Full wwPDB X-ray Structure Validation Report ⓘ

Sep 24, 2023 – 08:55 AM EDT

PDB ID	:	5UQY
Title	:	Crystal structure of Marburg virus GP in complex with the human survivor antibody MR78
Authors	:	Hashiguchi, T.; Fusco, M.L.; Hastie, K.M.; Bomholdt, Z.A.; Lee, J.E.; Flyak, A.I.; Matsuoka, R.; Kohda, D.; Yanagi, Y.; Hammel, M.; Crowe, J.E.; Saphire, E.O.
Deposited on	:	2017-02-08
Resolution	:	3.60 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 ⓘ 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 ⓘ) were used in the production of this report:

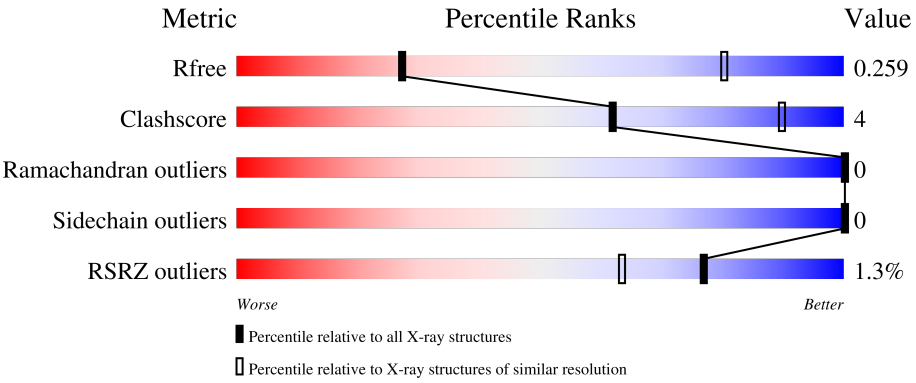
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.60 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	1257 (3.70-3.50)
Clashscore	141614	1353 (3.70-3.50)
Ramachandran outliers	138981	1307 (3.70-3.50)
Sidechain outliers	138945	1307 (3.70-3.50)
RSRZ outliers	127900	1161 (3.70-3.50)

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	250	51% 7% 42%
1	E	250	2% 52% 6% 42%
1	I	250	2% 50% 7% 43%
1	M	250	.% 49% 8% 43%

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Mol	Chain	Length	Quality of chain
2	B	237	47% 7% 46%
2	F	237	2% 34% 6% 60%
2	J	237	% 37% 59%
2	N	237	34% 5% 61%
3	C	211	2% 87% 13%
3	G	211	% 85% 15%
3	K	211	90% 10%
3	O	211	% 90% 10%
4	D	226	% 83% 14%
4	H	226	83% 14%
4	L	226	87% 12%
4	P	226	79% 14% 7%
5	Q	2	100%
5	R	2	100%
5	T	2	100%
5	W	2	100%
5	Y	2	100%
5	Z	2	100%
6	S	6	50% 33% 17%
6	U	6	33% 67%
7	V	4	75% 25%
7	X	4	50% 50%
8	a	5	40% 60%

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
10	MAN	M	305	-	-	-	X

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 21208 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called ENVELOPE GLYCOPROTEIN GP1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	145	Total	C	N	O	S	0	0	0
			1131	717	198	209	7			
1	E	144	Total	C	N	O	S	0	0	0
			1122	712	197	207	6			
1	I	142	Total	C	N	O	S	0	0	0
			1112	706	195	205	6			
1	M	142	Total	C	N	O	S	0	0	0
			1112	706	195	205	6			

- Molecule 2 is a protein called ENVELOPE GLYCOPROTEIN GP2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	127	Total	C	N	O	S	0	0	0
			962	608	167	182	5			
2	F	94	Total	C	N	O	S	0	0	0
			740	470	131	137	2			
2	J	97	Total	C	N	O	S	0	0	0
			752	477	133	140	2			
2	N	92	Total	C	N	O	S	0	0	0
			722	460	128	132	2			

There are 156 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	438	LEU	PHE	engineered mutation	UNP Q1PDC7
B	439	ALA	TRP	engineered mutation	UNP Q1PDC7
B	445	GLY	PHE	engineered mutation	UNP Q1PDC7
B	447	ASN	PHE	engineered mutation	UNP Q1PDC7
B	638	ASP	-	expression tag	UNP Q1PDC7
B	639	ASP	-	expression tag	UNP Q1PDC7
B	640	ASP	-	expression tag	UNP Q1PDC7
B	641	ASP	-	expression tag	UNP Q1PDC7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	642	LYS	-	expression tag	UNP Q1PDC7
B	643	ALA	-	expression tag	UNP Q1PDC7
B	644	GLY	-	expression tag	UNP Q1PDC7
B	645	TRP	-	expression tag	UNP Q1PDC7
B	646	SER	-	expression tag	UNP Q1PDC7
B	647	HIS	-	expression tag	UNP Q1PDC7
B	648	PRO	-	expression tag	UNP Q1PDC7
B	649	GLN	-	expression tag	UNP Q1PDC7
B	650	PHE	-	expression tag	UNP Q1PDC7
B	651	GLU	-	expression tag	UNP Q1PDC7
B	652	LYS	-	expression tag	UNP Q1PDC7
B	653	GLY	-	expression tag	UNP Q1PDC7
B	654	GLY	-	expression tag	UNP Q1PDC7
B	655	GLY	-	expression tag	UNP Q1PDC7
B	656	SER	-	expression tag	UNP Q1PDC7
B	657	GLY	-	expression tag	UNP Q1PDC7
B	658	GLY	-	expression tag	UNP Q1PDC7
B	659	GLY	-	expression tag	UNP Q1PDC7
B	660	SER	-	expression tag	UNP Q1PDC7
B	661	GLY	-	expression tag	UNP Q1PDC7
B	662	GLY	-	expression tag	UNP Q1PDC7
B	663	GLY	-	expression tag	UNP Q1PDC7
B	664	SER	-	expression tag	UNP Q1PDC7
B	665	TRP	-	expression tag	UNP Q1PDC7
B	666	SER	-	expression tag	UNP Q1PDC7
B	667	HIS	-	expression tag	UNP Q1PDC7
B	668	PRO	-	expression tag	UNP Q1PDC7
B	669	GLN	-	expression tag	UNP Q1PDC7
B	670	PHE	-	expression tag	UNP Q1PDC7
B	671	GLU	-	expression tag	UNP Q1PDC7
B	672	LYS	-	expression tag	UNP Q1PDC7
F	438	LEU	PHE	engineered mutation	UNP Q1PDC7
F	439	ALA	TRP	engineered mutation	UNP Q1PDC7
F	445	GLY	PHE	engineered mutation	UNP Q1PDC7
F	447	ASN	PHE	engineered mutation	UNP Q1PDC7
F	638	ASP	-	expression tag	UNP Q1PDC7
F	639	ASP	-	expression tag	UNP Q1PDC7
F	640	ASP	-	expression tag	UNP Q1PDC7
F	641	ASP	-	expression tag	UNP Q1PDC7
F	642	LYS	-	expression tag	UNP Q1PDC7
F	643	ALA	-	expression tag	UNP Q1PDC7
F	644	GLY	-	expression tag	UNP Q1PDC7

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Chain	Residue	Modelled	Actual	Comment	Reference
F	645	TRP	-	expression tag	UNP Q1PDC7
F	646	SER	-	expression tag	UNP Q1PDC7
F	647	HIS	-	expression tag	UNP Q1PDC7
F	648	PRO	-	expression tag	UNP Q1PDC7
F	649	GLN	-	expression tag	UNP Q1PDC7
F	650	PHE	-	expression tag	UNP Q1PDC7
F	651	GLU	-	expression tag	UNP Q1PDC7
F	652	LYS	-	expression tag	UNP Q1PDC7
F	653	GLY	-	expression tag	UNP Q1PDC7
F	654	GLY	-	expression tag	UNP Q1PDC7
F	655	GLY	-	expression tag	UNP Q1PDC7
F	656	SER	-	expression tag	UNP Q1PDC7
F	657	GLY	-	expression tag	UNP Q1PDC7
F	658	GLY	-	expression tag	UNP Q1PDC7
F	659	GLY	-	expression tag	UNP Q1PDC7
F	660	SER	-	expression tag	UNP Q1PDC7
F	661	GLY	-	expression tag	UNP Q1PDC7
F	662	GLY	-	expression tag	UNP Q1PDC7
F	663	GLY	-	expression tag	UNP Q1PDC7
F	664	SER	-	expression tag	UNP Q1PDC7
F	665	TRP	-	expression tag	UNP Q1PDC7
F	666	SER	-	expression tag	UNP Q1PDC7
F	667	HIS	-	expression tag	UNP Q1PDC7
F	668	PRO	-	expression tag	UNP Q1PDC7
F	669	GLN	-	expression tag	UNP Q1PDC7
F	670	PHE	-	expression tag	UNP Q1PDC7
F	671	GLU	-	expression tag	UNP Q1PDC7
F	672	LYS	-	expression tag	UNP Q1PDC7
J	438	LEU	PHE	engineered mutation	UNP Q1PDC7
J	439	ALA	TRP	engineered mutation	UNP Q1PDC7
J	445	GLY	PHE	engineered mutation	UNP Q1PDC7
J	447	ASN	PHE	engineered mutation	UNP Q1PDC7
J	638	ASP	-	expression tag	UNP Q1PDC7
J	639	ASP	-	expression tag	UNP Q1PDC7
J	640	ASP	-	expression tag	UNP Q1PDC7
J	641	ASP	-	expression tag	UNP Q1PDC7
J	642	LYS	-	expression tag	UNP Q1PDC7
J	643	ALA	-	expression tag	UNP Q1PDC7
J	644	GLY	-	expression tag	UNP Q1PDC7
J	645	TRP	-	expression tag	UNP Q1PDC7
J	646	SER	-	expression tag	UNP Q1PDC7
J	647	HIS	-	expression tag	UNP Q1PDC7

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Chain	Residue	Modelled	Actual	Comment	Reference
J	648	PRO	-	expression tag	UNP Q1PDC7
J	649	GLN	-	expression tag	UNP Q1PDC7
J	650	PHE	-	expression tag	UNP Q1PDC7
J	651	GLU	-	expression tag	UNP Q1PDC7
J	652	LYS	-	expression tag	UNP Q1PDC7
J	653	GLY	-	expression tag	UNP Q1PDC7
J	654	GLY	-	expression tag	UNP Q1PDC7
J	655	GLY	-	expression tag	UNP Q1PDC7
J	656	SER	-	expression tag	UNP Q1PDC7
J	657	GLY	-	expression tag	UNP Q1PDC7
J	658	GLY	-	expression tag	UNP Q1PDC7
J	659	GLY	-	expression tag	UNP Q1PDC7
J	660	SER	-	expression tag	UNP Q1PDC7
J	661	GLY	-	expression tag	UNP Q1PDC7
J	662	GLY	-	expression tag	UNP Q1PDC7
J	663	GLY	-	expression tag	UNP Q1PDC7
J	664	SER	-	expression tag	UNP Q1PDC7
J	665	TRP	-	expression tag	UNP Q1PDC7
J	666	SER	-	expression tag	UNP Q1PDC7
J	667	HIS	-	expression tag	UNP Q1PDC7
J	668	PRO	-	expression tag	UNP Q1PDC7
J	669	GLN	-	expression tag	UNP Q1PDC7
J	670	PHE	-	expression tag	UNP Q1PDC7
J	671	GLU	-	expression tag	UNP Q1PDC7
J	672	LYS	-	expression tag	UNP Q1PDC7
N	438	LEU	PHE	engineered mutation	UNP Q1PDC7
N	439	ALA	TRP	engineered mutation	UNP Q1PDC7
N	445	GLY	PHE	engineered mutation	UNP Q1PDC7
N	447	ASN	PHE	engineered mutation	UNP Q1PDC7
N	638	ASP	-	expression tag	UNP Q1PDC7
N	639	ASP	-	expression tag	UNP Q1PDC7
N	640	ASP	-	expression tag	UNP Q1PDC7
N	641	ASP	-	expression tag	UNP Q1PDC7
N	642	LYS	-	expression tag	UNP Q1PDC7
N	643	ALA	-	expression tag	UNP Q1PDC7
N	644	GLY	-	expression tag	UNP Q1PDC7
N	645	TRP	-	expression tag	UNP Q1PDC7
N	646	SER	-	expression tag	UNP Q1PDC7
N	647	HIS	-	expression tag	UNP Q1PDC7
N	648	PRO	-	expression tag	UNP Q1PDC7
N	649	GLN	-	expression tag	UNP Q1PDC7
N	650	PHE	-	expression tag	UNP Q1PDC7

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Chain	Residue	Modelled	Actual	Comment	Reference
N	651	GLU	-	expression tag	UNP Q1PDC7
N	652	LYS	-	expression tag	UNP Q1PDC7
N	653	GLY	-	expression tag	UNP Q1PDC7
N	654	GLY	-	expression tag	UNP Q1PDC7
N	655	GLY	-	expression tag	UNP Q1PDC7
N	656	SER	-	expression tag	UNP Q1PDC7
N	657	GLY	-	expression tag	UNP Q1PDC7
N	658	GLY	-	expression tag	UNP Q1PDC7
N	659	GLY	-	expression tag	UNP Q1PDC7
N	660	SER	-	expression tag	UNP Q1PDC7
N	661	GLY	-	expression tag	UNP Q1PDC7
N	662	GLY	-	expression tag	UNP Q1PDC7
N	663	GLY	-	expression tag	UNP Q1PDC7
N	664	SER	-	expression tag	UNP Q1PDC7
N	665	TRP	-	expression tag	UNP Q1PDC7
N	666	SER	-	expression tag	UNP Q1PDC7
N	667	HIS	-	expression tag	UNP Q1PDC7
N	668	PRO	-	expression tag	UNP Q1PDC7
N	669	GLN	-	expression tag	UNP Q1PDC7
N	670	PHE	-	expression tag	UNP Q1PDC7
N	671	GLU	-	expression tag	UNP Q1PDC7
N	672	LYS	-	expression tag	UNP Q1PDC7

- Molecule 3 is a protein called MR78 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	210	Total	C	N	O	S	0	0	0
			1632	1024	273	330	5			
3	G	210	Total	C	N	O	S	0	0	0
			1632	1024	273	330	5			
3	K	210	Total	C	N	O	S	0	0	0
			1632	1024	273	330	5			
3	O	210	Total	C	N	O	S	0	0	0
			1626	1021	270	330	5			

- Molecule 4 is a protein called MR78 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	218	Total	C	N	O	S	0	0	0
			1635	1045	259	326	5			
4	H	220	Total	C	N	O	S	0	0	0
			1640	1047	260	328	5			

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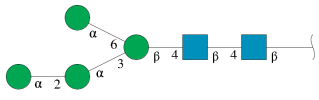
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	L	222	Total	C	N	O	S	0	0	0
			1655	1055	263	332	5			
4	P	211	Total	C	N	O	S	0	0	0
			1594	1019	252	318	5			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	Q	2	Total	C	N	O	0	0	0
			28	16	2	10			
5	R	2	Total	C	N	O	0	0	0
			28	16	2	10			
5	T	2	Total	C	N	O	0	0	0
			28	16	2	10			
5	W	2	Total	C	N	O	0	0	0
			28	16	2	10			
5	Y	2	Total	C	N	O	0	0	0
			28	16	2	10			
5	Z	2	Total	C	N	O	0	0	0
			28	16	2	10			

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



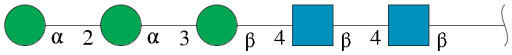
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	S	6	Total	C	N	O	0	0	0
			72	40	2	30			
6	U	6	Total	C	N	O	0	0	0
			72	40	2	30			

- Molecule 7 is an oligosaccharide called 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-gluco

pyranose.

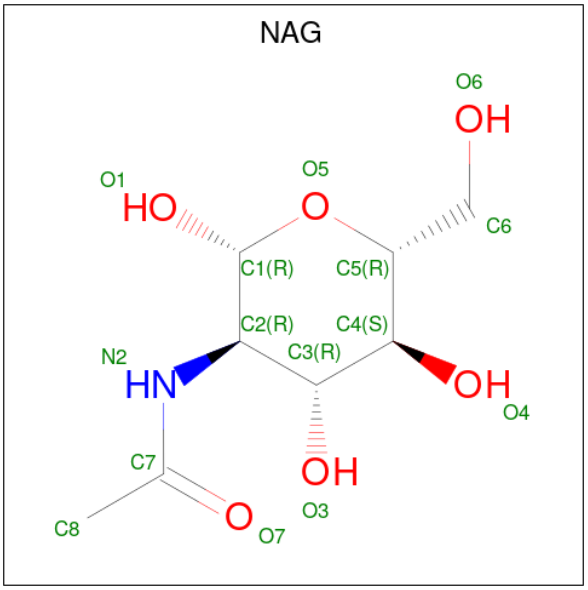
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	V	4	Total	C	N	O	0	0	0
			50	28	2	20			
7	X	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 8 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-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.



