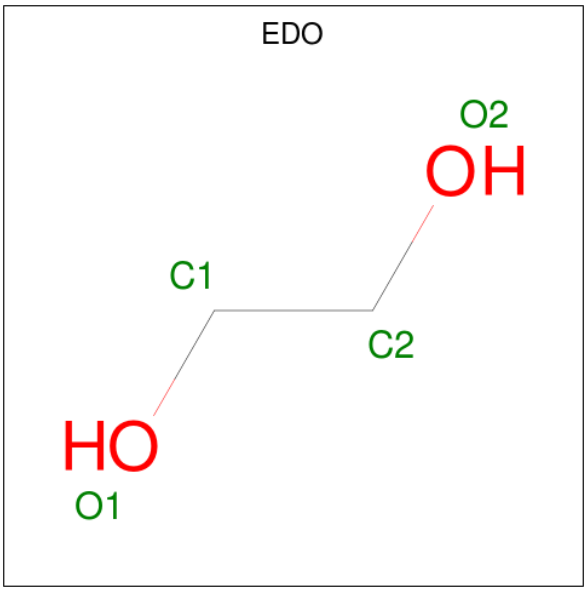
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	N	1	Total C N O 14 8 1 5	0	0
6	N	1	Total C N O 14 8 1 5	0	0
6	N	1	Total C N O 14 8 1 5	0	0
6	N	1	Total C N O 14 8 1 5	0	0
6	N	1	Total C N O 14 8 1 5	0	0
6	N	1	Total C N O 14 8 1 5	0	0

- Molecule 7 is AMMONIUM ION (three-letter code: NH4) (formula: H_4N).



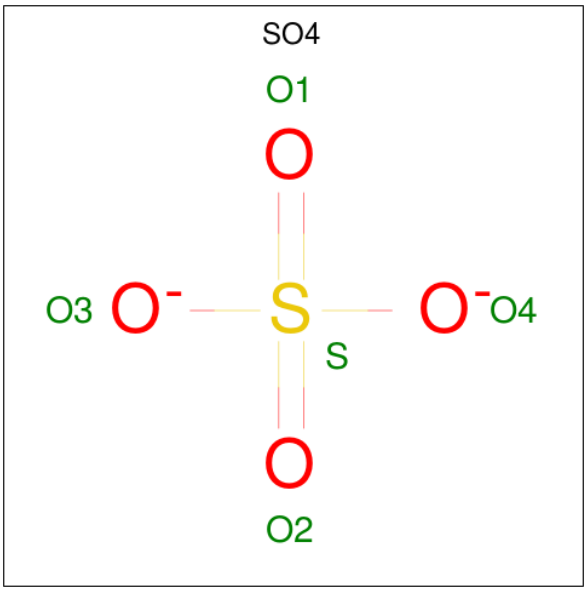
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	C	1	Total N 1 1	0	0
7	C	1	Total N 1 1	0	0
7	D	1	Total N 1 1	0	0
7	I	1	Total N 1 1	0	0

- Molecule 8 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 9 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	C	1	Total O S 5 4 1	0	0
9	D	1	Total O S 5 4 1	0	0
9	M	1	Total O S 5 4 1	0	0

- Molecule 10 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	C	11	Total O 11 11	0	0
10	D	15	Total O 15 15	0	0
10	G	8	Total O 8 8	0	0
10	H	4	Total O 4 4	0	0
10	I	1	Total O 1 1	0	0
10	L	5	Total O 5 5	0	0
10	M	12	Total O 12 12	0	0
10	N	16	Total O 16 16	0	0
10	Q	2	Total O 2 2	0	0

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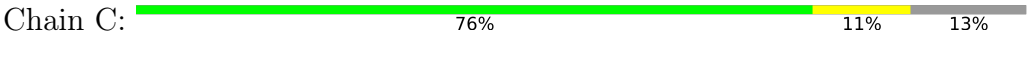
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	R	4	Total O 4 4	0	0
10	U	7	Total O 7 7	0	0
10	V	4	Total O 4 4	0	0

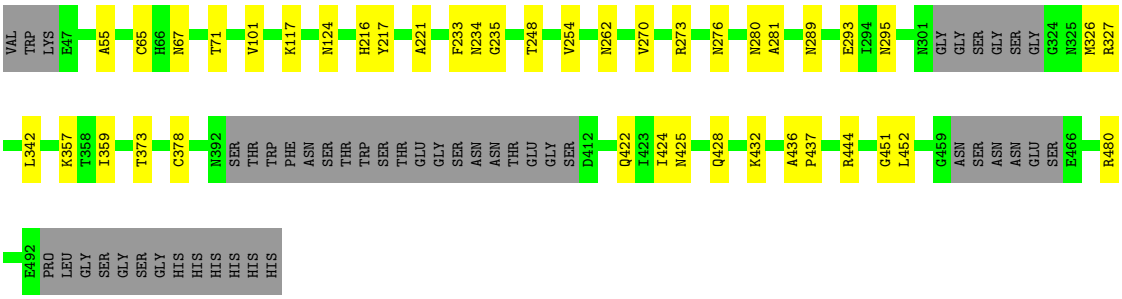
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Glycoprotein 120

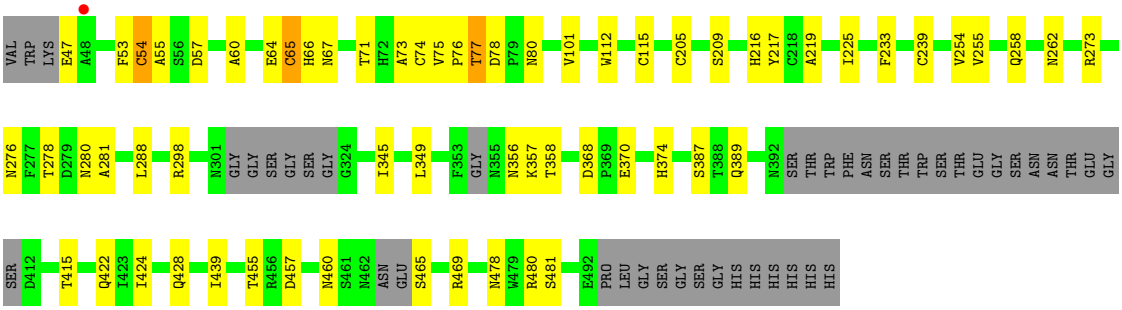
Chain C:





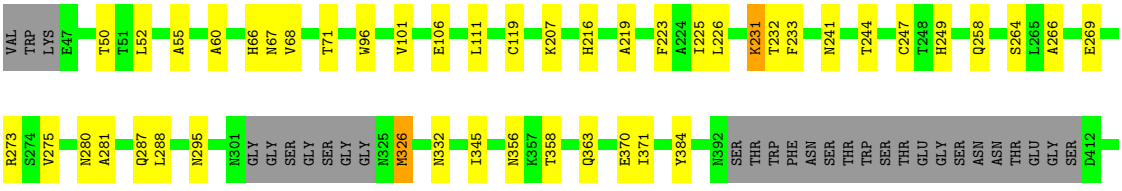
- Molecule 1: Glycoprotein 120

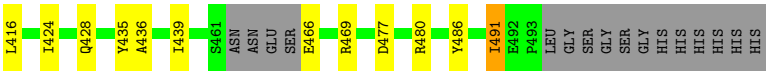
Chain D:



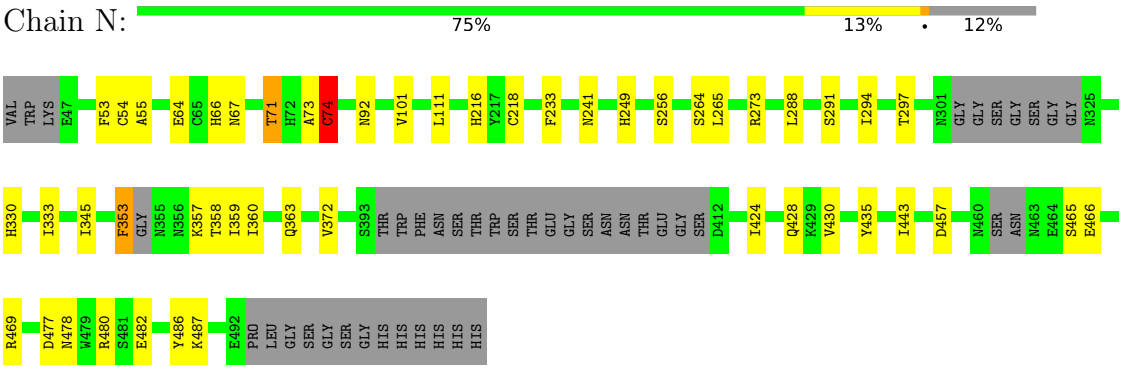
- Molecule 1: Glycoprotein 120

Chain M:

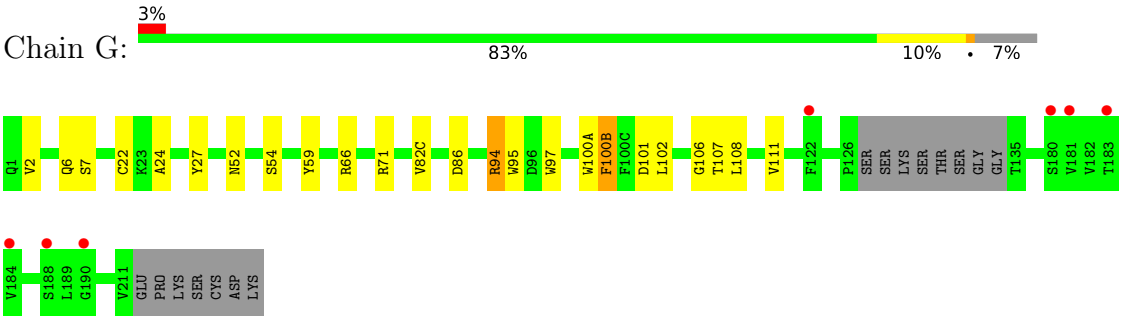




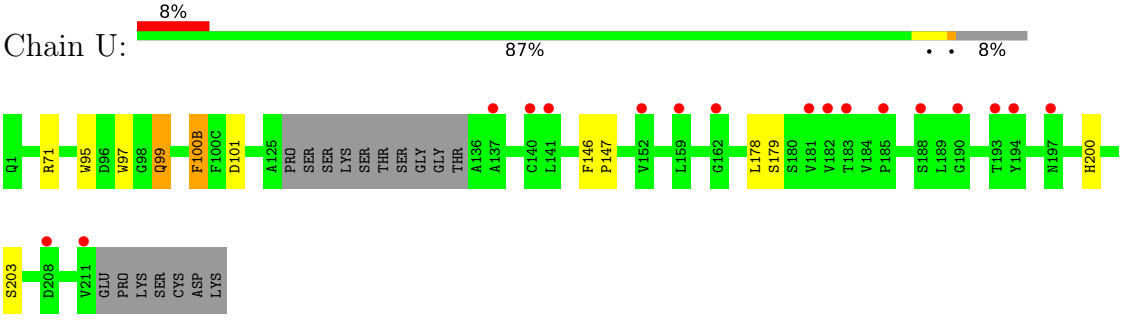
• Molecule 1: Glycoprotein 120



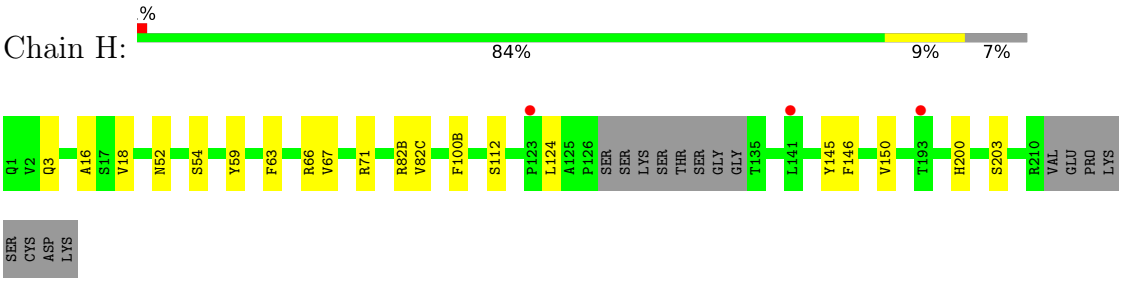
• Molecule 2: FH1 Fab Heavy Chain



• Molecule 2: FH1 Fab Heavy Chain

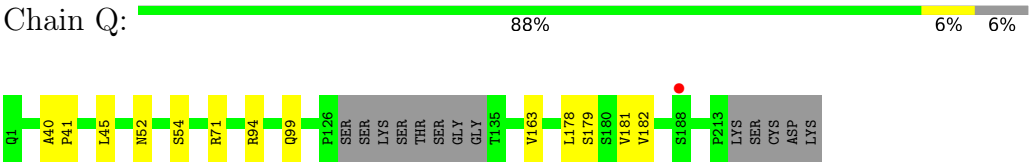


• Molecule 3: FH1 Fab Heavy Chain



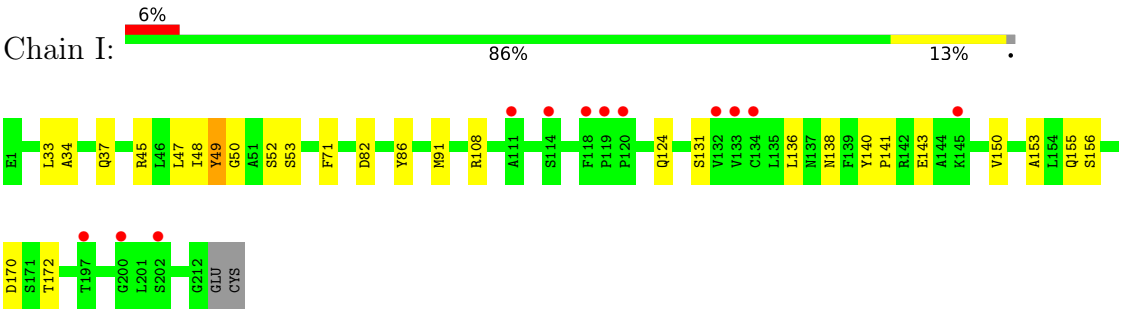
• Molecule 3: FH1 Fab Heavy Chain

Chain Q:



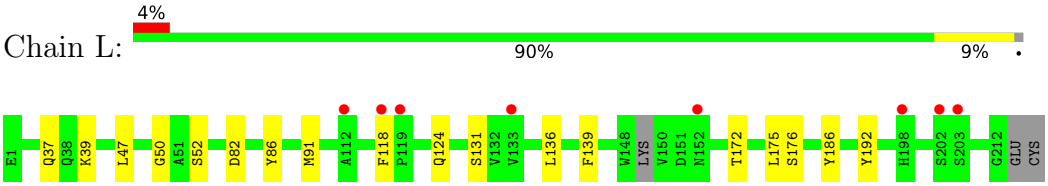
• Molecule 4: FH1 Fab Light Chain

Chain I:



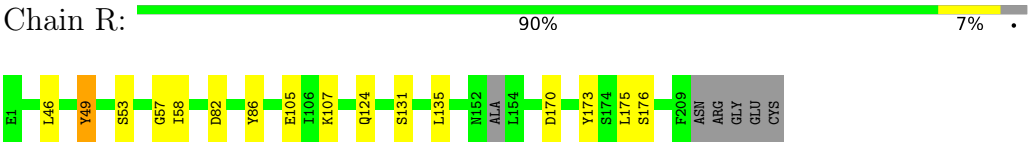
• Molecule 4: FH1 Fab Light Chain

Chain L:



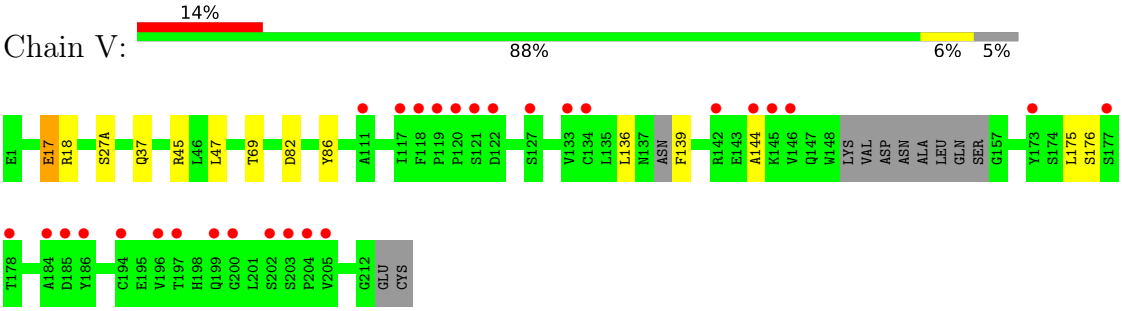
• Molecule 4: FH1 Fab Light Chain

Chain R:



• Molecule 4: FH1 Fab Light Chain

Chain V:

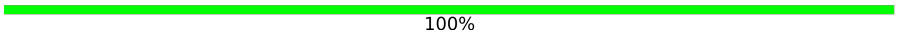


• Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:

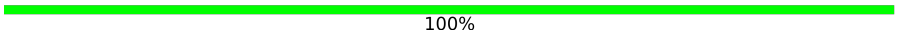
• Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain c:



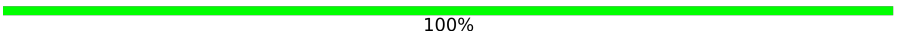
• Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain m:



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

Chain y:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	103.36Å 106.27Å 113.22Å 67.57° 76.67° 60.99°	Depositor
Resolution (Å)	50.18 – 3.55 50.18 – 3.55	Depositor EDS
% Data completeness (in resolution range)	76.8 (50.18-3.55) 76.9 (50.18-3.55)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.28 (at 3.57Å)	Xtriage
Refinement program	PHENIX 1.15.2_3472	Depositor
R, R_{free}	0.260 , 0.295 0.260 , 0.294	Depositor DCC
R_{free} test set	1842 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å^2)	61.8	Xtriage
Anisotropy	0.354	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 38.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.82	EDS
Total number of atoms	21960	wwPDB-VP
Average B, all atoms (Å^2)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.24% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, SO4, BMA, NH4, EDO, PCA

