wwPDB X-ray Structure Validation Summary Report (i)

Sep 26, 2023 – 08:07 PM EDT

PDB ID	:	6CCB
Title	:	Crystal structure of 253-11 SOSIP trimer in complex with 10-1074 Fab
Authors	:	Moyo, T.; Ereno-Orbea, J.; Dorfman, J.; Julien, J.P.
Deposited on	:	2018-02-06
Resolution	:	6.50 Å(reported)

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

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

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

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

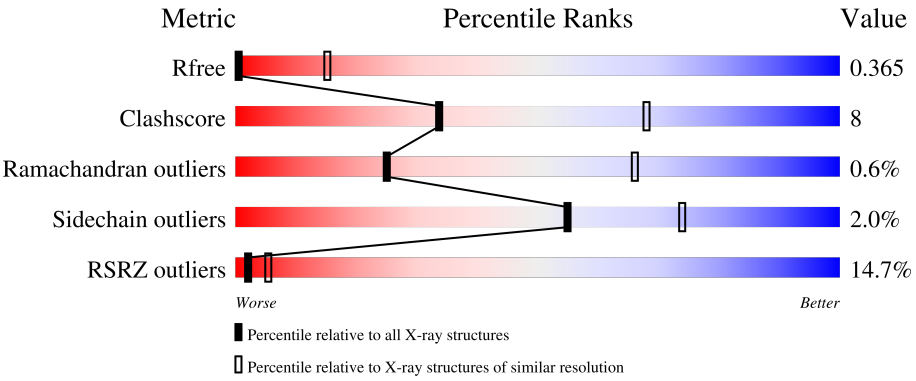
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 6.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1000 (9.00-3.90)
Clashscore	141614	1064 (9.00-3.90)
Ramachandran outliers	138981	1012 (9.00-3.88)
Sidechain outliers	138945	1010 (9.00-3.84)
RSRZ outliers	127900	1002 (9.00-3.80)

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	162	14% 60% 20% · 19%
1	B	162	12% 61% 19% · 19%
2	C	486	13% 65% 24% · 9%
2	G	486	12% 67% 22% · 9%
3	D	237	16% 78% 19% ·

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Mol	Chain	Length	Quality of chain
3	H	237	11% 74% 22%
4	E	215	16% 81% 17%
4	L	215	17% 82% 15%
5	F	6	33% 67%
6	I	10	30% 40% 30%
7	J	4	75% 25%
8	K	8	38% 38% 25%

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	F	1	-	-	-	X
6	NAG	I	1	-	-	-	X
7	MAN	J	4	-	-	-	X
8	NAG	K	1	-	-	-	X
8	MAN	K	5	-	-	-	X
8	MAN	K	6	-	-	-	X
8	MAN	K	8	-	-	-	X
9	NAG	A	701	-	-	-	X
9	NAG	A	702	-	-	-	X
9	NAG	B	701	-	-	-	X
9	NAG	B	702	-	-	-	X
9	NAG	C	602	-	-	-	X
9	NAG	C	603	-	-	-	X
9	NAG	C	604	-	-	-	X
9	NAG	C	605	-	-	-	X
9	NAG	C	606	-	-	-	X
9	NAG	C	625	-	-	-	X
9	NAG	C	626	-	-	-	X
9	NAG	C	627	-	-	-	X
9	NAG	C	628	-	-	-	X
9	NAG	C	629	-	-	-	X
9	NAG	C	630	-	-	-	X
9	NAG	G	602	-	-	-	X
9	NAG	G	603	-	-	-	X
9	NAG	G	604	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
9	NAG	G	605	-	-	-	X
9	NAG	G	610	-	-	-	X
9	NAG	G	620	-	-	-	X
9	NAG	G	621	-	-	-	X
9	NAG	G	622	-	-	-	X
9	NAG	G	623	-	-	-	X
9	NAG	G	624	-	-	-	X
9	NAG	G	625	-	-	-	X
9	NAG	G	626	-	-	-	X

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 16470 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 41.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	131	Total	C	N	O	S	0	0	0
			1047	663	178	201	5			
1	B	131	Total	C	N	O	S	0	0	0
			1047	663	178	201	5			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	605	CYS	THR	engineered mutation	UNP B2YFS0
A	665	GLY	-	expression tag	UNP B2YFS0
A	666	THR	-	expression tag	UNP B2YFS0
A	667	LYS	-	expression tag	UNP B2YFS0
A	668	HIS	-	expression tag	UNP B2YFS0
A	669	HIS	-	expression tag	UNP B2YFS0
A	670	HIS	-	expression tag	UNP B2YFS0
A	671	HIS	-	expression tag	UNP B2YFS0
A	672	HIS	-	expression tag	UNP B2YFS0
A	673	HIS	-	expression tag	UNP B2YFS0
B	605	CYS	THR	engineered mutation	UNP B2YFS0
B	665	GLY	-	expression tag	UNP B2YFS0
B	666	THR	-	expression tag	UNP B2YFS0
B	667	LYS	-	expression tag	UNP B2YFS0
B	668	HIS	-	expression tag	UNP B2YFS0
B	669	HIS	-	expression tag	UNP B2YFS0
B	670	HIS	-	expression tag	UNP B2YFS0
B	671	HIS	-	expression tag	UNP B2YFS0
B	672	HIS	-	expression tag	UNP B2YFS0
B	673	HIS	-	expression tag	UNP B2YFS0

- Molecule 2 is a protein called Glycoprotein 120.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	440	Total	C	N	O	S	0	0	0
			3438	2156	602	652	28			
2	G	440	Total	C	N	O	S	0	0	0
			3438	2156	602	652	28			

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	28	GLU	-	expression tag	UNP B2YFS0
C	29	THR	-	expression tag	UNP B2YFS0
C	30	GLY	-	expression tag	UNP B2YFS0
C	295	ASN	THR	engineered mutation	UNP B2YFS0
C	297	THR	ILE	engineered mutation	UNP B2YFS0
C	501	CYS	ALA	engineered mutation	UNP B2YFS0
C	507	GLY	-	expression tag	UNP B2YFS0
C	508	ARG	-	expression tag	UNP B2YFS0
C	509	ARG	-	expression tag	UNP B2YFS0
C	510	ARG	-	expression tag	UNP B2YFS0
C	511	ARG	-	expression tag	UNP B2YFS0
C	512	ARG	-	expression tag	UNP B2YFS0
C	513	ARG	-	expression tag	UNP B2YFS0
G	28	GLU	-	expression tag	UNP B2YFS0
G	29	THR	-	expression tag	UNP B2YFS0
G	30	GLY	-	expression tag	UNP B2YFS0
G	295	ASN	THR	engineered mutation	UNP B2YFS0
G	297	THR	ILE	engineered mutation	UNP B2YFS0
G	501	CYS	ALA	engineered mutation	UNP B2YFS0
G	507	GLY	-	expression tag	UNP B2YFS0
G	508	ARG	-	expression tag	UNP B2YFS0
G	509	ARG	-	expression tag	UNP B2YFS0
G	510	ARG	-	expression tag	UNP B2YFS0
G	511	ARG	-	expression tag	UNP B2YFS0
G	512	ARG	-	expression tag	UNP B2YFS0
G	513	ARG	-	expression tag	UNP B2YFS0

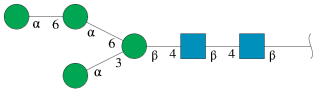
- Molecule 3 is a protein called 10-1074 FAB heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	230	Total	C	N	O	S	0	0	0
			1753	1108	293	345	7			
3	H	230	Total	C	N	O	S	0	0	0
			1753	1108	293	345	7			

- Molecule 4 is a protein called 10-1074 Fab light chain.

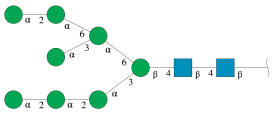
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	211	Total	C	N	O	S	0	0	0
			1607	1006	281	314	6			
4	L	211	Total	C	N	O	S	0	0	0
			1607	1006	281	314	6			

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	F	6	Total	C	N	O	0	0	0
			72	40	2	30			

- Molecule 6 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[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.

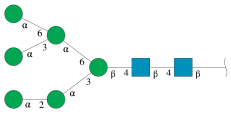


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	I	10	Total	C	N	O	0	0	0
			116	64	2	50			

- Molecule 7 is an oligosaccharide called 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.

