wwPDB X-ray Structure Validation Summary Report (i)

May 7, 2024 – 10:11 AM EDT

PDB ID	:	8SUF
Title	:	The complex of TOL-1 ectodomain bound to LAT-1 Lectin domain
Authors	:	Carmona Rosas, G.; Li, J.; Arac, D.; Ozkan, E.
Deposited on	:	2023-05-12
Resolution	:	4.00 Å(reported)

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

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

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

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

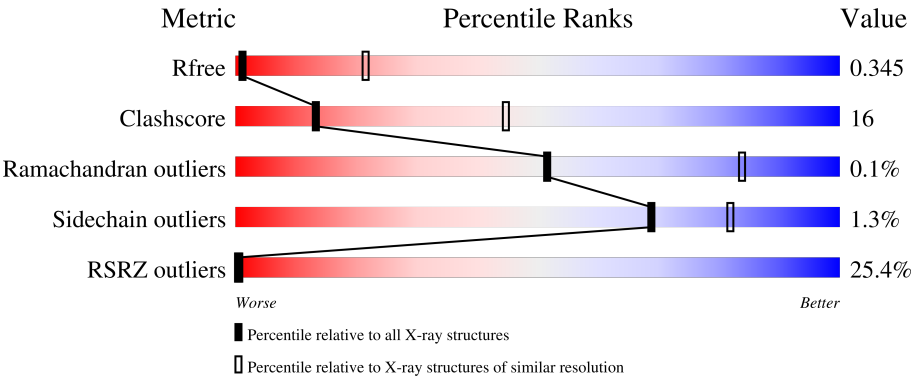
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.00 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	1087 (4.30-3.70)
Clashscore	141614	1148 (4.30-3.70)
Ramachandran outliers	138981	1108 (4.30-3.70)
Sidechain outliers	138945	1099 (4.30-3.70)
RSRZ outliers	127900	1028 (4.34-3.66)

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	1007	19% 57% 36% 7%
1	B	1007	23% 58% 33% • 7%
1	C	1007	21% 62% 30% 7%
1	D	1007	23% 57% 36% 7%
2	E	114	39% 71% 23% • 5%

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Mol	Chain	Length	Quality of chain
2	F	114	46% 71% 24% 5%
2	G	114	40% 68% 24% 6%
2	H	114	44% 67% 25% 8%
3	I	4	25% 25% 50%
3	M	4	25% 50% 25%
4	J	2	50% 50%
4	K	2	100%
4	N	2	100%
4	O	2	50% 50%
4	R	2	100%
5	L	4	25% 75%
6	P	5	60% 40%
7	Q	3	33% 67%

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
3	MAN	I	4	-	-	-	X
4	NAG	K	1	-	-	-	X
4	NAG	N	2	-	-	-	X
4	NAG	O	2	-	-	-	X
8	NAG	A	1102	-	-	-	X
8	NAG	A	1103	-	-	-	X
8	NAG	B	1102	-	-	-	X
8	NAG	B	1103	-	-	-	X
8	NAG	C	1101	-	-	-	X
8	NAG	D	1101	-	-	-	X

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 32993 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 TIR domain-containing protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	939	Total	C	N	O	S	0	0	0
			7315	4590	1278	1405	42			
1	B	935	Total	C	N	O	S	0	0	0
			7286	4570	1274	1401	41			
1	C	939	Total	C	N	O	S	0	0	0
			7315	4590	1278	1405	42			
1	D	939	Total	C	N	O	S	0	0	0
			7315	4590	1278	1405	42			

There are 144 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	ALA	-	expression tag	UNP Q9N5Z3
A	-5	ASP	-	expression tag	UNP Q9N5Z3
A	-4	PRO	-	expression tag	UNP Q9N5Z3
A	-3	HIS	-	expression tag	UNP Q9N5Z3
A	-2	HIS	-	expression tag	UNP Q9N5Z3
A	-1	HIS	-	expression tag	UNP Q9N5Z3
A	0	HIS	-	expression tag	UNP Q9N5Z3
A	1	HIS	-	expression tag	UNP Q9N5Z3
A	2	HIS	-	expression tag	UNP Q9N5Z3
A	3	GLY	-	expression tag	UNP Q9N5Z3
A	4	SER	-	expression tag	UNP Q9N5Z3
A	5	GLY	-	expression tag	UNP Q9N5Z3
A	6	LEU	-	expression tag	UNP Q9N5Z3
A	7	ASN	-	expression tag	UNP Q9N5Z3
A	8	ASP	-	expression tag	UNP Q9N5Z3
A	9	ILE	-	expression tag	UNP Q9N5Z3
A	10	PHE	-	expression tag	UNP Q9N5Z3
A	11	GLU	-	expression tag	UNP Q9N5Z3
A	12	ALA	-	expression tag	UNP Q9N5Z3
A	13	GLN	-	expression tag	UNP Q9N5Z3
A	14	LYS	-	expression tag	UNP Q9N5Z3