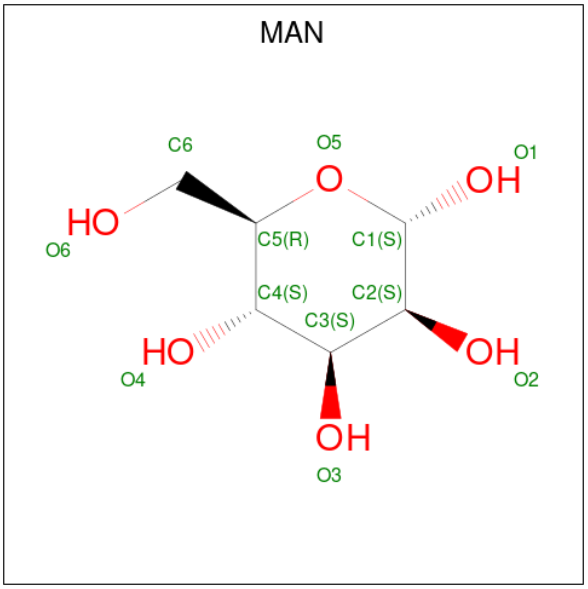
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	a	5	Total	C	N	O	0	0	0
			61	34	2	25			

- 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	E	1	Total C N O 14 8 1 5	0	0

- Molecule 10 is alpha-D-mannopyranose (three-letter code: MAN) (formula: $C_6H_{12}O_6$).



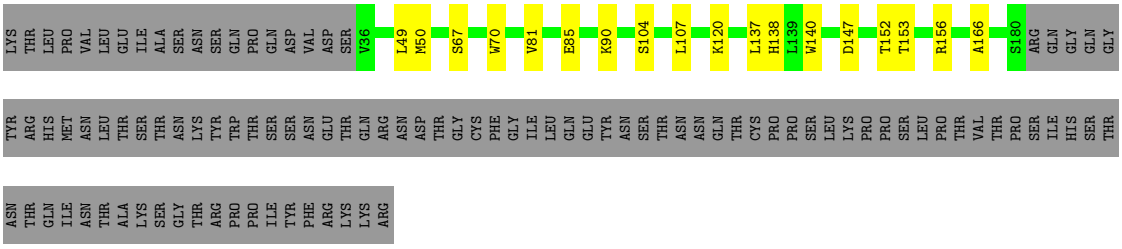
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	I	1	Total C O 11 6 5	0	0
10	M	1	Total C O 11 6 5	0	0

3 Residue-property plots (i)

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

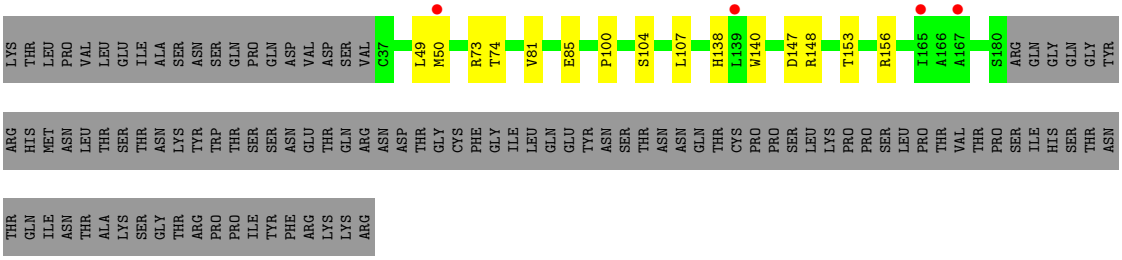
• Molecule 1: ENVELOPE GLYCOPROTEIN GP1

Chain A:



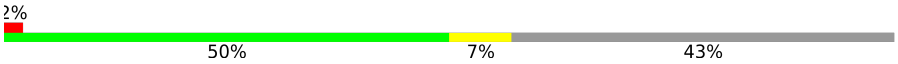
• Molecule 1: ENVELOPE GLYCOPROTEIN GP1

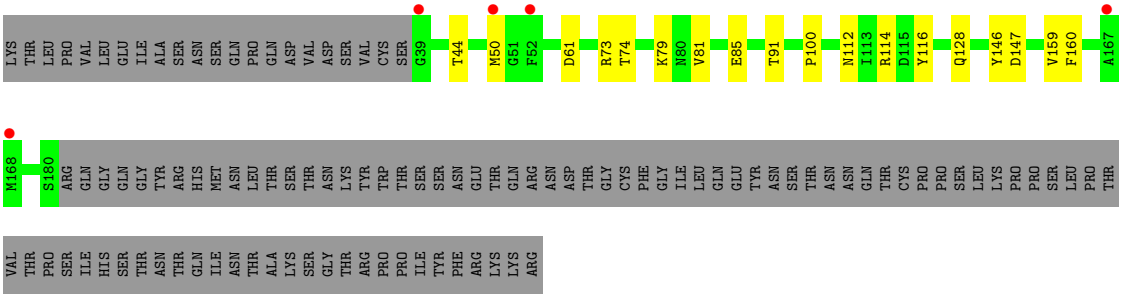
Chain E:



• Molecule 1: ENVELOPE GLYCOPROTEIN GP1

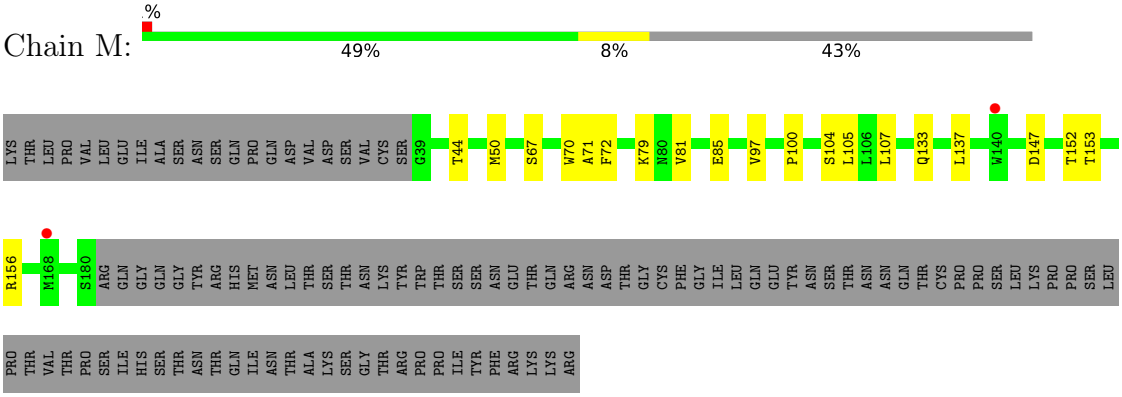
Chain I:





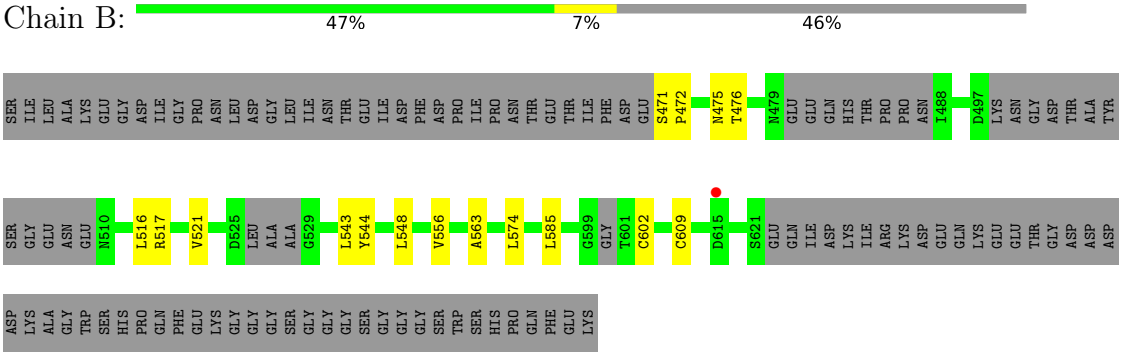
• Molecule 1: ENVELOPE GLYCOPROTEIN GP1

Chain M:



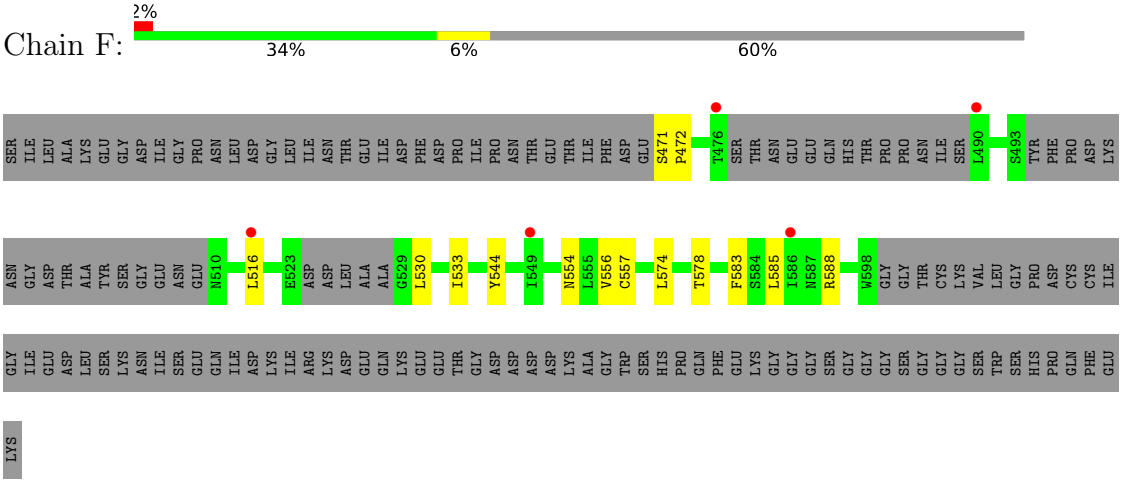
• Molecule 2: ENVELOPE GLYCOPROTEIN GP2

Chain B:



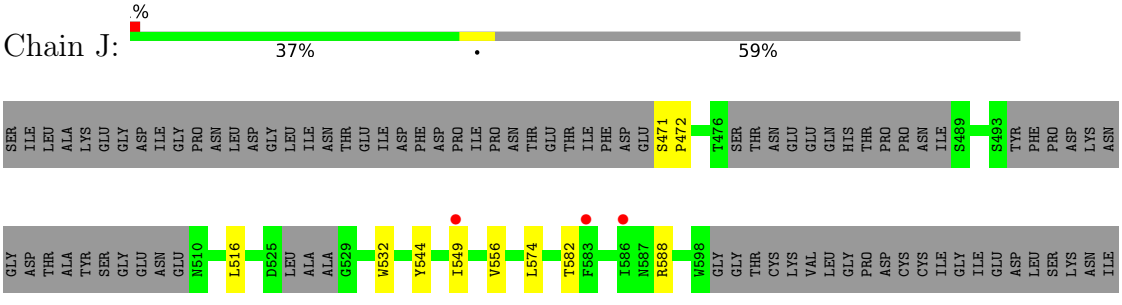
• Molecule 2: ENVELOPE GLYCOPROTEIN GP2

Chain F:



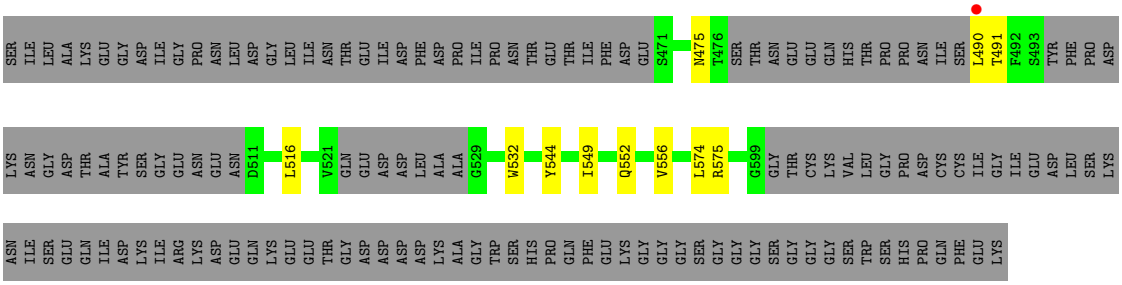
• Molecule 2: ENVELOPE GLYCOPROTEIN GP2

Chain J:



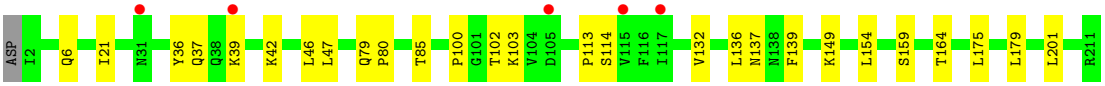
• Molecule 2: ENVELOPE GLYCOPROTEIN GP2

Chain N:



• Molecule 3: MR78 Fab light chain

Chain C:

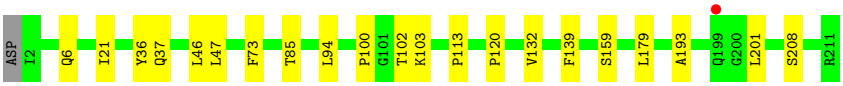


• Molecule 3: MR78 Fab light chain

Chain G:

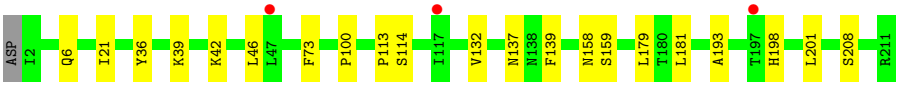
• Molecule 3: MR78 Fab light chain

Chain K:



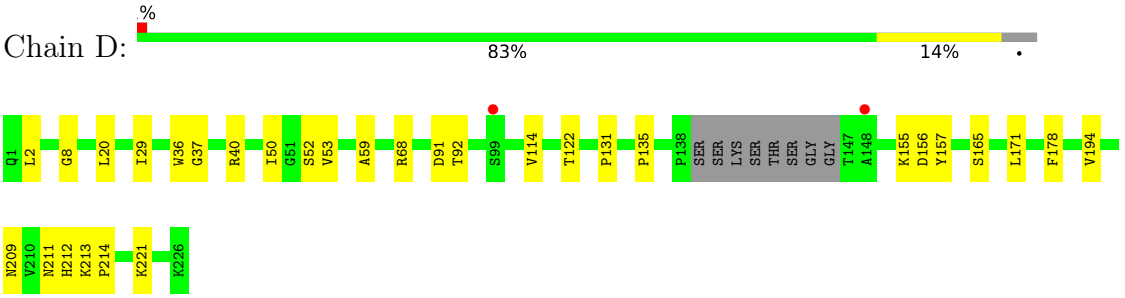
• Molecule 3: MR78 Fab light chain

Chain O:



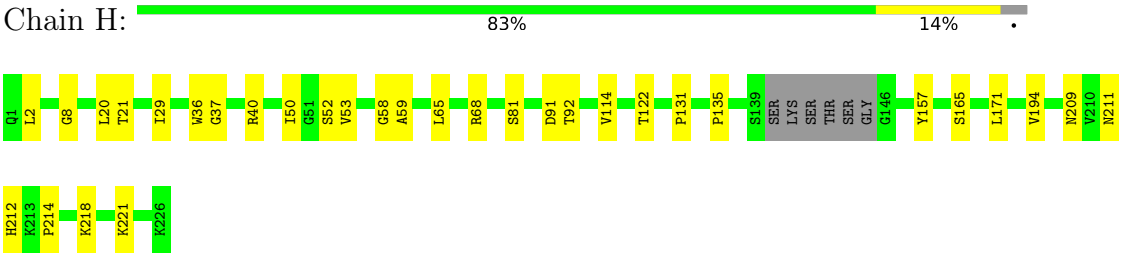
• Molecule 4: MR78 Fab heavy chain

Chain D:



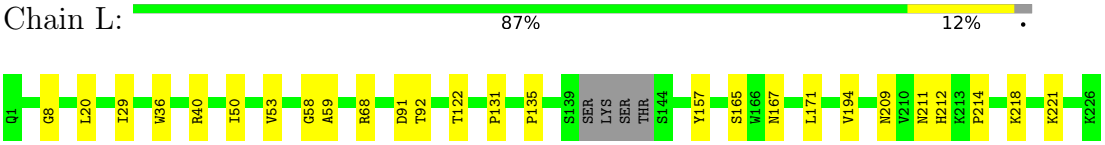
• Molecule 4: MR78 Fab heavy chain

Chain H:



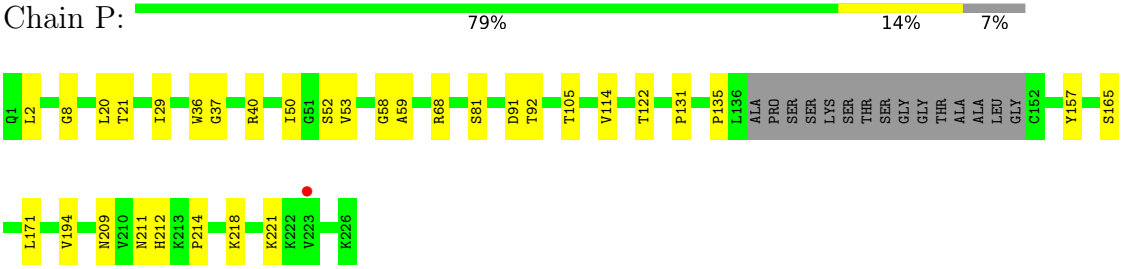
• Molecule 4: MR78 Fab heavy chain

Chain L:



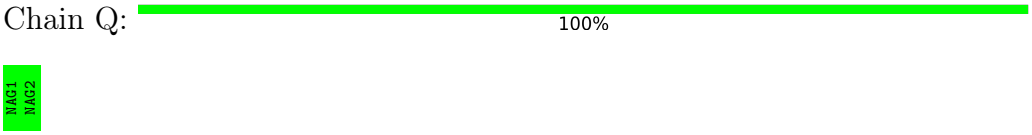
• Molecule 4: MR78 Fab heavy chain

Chain P:



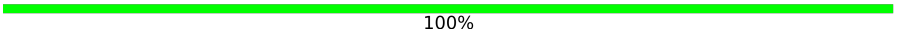
• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q:



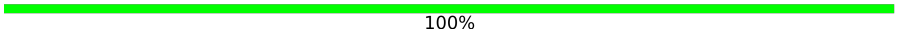
• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R:



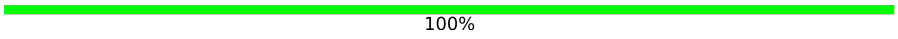
• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain T:



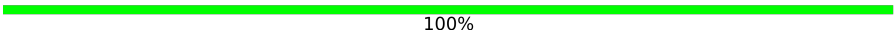
• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain W:



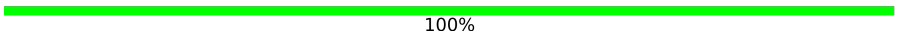
• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Y:



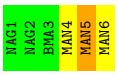
• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Z:



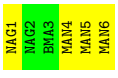
• Molecule 6: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain S:



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

Chain U:



• Molecule 7: 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

Chain V: 

• Molecule 7: 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

Chain X: 

• Molecule 8: alpha-D-mannopyranose-(1-2)-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

Chain a: 

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α, β, γ	204.65Å 204.65Å 192.96Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	84.74 – 3.60 130.53 – 3.60	Depositor EDS
% Data completeness (in resolution range)	99.4 (84.74-3.60) 99.4 (130.53-3.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.14	Depositor
$< I/\sigma(I) >$ [1]	2.23 (at 3.58Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.221 , 0.262 0.220 , 0.259	Depositor DCC
R_{free} test set	2674 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	105.0	Xtriage
Anisotropy	0.180	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 75.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.41$, $< L^2 > = 0.24$	Xtriage
Estimated twinning fraction	0.178 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	21208	wwPDB-VP
Average B, all atoms (Å^2)	106.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.65% 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: BMA, MAN, NAG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.25	0/1159	0.43	0/1571
1	E	0.25	0/1150	0.43	0/1559
1	I	0.25	0/1140	0.43	0/1545
1	M	0.24	0/1140	0.43	0/1545
2	B	0.24	0/976	0.42	0/1324
2	F	0.24	0/751	0.39	0/1017
2	J	0.24	0/763	0.40	0/1034
2	N	0.23	0/733	0.40	0/992
3	C	0.25	0/1667	0.45	0/2263
3	G	0.24	0/1667	0.45	0/2263
3	K	0.24	0/1667	0.45	0/2263
3	O	0.24	0/1661	0.45	0/2256
4	D	0.25	0/1680	0.45	0/2294
4	H	0.25	0/1685	0.45	0/2303
4	L	0.25	0/1700	0.45	0/2320
4	P	0.24	0/1638	0.44	0/2235
All	All	0.24	0/21177	0.44	0/28784

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	1131	0	1115	11	0
1	E	1122	0	1101	10	0
1	I	1112	0	1097	14	0
1	M	1112	0	1097	13	0
2	B	962	0	918	10	0
2	F	740	0	726	11	0
2	J	752	0	729	9	0
2	N	722	0	715	9	0
3	C	1632	0	1590	15	0
3	G	1632	0	1590	17	0
3	K	1632	0	1590	12	0
3	O	1626	0	1579	12	0
4	D	1635	0	1591	16	0
4	H	1640	0	1588	17	0
4	L	1655	0	1607	14	0
4	P	1594	0	1548	18	0
5	Q	28	0	25	0	0
5	R	28	0	25	0	0
5	T	28	0	25	0	0
5	W	28	0	25	0	0
5	Y	28	0	25	0	0
5	Z	28	0	25	0	0
6	S	72	0	61	1	0
6	U	72	0	61	1	0
7	V	50	0	43	0	0
7	X	50	0	43	1	0
8	a	61	0	52	0	0
9	E	14	0	13	0	0
10	I	11	0	10	0	0
10	M	11	0	10	0	0
All	All	21208	0	20624	184	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 4.

All (184) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:68:ARG:NH2	4:L:91:ASP:OD2	2.19	0.75
1:I:147:ASP:OD2	2:J:544:TYR:OH	2.07	0.71
1:A:147:ASP:OD2	2:B:544:TYR:OH	2.06	0.71
4:H:68:ARG:NH2	4:H:91:ASP:OD2	2.23	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:68:ARG:NH2	4:D:91:ASP:OD2	2.25	0.69
3:O:158:ASN:HD22	3:O:181:LEU:HD21	1.60	0.67
1:M:147:ASP:OD2	2:N:544:TYR:OH	2.11	0.67
4:P:8:GLY:HA3	4:P:20:LEU:HD23	1.78	0.65
4:D:135:PRO:HD3	4:D:221:LYS:HE2	1.79	0.65
4:H:8:GLY:HA3	4:H:20:LEU:HD23	1.79	0.64
1:M:100:PRO:HB2	4:P:58:GLY:HA3	1.80	0.64
4:D:8:GLY:HA3	4:D:20:LEU:HD23	1.79	0.63
4:L:8:GLY:HA3	4:L:20:LEU:HD23	1.81	0.62
2:B:517:ARG:HD3	2:B:548:LEU:HD13	1.82	0.61
3:O:113:PRO:HD2	3:O:201:LEU:HD13	1.83	0.61
2:J:588:ARG:HG3	1:M:44:THR:HG21	1.82	0.60
4:D:171:LEU:HD21	4:D:194:VAL:HG21	1.84	0.59
4:P:68:ARG:NH2	4:P:91:ASP:OD2	2.33	0.59
4:D:92:THR:HG23	4:D:122:THR:HA	1.85	0.58
3:G:120:PRO:HD3	3:G:132:VAL:HG22	1.83	0.58
4:H:92:THR:HG23	4:H:122:THR:HA	1.85	0.58
1:M:81:VAL:HG23	2:N:574:LEU:HD21	1.85	0.58
2:B:475:ASN:OD1	2:B:476:THR:N	2.37	0.57
3:O:132:VAL:HG23	3:O:179:LEU:HB3	1.87	0.57
3:C:113:PRO:HB3	3:C:139:PHE:HB3	1.87	0.57
3:G:6:GLN:HB2	3:G:100:PRO:HD2	1.87	0.56
1:E:81:VAL:HG23	2:F:574:LEU:HD21	1.86	0.56
4:P:171:LEU:HD21	4:P:194:VAL:HG21	1.88	0.56
4:P:53:VAL:HG12	4:P:59:ALA:HA	1.88	0.56
4:P:135:PRO:HD3	4:P:221:LYS:HE2	1.87	0.56
3:G:8:PRO:HD2	3:G:21:ILE:HG22	1.88	0.55
1:E:50:MET:HG2	1:E:85:GLU:HB2	1.87	0.55
3:K:120:PRO:HD3	3:K:132:VAL:HG22	1.88	0.55
3:C:113:PRO:HD2	3:C:201:LEU:HD13	1.88	0.55
3:K:113:PRO:HD2	3:K:201:LEU:HD13	1.87	0.55
3:G:113:PRO:HB3	3:G:139:PHE:HB3	1.88	0.55
3:G:21:ILE:HG21	3:G:102:THR:HG21	1.88	0.55
4:P:211:ASN:HD22	4:P:218:LYS:HG2	1.71	0.55
3:G:21:ILE:HG13	3:G:73:PHE:HB3	1.89	0.55
4:L:211:ASN:HD22	4:L:218:LYS:HG2	1.71	0.55
4:H:171:LEU:HD21	4:H:194:VAL:HG21	1.88	0.55
3:G:158:ASN:HD22	3:G:181:LEU:HD21	1.71	0.55
2:B:516:LEU:HD22	2:B:556:VAL:HG13	1.90	0.54
1:I:81:VAL:HG23	2:J:574:LEU:HD21	1.89	0.54
4:H:131:PRO:HB3	4:H:157:TYR:HB3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:VAL:HG23	2:B:574:LEU:HD21	1.90	0.53
3:K:21:ILE:HG13	3:K:73:PHE:HB3	1.90	0.53
3:K:113:PRO:HB3	3:K:139:PHE:HB3	1.89	0.53
3:C:21:ILE:HD12	3:C:102:THR:HG21	1.90	0.53
4:D:211:ASN:HD21	4:D:213:LYS:HG2	1.74	0.53
3:O:39:LYS:HB2	3:O:42:LYS:HG2	1.90	0.53
4:H:165:SER:HB3	4:H:209:ASN:HB2	1.91	0.53
3:G:36:TYR:CE1	3:G:46:LEU:HB3	2.44	0.53
4:P:92:THR:HG23	4:P:122:THR:HA	1.91	0.52
4:P:165:SER:HB3	4:P:209:ASN:HB2	1.90	0.52
4:D:29:ILE:HG13	4:D:36:TRP:CE2	2.45	0.52
4:H:211:ASN:HB2	4:H:218:LYS:HD2	1.91	0.51
4:L:92:THR:HG23	4:L:122:THR:HA	1.92	0.51
3:O:113:PRO:HB3	3:O:139:PHE:HB3	1.92	0.51
4:D:2:LEU:HB2	4:D:114:VAL:HG21	1.93	0.51
3:C:39:LYS:HB2	3:C:42:LYS:HG2	1.92	0.51
3:C:85:THR:HG22	3:C:103:LYS:HG2	1.92	0.51
3:G:54:LEU:HB2	3:G:58:VAL:HG21	1.93	0.51
1:I:128:GLN:HE21	3:K:94:LEU:HD23	1.76	0.51
4:L:165:SER:HB3	4:L:209:ASN:HB2	1.92	0.51
4:L:135:PRO:HD3	4:L:221:LYS:HE2	1.93	0.51
2:N:532:TRP:HH2	7:X:1:NAG:H83	1.76	0.51
4:D:131:PRO:HB3	4:D:157:TYR:HB3	1.94	0.50
3:K:21:ILE:HG21	3:K:102:THR:HG21	1.93	0.50
4:P:21:THR:HG22	4:P:81:SER:HB3	1.92	0.50
1:E:148:ARG:NH1	2:N:575:ARG:O	2.45	0.50
3:G:114:SER:HB2	3:G:137:ASN:HB3	1.94	0.50
3:O:21:ILE:HG13	3:O:73:PHE:HB3	1.94	0.50
2:F:516:LEU:HD22	2:F:556:VAL:HG13	1.93	0.50
4:L:29:ILE:HG13	4:L:36:TRP:CE2	2.46	0.50
4:L:171:LEU:HD21	4:L:194:VAL:HG21	1.93	0.49
1:I:100:PRO:HB2	4:L:58:GLY:HA3	1.94	0.49
3:K:6:GLN:HB2	3:K:100:PRO:HD2	1.94	0.49
4:L:131:PRO:HB3	4:L:157:TYR:HB3	1.94	0.49
1:I:79:LYS:HB3	2:J:574:LEU:HD22	1.93	0.49
3:C:6:GLN:HB2	3:C:100:PRO:HD2	1.94	0.49
1:E:147:ASP:OD2	2:F:544:TYR:OH	2.12	0.49
4:P:131:PRO:HB3	4:P:157:TYR:HB3	1.94	0.49
2:F:578:THR:HG22	1:I:114:ARG:HH22	1.78	0.49
2:B:521:VAL:HG13	2:B:543:LEU:HG	1.95	0.49
2:F:588:ARG:HG3	1:I:44:THR:HG21	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:212:HIS:CD2	4:D:214:PRO:HD2	2.48	0.48
1:I:50:MET:HG2	1:I:85:GLU:HB2	1.95	0.48
1:A:50:MET:HG2	1:A:85:GLU:HB2	1.95	0.48
4:H:21:THR:HG22	4:H:81:SER:HB3	1.94	0.48
2:N:490:LEU:N	2:N:552:GLN:HE22	2.10	0.48
3:C:114:SER:HB2	3:C:137:ASN:HB3	1.94	0.48
1:M:50:MET:HG2	1:M:85:GLU:HB2	1.94	0.48
2:F:583:PHE:HZ	2:F:588:ARG:HE	1.61	0.48
3:G:113:PRO:HD2	3:G:201:LEU:HD13	1.94	0.47
4:P:29:ILE:HG13	4:P:36:TRP:CE2	2.49	0.47
4:D:40:ARG:HB3	4:D:50:ILE:HD11	1.97	0.47
4:H:50:ILE:HG23	4:H:65:LEU:HD13	1.97	0.47
1:A:138:HIS:CE1	1:A:140:TRP:HB2	2.49	0.47
4:D:165:SER:HB3	4:D:209:ASN:HB2	1.96	0.47
4:L:212:HIS:CD2	4:L:214:PRO:HD2	2.49	0.47
3:K:85:THR:HG22	3:K:103:LYS:HG2	1.96	0.47
4:P:2:LEU:HB2	4:P:114:VAL:HG21	1.97	0.47
3:K:37:GLN:HB2	3:K:47:LEU:HD11	1.97	0.46
4:H:40:ARG:HB3	4:H:50:ILE:HD11	1.98	0.46
1:M:137:LEU:HD22	1:M:152:THR:HG22	1.97	0.46
3:K:36:TYR:CE1	3:K:46:LEU:HB3	2.50	0.46
3:C:159:SER:HB3	3:C:179:LEU:HD12	1.98	0.46
4:D:53:VAL:HG12	4:D:59:ALA:HA	1.97	0.46
3:G:37:GLN:HB2	3:G:47:LEU:HD11	1.98	0.46
2:J:516:LEU:HD22	2:J:556:VAL:HG13	1.97	0.46
2:J:532:TRP:HH2	6:U:1:NAG:H83	1.81	0.46
3:O:193:ALA:HB2	3:O:208:SER:HB3	1.98	0.46
4:L:53:VAL:HG12	4:L:59:ALA:HA	1.97	0.46
3:C:36:TYR:CE2	3:C:46:LEU:HB3	2.51	0.45
4:H:212:HIS:CD2	4:H:214:PRO:HD2	2.52	0.45
1:E:107:LEU:HD12	1:E:153:THR:HG21	1.99	0.45
4:H:53:VAL:HG12	4:H:59:ALA:HA	1.97	0.45
4:H:29:ILE:HG13	4:H:36:TRP:CE2	2.51	0.45
3:C:132:VAL:HG13	3:C:179:LEU:HB3	1.99	0.44
1:A:104:SER:HB3	1:A:156:ARG:HE	1.82	0.44
1:E:100:PRO:HB2	4:H:58:GLY:HA3	1.99	0.44
4:H:135:PRO:HD3	4:H:221:LYS:HE2	1.99	0.44
3:O:159:SER:HB3	3:O:179:LEU:HD12	1.98	0.44
1:E:73:ARG:HG2	1:E:74:THR:N	2.32	0.44
3:O:36:TYR:CE2	3:O:46:LEU:HB3	2.52	0.44
4:P:40:ARG:HB3	4:P:50:ILE:HD11	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:138:HIS:CE1	1:E:140:TRP:HB2	2.53	0.43
2:F:578:THR:HG22	1:I:114:ARG:NH2	2.32	0.43
3:C:164:THR:HG23	4:D:178:PHE:CD2	2.53	0.43
4:L:40:ARG:HB3	4:L:50:ILE:HD11	1.99	0.43
3:O:6:GLN:HB2	3:O:100:PRO:HD2	2.00	0.43
2:F:471:SER:HA	2:F:472:PRO:HD3	1.88	0.43
3:G:39:LYS:HB2	3:G:42:LYS:HG2	2.00	0.43
1:M:104:SER:HB3	1:M:156:ARG:HE	1.83	0.43
3:O:114:SER:HB2	3:O:137:ASN:HB3	2.00	0.43
2:F:530:LEU:HG	2:F:533:ILE:HD12	2.00	0.43
1:I:116:TYR:H	1:I:159:VAL:HG23	1.82	0.43
4:P:37:GLY:HA2	4:P:52:SER:HA	2.00	0.43
2:B:602:CYS:HB2	2:B:609:CYS:HB2	1.89	0.43
1:I:73:ARG:HG2	1:I:74:THR:N	2.32	0.43
4:D:37:GLY:HA2	4:D:52:SER:HA	2.01	0.43
3:G:193:ALA:HB2	3:G:208:SER:HB3	2.00	0.43
1:M:71:ALA:HB2	4:P:105:THR:HB	2.00	0.43
3:C:37:GLN:HB2	3:C:47:LEU:HD11	2.01	0.42
1:I:146:TYR:CE1	1:I:160:PHE:HB3	2.54	0.42
4:P:40:ARG:HH12	4:P:91:ASP:CG	2.22	0.42
2:J:471:SER:HA	2:J:472:PRO:HD3	1.86	0.42
3:O:198:HIS:HB3	3:O:201:LEU:HB2	2.00	0.42
3:C:79:GLN:HB3	3:C:80:PRO:HD2	2.00	0.42
1:A:67:SER:HA	1:A:70:TRP:CE3	2.54	0.42
1:A:166:ALA:HB2	2:B:563:ALA:HB2	2.00	0.42
2:J:516:LEU:HD23	2:J:549:ILE:HB	2.01	0.42
4:L:167:ASN:HD22	4:L:171:LEU:HB2	1.84	0.42
2:N:475:ASN:OD1	2:N:491:THR:OG1	2.37	0.42
1:E:49:LEU:HD11	2:F:585:LEU:HB3	2.01	0.42
1:M:107:LEU:HD12	1:M:153:THR:HG21	2.00	0.42
1:A:49:LEU:HD11	2:B:585:LEU:HB3	2.01	0.41
4:P:212:HIS:CD2	4:P:214:PRO:HD2	2.55	0.41
1:A:107:LEU:HD12	1:A:153:THR:HG21	2.01	0.41
3:C:149:LYS:HG2	3:C:154:LEU:HD22	2.02	0.41
1:E:104:SER:HB3	1:E:156:ARG:HE	1.85	0.41
3:G:59:PRO:HB2	3:G:61:ARG:HG2	2.02	0.41
3:K:159:SER:HB3	3:K:179:LEU:HD12	2.02	0.41
4:H:2:LEU:HB2	4:H:114:VAL:HG21	2.01	0.41
4:D:155:LYS:HG2	4:D:156:ASP:OD1	2.20	0.41
1:M:72:PHE:HB3	1:M:133:GLN:O	2.21	0.41
1:M:67:SER:HA	1:M:70:TRP:CE3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:S:4:MAN:H2	6:S:5:MAN:H2	1.81	0.41
4:H:37:GLY:HA2	4:H:52:SER:HA	2.02	0.41
1:I:61:ASP:HB3	1:I:91:THR:HG21	2.03	0.41
1:M:79:LYS:HB3	2:N:574:LEU:HD22	2.03	0.41
1:A:137:LEU:HD22	1:A:152:THR:HG22	2.03	0.41
2:F:554:ASN:HB2	2:F:557:CYS:HB2	2.03	0.41
3:G:85:THR:HG22	3:G:103:LYS:HG2	2.02	0.41
1:I:112:ASN:ND2	2:J:582:THR:HG23	2.36	0.41
3:K:193:ALA:HB2	3:K:208:SER:HB3	2.02	0.41
1:M:97:VAL:HG12	1:M:105:LEU:HD12	2.02	0.41
1:A:90:LYS:O	1:A:120:LYS:HB3	2.21	0.41
3:C:136:LEU:HB2	3:C:175:LEU:HB3	2.03	0.41
2:N:516:LEU:HD22	2:N:556:VAL:HG13	2.02	0.40
2:B:471:SER:HA	2:B:472:PRO:HD3	1.91	0.40
3:G:83:ILE:HD13	3:G:166:GLN:HB3	2.02	0.40
2:N:516:LEU:HD23	2:N:549:ILE:HB	2.04	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	143/250 (57%)	139 (97%)	4 (3%)	0	100	100
1	E	142/250 (57%)	138 (97%)	4 (3%)	0	100	100
1	I	140/250 (56%)	137 (98%)	3 (2%)	0	100	100
1	M	140/250 (56%)	136 (97%)	4 (3%)	0	100	100
2	B	117/237 (49%)	110 (94%)	7 (6%)	0	100	100
2	F	86/237 (36%)	81 (94%)	5 (6%)	0	100	100
2	J	89/237 (38%)	84 (94%)	5 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	N	84/237 (35%)	80 (95%)	4 (5%)	0	100	100
3	C	208/211 (99%)	203 (98%)	5 (2%)	0	100	100
3	G	208/211 (99%)	202 (97%)	6 (3%)	0	100	100
3	K	208/211 (99%)	204 (98%)	4 (2%)	0	100	100
3	O	208/211 (99%)	202 (97%)	6 (3%)	0	100	100
4	D	214/226 (95%)	202 (94%)	12 (6%)	0	100	100
4	H	216/226 (96%)	204 (94%)	12 (6%)	0	100	100
4	L	218/226 (96%)	205 (94%)	13 (6%)	0	100	100
4	P	207/226 (92%)	196 (95%)	11 (5%)	0	100	100
All	All	2628/3696 (71%)	2523 (96%)	105 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	124/222 (56%)	124 (100%)	0	100	100
1	E	121/222 (54%)	121 (100%)	0	100	100
1	I	121/222 (54%)	121 (100%)	0	100	100
1	M	121/222 (54%)	121 (100%)	0	100	100
2	B	103/202 (51%)	103 (100%)	0	100	100
2	F	80/202 (40%)	80 (100%)	0	100	100
2	J	80/202 (40%)	80 (100%)	0	100	100
2	N	78/202 (39%)	78 (100%)	0	100	100
3	C	188/189 (100%)	188 (100%)	0	100	100
3	G	188/189 (100%)	188 (100%)	0	100	100
3	K	188/189 (100%)	188 (100%)	0	100	100
3	O	187/189 (99%)	187 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	D	186/192 (97%)	186 (100%)	0	100	100
4	H	186/192 (97%)	186 (100%)	0	100	100
4	L	188/192 (98%)	188 (100%)	0	100	100
4	P	183/192 (95%)	183 (100%)	0	100	100
All	All	2322/3220 (72%)	2322 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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)