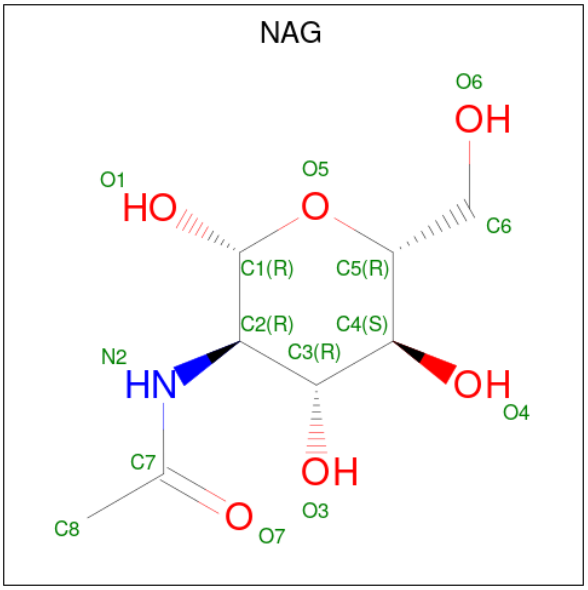
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
7	J	4	Total C N O 50 28 2 20	0	0	0

- Molecule 8 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]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
8	K	8	Total C N O 94 52 2 40	0	0	0

- Molecule 9 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total C N O 14 8 1 5	0	0
9	A	1	Total C N O 14 8 1 5	0	0
9	B	1	Total C N O 14 8 1 5	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	B	1	Total C N O 14 8 1 5	0	0
9	C	1	Total C N O 14 8 1 5	0	0
9	C	1	Total C N O 14 8 1 5	0	0
9	C	1	Total C N O 14 8 1 5	0	0
9	C	1	Total C N O 14 8 1 5	0	0
9	C	1	Total C N O 14 8 1 5	0	0
9	C	1	Total C N O 14 8 1 5	0	0
9	C	1	Total C N O 14 8 1 5	0	0
9	C	1	Total C N O 14 8 1 5	0	0
9	C	1	Total C N O 14 8 1 5	0	0
9	C	1	Total C N O 14 8 1 5	0	0
9	C	1	Total C N O 14 8 1 5	0	0
9	C	1	Total C N O 14 8 1 5	0	0
9	C	1	Total C N O 14 8 1 5	0	0
9	C	1	Total C N O 14 8 1 5	0	0
9	G	1	Total C N O 14 8 1 5	0	0
9	G	1	Total C N O 14 8 1 5	0	0
9	G	1	Total C N O 14 8 1 5	0	0
9	G	1	Total C N O 14 8 1 5	0	0
9	G	1	Total C N O 14 8 1 5	0	0
9	G	1	Total C N O 14 8 1 5	0	0

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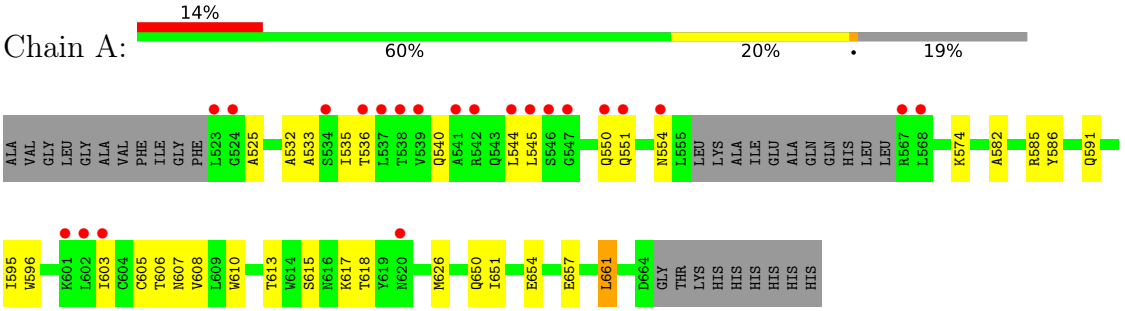
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	G	1	Total 14	C 8	N 1	O 5	0	0
9	G	1	Total 14	C 8	N 1	O 5	0	0
9	G	1	Total 14	C 8	N 1	O 5	0	0
9	G	1	Total 14	C 8	N 1	O 5	0	0
9	G	1	Total 14	C 8	N 1	O 5	0	0
9	G	1	Total 14	C 8	N 1	O 5	0	0
9	G	1	Total 14	C 8	N 1	O 5	0	0
9	G	1	Total 14	C 8	N 1	O 5	0	0

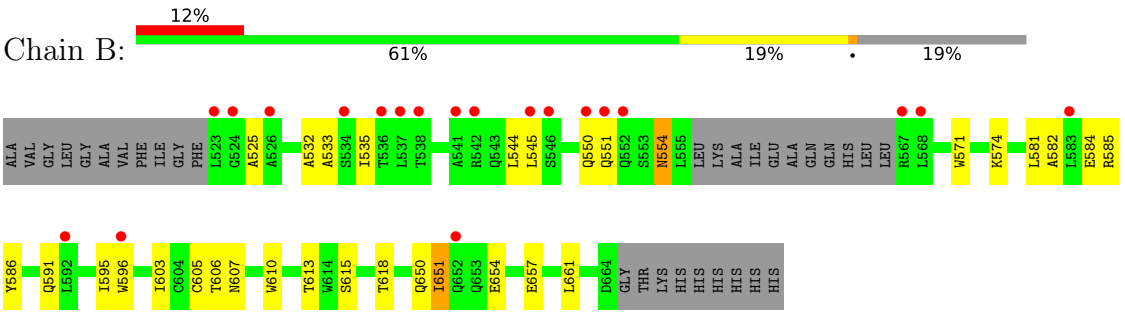
3 Residue-property plots (i)

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.