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	C	0.25	0/2440	0.42	0/3333
1	D	0.25	0/2489	0.44	0/3393
1	M	0.24	0/2455	0.43	0/3358
1	N	0.27	0/2462	0.50	1/3361 (0.0%)
2	G	0.25	0/1518	0.47	0/2084
2	U	0.25	0/1486	0.46	0/2039
3	H	0.25	0/1547	0.44	0/2120
3	Q	0.24	0/1641	0.44	0/2245
4	I	0.25	0/1416	0.45	0/1939
4	L	0.25	0/1456	0.43	0/1996
4	R	0.25	0/1473	0.43	0/2019
4	V	0.24	0/1371	0.43	0/1878
All	All	0.25	0/21754	0.45	1/29765 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	N	74	CYS	CA-CB-SG	-12.51	91.49	114.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2390	0	2159	30	0
1	D	2440	0	2222	46	0
1	M	2405	0	2180	34	0
1	N	2413	0	2183	36	0
2	G	1483	0	1225	15	0
2	U	1454	0	1203	14	0
3	H	1502	0	1276	11	0
3	Q	1595	0	1475	9	0
4	I	1391	0	1145	18	0
4	L	1424	0	1194	10	0
4	R	1439	0	1202	11	1
4	V	1344	0	1107	7	1
5	O	39	0	34	3	0
5	c	39	0	34	0	0
5	m	39	0	34	0	0
5	y	39	0	34	0	0
6	C	98	0	91	5	0
6	D	70	0	65	1	0
6	M	84	0	78	2	0
6	N	140	0	130	3	0
7	C	2	0	0	0	0
7	D	1	0	0	0	0
7	I	1	0	0	0	0
8	C	8	0	12	0	0
8	D	4	0	6	0	0
8	H	8	0	12	0	0
8	N	4	0	6	0	0
9	C	5	0	0	0	0
9	D	5	0	0	1	0
9	M	5	0	0	0	0
10	C	11	0	0	1	0
10	D	15	0	0	0	0
10	G	8	0	0	0	0
10	H	4	0	0	1	0
10	I	1	0	0	0	0
10	L	5	0	0	0	0
10	M	12	0	0	0	0
10	N	16	0	0	1	0
10	Q	2	0	0	0	0
10	R	4	0	0	0	0
10	U	7	0	0	0	0
10	V	4	0	0	0	0
All	All	21960	0	19107	231	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 6.

The worst 5 of 231 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:D:57:ASP:OD1	1:D:77:THR:OG1	1.83	0.96
1:M:358:THR:HG1	1:M:466:GLU:N	1.66	0.93
3:H:200:HIS:HD1	3:H:203:SER:HG	1.16	0.88
4:I:108:ARG:NH2	4:I:170:ASP:O	2.06	0.88
4:R:49:TYR:O	4:R:53:SER:OG	1.94	0.85

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)
4:R:57:GLY:O	4:V:45:ARG:NH1[1_565]	2.14	0.06

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	C	318/373 (85%)	302 (95%)	16 (5%)	0	100	100
1	D	319/373 (86%)	299 (94%)	20 (6%)	0	100	100
1	M	320/373 (86%)	302 (94%)	17 (5%)	1 (0%)	41	74
1	N	319/373 (86%)	305 (96%)	14 (4%)	0	100	100
2	G	206/225 (92%)	197 (96%)	8 (4%)	1 (0%)	29	67
2	U	204/225 (91%)	191 (94%)	13 (6%)	0	100	100
3	H	205/225 (91%)	195 (95%)	10 (5%)	0	100	100
3	Q	208/225 (92%)	202 (97%)	6 (3%)	0	100	100
4	I	207/211 (98%)	193 (93%)	14 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
4	L	204/211 (97%)	189 (93%)	14 (7%)	1 (0%)	29 67
4	R	201/211 (95%)	182 (90%)	19 (10%)	0	100 100
4	V	194/211 (92%)	183 (94%)	11 (6%)	0	100 100
All	All	2905/3236 (90%)	2740 (94%)	162 (6%)	3 (0%)	51 84

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	G	2	VAL
4	L	91	MET
1	M	269	GLU

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	C	244/328 (74%)	239 (98%)	5 (2%)	55 79
1	D	254/328 (77%)	249 (98%)	5 (2%)	55 79
1	M	247/328 (75%)	241 (98%)	6 (2%)	49 76
1	N	247/328 (75%)	243 (98%)	4 (2%)	62 83
2	G	124/190 (65%)	120 (97%)	4 (3%)	39 70
2	U	119/190 (63%)	116 (98%)	3 (2%)	47 75
3	H	130/191 (68%)	127 (98%)	3 (2%)	50 77
3	Q	166/191 (87%)	164 (99%)	2 (1%)	71 87
4	I	108/184 (59%)	107 (99%)	1 (1%)	78 90
4	L	118/184 (64%)	118 (100%)	0	100 100
4	R	129/184 (70%)	128 (99%)	1 (1%)	81 92
4	V	109/184 (59%)	108 (99%)	1 (1%)	78 90
All	All	1995/2810 (71%)	1960 (98%)	35 (2%)	59 81

5 of 35 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	Q	71	ARG
3	Q	94	ARG
2	U	99	GLN
2	G	94	ARG
2	G	71	ARG

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

Mol	Chain	Res	Type
1	D	66	HIS
2	U	52	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)

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

12 monosaccharides are modelled in this entry.

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	O	2	5	1/1/5/7	-	-
5	NAG	c	2	5	1/1/5/7	-	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	BMA	c	3	5	1/1/4/5	-	-
5	NAG	m	2	5	1/1/5/7	-	-
5	NAG	y	2	5	1/1/5/7	-	-

There are no bond length outliers.

There are no bond angle outliers.

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	O	2	NAG	C1
5	c	2	NAG	C1
5	c	3	BMA	C1
5	m	2	NAG	C1
5	y	2	NAG	C1

There are no torsion outliers.

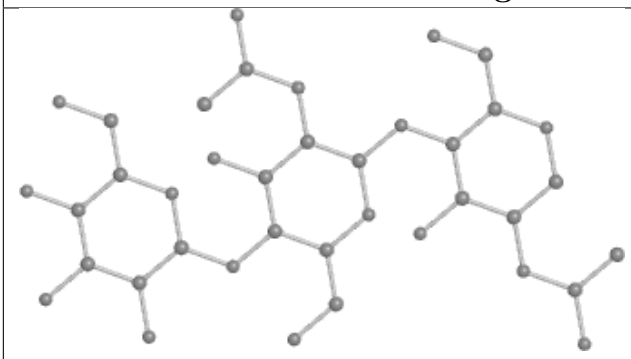
There are no ring outliers.