37 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	NAG	Q	1	1,5	14,14,15	0.30	0	17,19,21	0.41	0
5	NAG	Q	2	5	14,14,15	0.25	0	17,19,21	0.47	0
5	NAG	R	1	1,5	14,14,15	0.46	0	17,19,21	0.45	0
5	NAG	R	2	5	14,14,15	0.35	0	17,19,21	0.41	0
6	NAG	S	1	6,2	14,14,15	0.21	0	17,19,21	0.47	0
6	NAG	S	2	6	14,14,15	0.27	0	17,19,21	0.52	0
6	BMA	S	3	6	11,11,12	0.67	0	15,15,17	0.88	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	MAN	S	4	6	11,11,12	0.73	0	15,15,17	0.95	0
6	MAN	S	5	6	11,11,12	0.82	0	15,15,17	0.93	2 (13%)
6	MAN	S	6	6	11,11,12	0.91	1 (9%)	15,15,17	1.17	3 (20%)
5	NAG	T	1	1,5	14,14,15	0.33	0	17,19,21	0.37	0
5	NAG	T	2	5	14,14,15	0.24	0	17,19,21	0.48	0
6	NAG	U	1	6,2	14,14,15	0.23	0	17,19,21	0.47	0
6	NAG	U	2	6	14,14,15	0.27	0	17,19,21	0.46	0
6	BMA	U	3	6	11,11,12	0.61	0	15,15,17	0.77	0
6	MAN	U	4	6	11,11,12	1.09	1 (9%)	15,15,17	0.96	0
6	MAN	U	5	6	11,11,12	0.97	0	15,15,17	1.21	2 (13%)
6	MAN	U	6	6	11,11,12	0.73	0	15,15,17	1.13	2 (13%)
7	NAG	V	1	1,7	14,14,15	0.43	0	17,19,21	0.40	0
7	NAG	V	2	7	14,14,15	0.27	0	17,19,21	0.42	0
7	BMA	V	3	7	11,11,12	0.53	0	15,15,17	0.70	0
7	MAN	V	4	7	11,11,12	0.69	0	15,15,17	1.07	2 (13%)
5	NAG	W	1	1,5	14,14,15	0.33	0	17,19,21	0.36	0
5	NAG	W	2	5	14,14,15	0.31	0	17,19,21	0.47	0
7	NAG	X	1	7,2	14,14,15	0.18	0	17,19,21	0.47	0
7	NAG	X	2	7	14,14,15	0.24	0	17,19,21	0.45	0
7	BMA	X	3	7	11,11,12	0.73	0	15,15,17	0.79	0
7	MAN	X	4	7	11,11,12	0.78	0	15,15,17	0.96	1 (6%)
5	NAG	Y	1	1,5	14,14,15	0.30	0	17,19,21	0.41	0
5	NAG	Y	2	5	14,14,15	0.25	0	17,19,21	0.47	0
5	NAG	Z	1	1,5	14,14,15	0.35	0	17,19,21	0.49	0
5	NAG	Z	2	5	14,14,15	0.38	0	17,19,21	0.61	0
8	NAG	a	1	8,2	14,14,15	0.25	0	17,19,21	0.50	0
8	NAG	a	2	8	14,14,15	0.26	0	17,19,21	0.44	0
8	BMA	a	3	8	11,11,12	0.89	0	15,15,17	1.21	2 (13%)
8	MAN	a	4	8	11,11,12	0.75	0	15,15,17	1.01	1 (6%)
8	MAN	a	5	8	11,11,12	0.68	0	15,15,17	0.99	2 (13%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	Q	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	Q	2	5	-	0/6/23/26	0/1/1/1
5	NAG	R	1	1,5	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	R	2	5	-	0/6/23/26	0/1/1/1
6	NAG	S	1	6,2	-	2/6/23/26	0/1/1/1
6	NAG	S	2	6	-	0/6/23/26	0/1/1/1
6	BMA	S	3	6	-	0/2/19/22	0/1/1/1
6	MAN	S	4	6	-	1/2/19/22	0/1/1/1
6	MAN	S	5	6	-	2/2/19/22	0/1/1/1
6	MAN	S	6	6	-	2/2/19/22	0/1/1/1
5	NAG	T	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	T	2	5	-	0/6/23/26	0/1/1/1
6	NAG	U	1	6,2	-	0/6/23/26	0/1/1/1
6	NAG	U	2	6	-	0/6/23/26	0/1/1/1
6	BMA	U	3	6	-	2/2/19/22	0/1/1/1
6	MAN	U	4	6	-	0/2/19/22	0/1/1/1
6	MAN	U	5	6	-	0/2/19/22	0/1/1/1
6	MAN	U	6	6	-	0/2/19/22	0/1/1/1
7	NAG	V	1	1,7	-	0/6/23/26	0/1/1/1
7	NAG	V	2	7	-	0/6/23/26	0/1/1/1
7	BMA	V	3	7	-	1/2/19/22	0/1/1/1
7	MAN	V	4	7	-	2/2/19/22	0/1/1/1
5	NAG	W	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	W	2	5	-	0/6/23/26	0/1/1/1
7	NAG	X	1	7,2	-	2/6/23/26	0/1/1/1
7	NAG	X	2	7	-	0/6/23/26	0/1/1/1
7	BMA	X	3	7	-	2/2/19/22	0/1/1/1
7	MAN	X	4	7	-	1/2/19/22	0/1/1/1
5	NAG	Y	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	Y	2	5	-	0/6/23/26	0/1/1/1
5	NAG	Z	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	Z	2	5	-	0/6/23/26	0/1/1/1
8	NAG	a	1	8,2	-	2/6/23/26	0/1/1/1
8	NAG	a	2	8	-	0/6/23/26	0/1/1/1
8	BMA	a	3	8	-	1/2/19/22	0/1/1/1
8	MAN	a	4	8	-	1/2/19/22	0/1/1/1
8	MAN	a	5	8	-	0/2/19/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	S	6	MAN	C1-C2	2.53	1.58	1.52
6	U	4	MAN	C2-C3	2.00	1.55	1.52

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	U	6	MAN	C1-O5-C5	3.07	116.35	112.19
7	V	4	MAN	C1-O5-C5	2.61	115.72	112.19
8	a	5	MAN	C1-O5-C5	2.59	115.70	112.19
6	U	5	MAN	C1-O5-C5	2.56	115.66	112.19
8	a	3	BMA	O6-C6-C5	-2.43	102.97	111.29
6	S	6	MAN	C1-O5-C5	2.37	115.40	112.19
6	S	6	MAN	C1-C2-C3	2.30	112.49	109.67
6	S	6	MAN	O2-C2-C3	-2.28	105.56	110.14
7	X	4	MAN	O2-C2-C3	-2.26	105.60	110.14
6	U	6	MAN	O2-C2-C3	-2.26	105.61	110.14
6	S	5	MAN	O2-C2-C3	-2.21	105.70	110.14
6	U	5	MAN	O2-C2-C3	-2.18	105.76	110.14
7	V	4	MAN	O2-C2-C3	-2.15	105.82	110.14
8	a	3	BMA	O5-C5-C6	-2.12	103.89	107.20
6	S	5	MAN	C1-O5-C5	2.09	115.02	112.19
8	a	4	MAN	O3-C3-C2	2.05	113.92	109.99
8	a	5	MAN	O2-C2-C3	-2.03	106.08	110.14

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	V	4	MAN	O5-C5-C6-O6
5	Y	1	NAG	O5-C5-C6-O6
6	S	5	MAN	O5-C5-C6-O6
5	T	1	NAG	O5-C5-C6-O6
5	Q	1	NAG	O5-C5-C6-O6
7	V	4	MAN	C4-C5-C6-O6
6	U	3	BMA	O5-C5-C6-O6
6	U	3	BMA	C4-C5-C6-O6
5	Q	1	NAG	C4-C5-C6-O6
6	S	5	MAN	C4-C5-C6-O6
5	Y	1	NAG	C4-C5-C6-O6
5	T	1	NAG	C4-C5-C6-O6
6	S	1	NAG	O5-C5-C6-O6
6	S	1	NAG	C4-C5-C6-O6
7	X	3	BMA	O5-C5-C6-O6
8	a	4	MAN	O5-C5-C6-O6
7	X	4	MAN	O5-C5-C6-O6
5	W	1	NAG	C4-C5-C6-O6
6	S	4	MAN	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	W	1	NAG	O5-C5-C6-O6
8	a	1	NAG	C4-C5-C6-O6
8	a	3	BMA	O5-C5-C6-O6
7	X	1	NAG	C4-C5-C6-O6
8	a	1	NAG	O5-C5-C6-O6
6	S	6	MAN	C4-C5-C6-O6
6	S	6	MAN	O5-C5-C6-O6
7	X	1	NAG	O5-C5-C6-O6
5	R	1	NAG	C4-C5-C6-O6
7	X	3	BMA	C4-C5-C6-O6
5	R	1	NAG	O5-C5-C6-O6
7	V	3	BMA	O5-C5-C6-O6

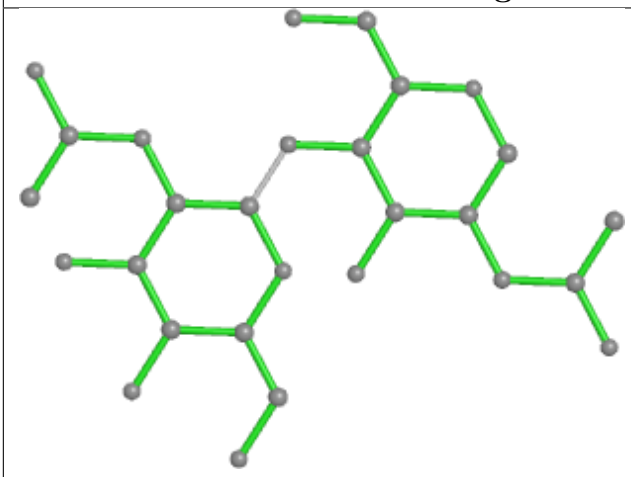
There are no ring outliers.