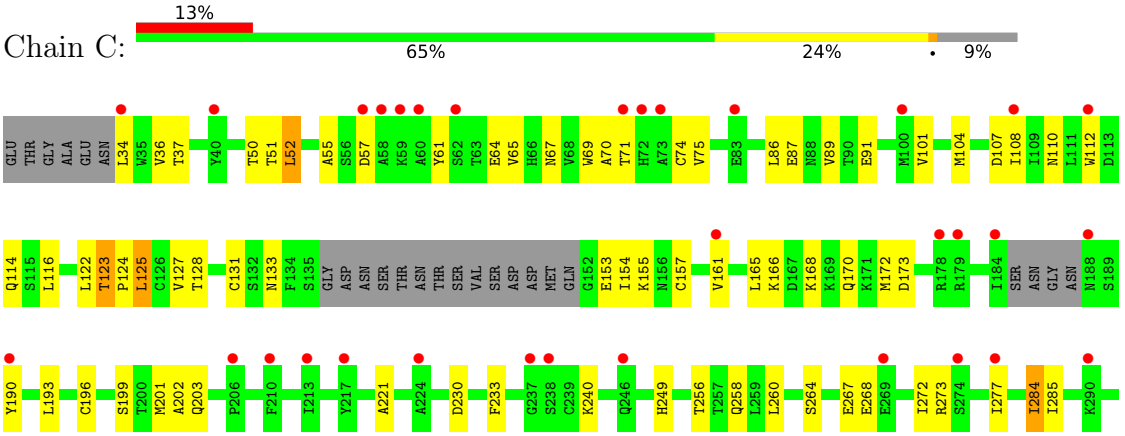
• Molecule 1: Glycoprotein 41

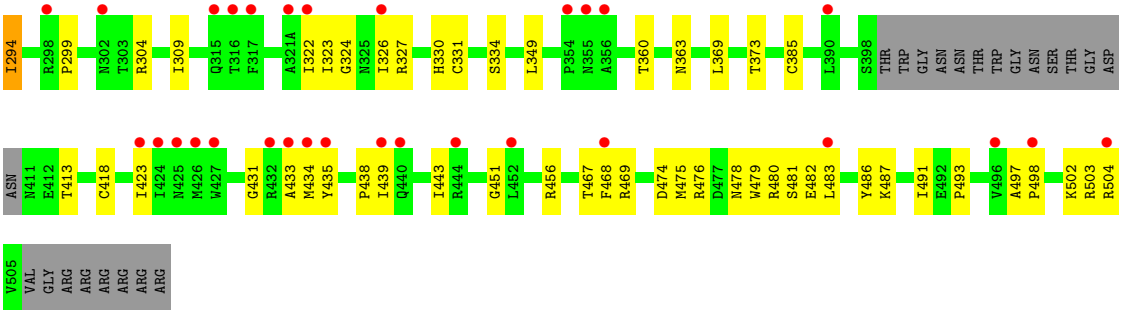


• Molecule 1: Glycoprotein 41

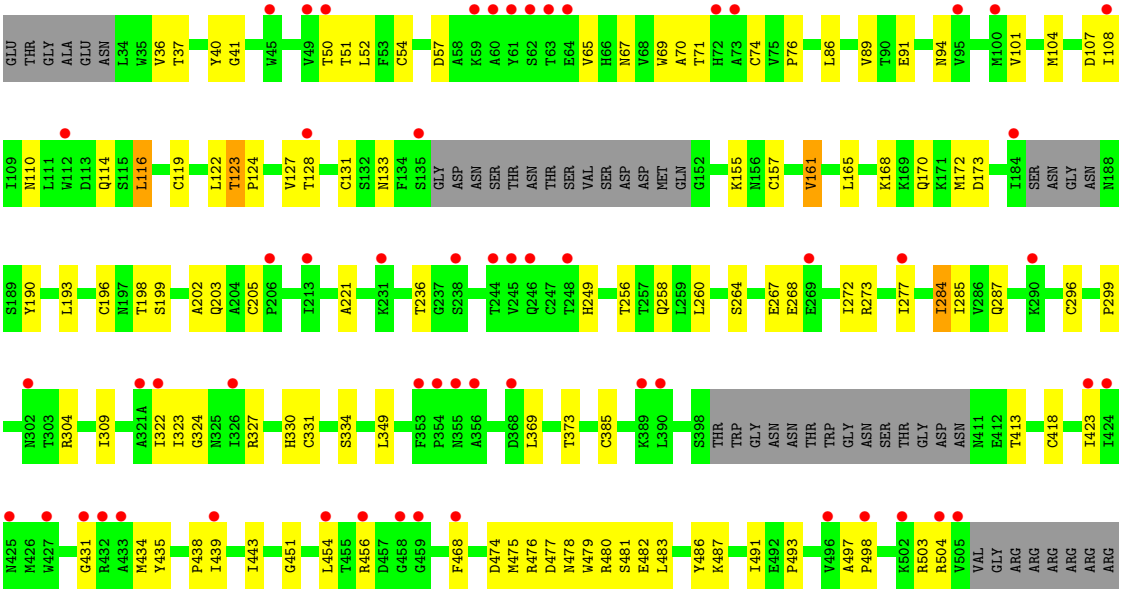


• Molecule 2: Glycoprotein 120

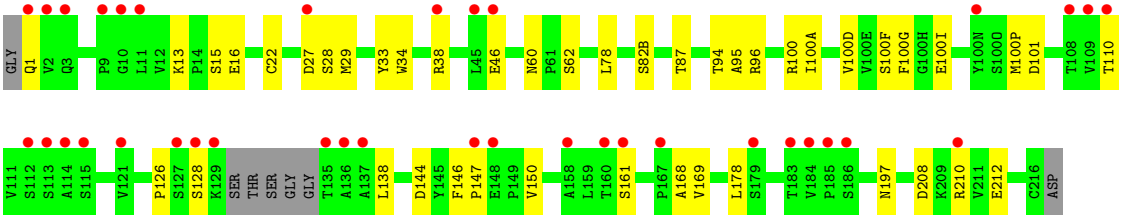




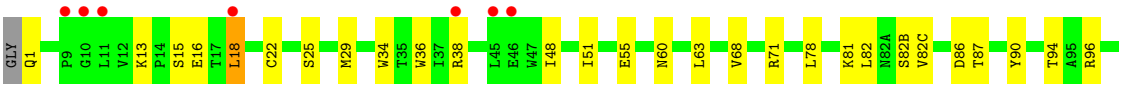
• Molecule 2: Glycoprotein 120

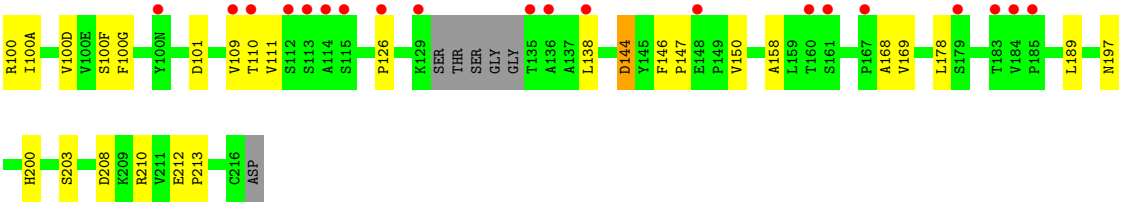


• Molecule 3: 10-1074 FAB heavy chain

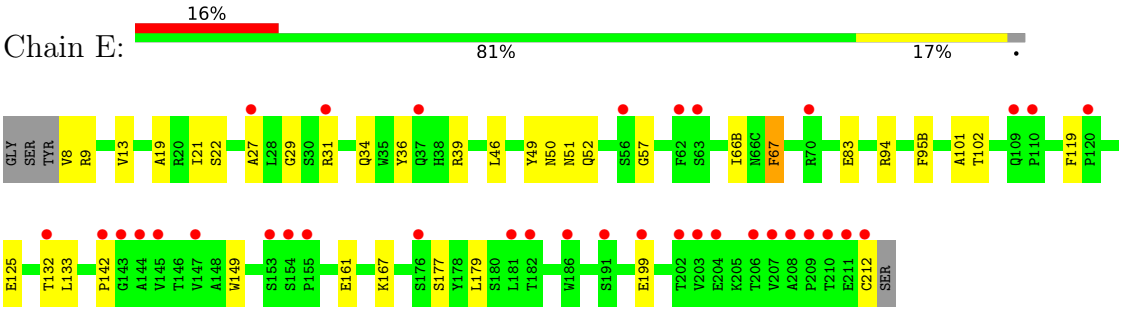


• Molecule 3: 10-1074 FAB heavy chain

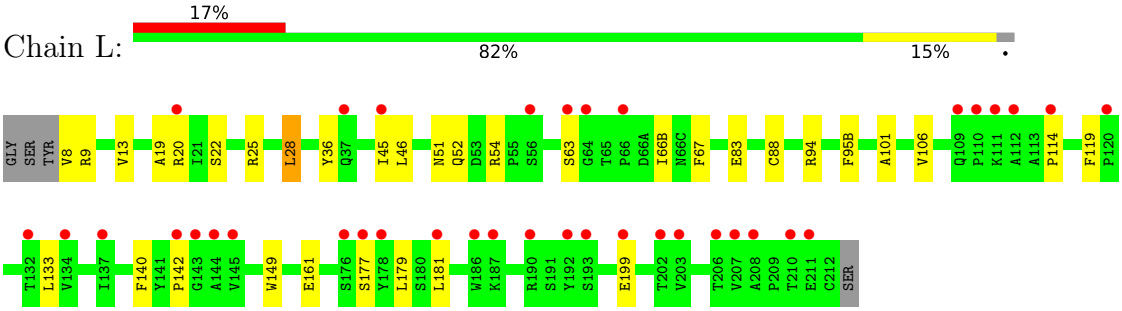




• Molecule 4: 10-1074 Fab light chain

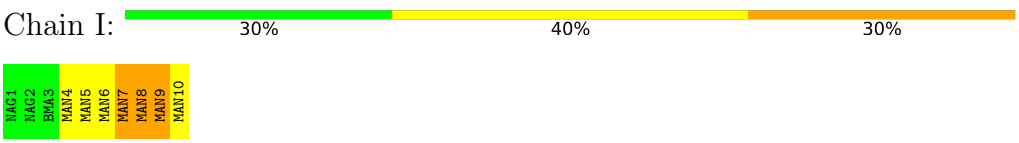


• Molecule 4: 10-1074 Fab light chain



• Molecule 5: alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

• Molecule 6: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[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

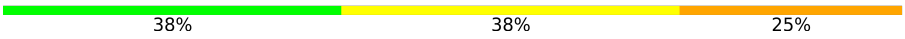


• Molecule 7: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:

• Molecule 8: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]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 K:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α, β, γ	237.28Å 237.28Å 282.04Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.55 – 6.50 39.55 – 6.50	Depositor EDS
% Data completeness (in resolution range)	99.3 (39.55-6.50) 99.3 (39.55-6.50)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.97 (at 6.65Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.298 , 0.366 0.296 , 0.365	Depositor DCC
R_{free} test set	1174 reflections (10.16%)	wwPDB-VP
Wilson B-factor (Å^2)	408.5	Xtriage
Anisotropy	0.133	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 500.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.000 for -2/3*h-1/3*k+2/3*l,-1/3*h-2/3*k-2/3*l,2/3*h-2/3*k+1/3*l 0.000 for -h,1/3*h-1/3*k+2/3*l,2/3*h+4/3*k+1/3*l 0.000 for -1/3*h+1/3*k-2/3*l,-k,-4/3*h-2/3*k+1/3*l 0.000 for -h,2/3*h+1/3*k-2/3*l,-2/3*h-4/3*k-1/3*l 0.000 for 1/3*h+2/3*k+2/3*l,-k,4/3*h+2/3*k-1/3*l 0.001 for -1/3*h-2/3*k-2/3*l,-2/3*h-1/3*k+2/3*l,-2/3*h+2/3*k-1/3*l 0.409 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.82	EDS
Total number of atoms	16470	wwPDB-VP
Average B, all atoms (Å^2)	479.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.02% 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, BMA, MAN

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	0.24	0/1063	0.51	1/1443 (0.1%)
1	B	0.23	0/1063	0.48	0/1443
2	C	0.25	0/3509	0.43	0/4765
2	G	0.24	0/3509	0.42	0/4765
3	D	0.24	0/1796	0.43	0/2450
3	H	0.24	0/1796	0.43	0/2450
4	E	0.24	0/1649	0.43	0/2250
4	L	0.24	0/1649	0.42	0/2250
All	All	0.24	0/16034	0.44	1/21816 (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	A	661	LEU	CA-CB-CG	5.85	128.75	115.30

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	A	1047	0	1038	29	0
1	B	1047	0	1038	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	3438	0	3359	77	0
2	G	3438	0	3359	72	0
3	D	1753	0	1719	28	0
3	H	1753	0	1719	37	0
4	E	1607	0	1550	21	0
4	L	1607	0	1550	18	0
5	F	72	0	61	0	0
6	I	116	0	97	3	0
7	J	50	0	43	0	0
8	K	94	0	79	1	0
9	A	28	0	26	0	0
9	B	28	0	26	0	0
9	C	196	0	182	2	0
9	G	196	0	182	1	0
All	All	16470	0	16028	275	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 8.

