Full wwPDB X-ray Structure Validation 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 Full wwPDB X-ray Structure Validation 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:

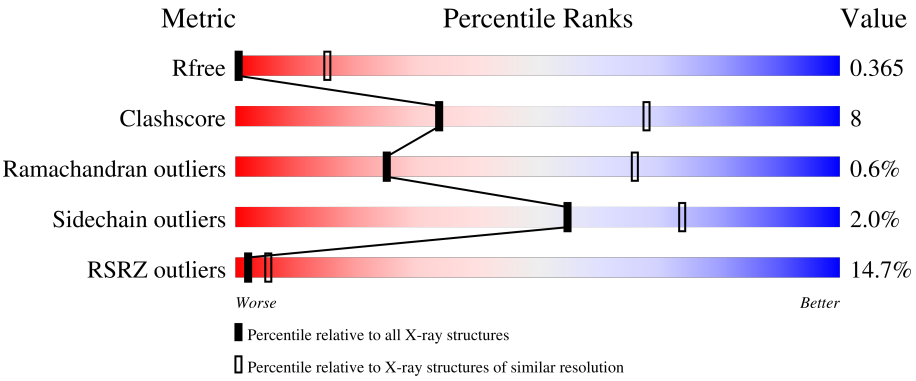
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

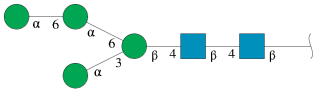
- Molecule 3 is a protein called 10-1074 FAB heavy chain.

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.

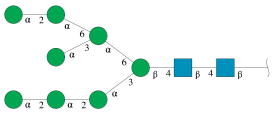
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	211	Total	C	N	O	S	0	0	0
			1607	1006	281	314	6			
4	L	211	Total	C	N	O	S	0	0	0
			1607	1006	281	314	6			

- 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.

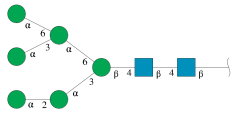


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	I	10	Total	C	N	O	0	0	0
			116	64	2	50			

- 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.

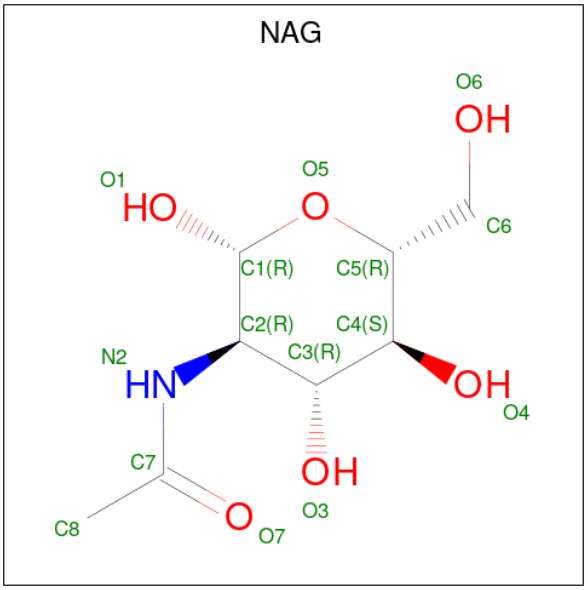
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
7	J	4	Total C N O 50 28 2 20	0	0	0

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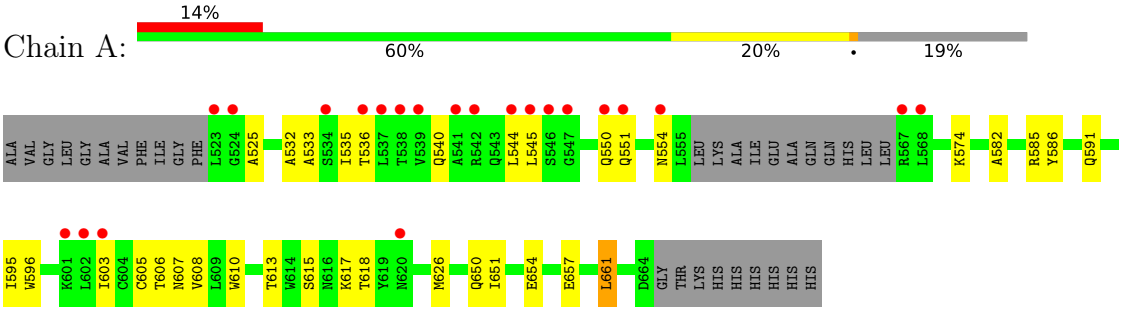
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	G	1	Total C N O 14 8 1 5	0	0
9	G	1	Total C N O 14 8 1 5	0	0
9	G	1	Total C N O 14 8 1 5	0	0
9	G	1	Total C N O 14 8 1 5	0	0
9	G	1	Total C N O 14 8 1 5	0	0
9	G	1	Total C N O 14 8 1 5	0	0
9	G	1	Total C N O 14 8 1 5	0	0
9	G	1	Total C N O 14 8 1 5	0	0

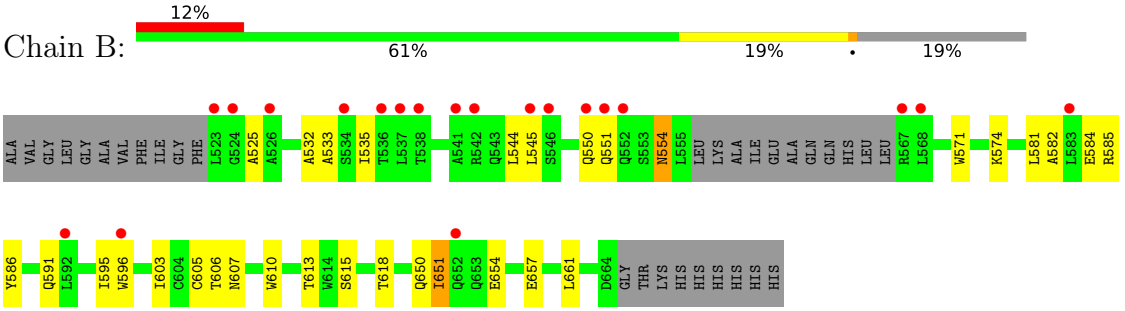
3 Residue-property plots (i)