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Chain	Residue	Modelled	Actual	Comment	Reference
A	15	ILE	-	expression tag	UNP Q9N5Z3
A	16	GLU	-	expression tag	UNP Q9N5Z3
A	17	TRP	-	expression tag	UNP Q9N5Z3
A	18	HIS	-	expression tag	UNP Q9N5Z3
A	19	GLU	-	expression tag	UNP Q9N5Z3
A	20	ALA	-	expression tag	UNP Q9N5Z3
A	21	ASP	-	expression tag	UNP Q9N5Z3
A	22	PRO	-	expression tag	UNP Q9N5Z3
A	23	GLY	-	expression tag	UNP Q9N5Z3
A	24	TYR	-	expression tag	UNP Q9N5Z3
A	25	THR	-	expression tag	UNP Q9N5Z3
A	997	ASP	-	expression tag	UNP Q9N5Z3
A	998	ILE	-	expression tag	UNP Q9N5Z3
A	999	GLN	-	expression tag	UNP Q9N5Z3
A	1000	HIS	-	expression tag	UNP Q9N5Z3
B	-6	ALA	-	expression tag	UNP Q9N5Z3
B	-5	ASP	-	expression tag	UNP Q9N5Z3
B	-4	PRO	-	expression tag	UNP Q9N5Z3
B	-3	HIS	-	expression tag	UNP Q9N5Z3
B	-2	HIS	-	expression tag	UNP Q9N5Z3
B	-1	HIS	-	expression tag	UNP Q9N5Z3
B	0	HIS	-	expression tag	UNP Q9N5Z3
B	1	HIS	-	expression tag	UNP Q9N5Z3
B	2	HIS	-	expression tag	UNP Q9N5Z3
B	3	GLY	-	expression tag	UNP Q9N5Z3
B	4	SER	-	expression tag	UNP Q9N5Z3
B	5	GLY	-	expression tag	UNP Q9N5Z3
B	6	LEU	-	expression tag	UNP Q9N5Z3
B	7	ASN	-	expression tag	UNP Q9N5Z3
B	8	ASP	-	expression tag	UNP Q9N5Z3
B	9	ILE	-	expression tag	UNP Q9N5Z3
B	10	PHE	-	expression tag	UNP Q9N5Z3
B	11	GLU	-	expression tag	UNP Q9N5Z3
B	12	ALA	-	expression tag	UNP Q9N5Z3
B	13	GLN	-	expression tag	UNP Q9N5Z3
B	14	LYS	-	expression tag	UNP Q9N5Z3
B	15	ILE	-	expression tag	UNP Q9N5Z3
B	16	GLU	-	expression tag	UNP Q9N5Z3
B	17	TRP	-	expression tag	UNP Q9N5Z3
B	18	HIS	-	expression tag	UNP Q9N5Z3
B	19	GLU	-	expression tag	UNP Q9N5Z3
B	20	ALA	-	expression tag	UNP Q9N5Z3

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Chain	Residue	Modelled	Actual	Comment	Reference
B	21	ASP	-	expression tag	UNP Q9N5Z3
B	22	PRO	-	expression tag	UNP Q9N5Z3
B	23	GLY	-	expression tag	UNP Q9N5Z3
B	24	TYR	-	expression tag	UNP Q9N5Z3
B	25	THR	-	expression tag	UNP Q9N5Z3
B	997	ASP	-	expression tag	UNP Q9N5Z3
B	998	ILE	-	expression tag	UNP Q9N5Z3
B	999	GLN	-	expression tag	UNP Q9N5Z3
B	1000	HIS	-	expression tag	UNP Q9N5Z3
C	-6	ALA	-	expression tag	UNP Q9N5Z3
C	-5	ASP	-	expression tag	UNP Q9N5Z3
C	-4	PRO	-	expression tag	UNP Q9N5Z3
C	-3	HIS	-	expression tag	UNP Q9N5Z3
C	-2	HIS	-	expression tag	UNP Q9N5Z3
C	-1	HIS	-	expression tag	UNP Q9N5Z3
C	0	HIS	-	expression tag	UNP Q9N5Z3
C	1	HIS	-	expression tag	UNP Q9N5Z3
C	2	HIS	-	expression tag	UNP Q9N5Z3
C	3	GLY	-	expression tag	UNP Q9N5Z3
C	4	SER	-	expression tag	UNP Q9N5Z3
C	5	GLY	-	expression tag	UNP Q9N5Z3
C	6	LEU	-	expression tag	UNP Q9N5Z3
C	7	ASN	-	expression tag	UNP Q9N5Z3
C	8	ASP	-	expression tag	UNP Q9N5Z3
C	9	ILE	-	expression tag	UNP Q9N5Z3
C	10	PHE	-	expression tag	UNP Q9N5Z3
C	11	GLU	-	expression tag	UNP Q9N5Z3
C	12	ALA	-	expression tag	UNP Q9N5Z3
C	13	GLN	-	expression tag	UNP Q9N5Z3
C	14	LYS	-	expression tag	UNP Q9N5Z3
C	15	ILE	-	expression tag	UNP Q9N5Z3
C	16	GLU	-	expression tag	UNP Q9N5Z3
C	17	TRP	-	expression tag	UNP Q9N5Z3
C	18	HIS	-	expression tag	UNP Q9N5Z3
C	19	GLU	-	expression tag	UNP Q9N5Z3
C	20	ALA	-	expression tag	UNP Q9N5Z3
C	21	ASP	-	expression tag	UNP Q9N5Z3
C	22	PRO	-	expression tag	UNP Q9N5Z3
C	23	GLY	-	expression tag	UNP Q9N5Z3
C	24	TYR	-	expression tag	UNP Q9N5Z3
C	25	THR	-	expression tag	UNP Q9N5Z3
C	997	ASP	-	expression tag	UNP Q9N5Z3