The worst 5 of 275 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:A:606:THR:HB	1:A:650:GLN:HE22	1.35	0.89
4:L:149:TRP:HE1	4:L:177:SER:HG	1.27	0.83
1:B:607:ASN:ND2	1:B:654:GLU:OE2	2.13	0.81
2:G:122:LEU:H	2:G:202:ALA:HA	1.46	0.80
1:A:585:ARG:NH2	2:C:491:ILE:O	2.14	0.80

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	127/162 (78%)	114 (90%)	12 (9%)	1 (1%)	19	60
1	B	127/162 (78%)	114 (90%)	12 (9%)	1 (1%)	19	60
2	C	432/486 (89%)	391 (90%)	37 (9%)	4 (1%)	17	57
2	G	432/486 (89%)	389 (90%)	41 (10%)	2 (0%)	29	69
3	D	226/237 (95%)	221 (98%)	5 (2%)	0	100	100
3	H	226/237 (95%)	217 (96%)	8 (4%)	1 (0%)	34	72
4	E	209/215 (97%)	198 (95%)	10 (5%)	1 (0%)	29	69
4	L	209/215 (97%)	197 (94%)	10 (5%)	2 (1%)	15	54
All	All	1988/2200 (90%)	1841 (93%)	135 (7%)	12 (1%)	25	66

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	554	ASN
1	B	554	ASN
2	C	154	ILE
3	H	144	ASP
2	C	153	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	A	114/137 (83%)	112 (98%)	2 (2%)	59	77
1	B	114/137 (83%)	111 (97%)	3 (3%)	46	66
2	C	388/426 (91%)	378 (97%)	10 (3%)	46	66
2	G	388/426 (91%)	380 (98%)	8 (2%)	53	72
3	D	202/206 (98%)	201 (100%)	1 (0%)	88	93
3	H	202/206 (98%)	200 (99%)	2 (1%)	76	86
4	E	175/178 (98%)	170 (97%)	5 (3%)	42	64
4	L	175/178 (98%)	170 (97%)	5 (3%)	42	64

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1758/1894 (93%)	1722 (98%)	36 (2%)	55 74

5 of 36 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	G	284	ILE
4	L	119	PHE
3	H	18	LEU
4	L	52	GLN
2	C	161	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	650	GLN
2	C	67	ASN
3	D	39	GLN
2	G	67	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)

28 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	F	1	5,2	14,14,15	0.36	0	17,19,21	0.59	0
5	NAG	F	2	5	14,14,15	0.27	0	17,19,21	0.57	0
5	BMA	F	3	5	11,11,12	1.23	2 (18%)	15,15,17	1.11	0
5	MAN	F	4	5	11,11,12	0.69	0	15,15,17	1.30	2 (13%)
5	MAN	F	5	5	11,11,12	0.69	0	15,15,17	0.97	2 (13%)
5	MAN	F	6	5	11,11,12	0.84	1 (9%)	15,15,17	0.80	1 (6%)
6	NAG	I	1	2,6	14,14,15	0.16	0	17,19,21	0.48	0
6	MAN	I	10	6	11,11,12	0.72	0	15,15,17	1.02	2 (13%)
6	NAG	I	2	6	14,14,15	0.21	0	17,19,21	0.55	0
6	BMA	I	3	6	11,11,12	0.68	0	15,15,17	0.96	0
6	MAN	I	4	6	11,11,12	1.10	1 (9%)	15,15,17	1.54	3 (20%)
6	MAN	I	5	6	11,11,12	0.62	0	15,15,17	1.22	2 (13%)
6	MAN	I	6	6	11,11,12	0.63	0	15,15,17	1.11	2 (13%)
6	MAN	I	7	6	11,11,12	0.63	0	15,15,17	1.23	2 (13%)
6	MAN	I	8	6	11,11,12	0.71	0	15,15,17	0.95	1 (6%)
6	MAN	I	9	6	11,11,12	0.66	0	15,15,17	0.95	1 (6%)
7	NAG	J	1	7,2	14,14,15	0.33	0	17,19,21	0.54	0
7	NAG	J	2	7	14,14,15	0.27	0	17,19,21	0.53	0
7	BMA	J	3	7	11,11,12	0.58	0	15,15,17	0.78	0
7	MAN	J	4	7	11,11,12	0.73	0	15,15,17	0.98	2 (13%)
8	NAG	K	1	8,2	14,14,15	0.19	0	17,19,21	0.49	0
8	NAG	K	2	8	14,14,15	0.21	0	17,19,21	0.54	0
8	BMA	K	3	8	11,11,12	0.72	0	15,15,17	0.94	0
8	MAN	K	4	8	11,11,12	1.06	1 (9%)	15,15,17	1.49	3 (20%)
8	MAN	K	5	8	11,11,12	0.62	0	15,15,17	1.12	2 (13%)
8	MAN	K	6	8	11,11,12	0.64	0	15,15,17	1.21	2 (13%)
8	MAN	K	7	8	11,11,12	0.69	0	15,15,17	0.98	2 (13%)
8	MAN	K	8	8	11,11,12	0.68	0	15,15,17	0.92	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	F	1	5,2	-	2/6/23/26	0/1/1/1
5	NAG	F	2	5	-	1/6/23/26	0/1/1/1
5	BMA	F	3	5	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	MAN	F	4	5	-	0/2/19/22	0/1/1/1
5	MAN	F	5	5	-	2/2/19/22	0/1/1/1
5	MAN	F	6	5	-	2/2/19/22	0/1/1/1
6	NAG	I	1	2,6	-	0/6/23/26	0/1/1/1
6	MAN	I	10	6	-	0/2/19/22	0/1/1/1
6	NAG	I	2	6	-	1/6/23/26	0/1/1/1
6	BMA	I	3	6	-	0/2/19/22	0/1/1/1
6	MAN	I	4	6	-	0/2/19/22	0/1/1/1
6	MAN	I	5	6	-	1/2/19/22	0/1/1/1
6	MAN	I	6	6	-	0/2/19/22	0/1/1/1
6	MAN	I	7	6	-	0/2/19/22	0/1/1/1
6	MAN	I	8	6	-	1/2/19/22	0/1/1/1
6	MAN	I	9	6	-	0/2/19/22	0/1/1/1
7	NAG	J	1	7,2	-	0/6/23/26	0/1/1/1
7	NAG	J	2	7	-	1/6/23/26	0/1/1/1
7	BMA	J	3	7	-	1/2/19/22	0/1/1/1
7	MAN	J	4	7	-	0/2/19/22	0/1/1/1
8	NAG	K	1	8,2	-	0/6/23/26	0/1/1/1
8	NAG	K	2	8	-	1/6/23/26	0/1/1/1
8	BMA	K	3	8	-	0/2/19/22	0/1/1/1
8	MAN	K	4	8	-	0/2/19/22	0/1/1/1
8	MAN	K	5	8	-	1/2/19/22	0/1/1/1
8	MAN	K	6	8	-	0/2/19/22	0/1/1/1
8	MAN	K	7	8	-	0/2/19/22	0/1/1/1
8	MAN	K	8	8	-	2/2/19/22	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	I	4	MAN	C1-C2	2.99	1.59	1.52
8	K	4	MAN	C1-C2	2.96	1.59	1.52
5	F	3	BMA	C4-C3	2.47	1.58	1.52
5	F	3	BMA	O5-C1	-2.18	1.40	1.43
5	F	6	MAN	O5-C1	-2.13	1.40	1.43

The worst 5 of 31 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	F	4	MAN	C1-O5-C5	3.99	117.60	112.19
6	I	5	MAN	C1-O5-C5	3.66	117.15	112.19
6	I	4	MAN	C1-C2-C3	3.42	113.87	109.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	K	5	MAN	C1-O5-C5	3.25	116.60	112.19
8	K	4	MAN	C1-O5-C5	3.12	116.42	112.19

There are no chirality outliers.

5 of 16 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	K	8	MAN	O5-C5-C6-O6
7	J	3	BMA	O5-C5-C6-O6
8	K	8	MAN	C4-C5-C6-O6
8	K	5	MAN	O5-C5-C6-O6
6	I	5	MAN	O5-C5-C6-O6

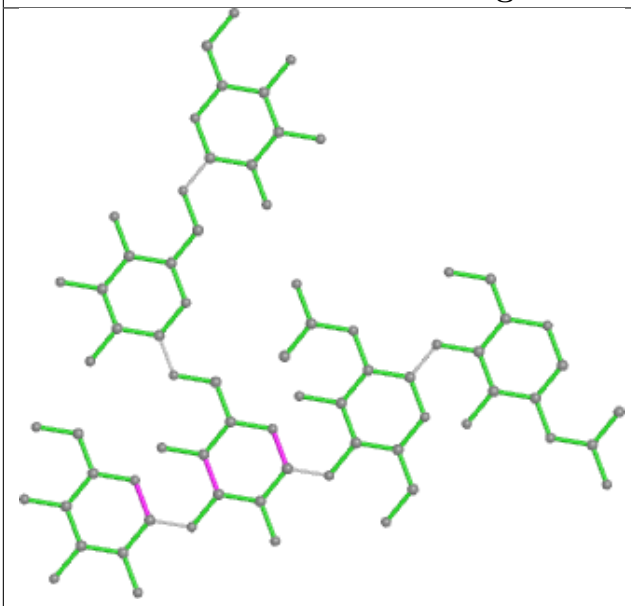
There are no ring outliers.