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

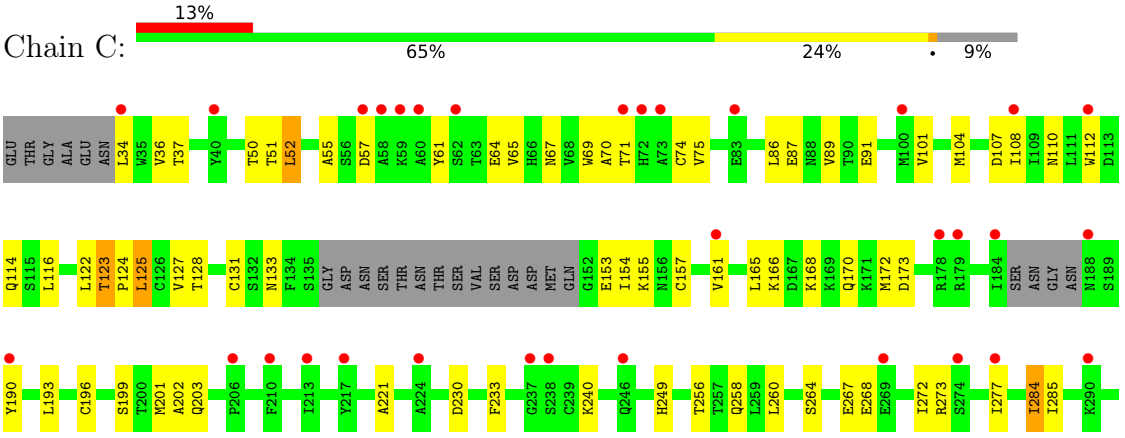
• Molecule 1: Glycoprotein 41

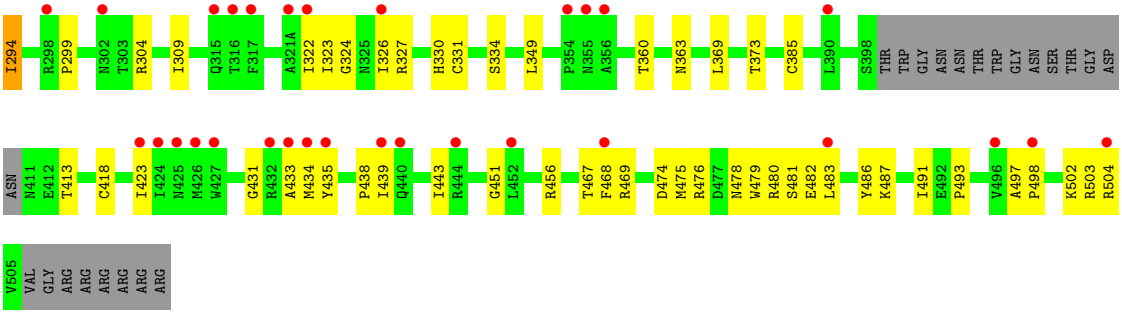


• Molecule 1: Glycoprotein 41



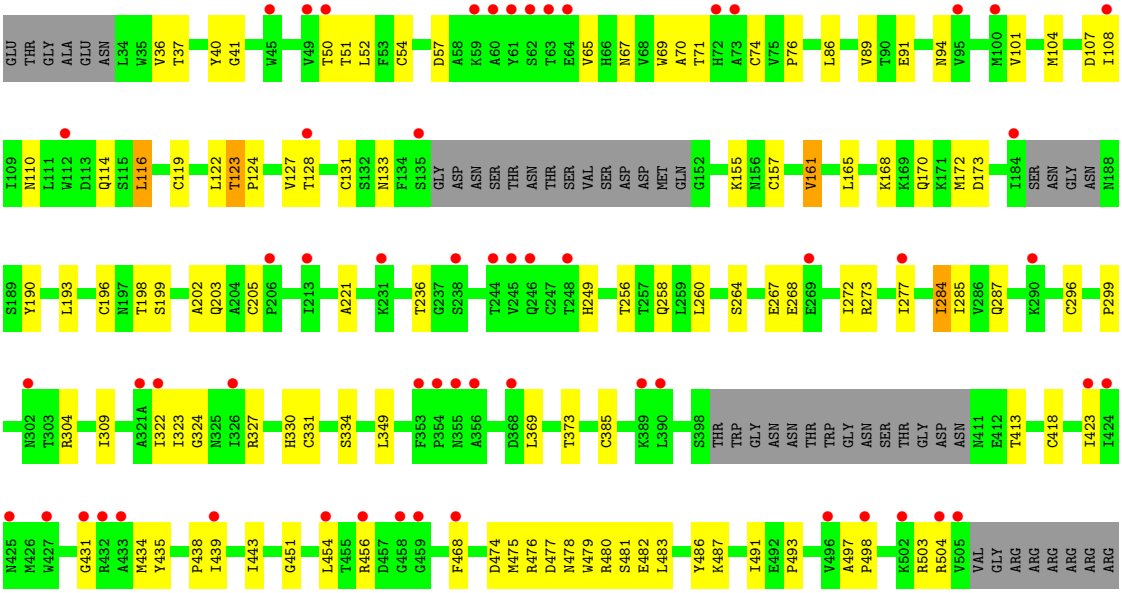
• Molecule 2: Glycoprotein 120





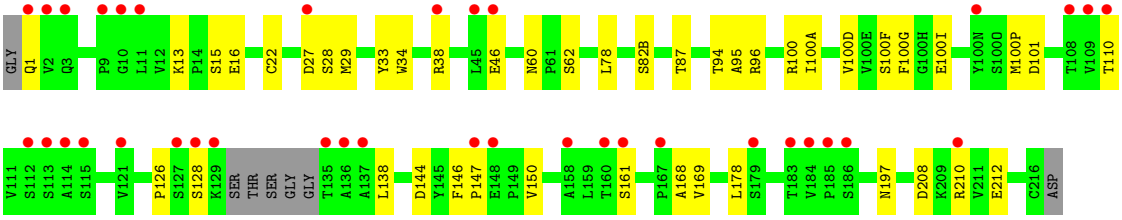
• Molecule 2: Glycoprotein 120

Chain G:



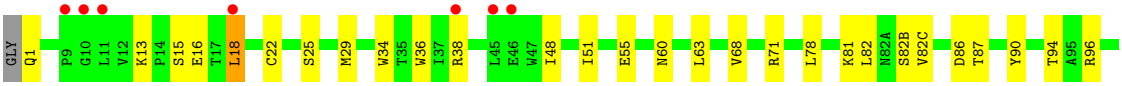
• Molecule 3: 10-1074 FAB heavy chain

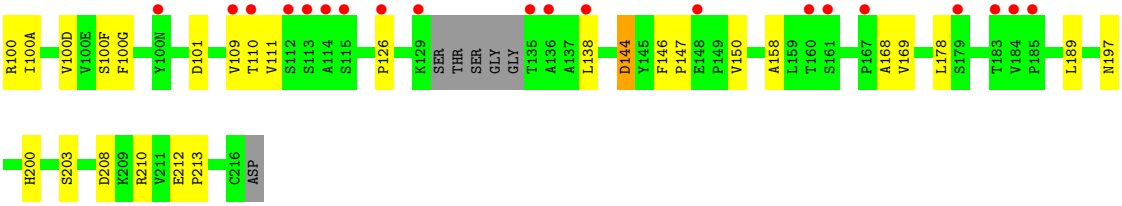
Chain D:



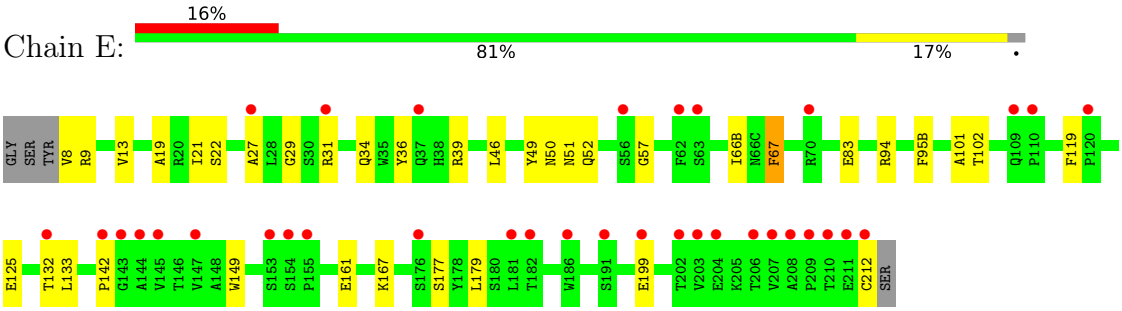
• Molecule 3: 10-1074 FAB heavy chain

Chain H:

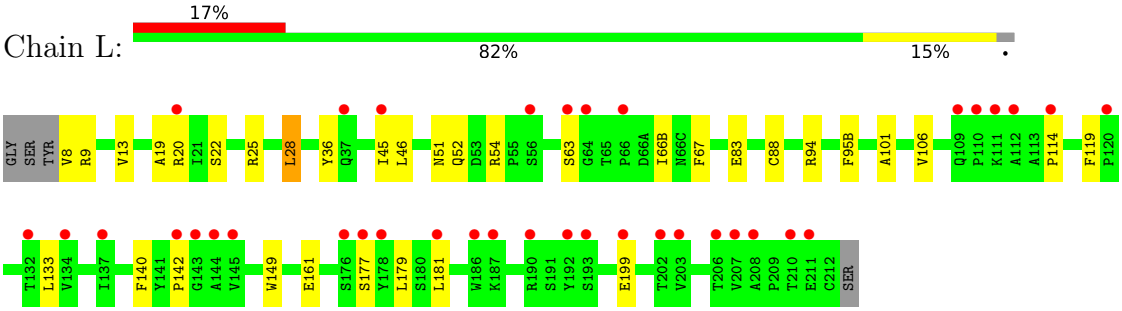




• Molecule 4: 10-1074 Fab light chain

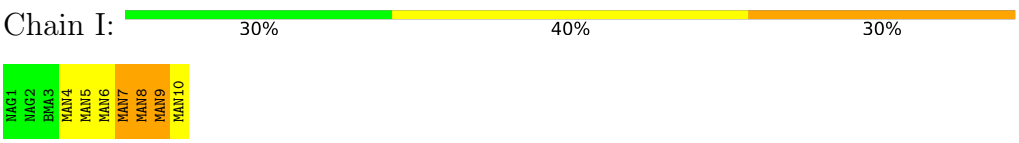


• Molecule 4: 10-1074 Fab light chain



• 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

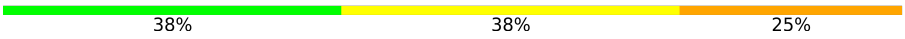


• Molecule 7: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

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.