1 monomer is involved in 1 short contact:

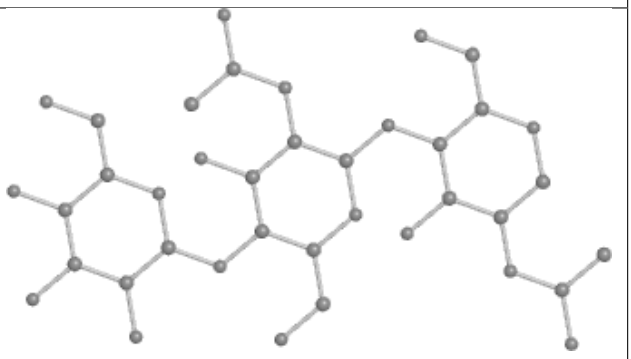
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	O	2	NAG	1	0

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

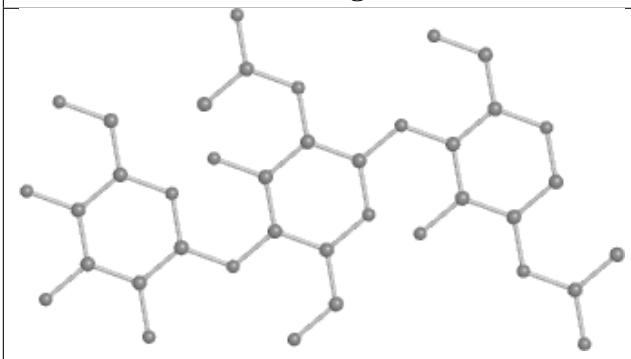
Oligosaccharide Chain O



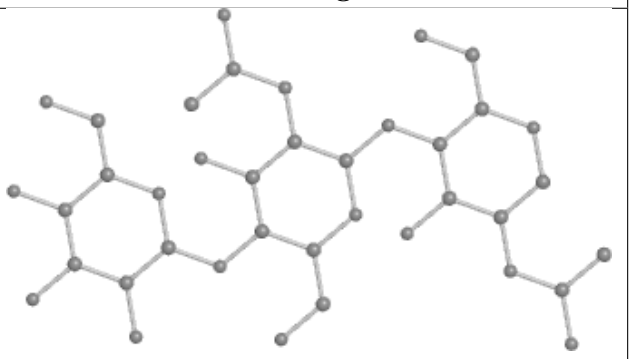
Bond lengths



Bond angles

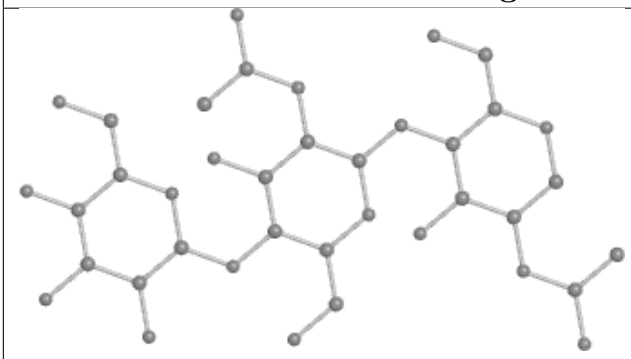


Torsions

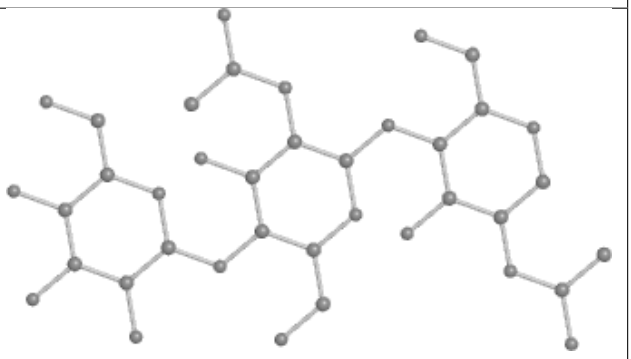


Rings

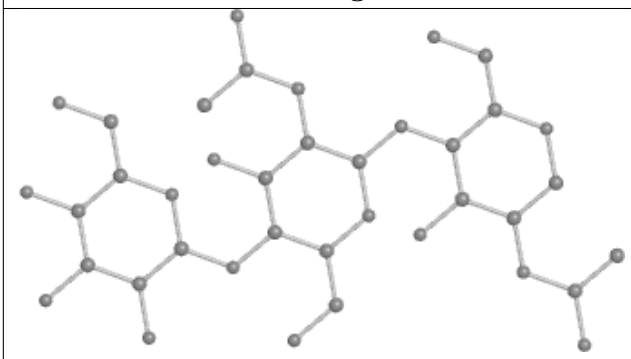
Oligosaccharide Chain c



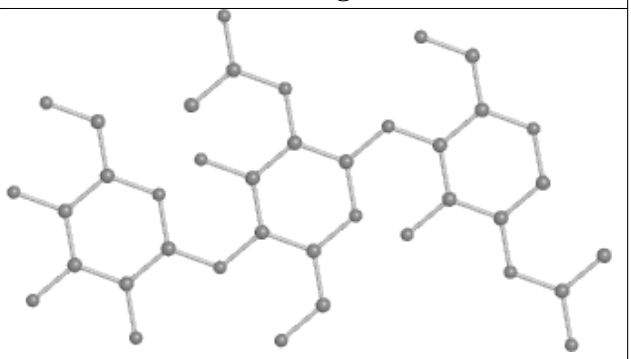
Bond lengths



Bond angles

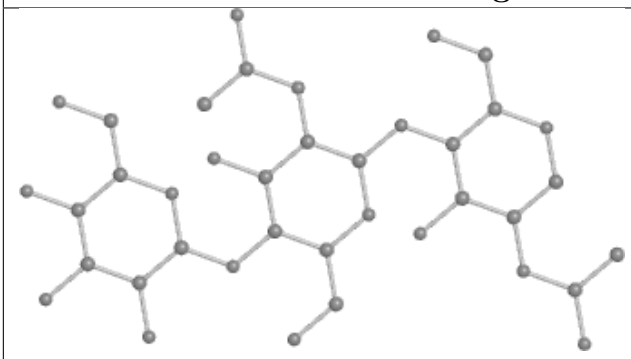


Torsions

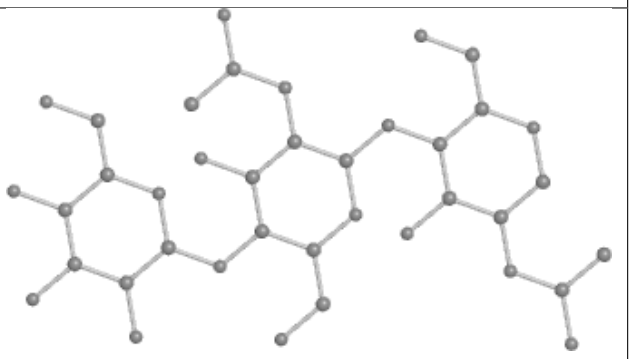


Rings

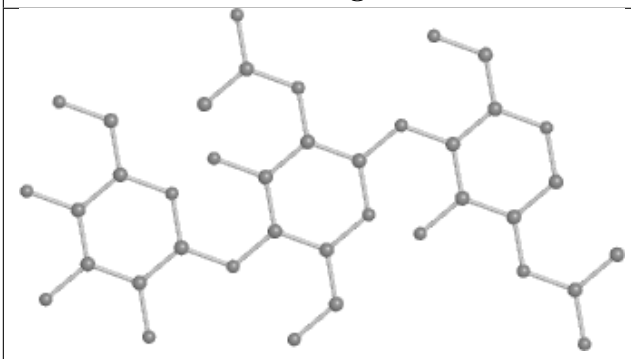
Oligosaccharide Chain m



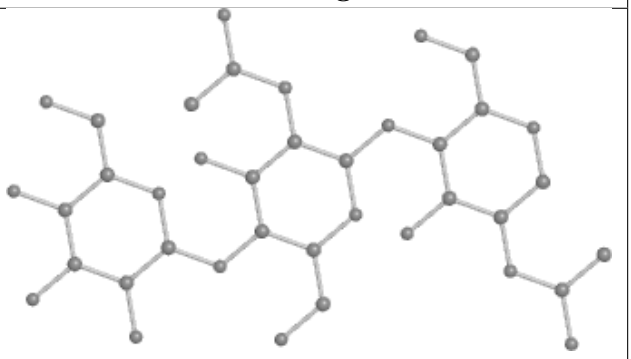
Bond lengths



Bond angles

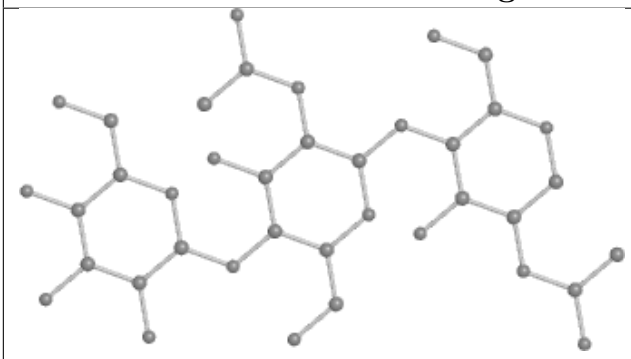


Torsions

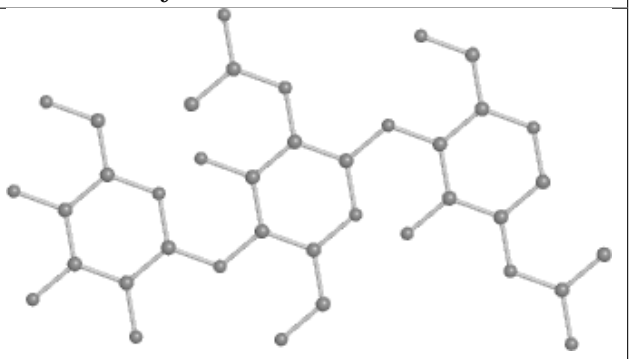


Rings

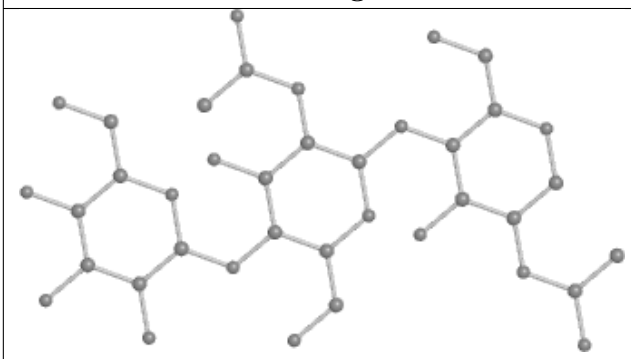