4 monomers are involved in 3 short contacts:

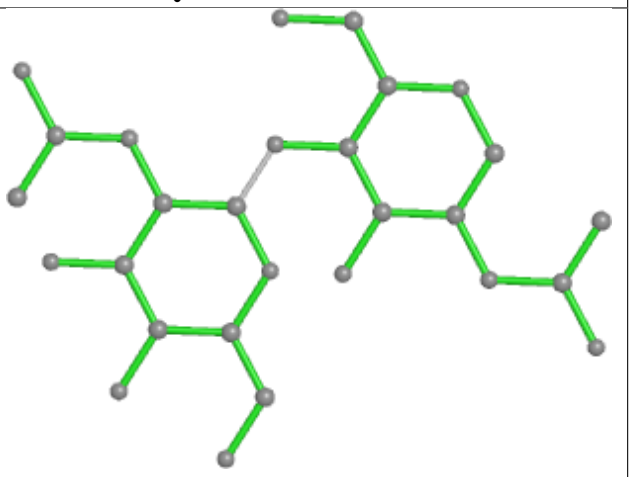
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	X	1	NAG	1	0
6	S	5	MAN	1	0
6	S	4	MAN	1	0
6	U	1	NAG	1	0

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

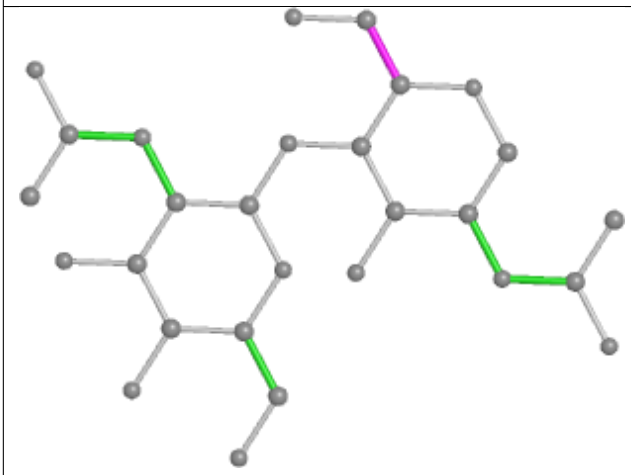
Oligosaccharide Chain Q



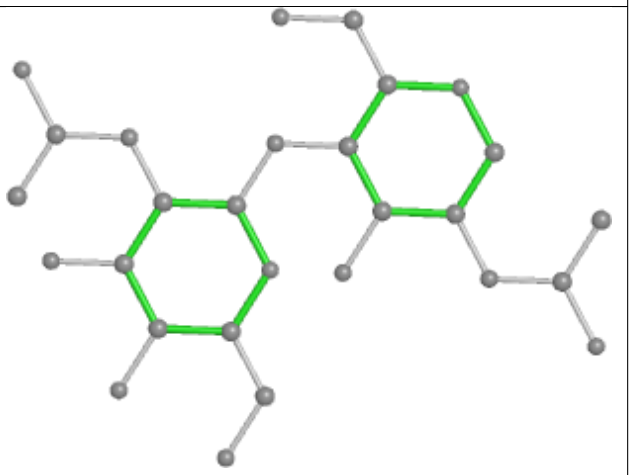
Bond lengths



Bond angles

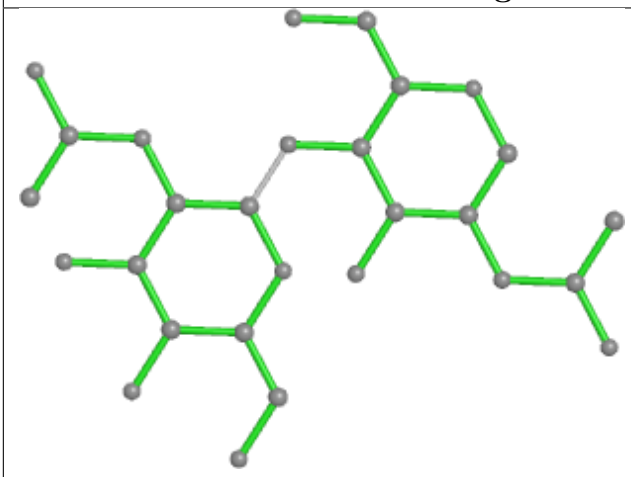


Torsions

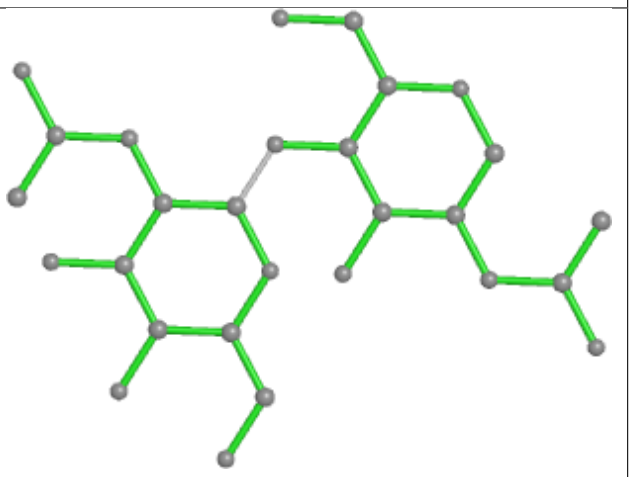


Rings

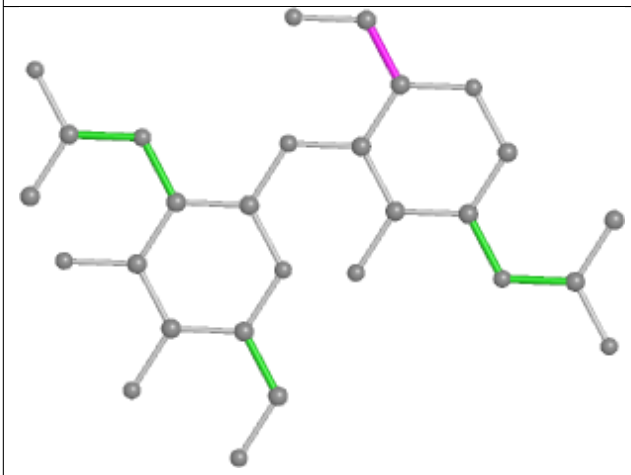
Oligosaccharide Chain R



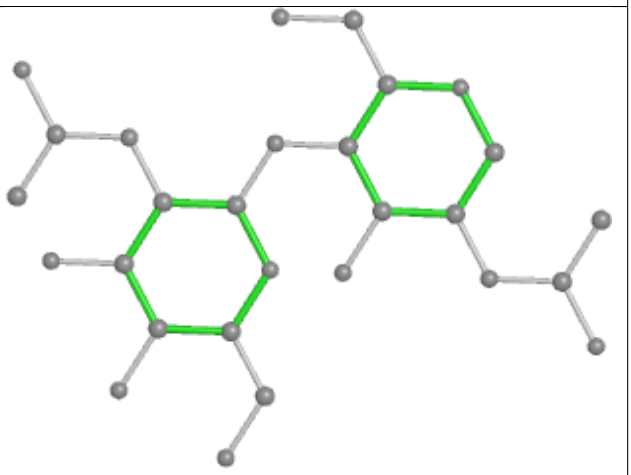
Bond lengths



Bond angles

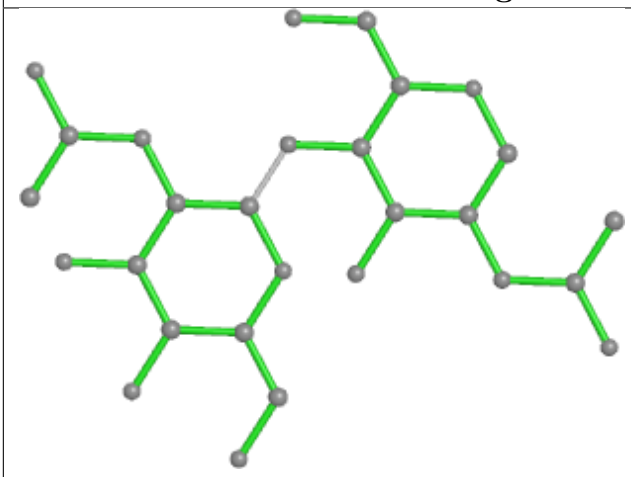


Torsions

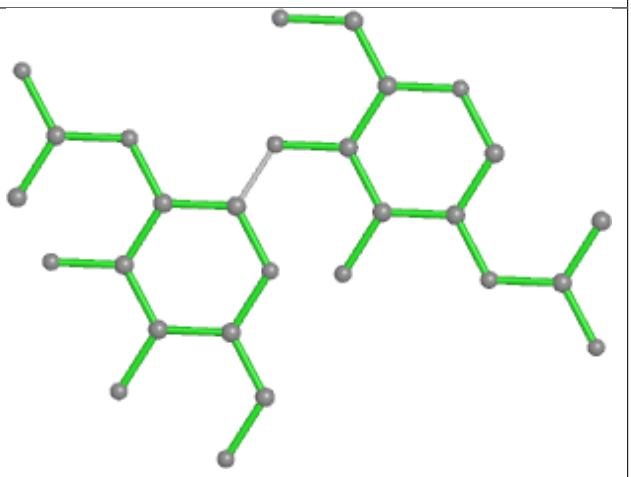


Rings

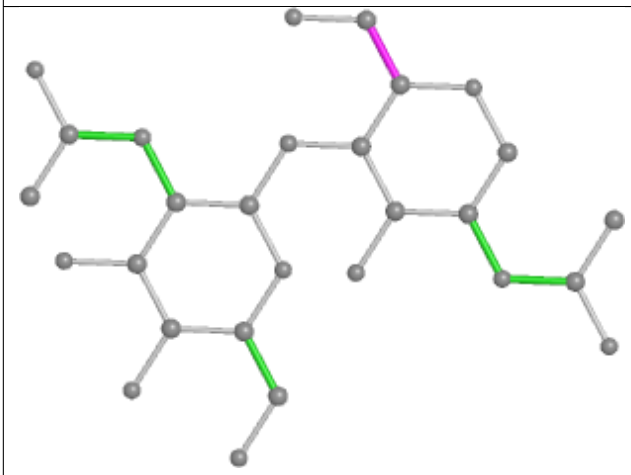
Oligosaccharide Chain T



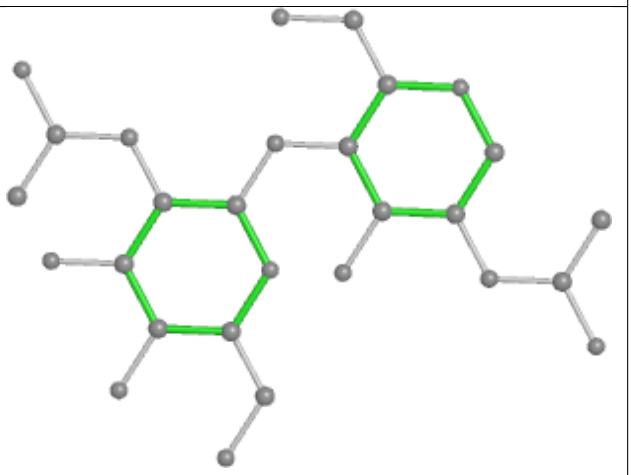
Bond lengths



Bond angles

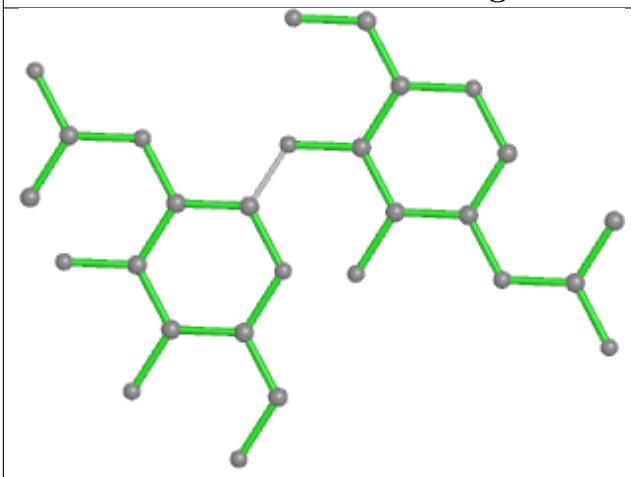


Torsions

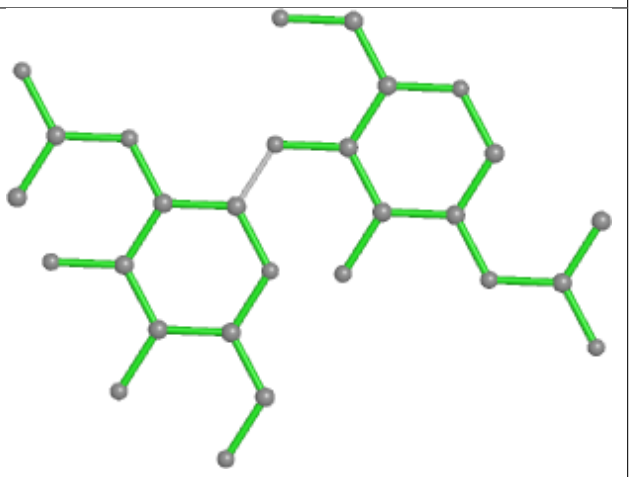


Rings

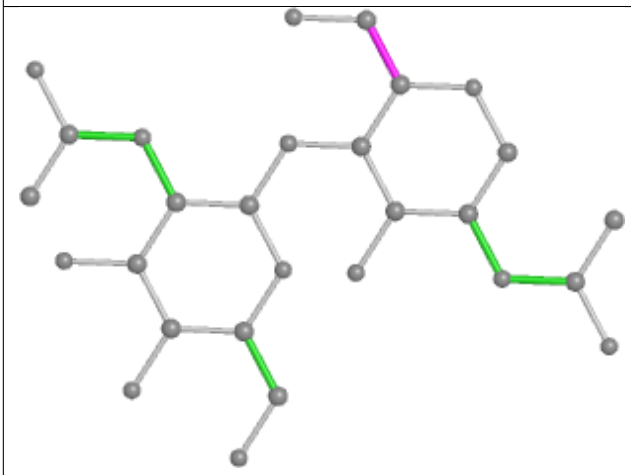
Oligosaccharide Chain W



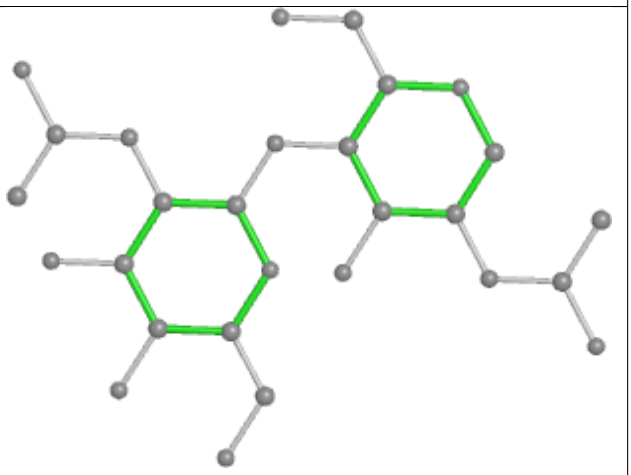
Bond lengths



Bond angles

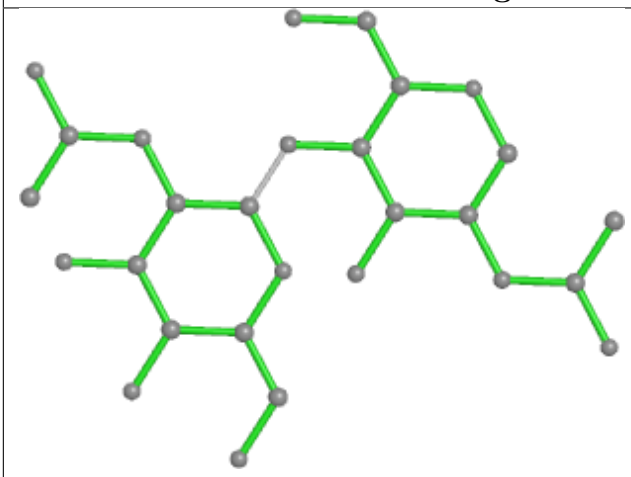


Torsions

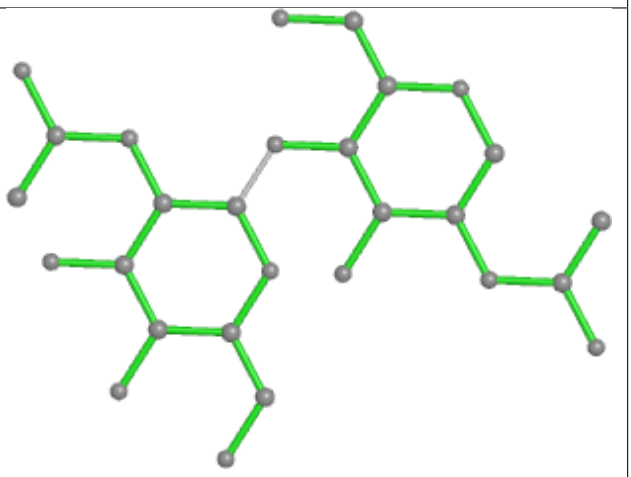


Rings

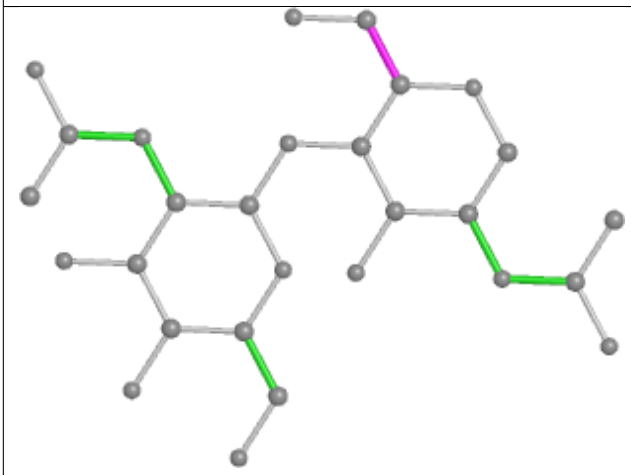
Oligosaccharide Chain Y



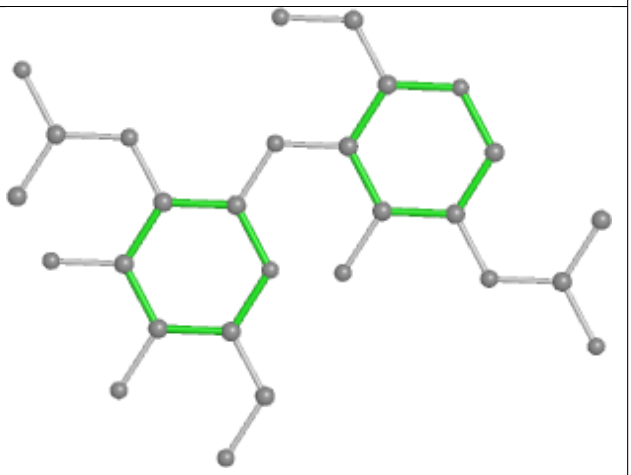
Bond lengths



Bond angles

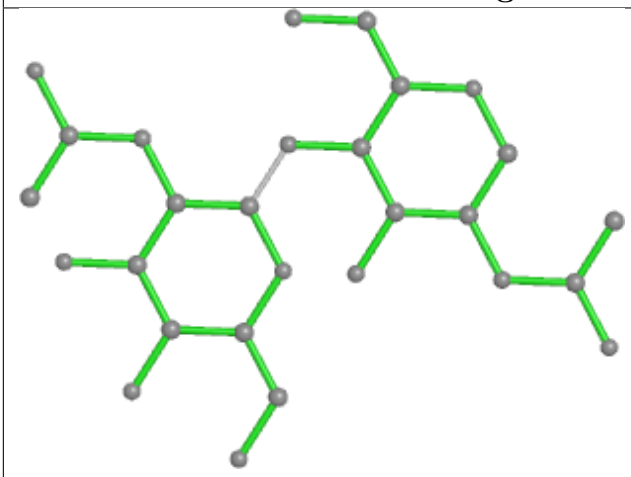


Torsions

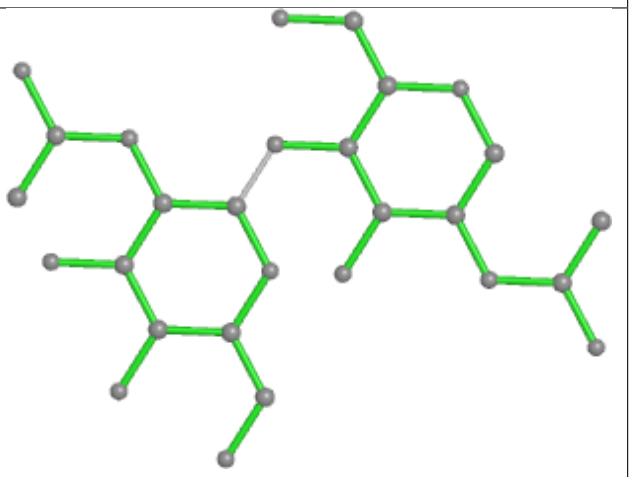


Rings

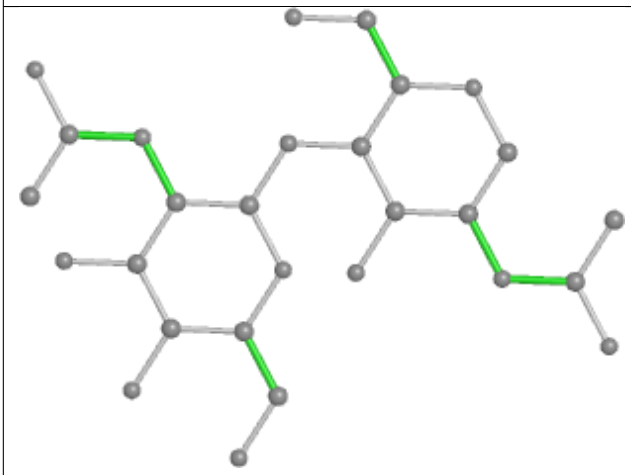
Oligosaccharide Chain Z



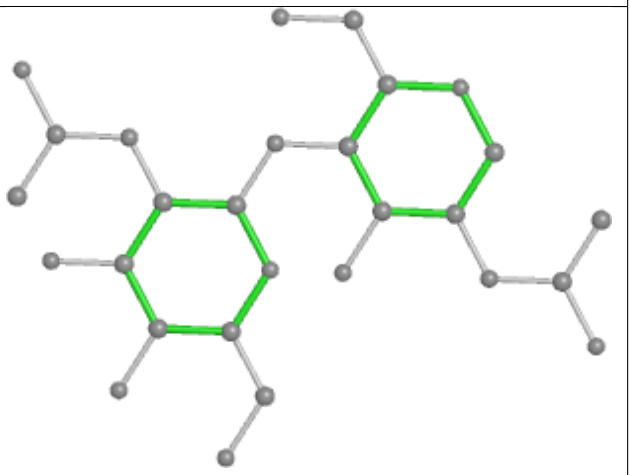
Bond lengths



Bond angles

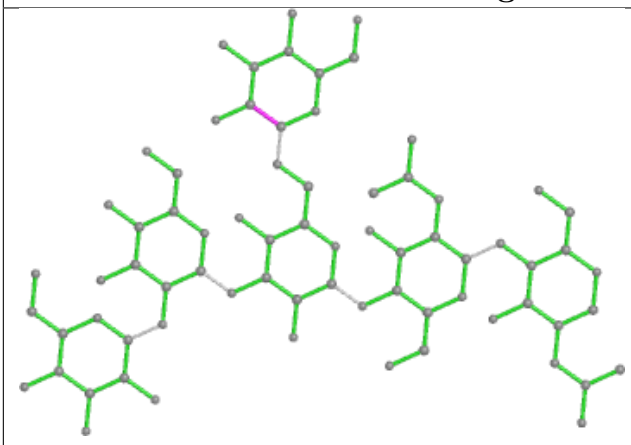


Torsions

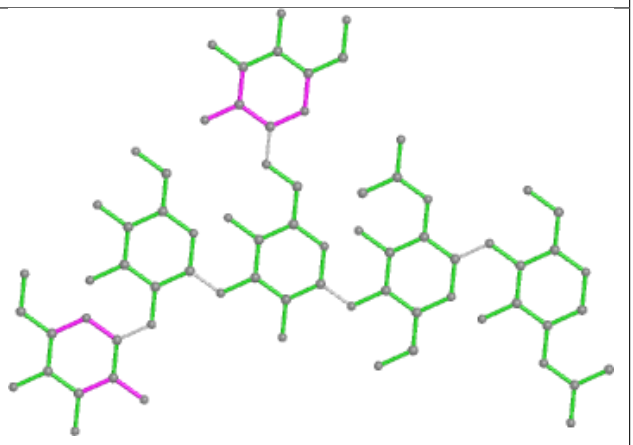


Rings

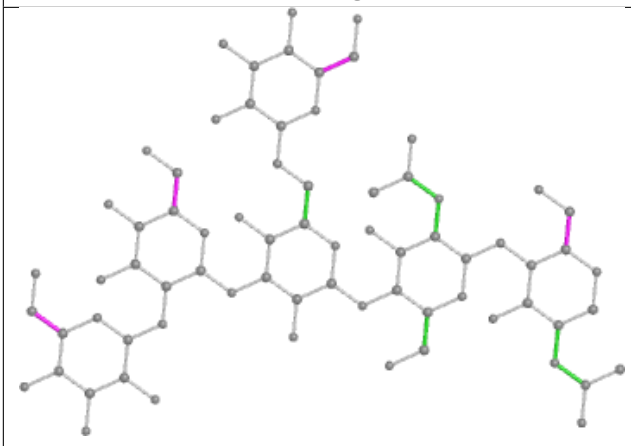
Oligosaccharide Chain S



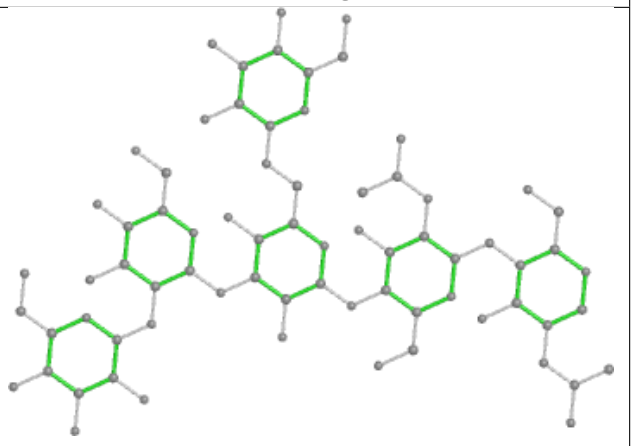
Bond lengths



Bond angles

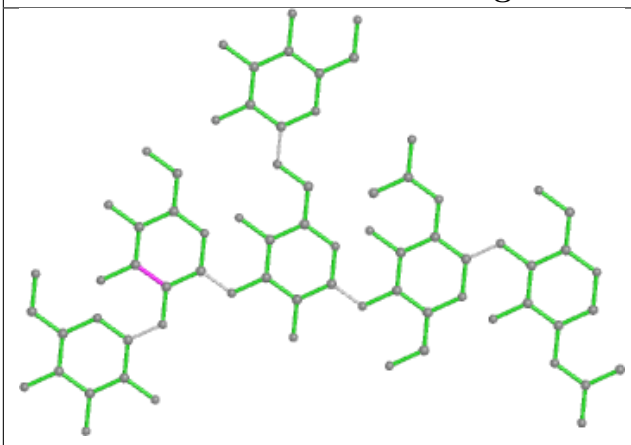


Torsions

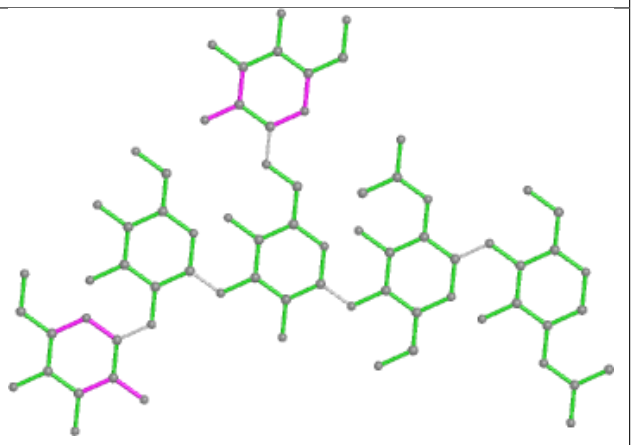


Rings

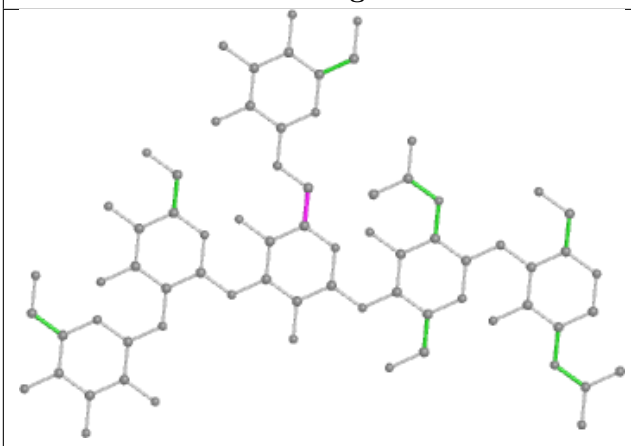
Oligosaccharide Chain U



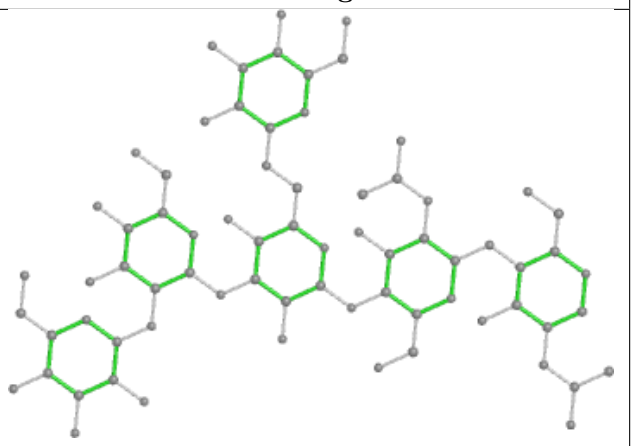
Bond lengths



Bond angles

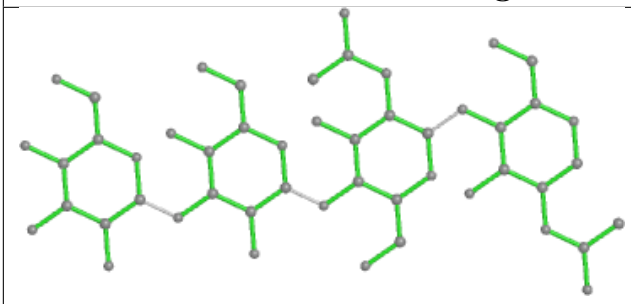


Torsions

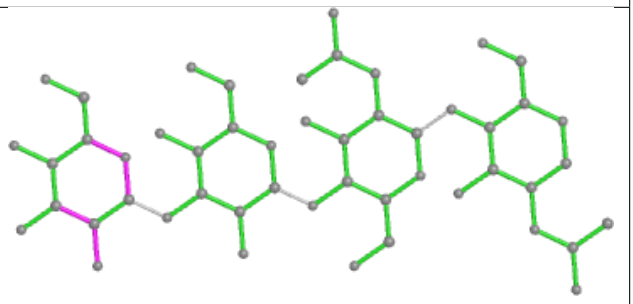


Rings

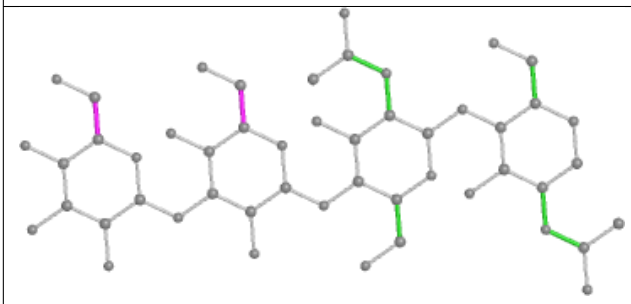
Oligosaccharide Chain V



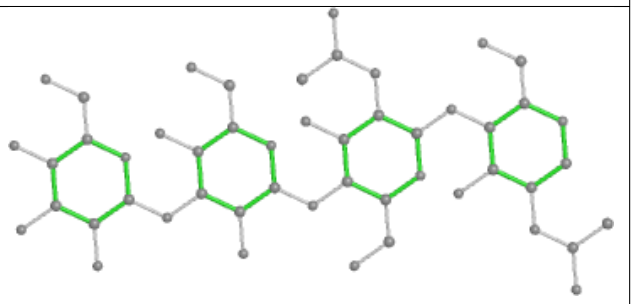
Bond lengths



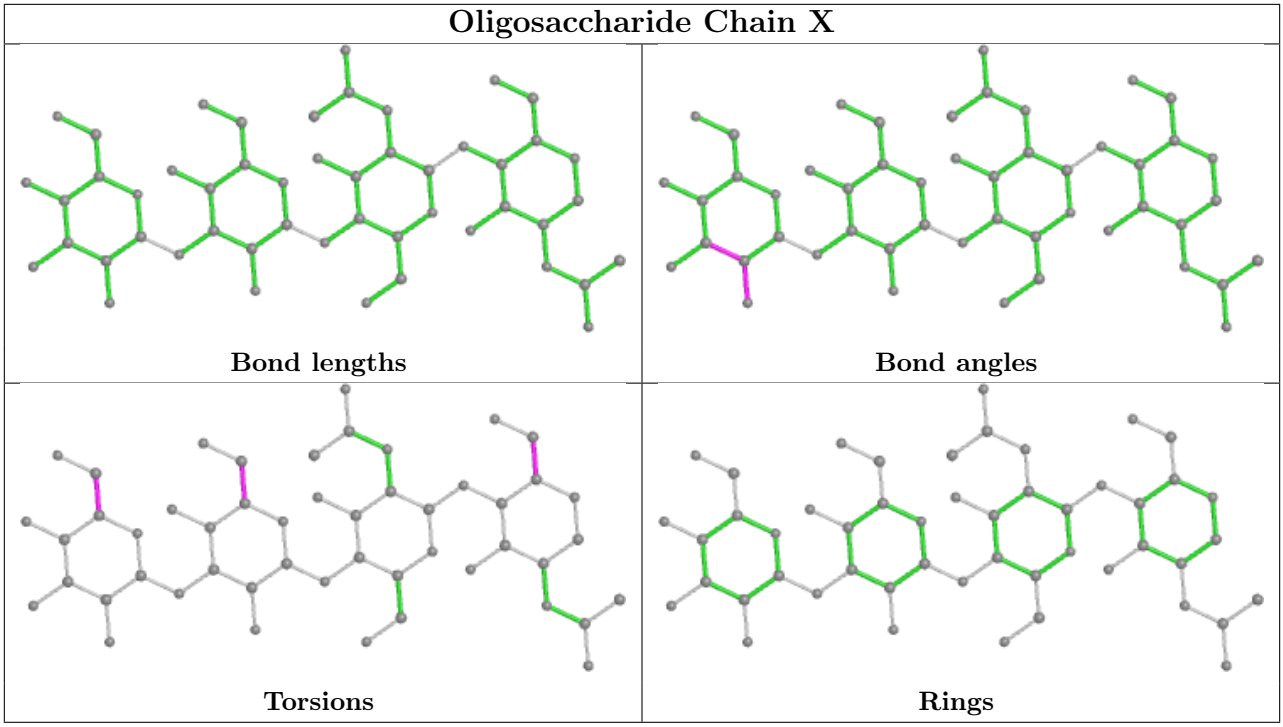
Bond angles

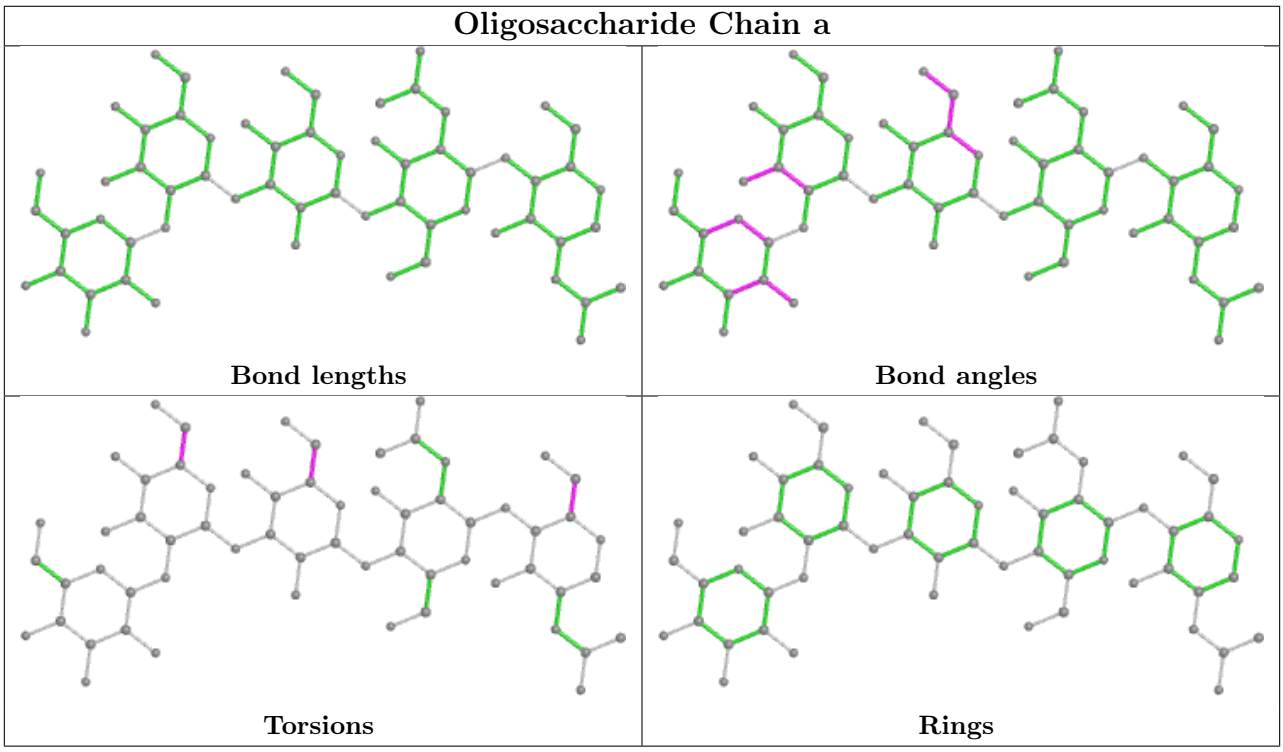


Torsions



Rings





5.6 Ligand geometry (i)

3 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	$\#\|Z\| > 2$