All (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
1:B:585:ARG:NH2	2:G:491:ILE:O	2.15	0.79
3:D:197:ASN:ND2	3:D:208:ASP:OD2	2.15	0.79
3:H:197:ASN:ND2	3:H:208:ASP:OD2	2.15	0.79
1:A:607:ASN:ND2	1:A:654:GLU:OE2	2.13	0.78
2:C:122:LEU:H	2:C:202:ALA:HA	1.50	0.77
1:A:550:GLN:HG3	1:A:551:GLN:HG2	1.66	0.77
1:B:550:GLN:HG3	1:B:551:GLN:HG2	1.66	0.76
4:E:149:TRP:HE1	4:E:177:SER:HG	1.34	0.76
1:A:608:VAL:HG23	1:A:650:GLN:HE21	1.50	0.75
3:H:38:ARG:HG3	3:H:48:ILE:HD11	1.68	0.74
1:B:574:LYS:NZ	2:G:107:ASP:OD2	2.17	0.72
2:G:198:THR:HG22	9:G:604:NAG:HN2	1.53	0.72
1:A:610:TRP:HB3	2:C:34:LEU:HB3	1.72	0.70
1:A:607:ASN:OD1	2:C:502:LYS:NZ	2.27	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:322:ILE:O	4:L:94:ARG:NH2	2.29	0.66
3:D:100(D):VAL:HG22	3:D:100(F):SER:H	1.61	0.65
1:A:574:LYS:NZ	2:C:107:ASP:OD2	2.21	0.64
1:B:610:TRP:HE3	2:G:36:VAL:HG12	1.64	0.63
2:C:101:VAL:HG13	2:C:479:TRP:HB2	1.79	0.63
2:G:161:VAL:HG23	2:G:170:GLN:HB3	1.79	0.63
2:G:101:VAL:HG13	2:G:479:TRP:HB2	1.79	0.63
2:G:477:ASP:OD1	2:G:480:ARG:NH1	2.31	0.63
2:G:477:ASP:HA	2:G:480:ARG:HD2	1.80	0.63
2:C:165:LEU:HB2	2:C:168:LYS:HB2	1.79	0.63
4:E:13:VAL:HG11	4:E:19:ALA:HB2	1.80	0.63
1:B:582:ALA:HB1	2:G:221:ALA:HB3	1.79	0.62
1:B:650:GLN:HG3	1:B:651:ILE:H	1.64	0.62
1:A:582:ALA:HB1	2:C:221:ALA:HB3	1.81	0.62
3:H:29:MET:O	3:H:71:ARG:NH1	2.32	0.62
3:D:100:ARG:NH1	3:D:100(A):ILE:O	2.33	0.62
2:C:322:ILE:O	4:E:94:ARG:NH2	2.33	0.62
2:C:91:GLU:OE2	2:C:487:LYS:NZ	2.33	0.61
2:G:165:LEU:HB2	2:G:168:LYS:HB2	1.81	0.61
3:H:36:TRP:HB3	3:H:48:ILE:HD12	1.81	0.61
4:L:28:LEU:HD22	4:L:94:ARG:HG3	1.82	0.61
4:E:29:GLY:H	4:E:67:PHE:HE2	1.47	0.61
1:A:610:TRP:HE3	2:C:36:VAL:HG12	1.66	0.60
1:A:657:GLU:O	1:A:661:LEU:HG	2.02	0.60
2:C:131:CYS:HA	2:C:157:CYS:HA	1.82	0.60
3:D:96:ARG:HD3	3:H:1:GLN:H1	1.66	0.60
2:G:172:MET:HE3	2:G:173:ASP:H	1.67	0.60
4:E:133:LEU:HB2	4:E:179:LEU:HB3	1.84	0.59
2:C:37:THR:OG1	2:C:497:ALA:O	2.20	0.59
2:G:267:GLU:HG3	2:G:268:GLU:HG2	1.82	0.59
4:L:133:LEU:HB2	4:L:179:LEU:HB3	1.84	0.59
2:G:91:GLU:OE2	2:G:487:LYS:NZ	2.36	0.59
1:A:650:GLN:O	1:A:654:GLU:N	2.30	0.59
2:C:277:ILE:O	2:C:456:ARG:NH1	2.35	0.59
1:A:606:THR:HB	1:A:650:GLN:NE2	2.13	0.59
2:G:131:CYS:HA	2:G:157:CYS:HA	1.85	0.59
2:G:277:ILE:O	2:G:456:ARG:NH1	2.35	0.58
4:L:36:TYR:HA	4:L:46:LEU:HA	1.85	0.58
3:H:60:ASN:HB3	3:H:63:LEU:HD13	1.84	0.58
4:L:9:ARG:NH1	4:L:22:SER:O	2.33	0.58
1:A:617:LYS:NZ	1:A:626:MET:SD	2.77	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:304:ARG:NH2	2:C:438:PRO:O	2.34	0.57
2:C:385:CYS:HA	2:C:418:CYS:HA	1.86	0.57
3:H:29:MET:HA	3:H:34:TRP:HZ2	1.70	0.57
3:H:100:ARG:NH1	3:H:100(A):ILE:O	2.38	0.57
2:C:256:THR:O	2:C:478:ASN:ND2	2.30	0.56
2:C:172:MET:HE3	2:C:173:ASP:H	1.69	0.56
2:C:264:SER:OG	2:C:482:GLU:OE1	2.23	0.56
2:G:116:LEU:HD11	2:G:434:MET:HB2	1.87	0.56
2:G:273:ARG:NH1	2:G:287:GLN:OE1	2.28	0.56
3:H:100(D):VAL:HG22	3:H:100(F):SER:H	1.71	0.56
4:L:13:VAL:HG11	4:L:19:ALA:HB2	1.88	0.55
4:E:133:LEU:HD22	4:E:179:LEU:HD23	1.87	0.55
2:C:133:ASN:OD1	2:C:155:LYS:NZ	2.39	0.55
2:C:285:ILE:HD11	2:C:481:SER:HB3	1.86	0.55
2:G:385:CYS:HA	2:G:418:CYS:HA	1.88	0.55
3:H:55:GLU:OE2	3:H:71:ARG:NH2	2.40	0.55
3:D:29:MET:HA	3:D:34:TRP:HZ2	1.71	0.55
1:A:544:LEU:HD21	2:C:493:PRO:HG3	1.88	0.54
4:E:36:TYR:HA	4:E:46:LEU:HA	1.88	0.54
3:H:38:ARG:HH12	3:H:82:LEU:HD22	1.72	0.54
2:C:267:GLU:HG3	2:C:268:GLU:HG2	1.87	0.54
2:C:52:LEU:H	2:C:52:LEU:HD23	1.73	0.54
2:G:299:PRO:HB2	2:G:327:ARG:HB2	1.89	0.54
4:L:179:LEU:HG	4:L:181:LEU:HD13	1.89	0.54
2:G:37:THR:OG1	2:G:497:ALA:O	2.25	0.54
2:G:285:ILE:HD11	2:G:481:SER:HB3	1.90	0.54
1:B:650:GLN:HG3	1:B:651:ILE:N	2.23	0.54
2:G:94:ASN:HA	2:G:236:THR:HG22	1.90	0.54
2:G:67:ASN:ND2	2:G:70:ALA:H	2.06	0.54
2:C:334:SER:HA	2:C:413:THR:HG22	1.89	0.53
4:E:66(B):ILE:HG13	3:H:158:ALA:HA	1.90	0.53
3:D:150:VAL:HB	3:D:178:LEU:HD21	1.91	0.53
4:E:9:ARG:NH1	4:E:22:SER:O	2.40	0.53
2:G:304:ARG:NH2	2:G:438:PRO:O	2.36	0.53
2:C:67:ASN:ND2	2:C:70:ALA:H	2.06	0.53
4:E:39:ARG:NH1	4:E:83:GLU:O	2.42	0.53
2:G:334:SER:HA	2:G:413:THR:HG22	1.91	0.53
1:B:606:THR:HB	1:B:650:GLN:OE1	2.08	0.53
2:G:264:SER:OG	2:G:482:GLU:OE1	2.23	0.53
2:G:476:ARG:HA	2:G:479:TRP:CD1	2.44	0.53
2:G:439:ILE:HB	2:G:443:ILE:HD11	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:545:LEU:HD13	1:A:586:TYR:CG	2.44	0.52
1:A:535:ILE:HG13	1:A:536:THR:HG23	1.90	0.52
3:D:87:THR:HG23	3:D:110:THR:HA	1.92	0.52
1:A:608:VAL:HG23	1:A:650:GLN:NE2	2.20	0.52
2:C:476:ARG:HA	2:C:479:TRP:CD1	2.45	0.51
4:L:8:VAL:HG12	4:L:101:ALA:HB3	1.93	0.51
3:H:87:THR:HG23	3:H:110:THR:HA	1.91	0.51
2:G:193:LEU:HB2	2:G:196:CYS:SG	2.51	0.51
2:C:203:GLN:HG3	2:C:435:TYR:HD2	1.75	0.51
4:L:114:PRO:HB3	4:L:140:PHE:HB3	1.92	0.51
3:D:13:LYS:HB2	3:D:16:GLU:OE2	2.11	0.50
1:B:545:LEU:HD13	1:B:586:TYR:CG	2.45	0.50
2:C:299:PRO:HB2	2:C:327:ARG:HB2	1.94	0.50
1:A:610:TRP:CE3	2:C:36:VAL:HG12	2.46	0.50
2:C:193:LEU:HB2	2:C:196:CYS:SG	2.51	0.50
2:G:474:ASP:OD2	2:G:476:ARG:NH1	2.44	0.50
2:G:67:ASN:HD21	2:G:70:ALA:H	1.59	0.50
2:G:474:ASP:OD1	2:G:475:MET:N	2.45	0.50
3:H:25:SER:HA	6:I:8:MAN:H61	1.94	0.49
1:A:545:LEU:HD13	1:A:586:TYR:CD2	2.47	0.49
3:D:22:CYS:HB3	3:D:78:LEU:HB3	1.93	0.49
2:C:503:ARG:HG2	2:C:504:ARG:H	1.77	0.49
3:H:150:VAL:HB	3:H:178:LEU:HD21	1.94	0.49
3:D:168:ALA:HB2	3:D:178:LEU:HB3	1.94	0.49
1:B:571:TRP:CE3	2:G:54:CYS:HB2	2.48	0.49
4:E:83:GLU:OE1	4:E:167:LYS:NZ	2.45	0.49
1:B:545:LEU:HD13	1:B:586:TYR:CD2	2.48	0.49
2:G:203:GLN:HG3	2:G:435:TYR:HD2	1.77	0.49
1:A:610:TRP:CD2	2:C:498:PRO:HB3	2.48	0.48
3:H:168:ALA:HB2	3:H:178:LEU:HB3	1.95	0.48
2:G:198:THR:OG1	2:G:199:SER:N	2.46	0.48
1:B:525:ALA:HB1	1:B:533:ALA:HA	1.96	0.48
2:C:193:LEU:HD22	2:C:423:ILE:HD11	1.95	0.48
3:D:1:GLN:N	3:H:96:ARG:HD3	2.29	0.48
3:D:33:TYR:HB2	3:D:95:ALA:HB3	1.95	0.48
2:G:86:LEU:HB3	2:G:89:VAL:HG21	1.96	0.48
2:G:133:ASN:OD1	2:G:155:LYS:NZ	2.45	0.48
2:C:87:GLU:HB2	9:C:601:NAG:H82	1.96	0.48
3:H:22:CYS:HB3	3:H:78:LEU:HB3	1.96	0.48
3:H:82:LEU:HD23	3:H:82(C):VAL:HG12	1.94	0.48
1:B:610:TRP:CG	2:G:498:PRO:HB3	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:330:HIS:HB3	3:D:100(G):PHE:HE2	1.79	0.48
3:H:126:PRO:HB3	3:H:138:LEU:HB3	1.95	0.48
3:H:13:LYS:HB2	3:H:16:GLU:OE2	2.14	0.48
2:C:128:THR:HG23	2:C:190:TYR:HB3	1.96	0.47
2:C:439:ILE:HB	2:C:443:ILE:HD11	1.95	0.47
2:C:474:ASP:OD2	2:C:476:ARG:NH1	2.46	0.47
2:G:193:LEU:HD22	2:G:423:ILE:HD11	1.95	0.47
1:B:581:LEU:HA	1:B:584:GLU:HB2	1.95	0.47
3:D:96:ARG:HD3	3:H:1:GLN:N	2.30	0.47
1:B:596:TRP:HA	1:B:651:ILE:HG21	1.96	0.47
2:G:110:ASN:O	2:G:114:GLN:HG2	2.15	0.47
2:G:256:THR:O	2:G:478:ASN:ND2	2.40	0.47
1:A:596:TRP:HA	1:A:651:ILE:HG21	1.96	0.46
2:C:240:LYS:HD2	9:C:606:NAG:H83	1.96	0.46
2:G:122:LEU:HG	2:G:203:GLN:H	1.79	0.46
2:G:503:ARG:HG2	2:G:504:ARG:H	1.79	0.46
2:C:474:ASP:OD1	2:C:475:MET:N	2.48	0.46
2:C:110:ASN:O	2:C:114:GLN:HG2	2.14	0.46
3:D:60:ASN:OD1	3:D:62:SER:OG	2.18	0.46
1:B:532:ALA:O	1:B:535:ILE:HG12	2.15	0.46
1:B:605:CYS:HA	2:G:37:THR:HG22	1.97	0.46
2:G:57:ASP:OD1	2:G:57:ASP:N	2.49	0.46
4:E:142:PRO:HD2	4:E:199:GLU:OE2	2.16	0.46
2:G:284:ILE:HG23	2:G:454:LEU:HB2	1.97	0.46
3:H:146:PHE:HA	3:H:147:PRO:HA	1.79	0.46
4:L:133:LEU:HD22	4:L:179:LEU:HD23	1.97	0.46
2:C:86:LEU:HB3	2:C:89:VAL:HG21	1.98	0.46
3:D:210:ARG:NH2	3:D:212:GLU:OE2	2.47	0.46
3:D:161:SER:OG	4:L:20:ARG:NH1	2.49	0.45
3:D:15:SER:HA	3:D:82(B):SER:HA	1.98	0.45
2:G:330:HIS:HB3	3:H:100(G):PHE:HE2	1.82	0.45
3:H:29:MET:HA	3:H:34:TRP:CZ2	2.51	0.45
4:L:25:ARG:NH2	4:L:88:CYS:O	2.50	0.45
1:A:536:THR:O	1:A:540:GLN:NE2	2.48	0.45
2:C:67:ASN:HD21	2:C:70:ALA:H	1.62	0.45
4:E:8:VAL:HG22	4:E:101:ALA:HB3	1.98	0.45
4:E:125:GLU:OE2	4:E:132:THR:N	2.49	0.45
2:C:201:MET:HA	2:C:433:ALA:HB3	1.98	0.45
2:C:323:ILE:HG22	2:C:324:GLY:H	1.81	0.45
2:G:199:SER:HB3	2:G:431:GLY:H	1.81	0.45
1:A:591:GLN:O	1:A:595:ILE:HG12	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:57:ASP:N	2:C:57:ASP:OD1	2.50	0.45
2:G:50:THR:OG1	2:G:51:THR:N	2.48	0.45
2:C:322:ILE:HD11	2:C:326:ILE:HD13	1.99	0.45
2:G:69:TRP:HE1	2:G:108:ILE:HD12	1.82	0.45
3:H:94:THR:OG1	3:H:101:ASP:OD1	2.34	0.45
2:G:369:LEU:O	2:G:373:THR:OG1	2.22	0.44
6:I:7:MAN:H62	6:I:8:MAN:H2	1.73	0.44
2:C:360:THR:HB	2:C:467:THR:HG22	1.98	0.44
2:C:69:TRP:HE1	2:C:108:ILE:HD12	1.83	0.44
3:H:210:ARG:NH2	3:H:212:GLU:OE2	2.50	0.44
2:C:369:LEU:O	2:C:373:THR:OG1	2.21	0.44
3:D:169:VAL:HG21	4:E:161:GLU:HB3	1.99	0.44
2:C:230:ASP:HB3	2:C:233:PHE:HB2	1.99	0.44
6:I:8:MAN:H2	6:I:9:MAN:H2	1.65	0.44
2:C:294:ILE:HD11	2:C:331:CYS:HB3	2.00	0.44
3:D:128:SER:OG	4:E:212:CYS:O	2.35	0.43
4:E:27:ALA:HB2	4:E:31:ARG:HD3	2.00	0.43
3:H:147:PRO:O	3:H:200:HIS:NE2	2.33	0.43
1:A:605:CYS:HA	2:C:37:THR:HG22	2.00	0.43
1:B:657:GLU:O	1:B:661:LEU:HG	2.17	0.43
2:C:166:LYS:HB2	2:C:166:LYS:HE3	1.88	0.43
2:G:249:HIS:ND1	2:G:486:TYR:OH	2.38	0.43
3:D:27:ASP:OD1	3:D:28:SER:N	2.47	0.43
2:G:260:LEU:HD12	2:G:451:GLY:HA3	1.99	0.43
3:H:51:ILE:HD11	3:H:55:GLU:HA	1.99	0.43
2:C:349:LEU:HD13	2:C:468:PHE:CE2	2.54	0.43
1:B:610:TRP:CD2	2:G:498:PRO:HB3	2.54	0.43
1:B:544:LEU:HD23	2:G:40:TYR:OH	2.19	0.43
1:B:613:THR:C	1:B:615:SER:H	2.22	0.43
2:G:272:ILE:HG22	2:G:284:ILE:HD11	2.00	0.43
2:C:123:THR:OG1	2:C:124:PRO:HD3	2.19	0.42
3:D:38:ARG:NE	3:D:46:GLU:OE2	2.52	0.42
2:G:41:GLY:H	2:G:493:PRO:HB2	1.83	0.42
2:G:101:VAL:HG22	2:G:483:LEU:HD12	2.01	0.42
4:E:34:GLN:HG3	4:E:49:TYR:HA	2.01	0.42
2:C:112:TRP:O	2:C:116:LEU:HG	2.19	0.42
2:C:122:LEU:HD22	2:C:125:LEU:HD23	2.00	0.42
2:G:123:THR:OG1	2:G:124:PRO:HD3	2.19	0.42
4:L:142:PRO:HD2	4:L:199:GLU:OE2	2.20	0.42
2:C:249:HIS:ND1	2:C:486:TYR:OH	2.39	0.42
2:C:363:ASN:O	2:C:469:ARG:NH1	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:55:ALA:HA	2:C:75:VAL:O	2.20	0.42
2:C:61:TYR:HB3	2:C:64:GLU:O	2.18	0.42
2:G:323:ILE:HG22	2:G:324:GLY:H	1.84	0.42
3:D:100(G):PHE:HB2	3:D:100(I):GLU:HG3	2.02	0.42
3:D:126:PRO:HB3	3:D:138:LEU:HB3	2.02	0.42
2:G:128:THR:HG23	2:G:190:TYR:HB3	2.02	0.42
1:B:610:TRP:CE3	2:G:36:VAL:HG12	2.51	0.41
3:H:15:SER:HA	3:H:82(B):SER:HA	2.01	0.41
1:B:554:ASN:OD1	2:G:76:PRO:HD3	2.20	0.41
2:C:116:LEU:HD22	2:C:434:MET:HG3	2.01	0.41
1:A:574:LYS:HD3	2:C:52:LEU:O	2.19	0.41
1:B:574:LYS:HD3	2:G:52:LEU:O	2.20	0.41
2:C:260:LEU:HD12	2:C:451:GLY:HA3	2.01	0.41
2:C:476:ARG:O	2:C:480:ARG:HG3	2.20	0.41
4:E:36:TYR:CE2	4:E:46:LEU:HB3	2.56	0.41
3:H:18:LEU:HD11	3:H:109:VAL:HG11	2.02	0.41
1:A:613:THR:C	1:A:615:SER:H	2.24	0.41
3:D:94:THR:OG1	3:D:101:ASP:OD1	2.38	0.41
4:E:21:ILE:HG23	4:E:102:THR:HG21	2.01	0.41
3:H:200:HIS:HB3	3:H:203:SER:HG	1.85	0.41
2:C:233:PHE:HD2	2:C:273:ARG:HH21	1.69	0.41
3:D:146:PHE:HA	3:D:147:PRO:HA	1.79	0.41
2:G:296:CYS:HA	2:G:331:CYS:HA	2.03	0.41
3:H:68:VAL:HB	3:H:81:LYS:HB2	2.02	0.41
4:L:54:ARG:HH21	4:L:63:SER:HA	1.85	0.41
8:K:6:MAN:H62	8:K:8:MAN:H2	1.79	0.41
1:A:525:ALA:HB1	1:A:533:ALA:HA	2.02	0.41
2:C:50:THR:OG1	2:C:51:THR:N	2.52	0.41
2:C:101:VAL:HG22	2:C:483:LEU:HD12	2.03	0.41
2:C:272:ILE:HG23	2:C:284:ILE:HD11	2.03	0.41
2:G:104:MET:O	2:G:108:ILE:HG12	2.21	0.41
2:C:108:ILE:O	2:C:112:TRP:HD1	2.04	0.41
2:C:122:LEU:HG	2:C:203:GLN:H	1.86	0.41
4:E:57:GLY:HA2	4:L:45:ILE:HD13	2.02	0.41
2:G:349:LEU:HD13	2:G:468:PHE:CE2	2.55	0.41
2:C:122:LEU:HD23	2:C:122:LEU:HA	1.92	0.41
3:H:86:ASP:HB2	3:H:111:VAL:HG21	2.03	0.41
1:A:532:ALA:O	1:A:535:ILE:HG12	2.21	0.40
2:C:199:SER:HB3	2:C:431:GLY:H	1.86	0.40
3:H:189:LEU:HD21	3:H:213:PRO:HG3	2.03	0.40
2:G:119:CYS:SG	2:G:205:CYS:N	2.94	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:273:ARG:O	2:G:284:ILE:HD12	2.21	0.40
1:B:591:GLN:O	1:B:595:ILE:HG12	2.21	0.40
2:C:104:MET:O	2:C:108:ILE:HG12	2.21	0.40
2:G:478:ASN:O	2:G:481:SER:OG	2.35	0.40
4:L:83:GLU:HB2	4:L:106:VAL:HG23	2.02	0.40
2:C:170:GLN:HG2	2:C:172:MET:HG2	2.04	0.40
3:D:29:MET:HA	3:D:34:TRP:CZ2	2.55	0.40
3:D:100(P):MET:N	3:D:100(P):MET:SD	2.95	0.40
3:H:38:ARG:HG2	3:H:90:TYR:CD1	2.56	0.40
3:H:169:VAL:HG21	4:L:161:GLU:HB3	2.02	0.40