5 monomers are involved in 4 short contacts:

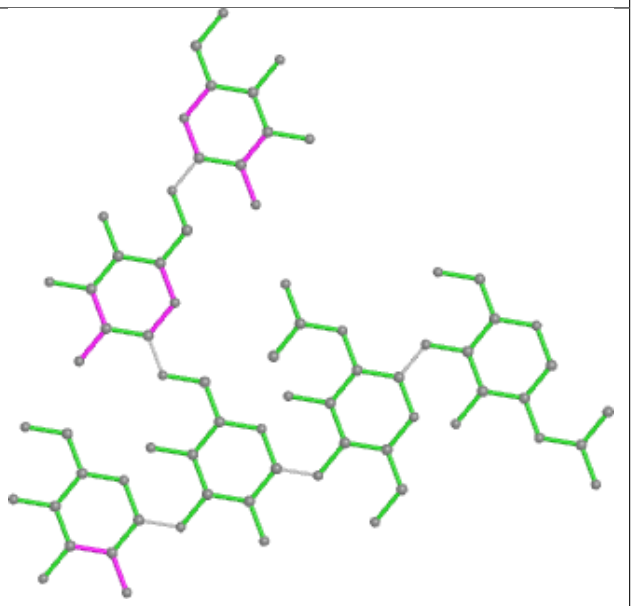
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	K	8	MAN	1	0
6	I	7	MAN	1	0
8	K	6	MAN	1	0
6	I	9	MAN	1	0
6	I	8	MAN	3	0