10	MAN	I	305	-	11,11,12	0.66	0	15,15,17	1.19	3 (20%)
10	MAN	M	305	-	11,11,12	0.97	1 (9%)	15,15,17	1.25	3 (20%)
9	NAG	E	303	1	14,14,15	0.35	0	17,19,21	0.42	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
10	MAN	I	305	-	-	2/2/19/22	0/1/1/1
10	MAN	M	305	-	-	2/2/19/22	0/1/1/1
9	NAG	E	303	1	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	M	305	MAN	O5-C1	-2.10	1.40	1.43

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	M	305	MAN	O5-C1-C2	2.47	114.59	110.77
10	I	305	MAN	C1-O5-C5	2.25	115.24	112.19
10	I	305	MAN	O2-C2-C3	-2.20	105.73	110.14
10	M	305	MAN	O2-C2-C3	-2.16	105.82	110.14
10	I	305	MAN	O5-C1-C2	2.09	114.00	110.77
10	M	305	MAN	C1-O5-C5	2.03	114.94	112.19

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	E	303	NAG	O5-C5-C6-O6
9	E	303	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
10	M	305	MAN	O5-C5-C6-O6
10	I	305	MAN	C4-C5-C6-O6
10	I	305	MAN	O5-C5-C6-O6
10	M	305	MAN	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	145/250 (58%)	0.14	0 100 100	55, 86, 119, 147	0
1	E	144/250 (57%)	0.48	4 (2%) 53 37	70, 94, 132, 148	0
1	I	142/250 (56%)	0.60	5 (3%) 44 29	70, 99, 133, 149	0
1	M	142/250 (56%)	0.49	2 (1%) 75 61	94, 116, 139, 155	0
2	B	127/237 (53%)	0.11	1 (0%) 86 75	73, 110, 158, 174	0
2	F	94/237 (39%)	0.49	5 (5%) 26 16	79, 120, 149, 158	0
2	J	97/237 (40%)	0.51	3 (3%) 49 33	80, 120, 149, 176	0
2	N	92/237 (38%)	0.35	1 (1%) 80 68	93, 124, 150, 173	0
3	C	210/211 (99%)	0.36	5 (2%) 59 42	72, 116, 136, 149	0
3	G	210/211 (99%)	0.43	3 (1%) 75 61	68, 99, 128, 161	0
3	K	210/211 (99%)	0.35	1 (0%) 91 83	61, 95, 124, 141	0
3	O	210/211 (99%)	0.17	3 (1%) 75 61	110, 138, 158, 168	0
4	D	218/226 (96%)	0.30	2 (0%) 84 73	59, 86, 127, 155	0
4	H	220/226 (97%)	0.35	0 100 100	59, 82, 111, 128	0
4	L	222/226 (98%)	0.26	0 100 100	57, 80, 124, 151	0
4	P	211/226 (93%)	0.12	1 (0%) 91 83	99, 126, 148, 174	0
All	All	2694/3696 (72%)	0.33	36 (1%) 77 63	55, 105, 145, 176	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	476	THR	4.0
2	J	583	PHE	3.6
3	G	30	SER	3.3
3	C	105	ASP	3.0
1	E	50	MET	2.9

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Mol	Chain	Res	Type	RSRZ
3	C	117	ILE	2.9
3	K	199	GLN	2.7
3	O	197	THR	2.6
1	E	139	LEU	2.6
1	I	50	MET	2.6
4	D	148	ALA	2.5
2	J	549	ILE	2.5
3	C	31	ASN	2.4
1	M	168	MET	2.4
1	I	39	GLY	2.4
3	O	47	LEU	2.3
3	O	117	ILE	2.3
2	N	490	LEU	2.3
2	B	615	ASP	2.2
3	C	115	VAL	2.2
2	J	586	ILE	2.2
2	F	586	ILE	2.2
3	G	148	TRP	2.2
2	F	516	LEU	2.2
1	I	167	ALA	2.2
3	C	39	LYS	2.1
4	D	99	SER	2.1
3	G	29	ILE	2.1
1	I	168	MET	2.1