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

All (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
2	C	258	GLN
4	E	51	ASN
2	G	258	GLN
4	L	51	ASN
4	L	66(B)	ILE
2	C	309	ILE
2	G	309	ILE

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
All	All	1758/1894 (93%)	1722 (98%)	36 (2%)	55	74

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	603	ILE
1	A	618	THR
1	B	603	ILE
1	B	618	THR

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Mol	Chain	Res	Type
1	B	651	ILE
2	C	52	LEU
2	C	65	VAL
2	C	71	THR
2	C	74	CYS
2	C	123	THR
2	C	125	LEU
2	C	127	VAL
2	C	161	VAL
2	C	284	ILE
2	C	294	ILE
3	D	144	ASP
4	E	50	ASN
4	E	52	GLN
4	E	67	PHE
4	E	95(B)	PHE
4	E	119	PHE
2	G	65	VAL
2	G	71	THR
2	G	74	CYS
2	G	116	LEU
2	G	123	THR
2	G	127	VAL
2	G	161	VAL
2	G	284	ILE
3	H	18	LEU
3	H	144	ASP
4	L	28	LEU
4	L	52	GLN
4	L	67	PHE
4	L	95(B)	PHE
4	L	119	PHE

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

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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

All (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
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
8	K	4	MAN	C1-C2-C3	3.09	113.47	109.67
6	I	6	MAN	C1-O5-C5	3.06	116.34	112.19
6	I	4	MAN	C1-O5-C5	3.03	116.30	112.19
6	I	7	MAN	C1-O5-C5	2.99	116.25	112.19
8	K	6	MAN	C1-O5-C5	2.91	116.13	112.19
6	I	5	MAN	O2-C2-C3	-2.55	105.02	110.14
6	I	8	MAN	O2-C2-C3	-2.55	105.02	110.14
5	F	6	MAN	O2-C2-C3	-2.31	105.51	110.14
6	I	4	MAN	O5-C1-C2	2.26	114.26	110.77
6	I	6	MAN	O2-C2-C3	-2.25	105.62	110.14
5	F	4	MAN	O2-C2-C3	-2.23	105.67	110.14
6	I	9	MAN	O2-C2-C3	-2.22	105.69	110.14
6	I	10	MAN	O2-C2-C3	-2.21	105.70	110.14
8	K	8	MAN	O2-C2-C3	-2.21	105.71	110.14
5	F	5	MAN	C1-O5-C5	2.20	115.18	112.19
8	K	5	MAN	O2-C2-C3	-2.20	105.72	110.14
8	K	7	MAN	O2-C2-C3	-2.17	105.79	110.14
8	K	6	MAN	O2-C2-C3	-2.15	105.84	110.14
8	K	4	MAN	O5-C1-C2	2.14	114.08	110.77
7	J	4	MAN	O2-C2-C3	-2.14	105.85	110.14
5	F	5	MAN	O2-C2-C3	-2.13	105.88	110.14
6	I	10	MAN	C1-O5-C5	2.12	115.06	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	J	4	MAN	C1-O5-C5	2.12	115.06	112.19
6	I	7	MAN	O2-C2-C3	-2.10	105.94	110.14
8	K	7	MAN	C1-O5-C5	2.01	114.91	112.19
8	K	8	MAN	C1-O5-C5	2.00	114.90	112.19

There are no chirality outliers.