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Chain	Residue	Modelled	Actual	Comment	Reference
C	998	ILE	-	expression tag	UNP Q9N5Z3
C	999	GLN	-	expression tag	UNP Q9N5Z3
C	1000	HIS	-	expression tag	UNP Q9N5Z3
D	-6	ALA	-	expression tag	UNP Q9N5Z3
D	-5	ASP	-	expression tag	UNP Q9N5Z3
D	-4	PRO	-	expression tag	UNP Q9N5Z3
D	-3	HIS	-	expression tag	UNP Q9N5Z3
D	-2	HIS	-	expression tag	UNP Q9N5Z3
D	-1	HIS	-	expression tag	UNP Q9N5Z3
D	0	HIS	-	expression tag	UNP Q9N5Z3
D	1	HIS	-	expression tag	UNP Q9N5Z3
D	2	HIS	-	expression tag	UNP Q9N5Z3
D	3	GLY	-	expression tag	UNP Q9N5Z3
D	4	SER	-	expression tag	UNP Q9N5Z3
D	5	GLY	-	expression tag	UNP Q9N5Z3
D	6	LEU	-	expression tag	UNP Q9N5Z3
D	7	ASN	-	expression tag	UNP Q9N5Z3
D	8	ASP	-	expression tag	UNP Q9N5Z3
D	9	ILE	-	expression tag	UNP Q9N5Z3
D	10	PHE	-	expression tag	UNP Q9N5Z3
D	11	GLU	-	expression tag	UNP Q9N5Z3
D	12	ALA	-	expression tag	UNP Q9N5Z3
D	13	GLN	-	expression tag	UNP Q9N5Z3
D	14	LYS	-	expression tag	UNP Q9N5Z3
D	15	ILE	-	expression tag	UNP Q9N5Z3
D	16	GLU	-	expression tag	UNP Q9N5Z3
D	17	TRP	-	expression tag	UNP Q9N5Z3
D	18	HIS	-	expression tag	UNP Q9N5Z3
D	19	GLU	-	expression tag	UNP Q9N5Z3
D	20	ALA	-	expression tag	UNP Q9N5Z3
D	21	ASP	-	expression tag	UNP Q9N5Z3
D	22	PRO	-	expression tag	UNP Q9N5Z3
D	23	GLY	-	expression tag	UNP Q9N5Z3
D	24	TYR	-	expression tag	UNP Q9N5Z3
D	25	THR	-	expression tag	UNP Q9N5Z3
D	997	ASP	-	expression tag	UNP Q9N5Z3
D	998	ILE	-	expression tag	UNP Q9N5Z3
D	999	GLN	-	expression tag	UNP Q9N5Z3
D	1000	HIS	-	expression tag	UNP Q9N5Z3

- Molecule 2 is a protein called Latrophilin-like protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	108	Total	C	N	O	S	0	0	0
			815	507	133	166	9			
2	F	108	Total	C	N	O	S	0	0	0
			815	507	133	166	9			
2	G	107	Total	C	N	O	S	0	0	0
			808	502	132	165	9			
2	H	105	Total	C	N	O	S	0	0	0
			794	492	130	163	9			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	29	ALA	-	expression tag	UNP G5EDW2
E	30	ASP	-	expression tag	UNP G5EDW2
E	137	HIS	-	expression tag	UNP G5EDW2
E	138	HIS	-	expression tag	UNP G5EDW2
E	139	HIS	-	expression tag	UNP G5EDW2
E	140	HIS	-	expression tag	UNP G5EDW2
E	141	HIS	-	expression tag	UNP G5EDW2
E	142	HIS	-	expression tag	UNP G5EDW2
F	29	ALA	-	expression tag	UNP G5EDW2
F	30	ASP	-	expression tag	UNP G5EDW2
F	137	HIS	-	expression tag	UNP G5EDW2
F	138	HIS	-	expression tag	UNP G5EDW2
F	139	HIS	-	expression tag	UNP G5EDW2
F	140	HIS	-	expression tag	UNP G5EDW2
F	141	HIS	-	expression tag	UNP G5EDW2
F	142	HIS	-	expression tag	UNP G5EDW2
G	29	ALA	-	expression tag	UNP G5EDW2
G	30	ASP	-	expression tag	UNP G5EDW2
G	137	HIS	-	expression tag	UNP G5EDW2
G	138	HIS	-	expression tag	UNP G5EDW2
G	139	HIS	-	expression tag	UNP G5EDW2
G	140	HIS	-	expression tag	UNP G5EDW2
G	141	HIS	-	expression tag	UNP G5EDW2
G	142	HIS	-	expression tag	UNP G5EDW2
H	29	ALA	-	expression tag	UNP G5EDW2
H	30	ASP	-	expression tag	UNP G5EDW2
H	137	HIS	-	expression tag	UNP G5EDW2
H	138	HIS	-	expression tag	UNP G5EDW2
H	139	HIS	-	expression tag	UNP G5EDW2
H	140	HIS	-	expression tag	UNP G5EDW2
H	141	HIS	-	expression tag	UNP G5EDW2
H	142	HIS	-	expression tag	UNP G5EDW2

- Molecule 3 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
3	I	4	Total	C	N	O	0	0	0
			50	28	2	20			
3	M	4	Total	C	N	O	0	0	0
			50	28	2	20			

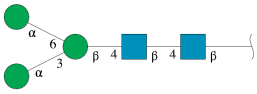
- Molecule 4 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	J	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	K	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	N	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	O	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	R	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 5 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-glucopyranose.