1	I	52	PHE	2.1
2	F	490	LEU	2.1
2	F	549	ILE	2.1
1	M	140	TRP	2.1
1	E	165	ILE	2.0
4	P	223	VAL	2.0
1	E	167	ALA	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)

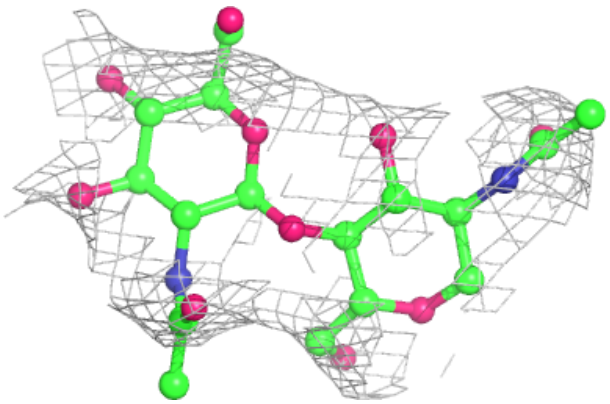
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

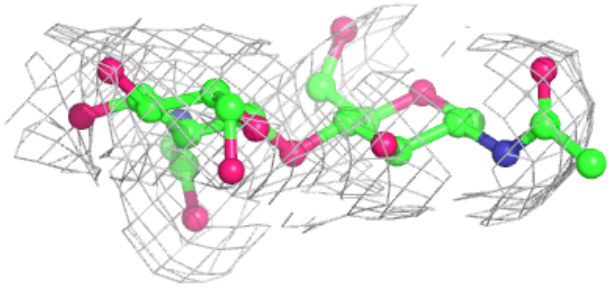
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	NAG	Z	2	14/15	0.59	0.30	148,168,184,187	0
5	NAG	W	2	14/15	0.67	0.23	101,164,178,181	0
7	BMA	V	3	11/12	0.74	0.20	143,162,184,184	0
6	MAN	U	6	11/12	0.75	0.21	107,150,161,168	0
6	MAN	S	6	11/12	0.77	0.25	98,121,144,159	0
7	MAN	V	4	11/12	0.78	0.29	116,160,172,172	0
7	MAN	X	4	11/12	0.78	0.23	141,152,161,171	0
5	NAG	Y	2	14/15	0.82	0.24	125,157,178,198	0
8	MAN	a	4	11/12	0.82	0.25	167,178,185,195	0
5	NAG	R	2	14/15	0.83	0.17	119,161,166,173	0
6	MAN	U	4	11/12	0.84	0.31	139,150,160,161	0
5	NAG	Y	1	14/15	0.85	0.25	122,137,150,152	0
8	BMA	a	3	11/12	0.85	0.22	143,167,178,180	0
5	NAG	Q	2	14/15	0.85	0.25	94,123,152,155	0
7	BMA	X	3	11/12	0.86	0.17	89,135,147,164	0
5	NAG	Z	1	14/15	0.86	0.15	131,149,167,169	0
8	MAN	a	5	11/12	0.86	0.14	111,156,169,170	0
7	NAG	V	2	14/15	0.87	0.24	115,138,152,156	0
6	BMA	S	3	11/12	0.87	0.21	129,143,167,173	0
5	NAG	R	1	14/15	0.88	0.16	109,132,148,159	0
6	BMA	U	3	11/12	0.88	0.16	111,118,133,145	0
6	MAN	S	5	11/12	0.88	0.22	116,129,139,141	0
6	MAN	U	5	11/12	0.89	0.20	129,138,146,157	0
7	NAG	X	2	14/15	0.90	0.24	88,101,119,124	0
6	MAN	S	4	11/12	0.90	0.27	119,131,156,166	0
5	NAG	T	2	14/15	0.90	0.19	118,143,154,159	0
5	NAG	W	1	14/15	0.91	0.16	146,161,166,172	0
6	NAG	S	2	14/15	0.91	0.35	90,104,122,125	0
8	NAG	a	2	14/15	0.91	0.34	110,122,148,152	0
7	NAG	V	1	14/15	0.92	0.25	104,113,126,141	0
8	NAG	a	1	14/15	0.92	0.46	108,126,155,155	0
6	NAG	U	2	14/15	0.92	0.26	82,102,128,131	0
5	NAG	T	1	14/15	0.94	0.24	97,105,130,157	0
6	NAG	S	1	14/15	0.95	0.32	75,87,93,99	0
5	NAG	Q	1	14/15	0.95	0.25	82,103,124,127	0
6	NAG	U	1	14/15	0.95	0.29	96,106,115,119	0
7	NAG	X	1	14/15	0.95	0.32	88,107,118,123	0

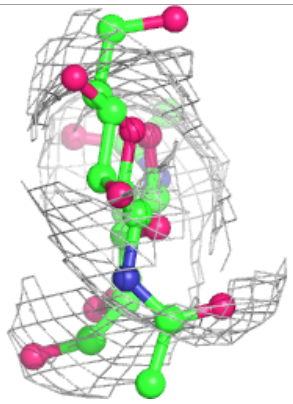
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain Q:

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

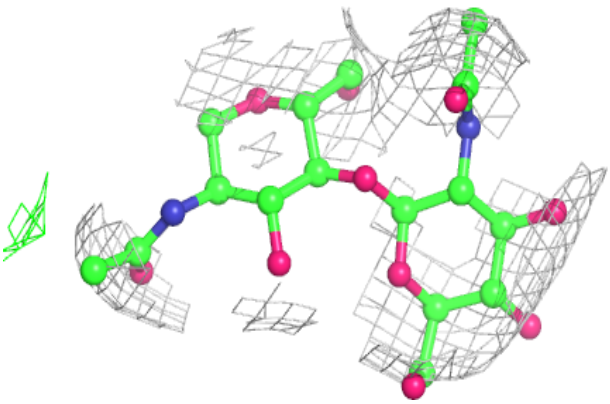


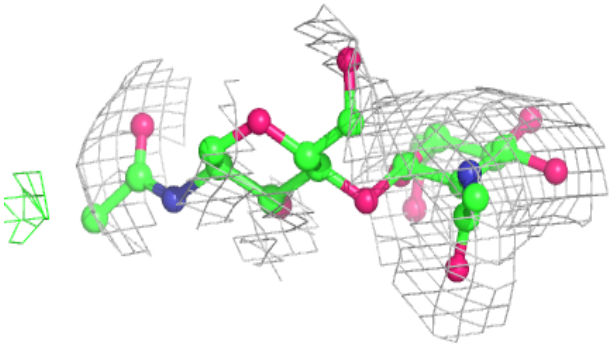


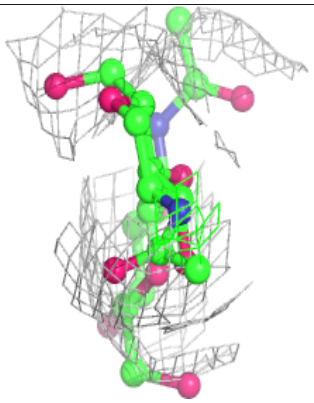


Electron density around Chain R:

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

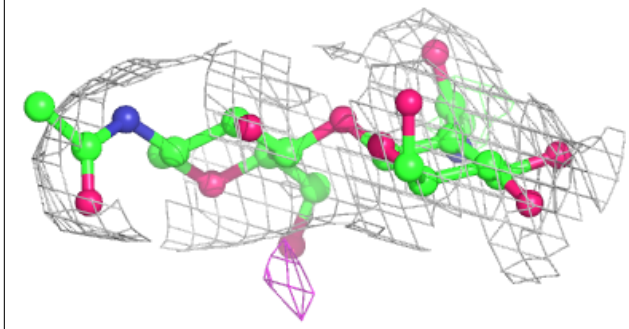


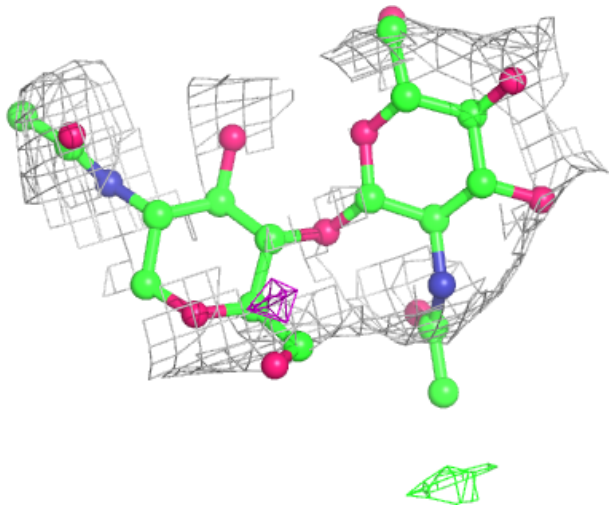


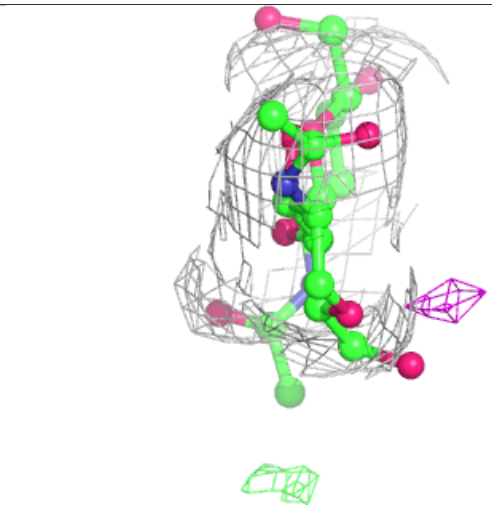


Electron density around Chain T:

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

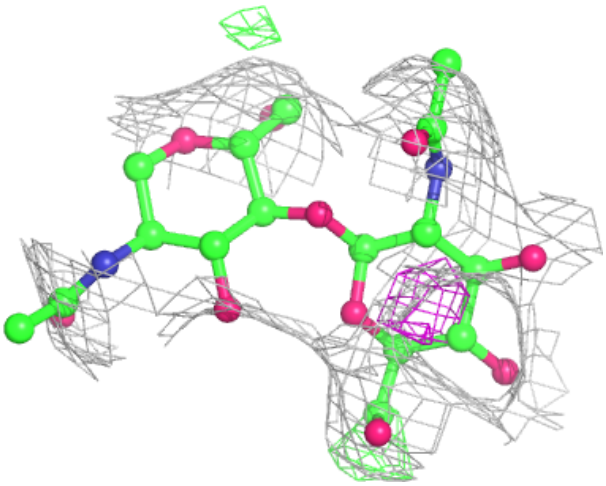


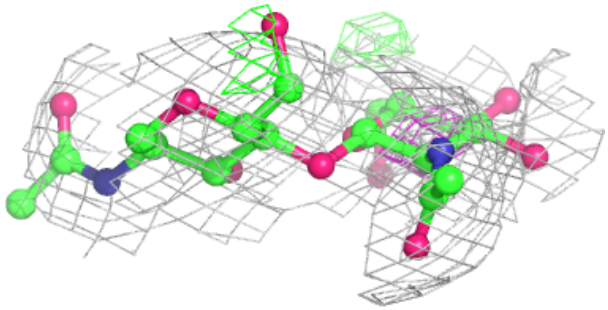


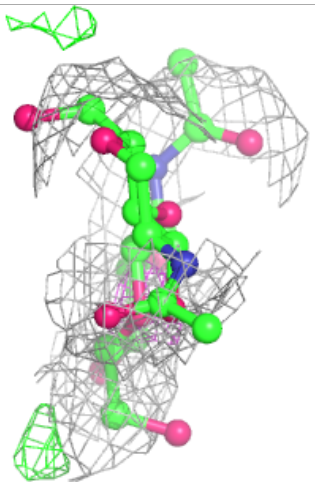


Electron density around Chain W:

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

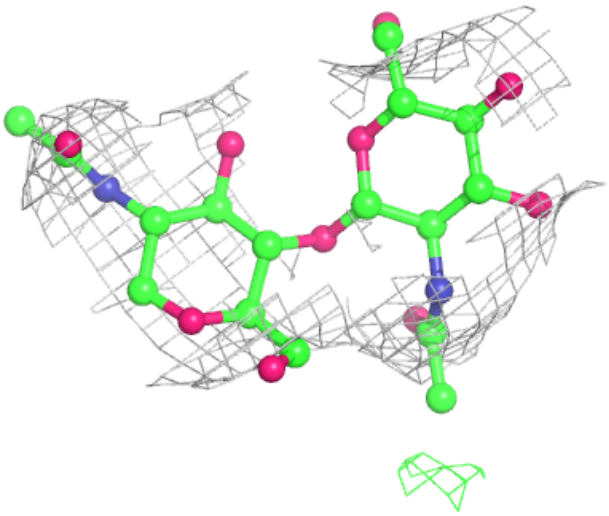


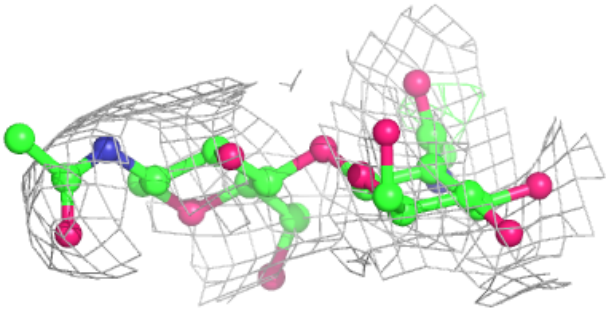


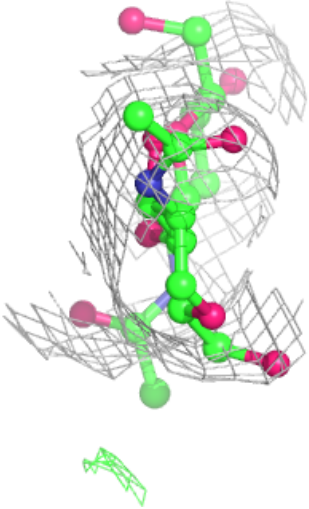


Electron density around Chain Y:

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

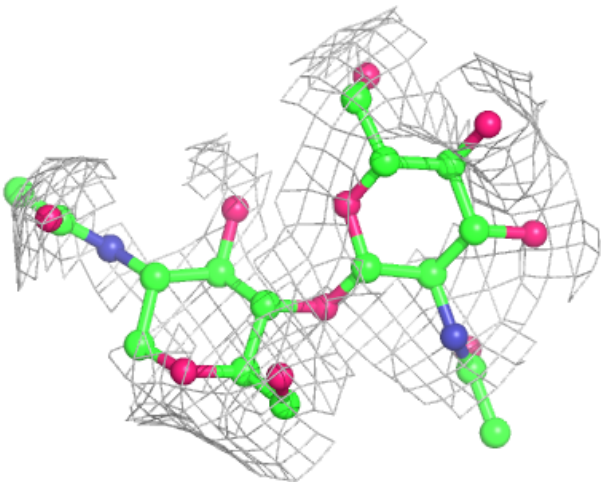


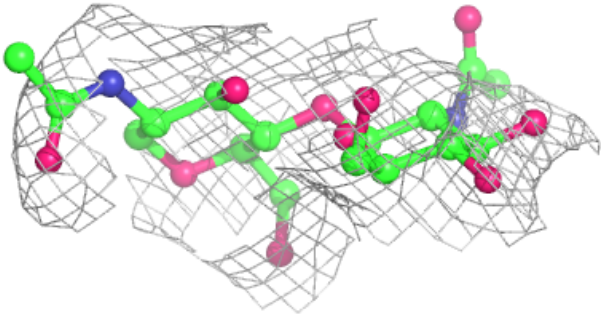


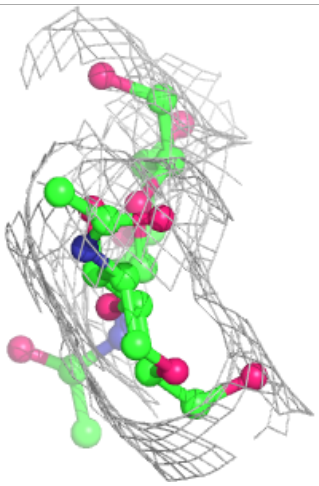


Electron density around Chain Z:

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

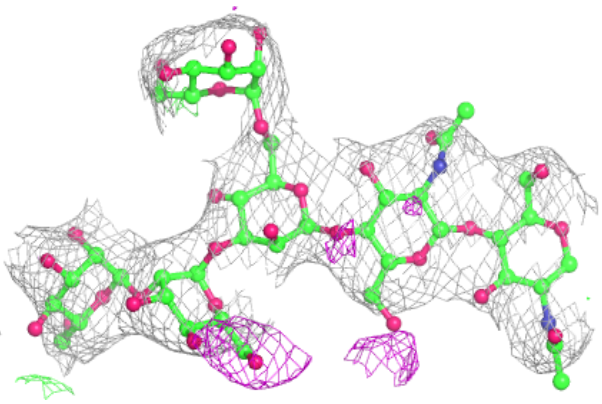


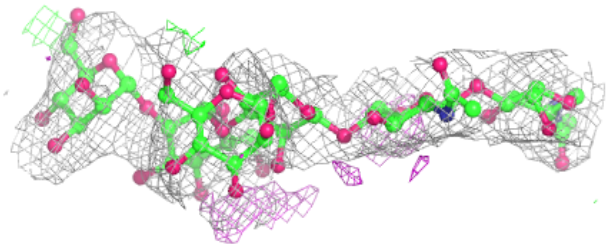


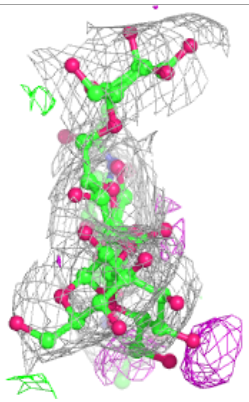


Electron density around Chain S:

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

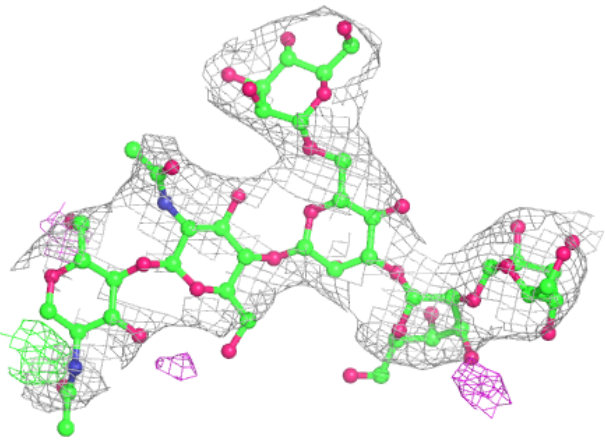


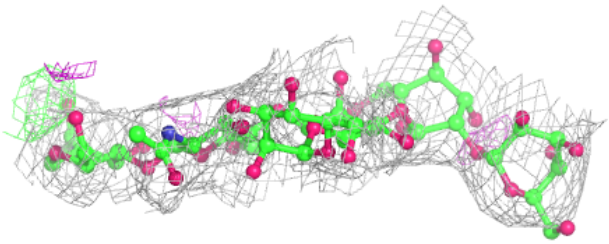


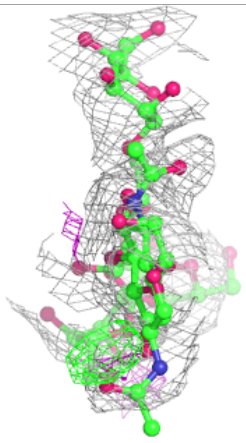


Electron density around Chain U:

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

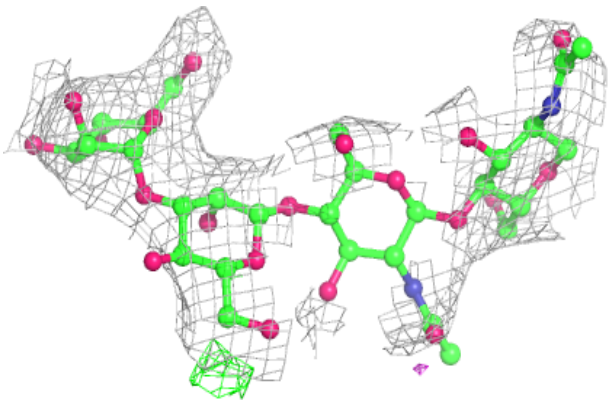


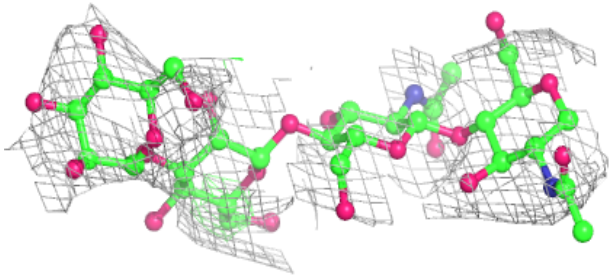




Electron density around Chain V:

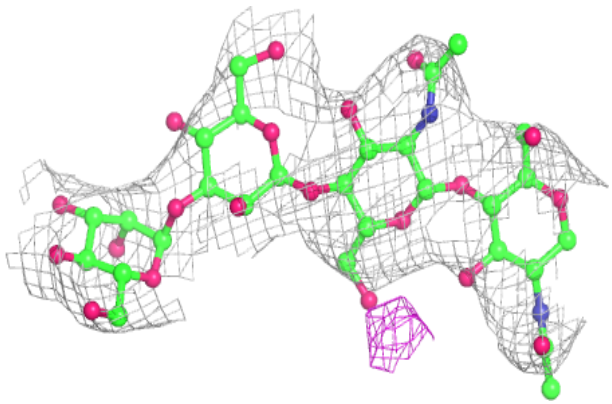
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

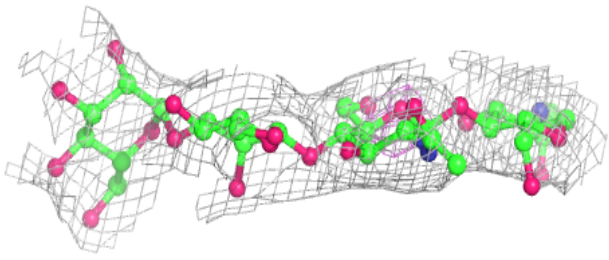


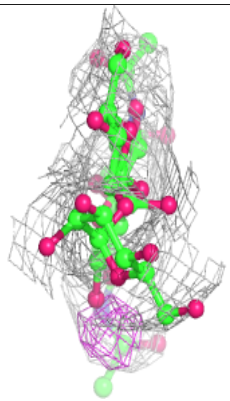


Electron density around Chain X:

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

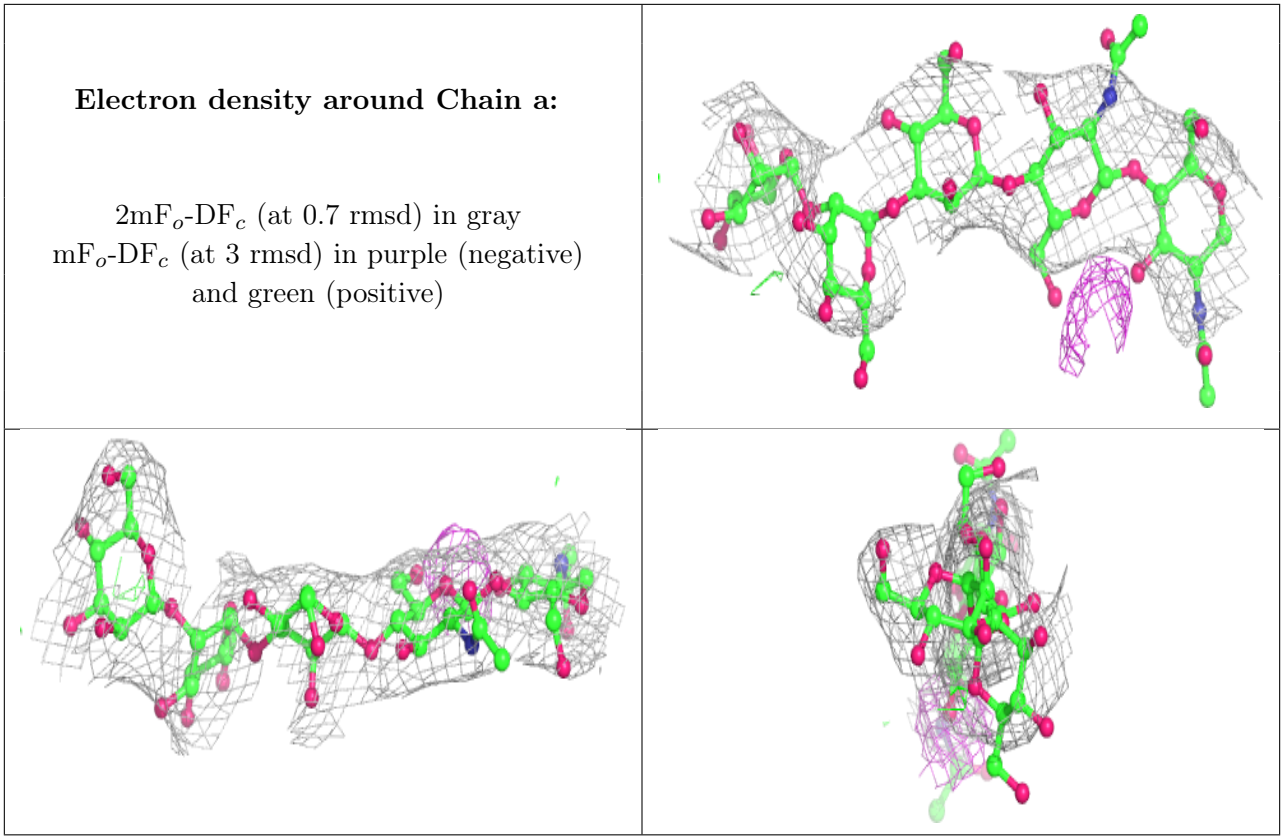






Electron density around Chain a:

$2mF_o$-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
10	MAN	M	305	11/12	0.69	0.41	152,184,193,196	0
10	MAN	I	305	11/12	0.72	0.21	115,144,163,168	0
9	NAG	E	303	14/15	0.76	0.25	119,150,167,170	0

6.5 Other polymers

There are no such residues in this entry.