All (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
5	F	1	NAG	O5-C5-C6-O6
5	F	1	NAG	C4-C5-C6-O6
6	I	8	MAN	O5-C5-C6-O6
5	F	6	MAN	C4-C5-C6-O6
5	F	2	NAG	C3-C2-N2-C7
6	I	2	NAG	C3-C2-N2-C7
7	J	2	NAG	C3-C2-N2-C7
8	K	2	NAG	C3-C2-N2-C7
5	F	5	MAN	O5-C5-C6-O6
5	F	5	MAN	C4-C5-C6-O6
5	F	6	MAN	O5-C5-C6-O6

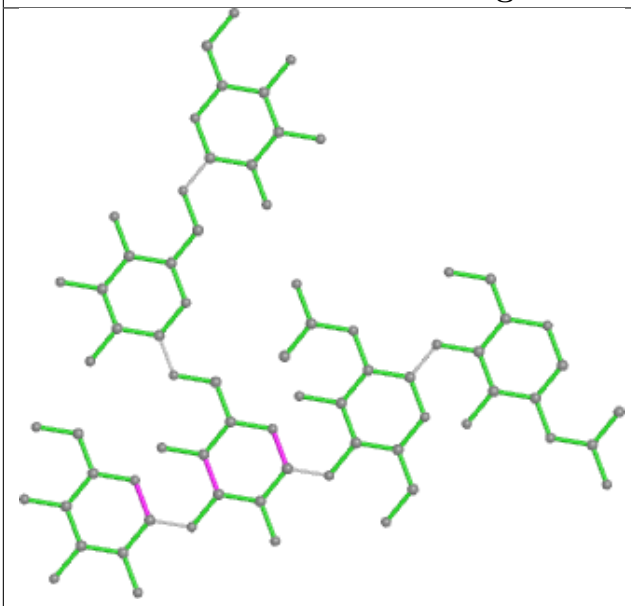
There are no ring outliers.

5 monomers are involved in 4 short contacts:

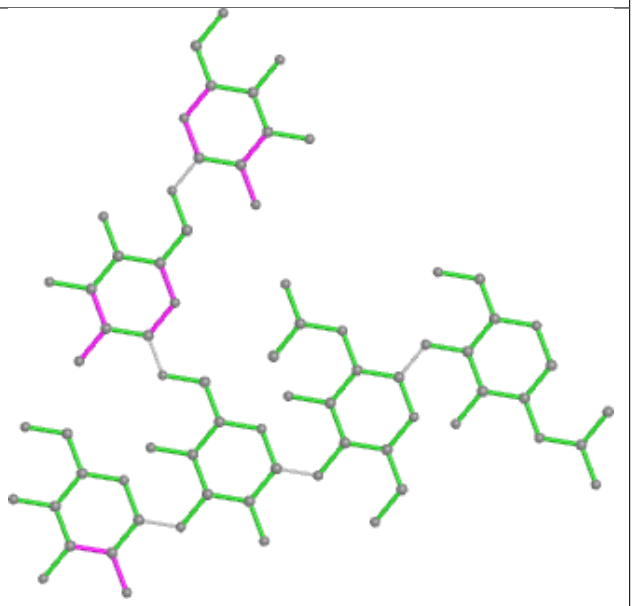
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	K	8	MAN	1	0
6	I	7	MAN	1	0
8	K	6	MAN	1	0
6	I	9	MAN	1	0
6	I	8	MAN	3	0