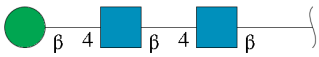
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	L	4	Total	C	N	O	0	0	0
			50	28	2	20			

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



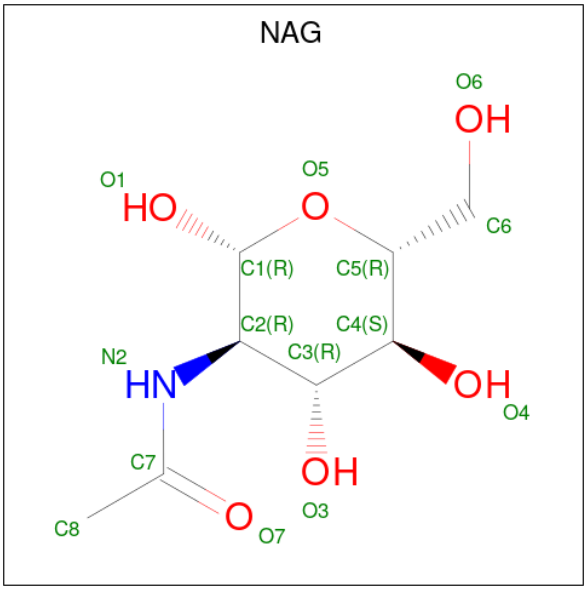
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
6	P	5	61	34	2	25	0	0	0

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



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

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



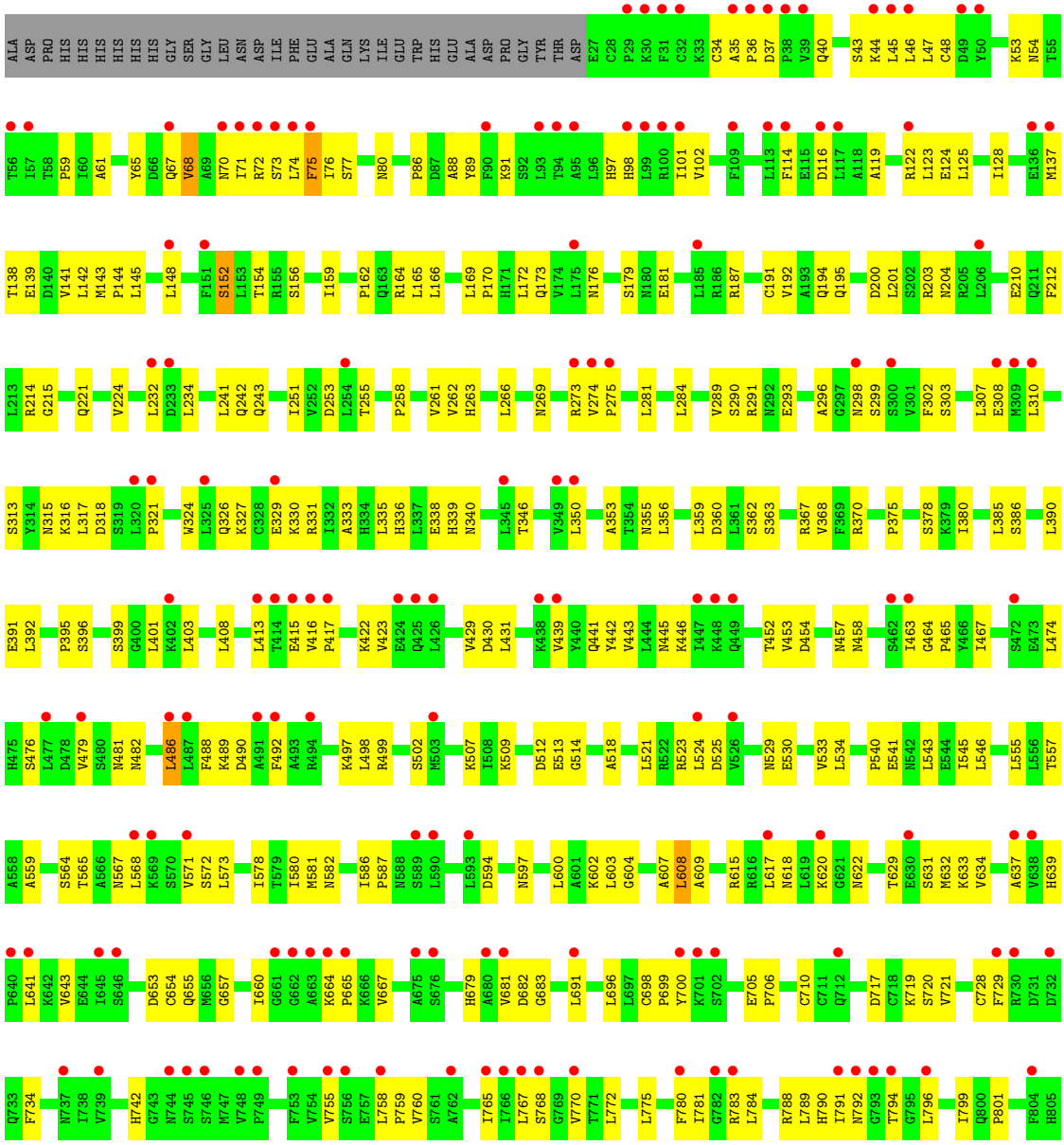
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	N	O	0	0
			14	8	1	5		
8	A	1	Total	C	N	O	0	0
			14	8	1	5		
8	A	1	Total	C	N	O	0	0
			14	8	1	5		
8	B	1	Total	C	N	O	0	0
			14	8	1	5		
8	B	1	Total	C	N	O	0	0
			14	8	1	5		
8	B	1	Total	C	N	O	0	0
			14	8	1	5		
8	C	1	Total	C	N	O	0	0
			14	8	1	5		
8	C	1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