Oligosaccharide Chain y



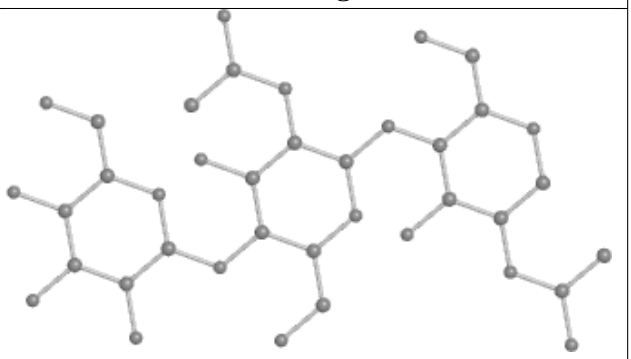
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry (i)

Of 41 ligands modelled in this entry, 4 are modelled with single atom - leaving 37 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	C	326/373 (87%)	-0.50	0 100 100	30, 62, 95, 128	0
1	D	329/373 (88%)	-0.55	1 (0%) 94 88	26, 60, 89, 114	0
1	M	328/373 (87%)	-0.50	0 100 100	27, 60, 93, 106	0
1	N	329/373 (88%)	-0.50	0 100 100	29, 62, 92, 117	0
2	G	209/225 (92%)	-0.19	7 (3%) 46 32	36, 65, 130, 141	0
2	U	207/225 (92%)	0.14	17 (8%) 11 8	35, 60, 164, 172	0
3	H	209/225 (92%)	-0.42	3 (1%) 75 60	29, 59, 117, 137	0
3	Q	212/225 (94%)	-0.49	1 (0%) 91 83	35, 62, 100, 114	0
4	I	209/211 (99%)	-0.12	12 (5%) 23 14	37, 87, 143, 152	0
4	L	208/211 (98%)	-0.30	8 (3%) 40 27	31, 73, 123, 127	0
4	R	205/211 (97%)	-0.48	0 100 100	32, 74, 108, 121	0
4	V	200/211 (94%)	0.24	29 (14%) 2 2	32, 81, 169, 186	0
All	All	2971/3236 (91%)	-0.34	78 (2%) 56 39	26, 64, 137, 186	0