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

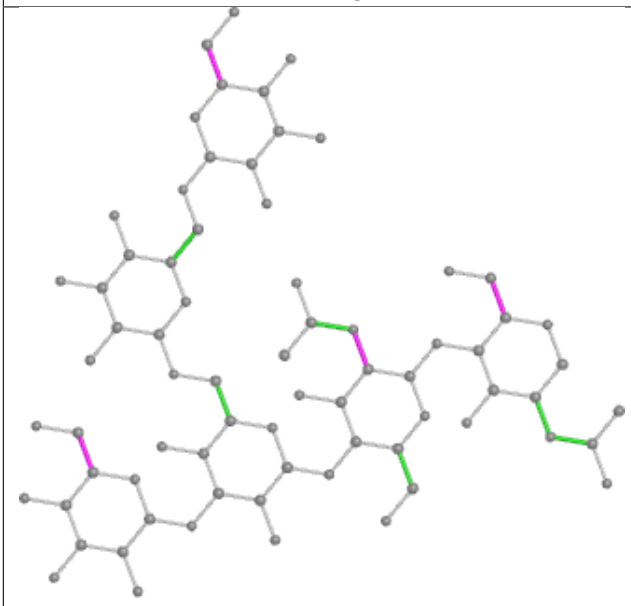
Oligosaccharide Chain F



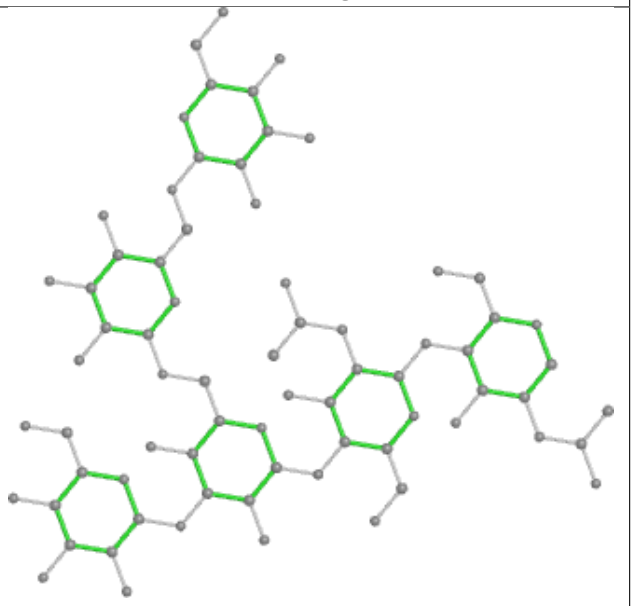
Bond lengths



Bond angles

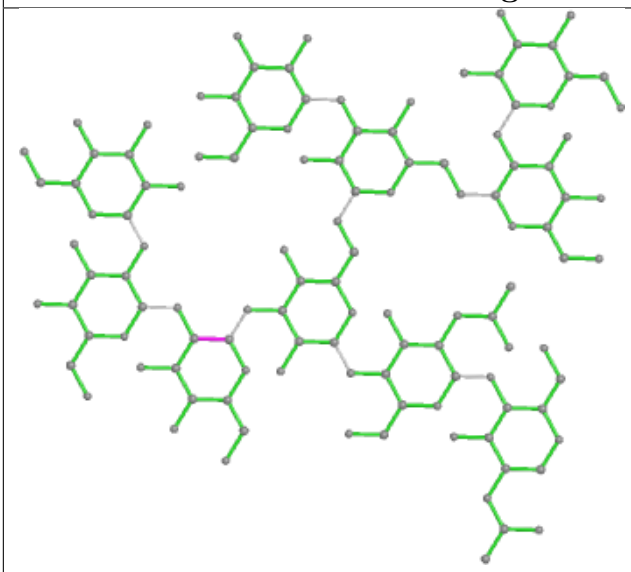


Torsions

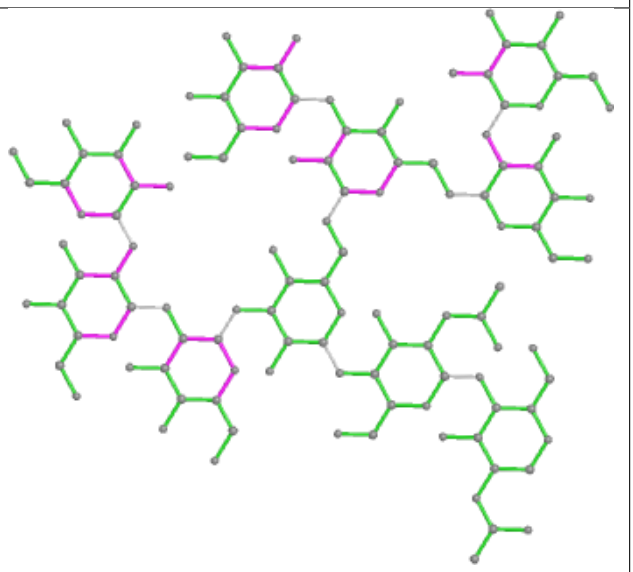


Rings

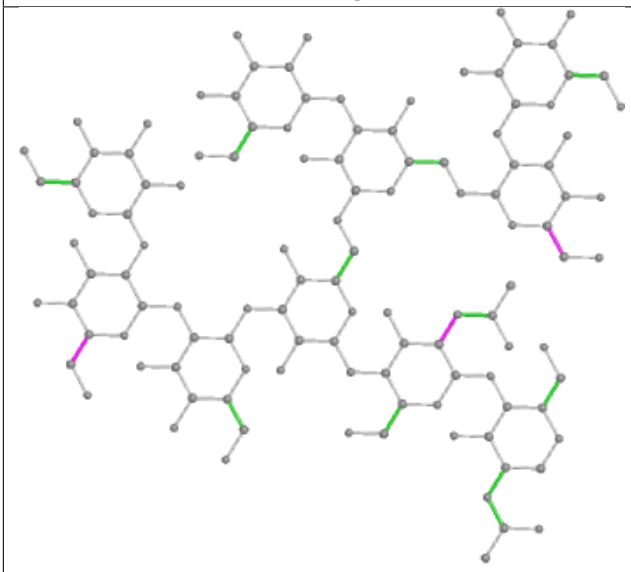
Oligosaccharide Chain I



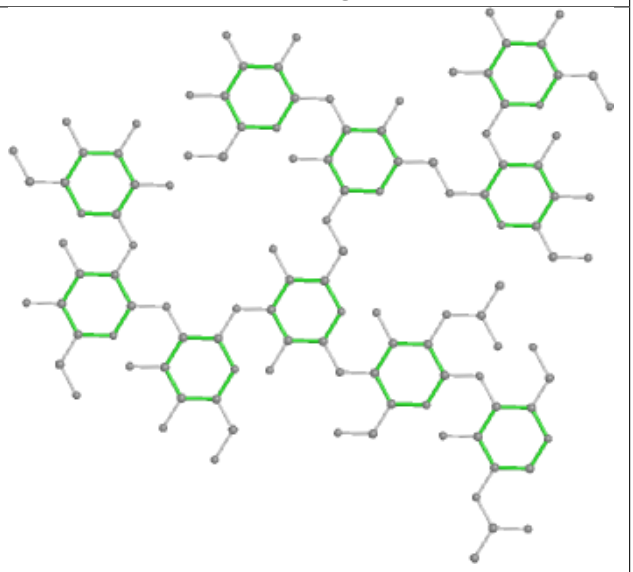
Bond lengths



Bond angles

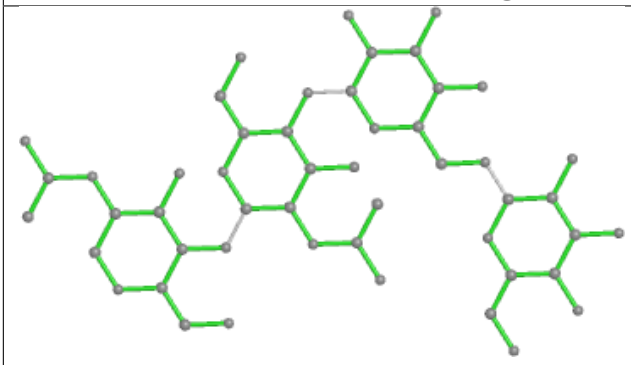


Torsions

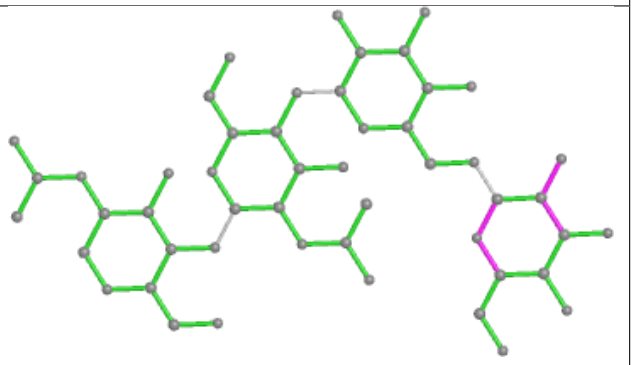


Rings

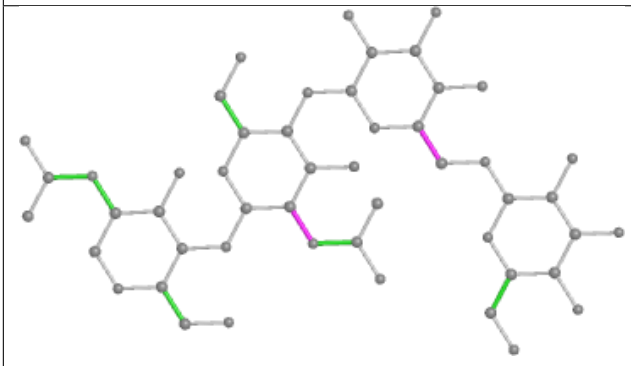
Oligosaccharide Chain J



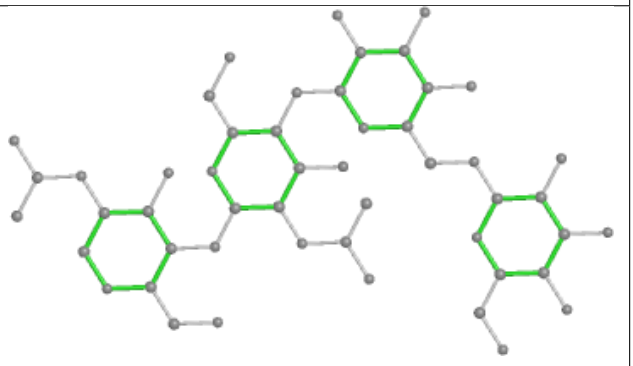
Bond lengths



Bond angles

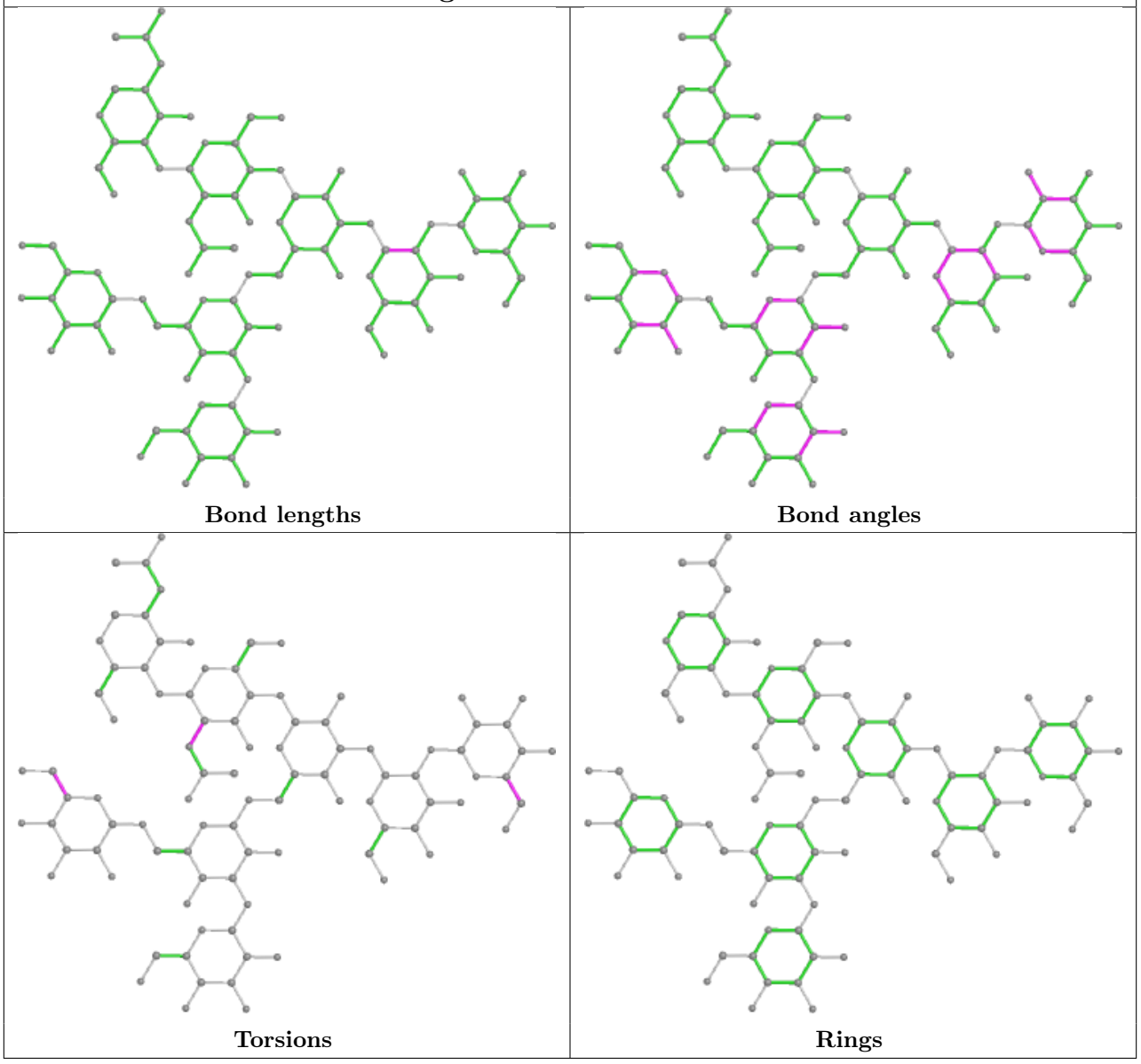


Torsions



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.

All (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
9	G	603	NAG	O5-C5-C6-O6
9	A	701	NAG	O5-C5-C6-O6
9	C	606	NAG	O5-C5-C6-O6
9	G	602	NAG	O5-C5-C6-O6
9	G	605	NAG	O5-C5-C6-O6
9	G	620	NAG	O5-C5-C6-O6
9	G	624	NAG	O5-C5-C6-O6
9	C	603	NAG	C4-C5-C6-O6
9	C	605	NAG	O5-C5-C6-O6
9	G	604	NAG	O5-C5-C6-O6
9	B	701	NAG	C4-C5-C6-O6
9	G	603	NAG	C4-C5-C6-O6
9	C	606	NAG	C4-C5-C6-O6
9	G	605	NAG	C4-C5-C6-O6
9	G	620	NAG	C4-C5-C6-O6
9	C	604	NAG	O5-C5-C6-O6
9	C	624	NAG	O5-C5-C6-O6
9	G	601	NAG	C4-C5-C6-O6
9	G	602	NAG	C4-C5-C6-O6
9	C	601	NAG	C4-C5-C6-O6
9	C	625	NAG	C4-C5-C6-O6
9	A	701	NAG	C4-C5-C6-O6
9	G	624	NAG	C4-C5-C6-O6
9	C	604	NAG	C4-C5-C6-O6
9	C	626	NAG	O5-C5-C6-O6
9	C	624	NAG	C4-C5-C6-O6
9	C	605	NAG	C4-C5-C6-O6
9	G	604	NAG	C4-C5-C6-O6
9	C	626	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
9	G	619	NAG	O5-C5-C6-O6
9	G	624	NAG	C1-C2-N2-C7
9	C	602	NAG	O5-C5-C6-O6
9	G	610	NAG	O5-C5-C6-O6
9	C	602	NAG	C3-C2-N2-C7
9	G	619	NAG	C4-C5-C6-O6
9	G	621	NAG	C4-C5-C6-O6
9	G	621	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