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

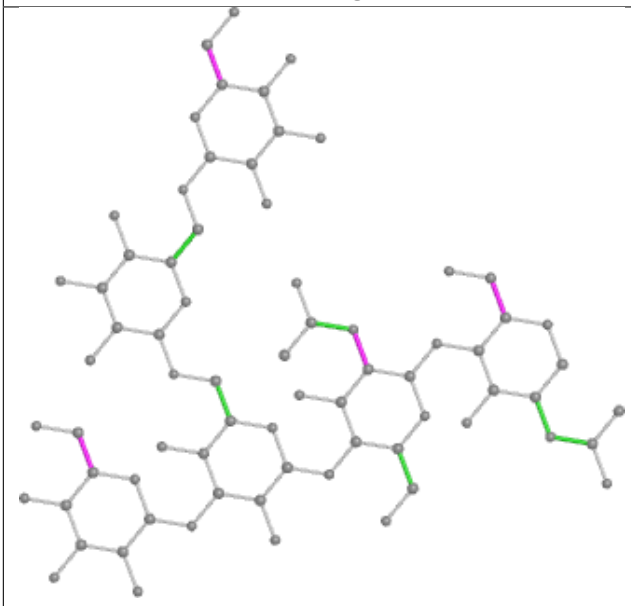
Oligosaccharide Chain F



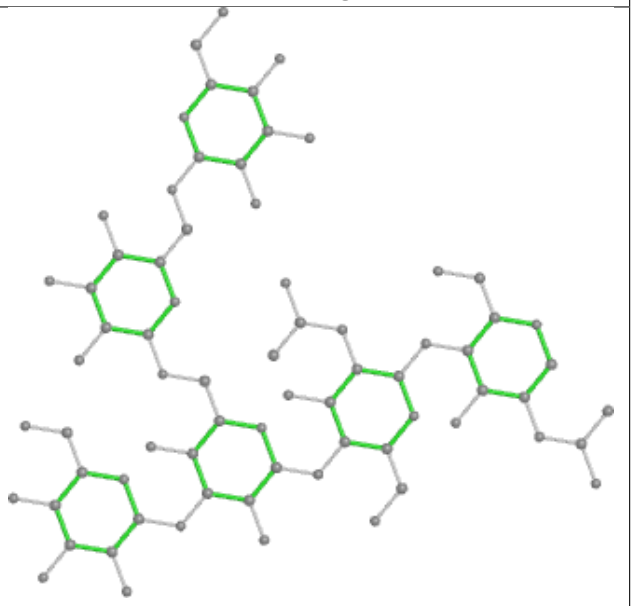
Bond lengths



Bond angles

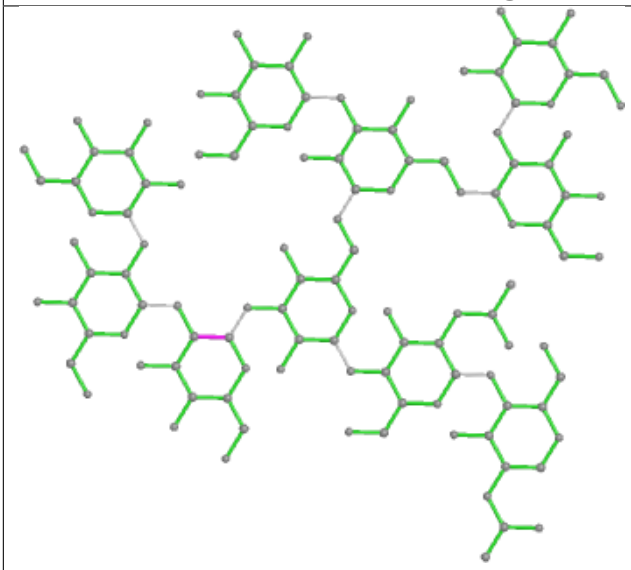


Torsions

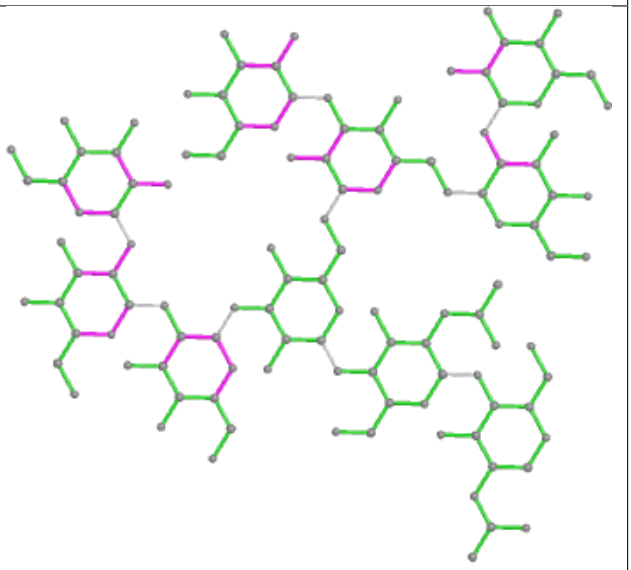


Rings

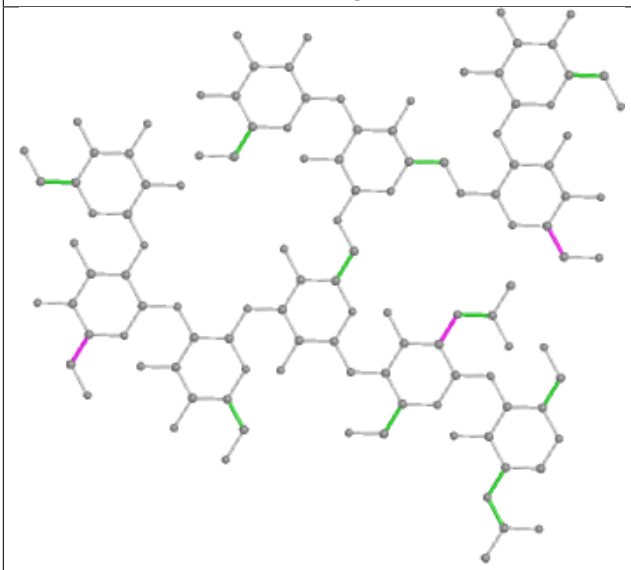
Oligosaccharide Chain I



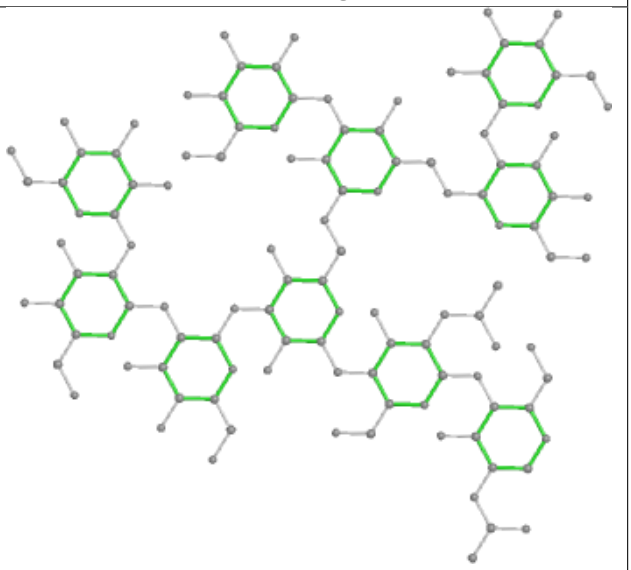
Bond lengths



Bond angles

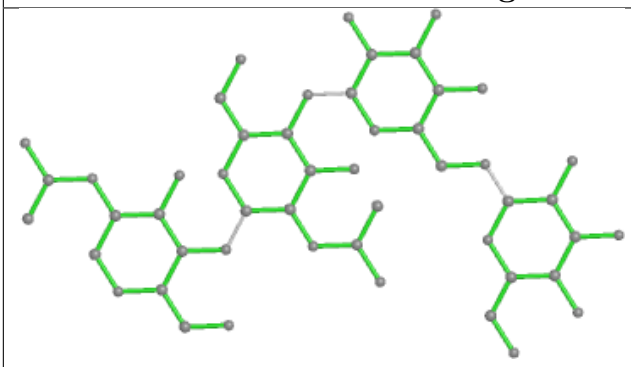


Torsions

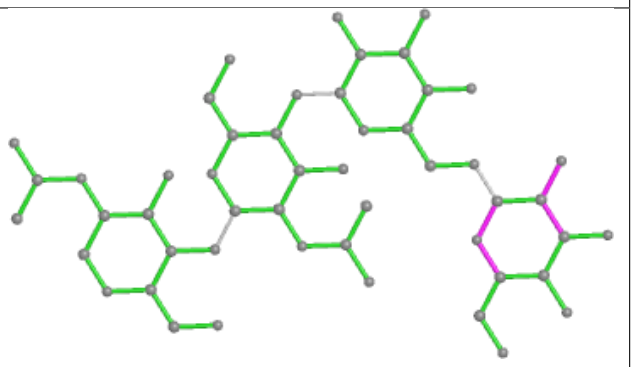


Rings

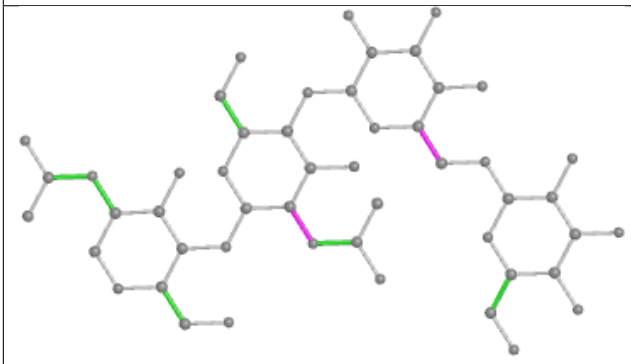
Oligosaccharide Chain J



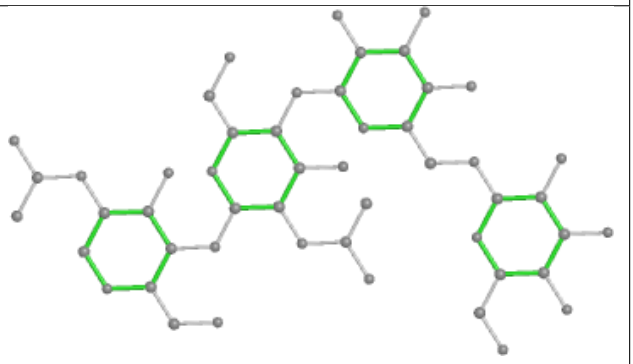
Bond lengths



Bond angles

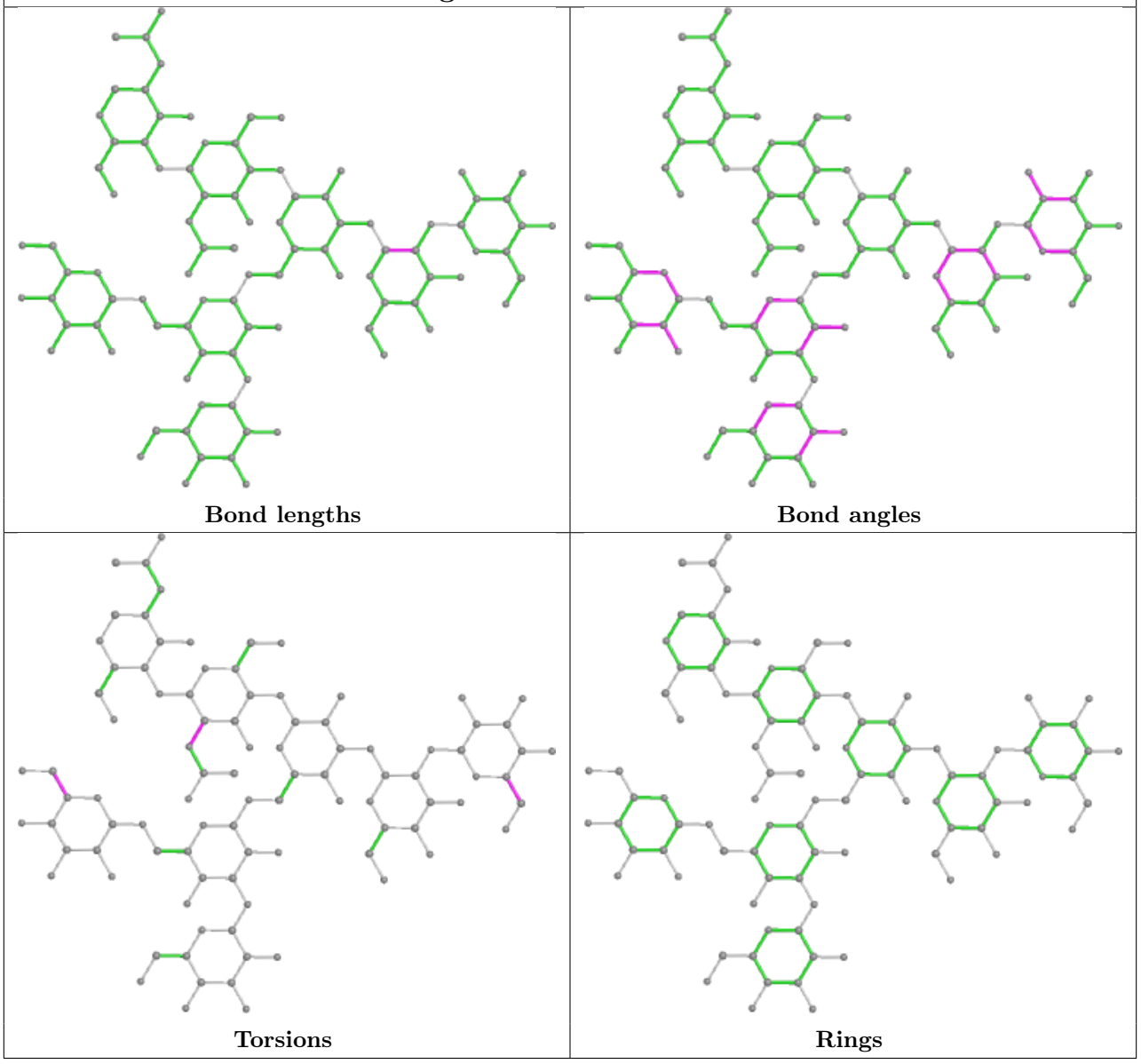


Torsions



Rings

Oligosaccharide Chain K



5.6 Ligand geometry (i)

32 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	$\#\|Z\|>2$
9	NAG	G	623	2	14,14,15	0.27	0	17,19,21	0.48	0
9	NAG	G	603	2	14,14,15	0.23	0	17,19,21	0.43	0
9	NAG	G	626	2	14,14,15	0.29	0	17,19,21	0.40	0
9	NAG	C	604	2	14,14,15	0.21	0	17,19,21	0.40	0
9	NAG	G	622	2	14,14,15	0.23	0	17,19,21	0.42	0
9	NAG	C	627	2	14,14,15	0.22	0	17,19,21	0.41	0
9	NAG	C	630	2	14,14,15	0.16	0	17,19,21	0.53	0
9	NAG	G	604	2	14,14,15	0.21	0	17,19,21	0.39	0
9	NAG	G	602	2	14,14,15	0.24	0	17,19,21	0.44	0
9	NAG	C	603	2	14,14,15	0.23	0	17,19,21	0.44	0
9	NAG	G	610	2	14,14,15	0.24	0	17,19,21	0.40	0
9	NAG	C	628	2	14,14,15	0.19	0	17,19,21	0.35	0
9	NAG	G	625	2	14,14,15	0.29	0	17,19,21	0.42	0
9	NAG	G	619	2	14,14,15	0.19	0	17,19,21	0.40	0
9	NAG	G	621	2	14,14,15	0.21	0	17,19,21	0.47	0
9	NAG	G	620	2	14,14,15	0.19	0	17,19,21	0.40	0
9	NAG	A	701	1	14,14,15	0.29	0	17,19,21	0.44	0
9	NAG	C	613	2	14,14,15	0.23	0	17,19,21	0.37	0
9	NAG	C	605	2	14,14,15	0.20	0	17,19,21	0.38	0
9	NAG	C	602	2	14,14,15	0.38	0	17,19,21	0.52	0
9	NAG	C	606	2	14,14,15	0.20	0	17,19,21	0.40	0
9	NAG	C	625	2	14,14,15	0.22	0	17,19,21	0.41	0
9	NAG	C	624	2	14,14,15	0.21	0	17,19,21	0.42	0
9	NAG	G	605	2	14,14,15	0.21	0	17,19,21	0.41	0
9	NAG	G	601	2	14,14,15	0.21	0	17,19,21	0.43	0
9	NAG	C	626	2	14,14,15	0.25	0	17,19,21	0.44	0
9	NAG	B	702	1	14,14,15	0.98	2 (14%)	17,19,21	1.19	1 (5%)
9	NAG	C	629	2	14,14,15	0.27	0	17,19,21	0.49	0
9	NAG	G	624	2	14,14,15	0.21	0	17,19,21	0.77	0
9	NAG	A	702	1	14,14,15	1.05	2 (14%)	17,19,21	1.19	1 (5%)
9	NAG	B	701	1	14,14,15	0.28	0	17,19,21	0.45	0
9	NAG	C	601	2	14,14,15	0.20	0	17,19,21	0.41	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
9	NAG	G	623	2	-	0/6/23/26	0/1/1/1
9	NAG	G	603	2	-	2/6/23/26	0/1/1/1
9	NAG	G	626	2	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	NAG	C	604	2	-	2/6/23/26	0/1/1/1
9	NAG	G	622	2	-	0/6/23/26	0/1/1/1
9	NAG	C	627	2	-	0/6/23/26	0/1/1/1
9	NAG	C	630	2	-	0/6/23/26	0/1/1/1
9	NAG	G	604	2	-	2/6/23/26	0/1/1/1
9	NAG	G	602	2	-	2/6/23/26	0/1/1/1
9	NAG	C	603	2	-	2/6/23/26	0/1/1/1
9	NAG	G	610	2	-	1/6/23/26	0/1/1/1
9	NAG	C	628	2	-	0/6/23/26	0/1/1/1
9	NAG	G	625	2	-	0/6/23/26	0/1/1/1
9	NAG	G	619	2	-	2/6/23/26	0/1/1/1
9	NAG	G	621	2	-	2/6/23/26	0/1/1/1
9	NAG	G	620	2	-	2/6/23/26	0/1/1/1
9	NAG	A	701	1	-	2/6/23/26	0/1/1/1
9	NAG	C	613	2	-	0/6/23/26	0/1/1/1
9	NAG	C	605	2	-	2/6/23/26	0/1/1/1
9	NAG	C	602	2	-	2/6/23/26	0/1/1/1
9	NAG	C	606	2	-	2/6/23/26	0/1/1/1
9	NAG	C	625	2	-	2/6/23/26	0/1/1/1
9	NAG	C	624	2	-	2/6/23/26	0/1/1/1
9	NAG	G	605	2	-	2/6/23/26	0/1/1/1
9	NAG	G	601	2	-	2/6/23/26	0/1/1/1
9	NAG	C	626	2	-	2/6/23/26	0/1/1/1
9	NAG	B	702	1	-	0/6/23/26	0/1/1/1
9	NAG	C	629	2	-	0/6/23/26	0/1/1/1
9	NAG	G	624	2	-	3/6/23/26	0/1/1/1
9	NAG	A	702	1	-	0/6/23/26	0/1/1/1
9	NAG	B	701	1	-	2/6/23/26	0/1/1/1
9	NAG	C	601	2	-	2/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	702	NAG	C1-C2	2.82	1.56	1.52
9	B	702	NAG	O5-C1	2.81	1.48	1.43
9	A	702	NAG	O5-C1	2.62	1.47	1.43
9	B	702	NAG	C1-C2	2.22	1.55	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	B	702	NAG	C1-O5-C5	4.81	118.71	112.19
9	A	702	NAG	C1-O5-C5	4.66	118.51	112.19