The worst 5 of 78 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	V	133	VAL	9.2
4	V	145	LYS	9.1
2	U	140	CYS	8.4
4	V	134	CYS	8.2
4	V	144	ALA	7.8

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

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	PCA	U	1	8/9	0.90	0.17	70,77,82,91	0
2	PCA	G	1	8/9	0.92	0.14	64,67,78,79	0

6.3 Carbohydrates (i)

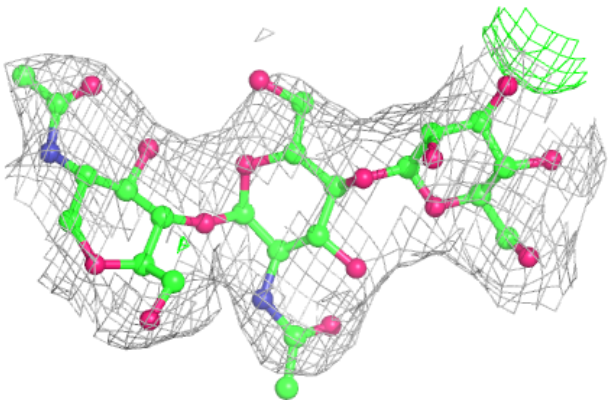
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

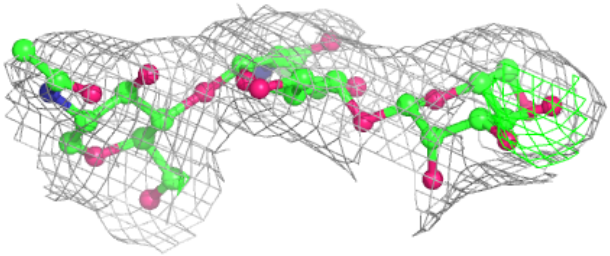
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	BMA	m	3	11/12	0.79	0.22	50,62,72,74	0
5	NAG	y	1	14/15	0.80	0.27	54,66,77,78	0
5	BMA	c	3	11/12	0.82	0.19	55,70,80,84	0
5	BMA	O	3	11/12	0.87	0.18	49,56,70,84	0
5	NAG	m	1	14/15	0.90	0.17	51,64,72,74	0
5	NAG	m	2	14/15	0.90	0.20	59,74,81,86	0
5	NAG	c	2	14/15	0.92	0.17	60,68,82,85	0
5	NAG	O	1	14/15	0.93	0.23	46,54,62,67	0
5	NAG	c	1	14/15	0.93	0.20	46,50,64,66	0
5	BMA	y	3	11/12	0.94	0.12	56,61,78,87	0
5	NAG	y	2	14/15	0.95	0.15	58,70,79,86	0
5	NAG	O	2	14/15	0.95	0.18	54,65,74,83	0

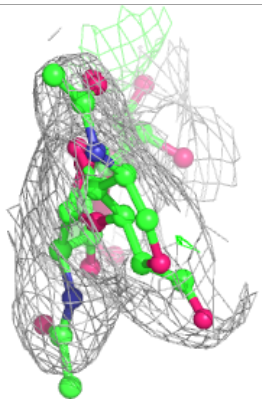
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain O:

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

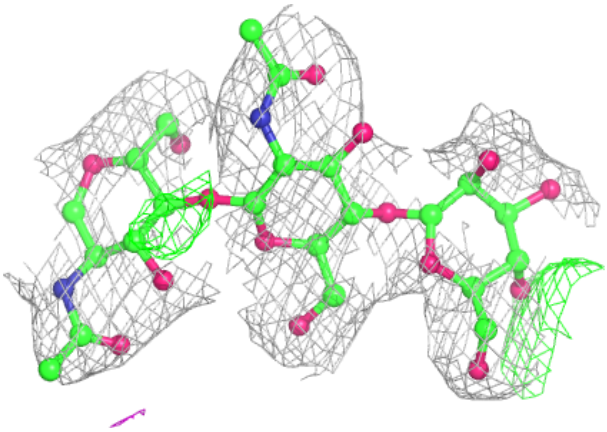


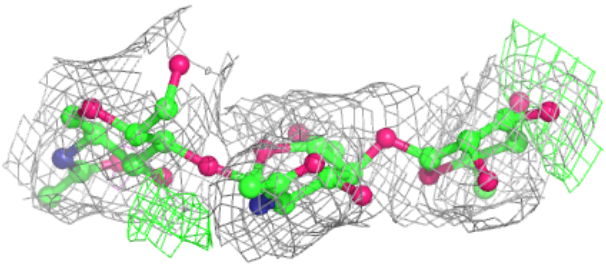


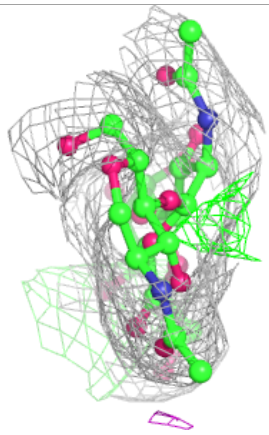


Electron density around Chain c:

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

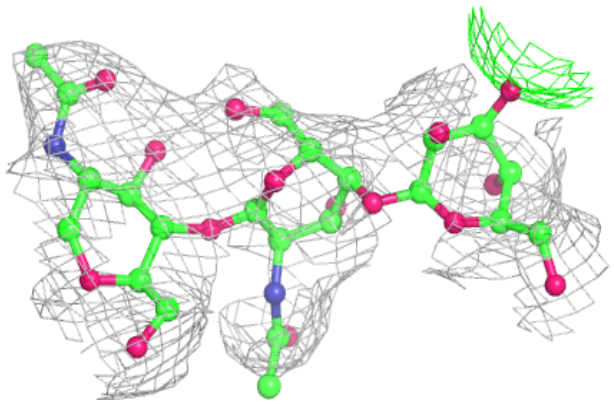


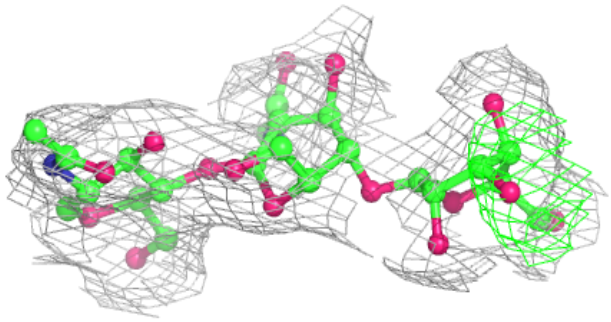


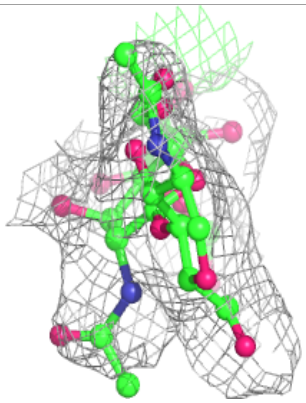


Electron density around Chain m:

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

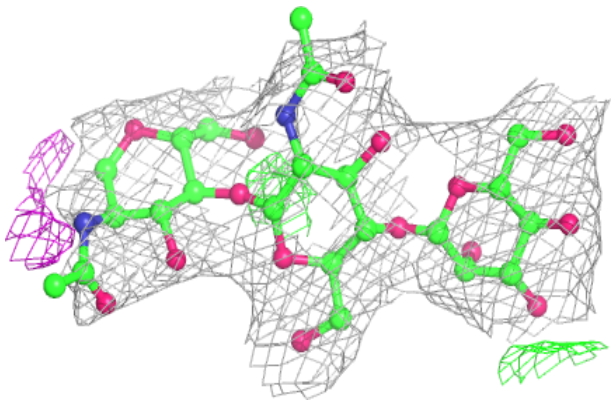


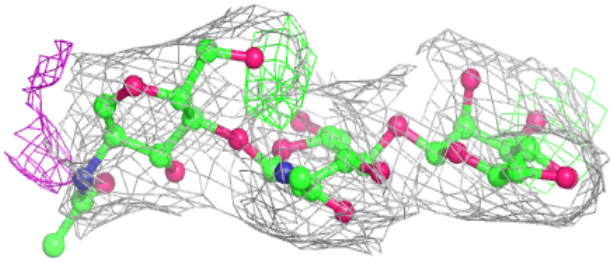


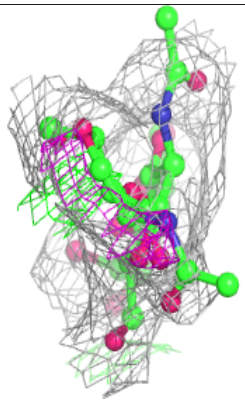


Electron density around Chain y:

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







6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	NAG	M	605	14/15	0.70	0.22	92,99,109,110	0
6	NAG	M	603	14/15	0.72	0.39	94,125,140,144	0
6	NAG	M	602	14/15	0.73	0.32	90,97,106,109	0
6	NAG	N	603	14/15	0.73	0.20	84,98,107,107	0
6	NAG	D	603	14/15	0.75	0.28	103,123,132,136	0
8	EDO	C	610	4/4	0.75	0.27	69,72,73,77	0
6	NAG	M	604	14/15	0.77	0.32	107,114,130,130	0
6	NAG	N	608	14/15	0.78	0.46	146,163,168,171	0
6	NAG	C	602	14/15	0.78	0.30	96,105,110,127	0
6	NAG	C	604	14/15	0.81	0.36	106,116,130,135	0
6	NAG	N	607	14/15	0.81	0.36	94,110,128,133	0
6	NAG	C	607	14/15	0.83	0.15	93,107,114,117	0
6	NAG	N	601	14/15	0.83	0.31	68,80,85,88	0
6	NAG	N	609	14/15	0.84	0.18	82,93,99,102	0
6	NAG	D	605	14/15	0.84	0.20	62,86,95,96	0
6	NAG	M	601	14/15	0.85	0.25	81,88,101,108	0
6	NAG	N	605	14/15	0.85	0.23	84,108,134,140	0
6	NAG	N	610	14/15	0.85	0.18	65,105,110,113	0
6	NAG	C	605	14/15	0.85	0.17	76,85,89,90	0
8	EDO	H	301	4/4	0.85	0.18	50,53,64,66	0
6	NAG	C	603	14/15	0.86	0.28	101,109,118,132	0
6	NAG	N	604	14/15	0.87	0.17	70,85,93,98	0
6	NAG	N	606	14/15	0.87	0.30	74,91,109,110	0
8	EDO	C	611	4/4	0.88	0.21	50,62,69,75	0
6	NAG	N	602	14/15	0.89	0.25	89,97,108,123	0
6	NAG	D	604	14/15	0.89	0.16	82,88,97,98	0
6	NAG	C	606	14/15	0.89	0.17	85,94,104,110	0
6	NAG	D	602	14/15	0.91	0.23	82,98,108,115	0
8	EDO	N	611	4/4	0.91	0.19	69,70,75,80	0
6	NAG	D	601	14/15	0.92	0.20	62,77,84,92	0
6	NAG	C	601	14/15	0.92	0.17	58,69,73,75	0
9	SO4	C	612	5/5	0.92	0.23	79,94,107,113	0
8	EDO	D	607	4/4	0.93	0.20	42,55,57,62	0
7	NH4	D	606	1/1	0.94	0.39	17,17,17,17	0
8	EDO	H	302	4/4	0.94	0.12	33,37,38,38	0
6	NAG	M	606	14/15	0.95	0.19	64,80,90,101	0
7	NH4	C	609	1/1	0.95	0.40	4,4,4,4	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
9	SO4	D	608	5/5	0.96	0.15	62,63,66,70	0
7	NH4	C	608	1/1	0.97	0.37	24,24,24,24	0
7	NH4	I	301	1/1	0.97	0.42	21,21,21,21	0
9	SO4	M	607	5/5	0.97	0.14	66,68,83,88	0

6.5 Other polymers (i)

There are no such residues in this entry.