All (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
1	A	545	LEU	7.3
3	D	184	VAL	7.3
4	E	208	ALA	7.3
1	A	538	THR	7.2
4	E	212	CYS	7.2
4	E	144	ALA	7.1
1	A	541	ALA	6.9
4	L	110	PRO	6.8
1	B	524	GLY	6.8
4	E	210	THR	6.7
1	A	542	ARG	6.6

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Mol	Chain	Res	Type	RSRZ
4	E	207	VAL	6.6
3	D	113	SER	6.5
3	D	11	LEU	6.5
4	E	145	VAL	6.3
2	G	64	GLU	6.2
4	L	145	VAL	6.0
2	G	63	THR	5.9
1	B	545	LEU	5.8
2	G	72	HIS	5.8
3	D	110	THR	5.7
3	D	10	GLY	5.7
4	L	111	LYS	5.5
2	C	72	HIS	5.4
3	D	183	THR	5.3
2	G	290	LYS	5.2
3	D	127	SER	5.2
3	D	148	GLU	5.2
1	A	602	LEU	5.1
4	L	207	VAL	5.0
2	G	61	TYR	5.0
4	E	153	SER	5.0
2	C	355	ASN	4.9
2	G	326	ILE	4.9
2	C	58	ALA	4.8
3	H	161	SER	4.7
2	G	354	PRO	4.7
2	C	354	PRO	4.7
3	D	46	GLU	4.7
3	D	45	LEU	4.6
2	G	427	TRP	4.6
4	L	176	SER	4.6
2	C	427	TRP	4.6
3	H	183	THR	4.5
1	A	550	GLN	4.5
1	B	538	THR	4.5
2	G	60	ALA	4.5
1	A	551	GLN	4.5
3	D	185	PRO	4.4
4	E	110	PRO	4.4
2	G	322	ILE	4.4
2	C	57	ASP	4.4
3	D	1	GLN	4.4

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Mol	Chain	Res	Type	RSRZ
2	G	432	ARG	4.4
2	C	40	TYR	4.3
3	D	129	LYS	4.3
3	D	167	PRO	4.3
4	E	209	PRO	4.3
2	C	432	ARG	4.3
2	G	112	TRP	4.3
2	C	326	ILE	4.2
4	L	144	ALA	4.2
1	B	541	ALA	4.2
1	B	542	ARG	4.2
4	E	154	SER	4.2
2	C	238	SER	4.2
2	G	321(A)	ALA	4.2
2	G	184	ILE	4.1
4	L	37	GLN	4.1
2	C	424	ILE	4.1
4	L	211	GLU	4.1
3	D	100(N)	TYR	4.1
3	H	185	PRO	4.1
2	C	322	ILE	4.1
1	B	567	ARG	4.0
3	H	114	ALA	4.0
2	C	496	VAL	4.0
4	L	186	TRP	3.9
4	E	27	ALA	3.9
2	G	496	VAL	3.9
3	H	11	LEU	3.9
2	G	277	ILE	3.9
4	L	199	GLU	3.9
3	D	147	PRO	3.8
4	L	112	ALA	3.8
2	C	59	LYS	3.8
2	G	238	SER	3.8
1	A	537	LEU	3.8
2	G	431	GLY	3.8
3	D	160	THR	3.8
2	G	355	ASN	3.8
1	A	603	ILE	3.7
3	D	2	VAL	3.7
4	E	203	VAL	3.7
3	D	115	SER	3.6

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Mol	Chain	Res	Type	RSRZ
3	D	9	PRO	3.6
2	C	434	MET	3.6
4	L	143	GLY	3.6
4	E	186	TRP	3.6
4	E	182	THR	3.6
3	D	136	ALA	3.5
1	B	552	GLN	3.5
4	E	155	PRO	3.5
1	B	568	LEU	3.5
2	C	356	ALA	3.5
2	C	321(A)	ALA	3.5
4	E	109	GLN	3.5
1	B	550	GLN	3.5
2	C	62	SER	3.4
2	G	468	PHE	3.4
2	C	433	ALA	3.4
2	C	425	ASN	3.4
3	D	109	VAL	3.4
3	H	9	PRO	3.4
1	B	536	THR	3.4
3	H	38	ARG	3.4
3	D	128	SER	3.3
3	D	108	THR	3.3
4	L	206	THR	3.3
3	H	160	THR	3.3
3	D	137	ALA	3.3
1	A	568	LEU	3.3
1	B	523	LEU	3.2
1	A	546	SER	3.2
2	C	179	ARG	3.2
3	H	110	THR	3.2
1	A	547	GLY	3.2
2	C	423	ILE	3.2
3	D	186	SER	3.2
3	D	27	ASP	3.2
2	C	210	PHE	3.2
4	L	132	THR	3.2
2	G	456	ARG	3.2
4	L	203	VAL	3.1
1	A	536	THR	3.1
4	L	210	THR	3.1
2	C	468	PHE	3.1

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Mol	Chain	Res	Type	RSRZ
2	G	302	ASN	3.0
2	G	244	THR	3.0
3	D	112	SER	3.0
2	G	245	VAL	3.0
2	C	83	GLU	3.0
3	D	135	THR	3.0
3	D	161	SER	3.0
1	A	524	GLY	3.0
2	C	504	ARG	3.0
4	E	206	THR	3.0
4	L	137	ILE	3.0
2	C	277	ILE	2.9
2	C	184	ILE	2.9
3	H	135	THR	2.9
2	C	112	TRP	2.9
3	D	38	ARG	2.9
3	H	10	GLY	2.9
2	G	389	LYS	2.9
2	C	498	PRO	2.9
3	H	113	SER	2.9
3	D	210	ARG	2.8
2	G	206	PRO	2.8
1	A	554	ASN	2.8
2	C	302	ASN	2.8
3	H	136	ALA	2.8
2	G	45	TRP	2.8
2	C	213	ILE	2.8
2	C	315	GLN	2.8
3	H	148	GLU	2.8
2	C	100	MET	2.8
4	L	192	TYR	2.8
2	C	440	GLN	2.7
2	G	458	GLY	2.7
3	H	115	SER	2.7
3	H	100(N)	TYR	2.7
1	B	583	LEU	2.7
2	G	49	VAL	2.7
1	A	601	LYS	2.7
2	C	108	ILE	2.7
1	A	544	LEU	2.7
1	B	534	SER	2.7
4	E	37	GLN	2.7

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Mol	Chain	Res	Type	RSRZ
4	E	56	SER	2.7
2	C	190	TYR	2.7
4	E	176	SER	2.6
4	L	66	PRO	2.6
4	E	199	GLU	2.6
3	H	45	LEU	2.6
2	C	217	TYR	2.6
3	H	112	SER	2.6
1	A	523	LEU	2.6
2	C	161	VAL	2.6
2	G	498	PRO	2.6
2	G	502	LYS	2.6
4	L	181	LEU	2.6
3	H	126	PRO	2.6
4	L	208	ALA	2.6
4	L	190	ARG	2.6
2	C	290	LYS	2.6
2	C	60	ALA	2.6
2	C	188	ASN	2.6
2	G	246	GLN	2.6
2	C	73	ALA	2.5
3	D	179	SER	2.5
4	L	142	PRO	2.5
2	G	504	ARG	2.5
4	E	142	PRO	2.5
2	C	439	ILE	2.5
2	G	425	ASN	2.5
2	C	178	ARG	2.5
2	G	213	ILE	2.5
2	C	206	PRO	2.5
2	C	426	MET	2.5
2	G	424	ILE	2.5
3	H	18	LEU	2.5
4	L	64	GLY	2.5
2	G	423	ILE	2.4
1	A	534	SER	2.4
2	G	459	GLY	2.4
4	L	20	ARG	2.4
3	H	179	SER	2.4
3	H	109	VAL	2.4
2	G	95	VAL	2.4
2	C	317	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
2	G	368	ASP	2.4
1	B	551	GLN	2.4
1	B	526	ALA	2.4
4	L	109	GLN	2.3
3	H	167	PRO	2.3
4	L	120	PRO	2.3
1	B	537	LEU	2.3
2	C	237	GLY	2.3
4	E	63	SER	2.3
2	G	108	ILE	2.3
3	D	121	VAL	2.3
1	B	592	LEU	2.3
2	G	135	SER	2.3
2	C	316	THR	2.3
2	C	274	SER	2.3
2	G	73	ALA	2.3
2	G	353	PHE	2.3
2	C	435	TYR	2.2
2	G	128	THR	2.2
4	L	193	SER	2.2
2	G	269	GLU	2.2
2	G	248	THR	2.2
4	L	63	SER	2.2
4	L	178	TYR	2.2
2	G	100	MET	2.2
2	G	439	ILE	2.2
2	G	231	LYS	2.2
2	G	433	ALA	2.2
4	E	202	THR	2.2
2	G	390	LEU	2.2
4	E	147	VAL	2.2
4	L	202	THR	2.2
4	E	191	SER	2.2
1	B	596	TRP	2.2
2	C	34	LEU	2.2
1	B	546	SER	2.2
3	H	129	LYS	2.2
2	G	50	THR	2.2
4	L	56	SER	2.2
2	C	269	GLU	2.1
4	L	114	PRO	2.1
3	D	158	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
4	E	181	LEU	2.1
4	L	45	ILE	2.1
1	A	539	VAL	2.1
2	C	246	GLN	2.1
2	G	454	LEU	2.1
4	E	132	THR	2.1
4	L	177	SER	2.1
4	E	31	ARG	2.1
4	L	187	LYS	2.1
4	L	134	VAL	2.1
2	G	356	ALA	2.1
3	H	138	LEU	2.1
2	C	224	ALA	2.1
3	D	3	GLN	2.1
2	G	505	VAL	2.1
2	G	59	LYS	2.1
3	H	46	GLU	2.1
2	C	390	LEU	2.1
4	E	70	ARG	2.1
2	C	452	LEU	2.1
1	B	652	GLN	2.0
4	E	120	PRO	2.0
2	C	71	THR	2.0
2	C	483	LEU	2.0
1	A	620	ASN	2.0
1	A	567	ARG	2.0
2	C	298	ARG	2.0
4	E	204	GLU	2.0
4	E	62	PHE	2.0
2	C	444	ARG	2.0