There are no chirality outliers.

5 of 42 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	G	601	NAG	O5-C5-C6-O6
9	B	701	NAG	O5-C5-C6-O6
9	C	601	NAG	O5-C5-C6-O6
9	C	625	NAG	O5-C5-C6-O6
9	C	603	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
9	G	604	NAG	1	0
9	C	606	NAG	1	0
9	C	601	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

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	A	131/162 (80%)	1.07	22 (16%)	1	4	305, 489, 584, 661	0
1	B	131/162 (80%)	0.97	20 (15%)	2	5	315, 484, 580, 673	0
2	C	440/486 (90%)	0.81	62 (14%)	2	6	216, 460, 586, 659	0
2	G	440/486 (90%)	0.85	58 (13%)	3	6	274, 461, 582, 686	0
3	D	230/237 (97%)	0.87	37 (16%)	1	4	283, 477, 587, 658	0
3	H	230/237 (97%)	0.64	27 (11%)	4	8	285, 477, 584, 679	0
4	E	211/215 (98%)	0.98	35 (16%)	1	4	362, 504, 633, 694	0
4	L	211/215 (98%)	0.89	37 (17%)	1	4	355, 506, 620, 683	0
All	All	2024/2200 (92%)	0.86	298 (14%)	2	5	216, 478, 595, 694	0

The worst 5 of 298 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	H	184	VAL	10.6
4	E	211	GLU	10.0
4	E	143	GLY	9.8
3	D	114	ALA	8.1
2	G	62	SER	7.8

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

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

6.3 Carbohydrates

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,

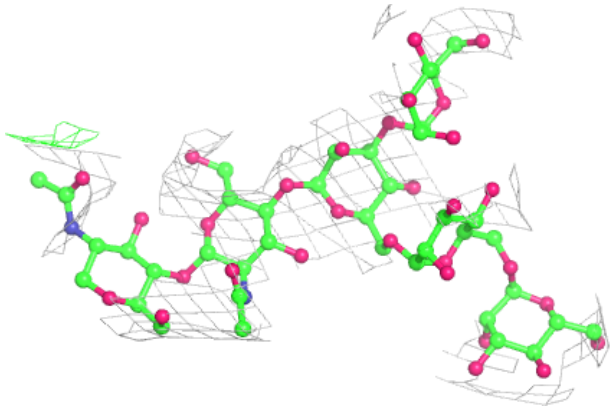
median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

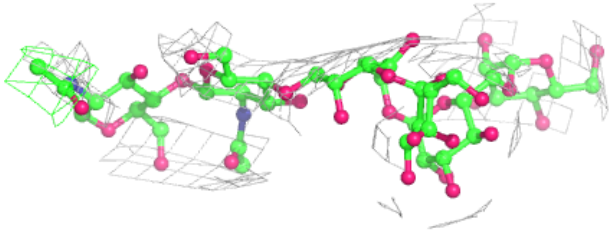
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
8	MAN	K	6	11/12	0.56	0.42	439,456,462,469	0
8	BMA	K	3	11/12	0.62	0.30	472,490,501,501	0
6	BMA	I	3	11/12	0.63	0.29	466,483,494,494	0
8	MAN	K	5	11/12	0.64	0.44	507,510,523,531	0
6	MAN	I	7	11/12	0.66	0.32	422,439,445,451	0
7	BMA	J	3	11/12	0.71	0.33	452,452,452,452	0
6	NAG	I	1	14/15	0.71	0.64	402,413,430,435	0
5	NAG	F	2	14/15	0.74	0.35	498,514,535,540	0
7	MAN	J	4	11/12	0.74	0.47	551,551,551,551	0
8	NAG	K	1	14/15	0.74	0.60	391,402,420,425	0
8	MAN	K	8	11/12	0.74	0.64	476,489,512,522	0
5	NAG	F	1	14/15	0.75	0.43	431,442,459,464	0
7	NAG	J	2	14/15	0.76	0.39	448,465,485,491	0
6	MAN	I	5	11/12	0.76	0.31	485,489,502,510	0
6	MAN	I	9	11/12	0.78	0.35	495,495,495,495	0
6	MAN	I	6	11/12	0.81	0.34	437,443,447,448	0
7	NAG	J	1	14/15	0.81	0.56	408,418,436,441	0
6	MAN	I	10	11/12	0.83	0.37	433,435,444,450	0
5	MAN	F	5	11/12	0.83	0.40	528,543,549,551	0
8	MAN	K	7	11/12	0.84	0.32	501,501,501,501	0
8	NAG	K	2	14/15	0.84	0.34	389,406,426,432	0
5	BMA	F	3	11/12	0.85	0.41	469,486,501,503	0
6	NAG	I	2	14/15	0.86	0.32	398,414,435,441	0
5	MAN	F	6	11/12	0.87	0.34	438,438,438,438	0
6	MAN	I	4	11/12	0.88	0.20	432,437,455,475	0
8	MAN	K	4	11/12	0.88	0.23	480,485,503,523	0
5	MAN	F	4	11/12	0.88	0.26	479,497,502,512	0
6	MAN	I	8	11/12	0.93	0.25	469,481,505,514	0

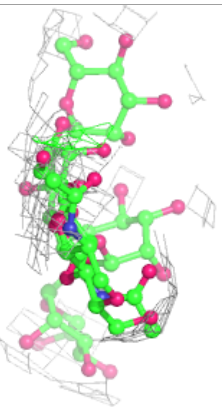
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain F:

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

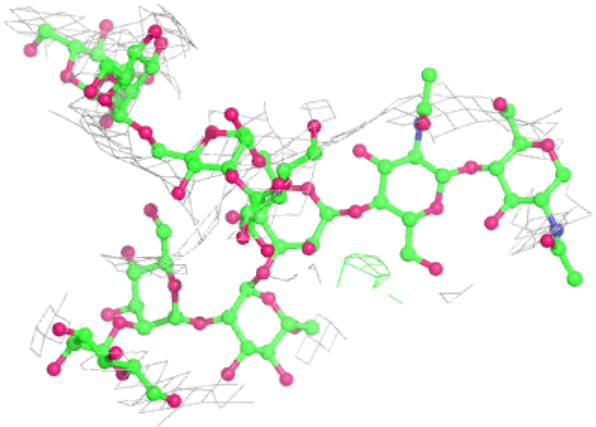


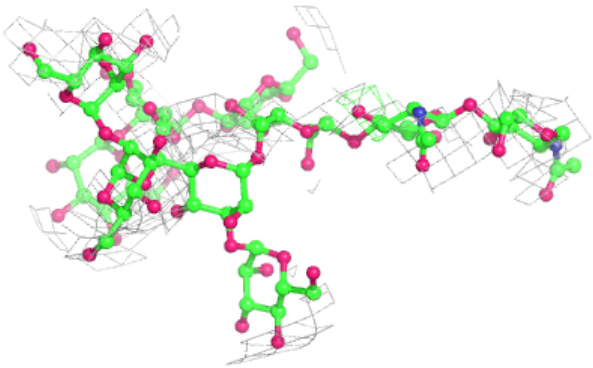


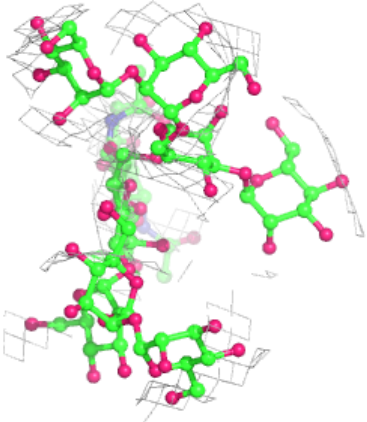


Electron density around Chain I:

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

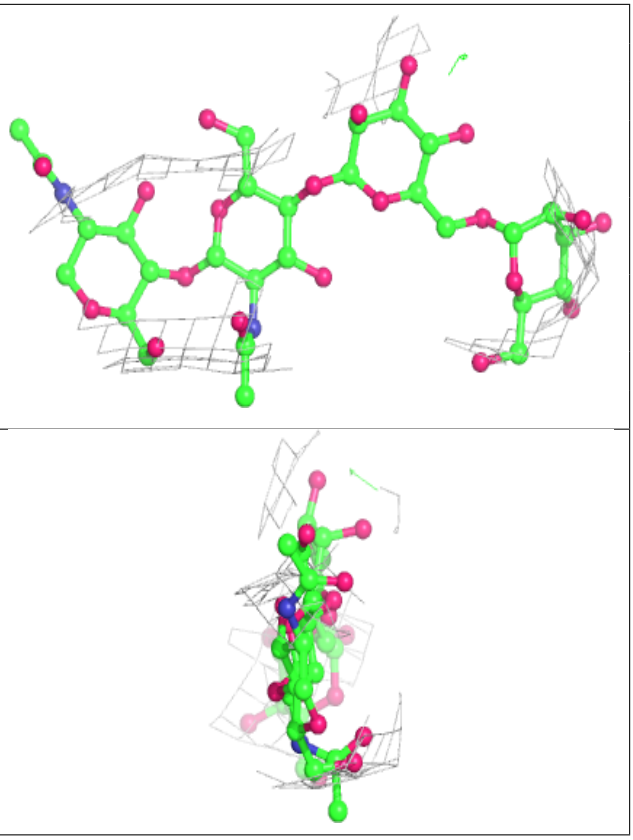


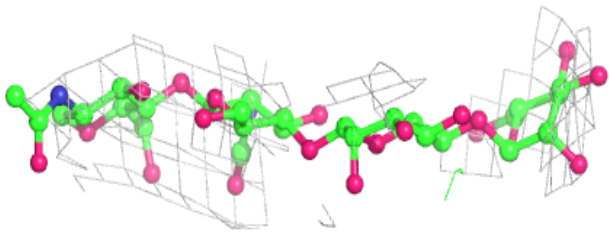




Electron density around Chain J:

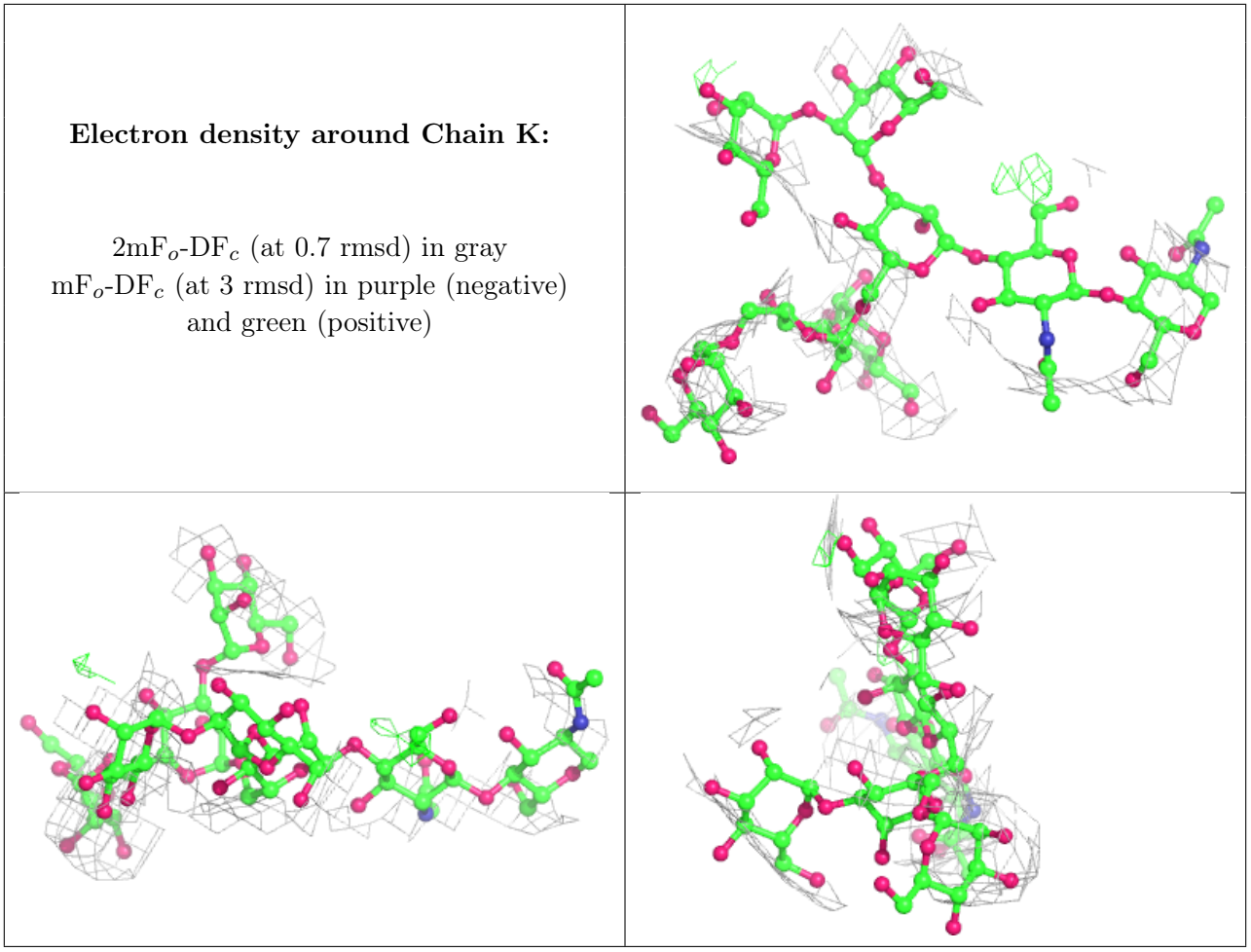
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





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

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
9	NAG	C	627	14/15	-0.40	1.80	576,576,576,576	0
9	NAG	G	622	14/15	0.05	1.03	576,576,576,576	0
9	NAG	C	630	14/15	0.14	0.79	530,530,530,530	0
9	NAG	G	623	14/15	0.17	0.90	579,579,579,579	0
9	NAG	G	603	14/15	0.20	0.53	527,527,527,527	0
9	NAG	G	602	14/15	0.21	0.61	447,447,447,447	0
9	NAG	C	603	14/15	0.24	0.49	495,495,495,495	0
9	NAG	C	629	14/15	0.38	0.55	598,598,598,598	0
9	NAG	G	626	14/15	0.39	0.64	476,476,476,476	0
9	NAG	C	604	14/15	0.40	0.71	557,557,557,557	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
9	NAG	C	605	14/15	0.43	0.69	494,494,494,494	0
9	NAG	G	605	14/15	0.46	0.59	516,516,516,516	0
9	NAG	A	701	14/15	0.46	0.70	625,625,625,625	0
9	NAG	G	624	14/15	0.52	0.63	538,538,538,538	0
9	NAG	G	604	14/15	0.52	0.90	600,600,600,600	0
9	NAG	B	702	14/15	0.54	0.83	570,570,570,570	0
9	NAG	C	602	14/15	0.54	0.50	438,438,438,438	0
9	NAG	C	606	14/15	0.57	0.44	549,549,549,549	0
9	NAG	G	621	14/15	0.58	0.57	415,415,415,415	0
9	NAG	A	702	14/15	0.65	0.60	583,583,583,583	0
9	NAG	C	626	14/15	0.67	0.58	420,420,420,420	0
9	NAG	G	620	14/15	0.68	0.58	449,449,449,449	0
9	NAG	C	628	14/15	0.68	0.52	487,487,487,487	0
9	NAG	G	601	14/15	0.69	0.32	525,525,525,525	0
9	NAG	B	701	14/15	0.70	0.40	601,601,601,601	0
9	NAG	G	625	14/15	0.73	0.52	458,458,458,458	0
9	NAG	C	625	14/15	0.75	0.43	429,429,429,429	0
9	NAG	G	619	14/15	0.77	0.35	465,465,465,465	0
9	NAG	G	610	14/15	0.79	0.46	507,507,507,507	0
9	NAG	C	601	14/15	0.80	0.24	547,547,547,547	0
9	NAG	C	613	14/15	0.80	0.50	488,488,488,488	0
9	NAG	C	624	14/15	0.85	0.46	484,484,484,484	0

6.5 Other polymers (i)

There are no such residues in this entry.