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)

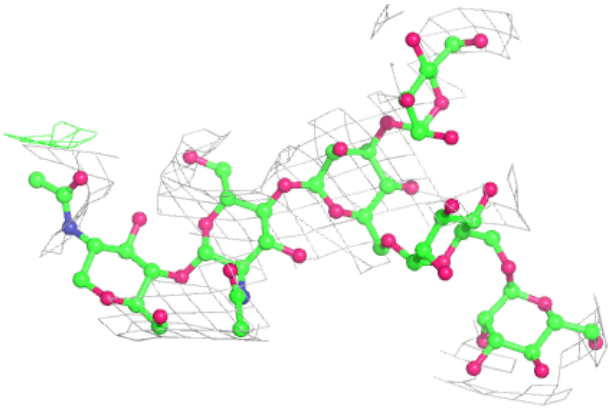
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

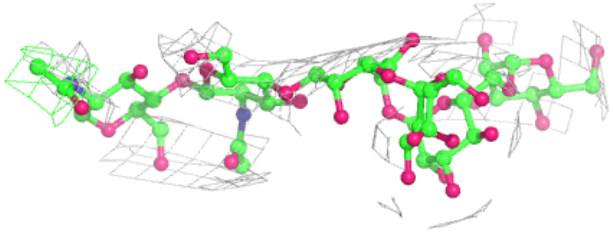
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
8	MAN	K	6	11/12	0.56	0.42	439,456,462,469	0
8	BMA	K	3	11/12	0.62	0.30	472,490,501,501	0
6	BMA	I	3	11/12	0.63	0.29	466,483,494,494	0
8	MAN	K	5	11/12	0.64	0.44	507,510,523,531	0
6	MAN	I	7	11/12	0.66	0.32	422,439,445,451	0
7	BMA	J	3	11/12	0.71	0.33	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

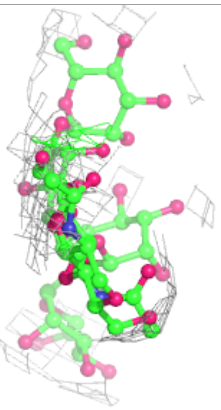
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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)

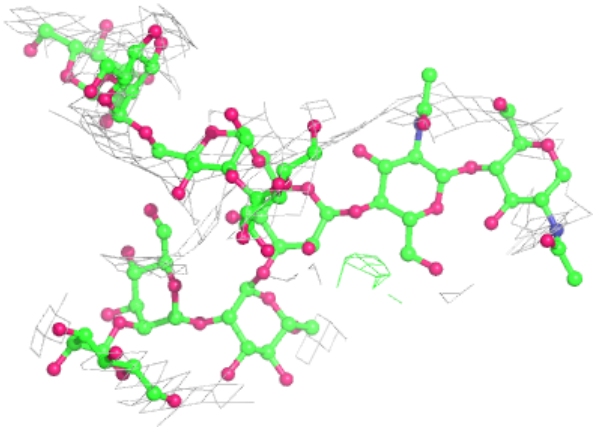


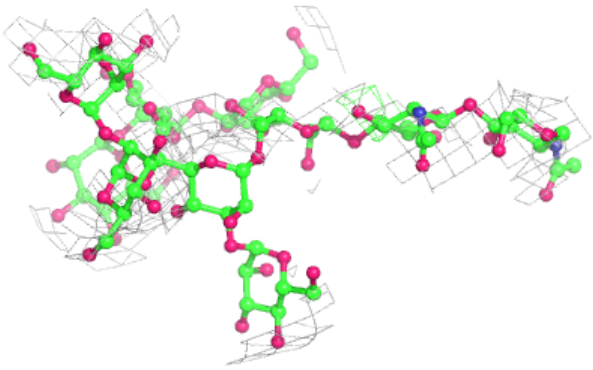


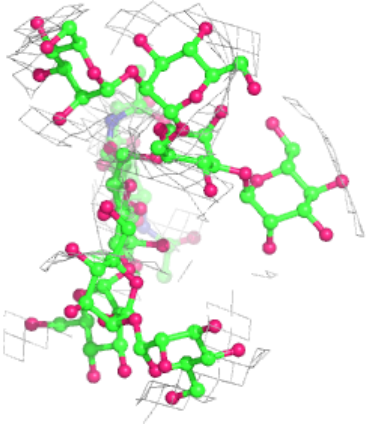


Electron density around Chain I:

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

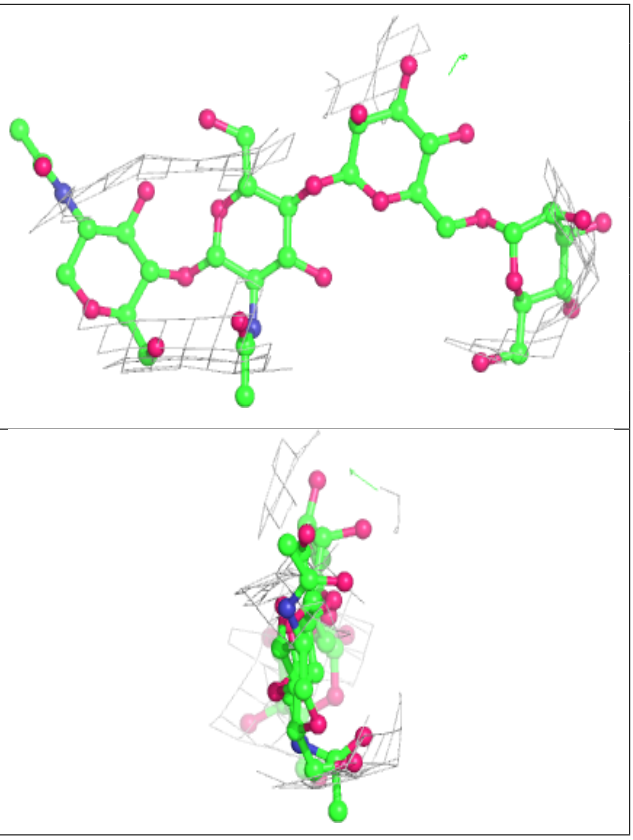


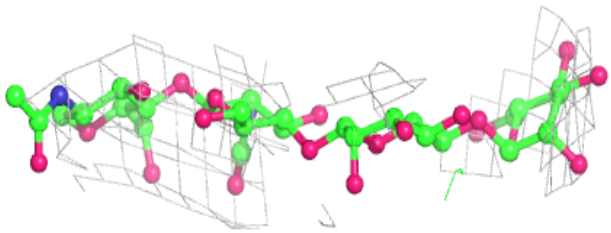




Electron density around Chain J:

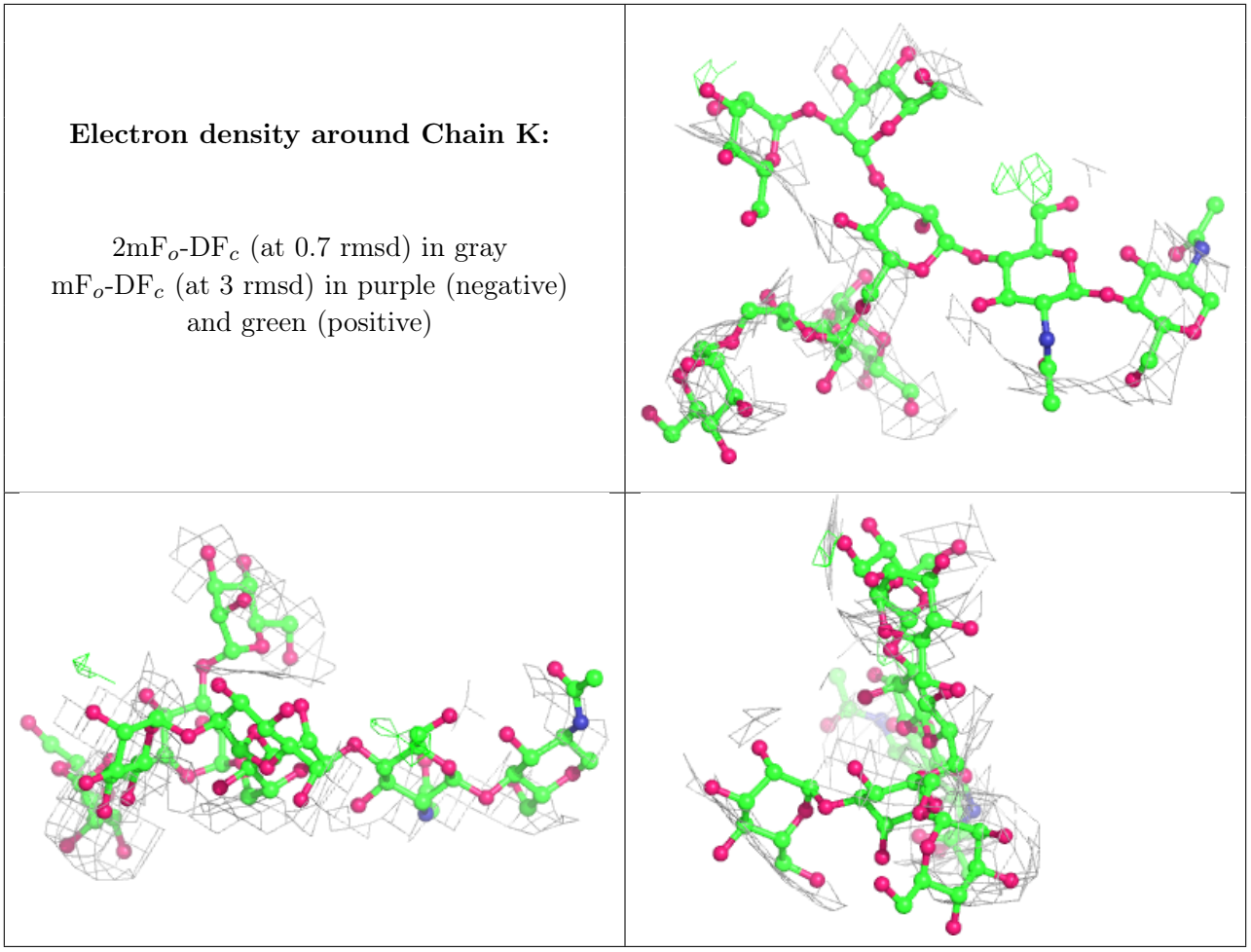
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





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.