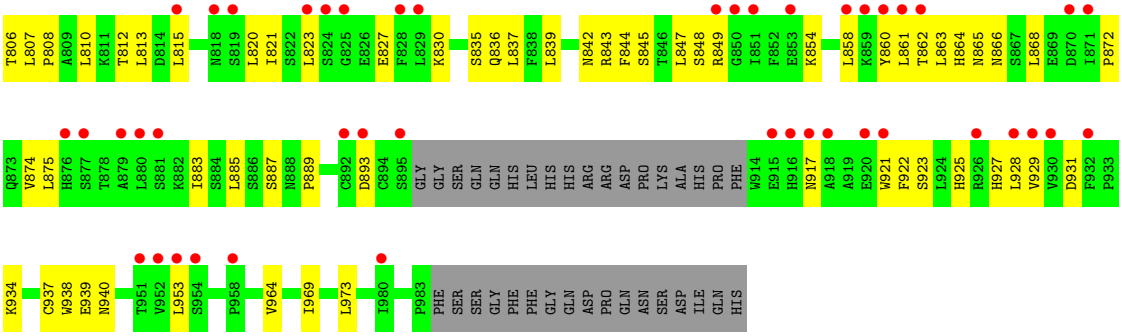
3 Residue-property plots (i)

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: TIR domain-containing protein

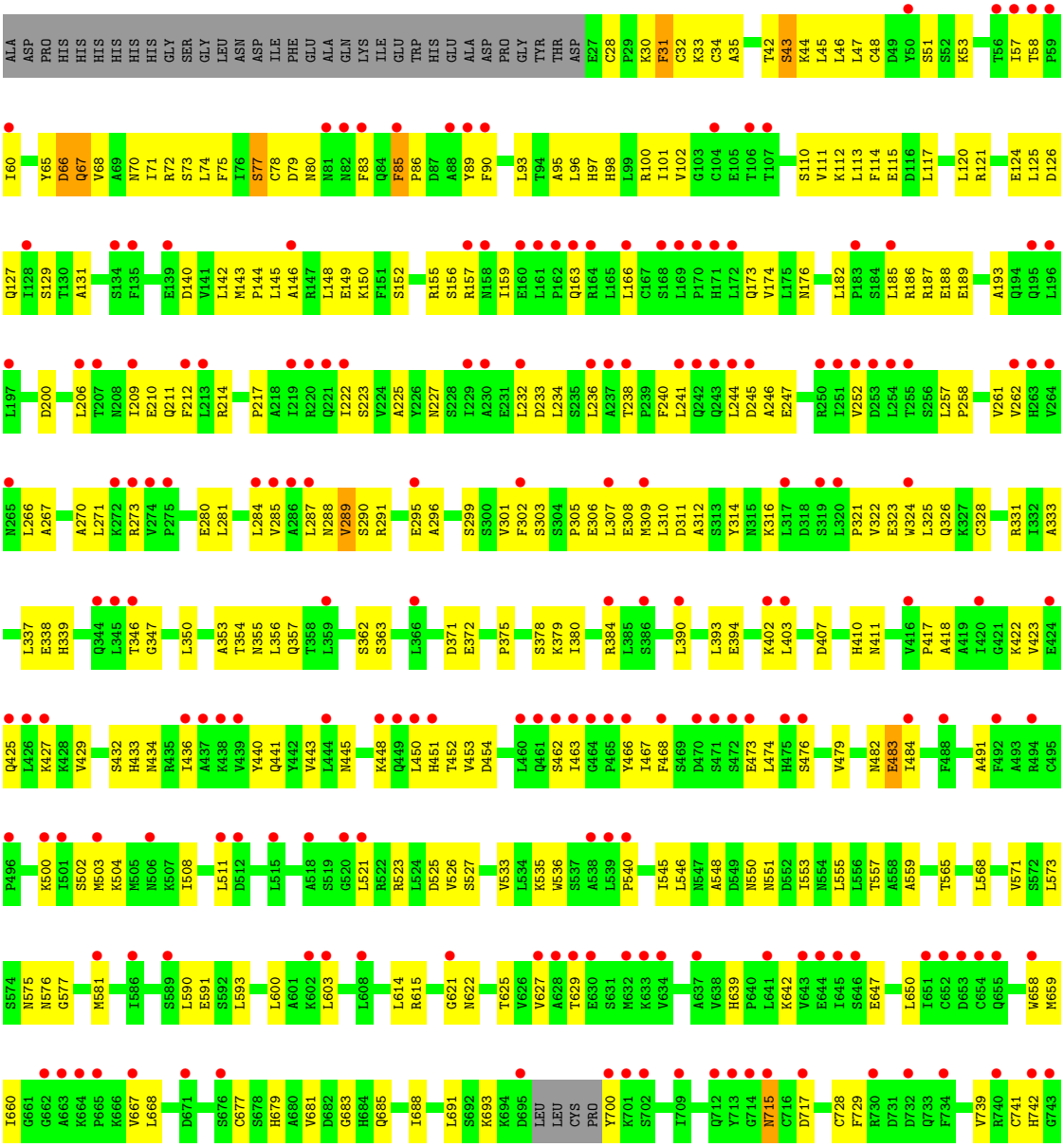
Chain A:

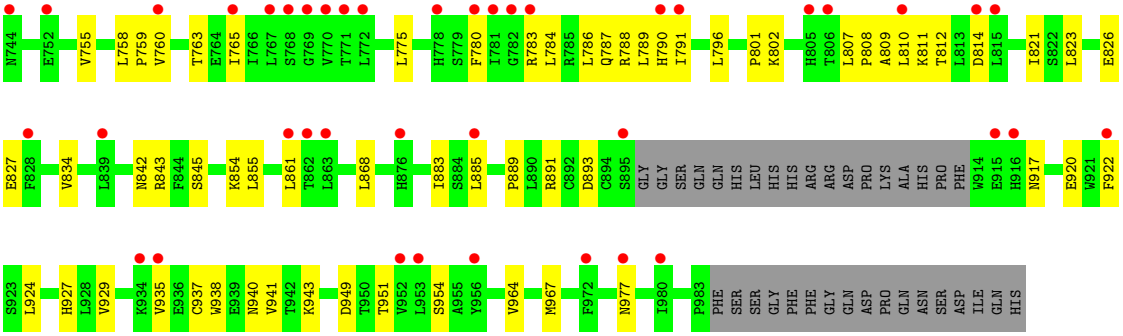




• Molecule 1: TIR domain-containing protein

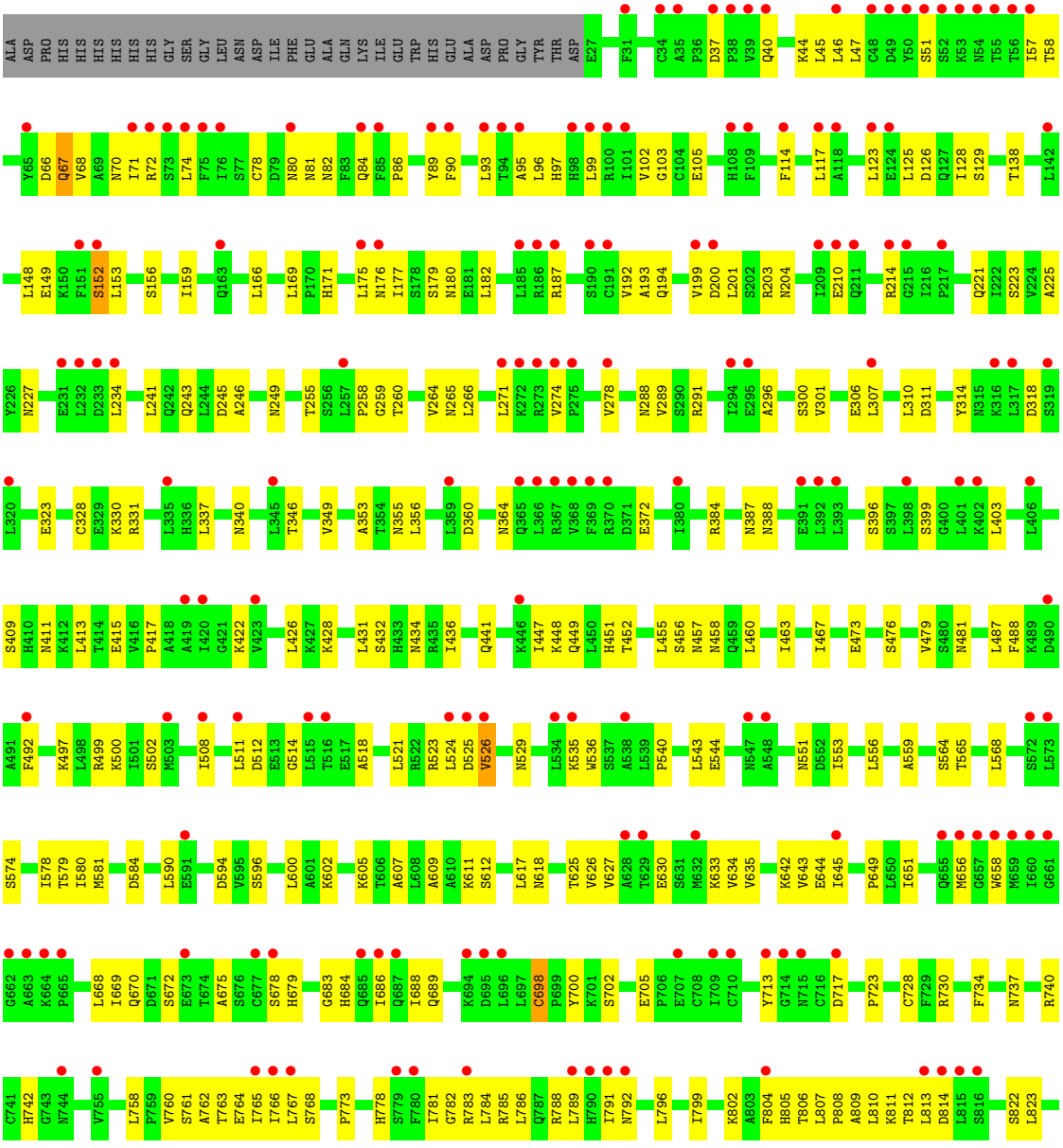
Chain B:

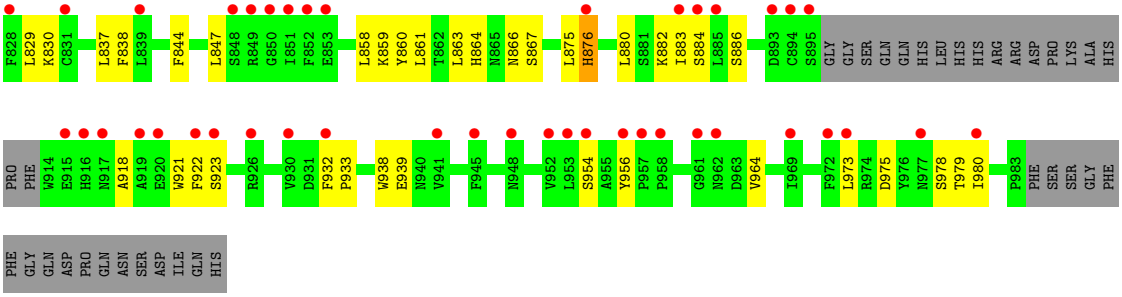




• Molecule 1: TIR domain-containing protein

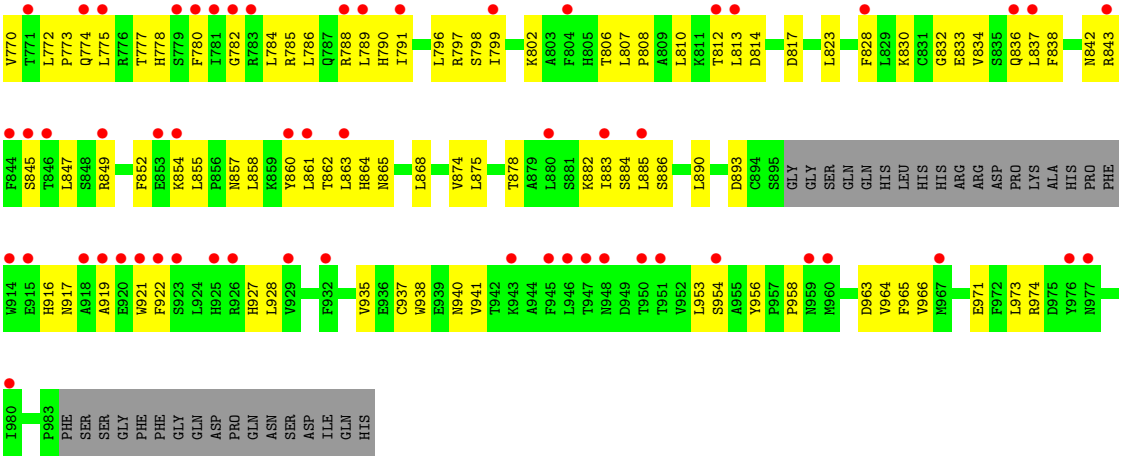
Chain C:





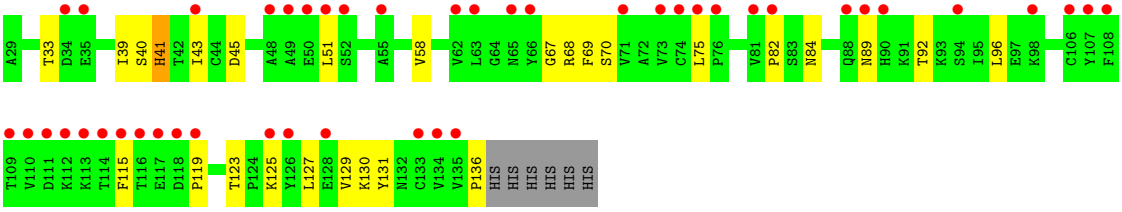
• Molecule 1: TIR domain-containing protein

Chain D:



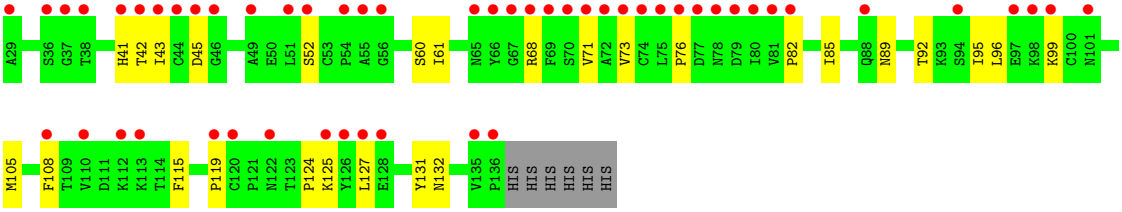
• Molecule 2: Latrophilin-like protein 1

Chain E:



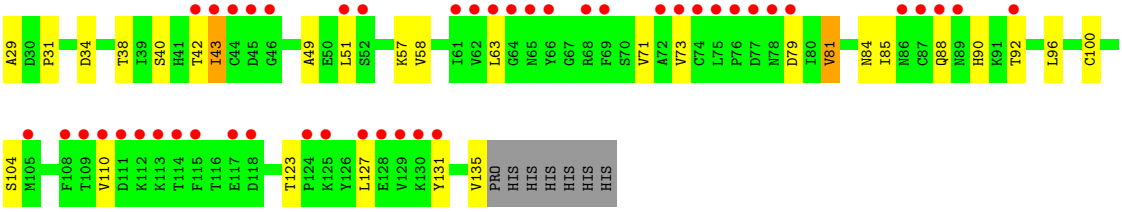
• Molecule 2: Latrophilin-like protein 1

Chain F:



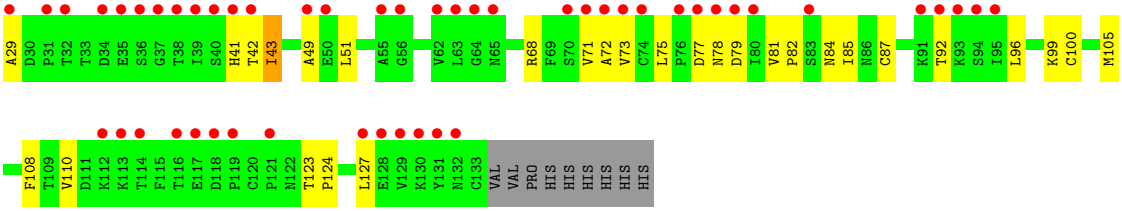
• Molecule 2: Latrophilin-like protein 1

Chain G:



• Molecule 2: Latrophilin-like protein 1

Chain H:

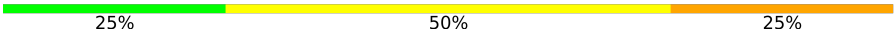


• Molecule 3: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:

• Molecule 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 M:

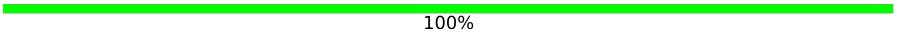


• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:

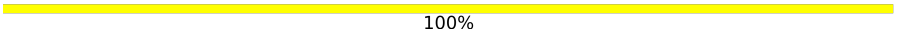
• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:



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

Chain N:

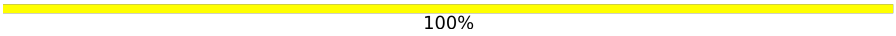


• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:

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

Chain R:

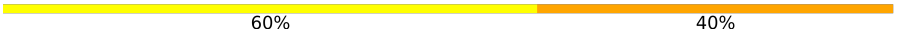


• Molecule 5: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L:

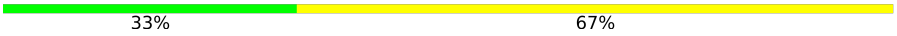
• Molecule 6: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P:



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

Chain Q:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	74.15Å 316.75Å 172.44Å 90.00° 90.16° 90.00°	Depositor
Resolution (Å)	74.15 – 4.00 172.44 – 4.00	Depositor EDS
% Data completeness (in resolution range)	55.5 (74.15-4.00) 55.6 (172.44-4.00)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.11	Depositor
$< I/\sigma(I) >$ [1]	2.13 (at 4.02Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.288 , 0.338 0.293 , 0.345	Depositor DCC
R_{free} test set	1861 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	139.9	Xtriage
Anisotropy	0.112	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 381.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.25$	Xtriage
Estimated twinning fraction	0.177 for h,-k,-l	Xtriage
F_o,F_c correlation	0.83	EDS
Total number of atoms	32993	wwPDB-VP
Average B, all atoms (Å^2)	220.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.43% 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	0.35	0/7436	0.66	0/10087
1	B	0.36	0/7405	0.67	0/10042
1	C	0.36	0/7436	0.68	0/10087
1	D	0.36	0/7436	0.66	1/10087 (0.0%)
2	E	0.29	0/831	0.54	0/1131
2	F	0.26	0/831	0.51	0/1131
2	G	0.29	0/823	0.58	0/1119
2	H	0.28	0/809	0.58	0/1099
All	All	0.35	0/33007	0.66	1/44783 (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	D	160	GLU	C-N-CA	6.22	137.24	121.70

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	7315	0	7381	262	0
1	B	7286	0	7348	253	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	7315	0	7383	217	1
1	D	7315	0	7385	283	0
2	E	815	0	786	18	0
2	F	815	0	786	15	0
2	G	808	0	779	22	0
2	H	794	0	761	32	0
3	I	50	0	43	2	0
3	M	50	0	43	5	0
4	J	28	0	25	0	0
4	K	28	0	25	0	0
4	N	28	0	25	0	0
4	O	28	0	25	2	0
4	R	28	0	25	0	0
5	L	50	0	43	0	0
6	P	61	0	52	5	0
7	Q	39	0	34	0	0
8	A	42	0	39	3	0
8	B	42	0	39	2	0
8	C	28	0	26	1	0
8	D	28	0	26	2	0
All	All	32993	0	33079	1072	1

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

The worst 5 of 1072 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:407:ASP:HA	1:D:430:ASP:HB3	1.48	0.94
1:D:410:HIS:H	1:D:433:HIS:HB2	1.31	0.94
1:C:581:MET:HG3	1:C:600:LEU:HD21	1.50	0.91
1:A:86:PRO:HG2	1:A:89:TYR:HB2	1.53	0.90
1:A:799:ILE:HD12	1:A:823:LEU:HD21	1.51	0.89

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:927:HIS:NE2	1:C:702:SER:OG[2_654]	2.09	0.11

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	935/1007 (93%)	813 (87%)	122 (13%)	0	100	100
1	B	929/1007 (92%)	805 (87%)	123 (13%)	1 (0%)	51	84
1	C	935/1007 (93%)	802 (86%)	132 (14%)	1 (0%)	51	84
1	D	935/1007 (93%)	812 (87%)	122 (13%)	1 (0%)	51	84
2	E	106/114 (93%)	101 (95%)	5 (5%)	0	100	100
2	F	106/114 (93%)	101 (95%)	5 (5%)	0	100	100
2	G	105/114 (92%)	101 (96%)	4 (4%)	0	100	100
2	H	103/114 (90%)	98 (95%)	5 (5%)	0	100	100
All	All	4154/4484 (93%)	3633 (88%)	518 (12%)	3 (0%)	51	84

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	325	LEU
1	B	346	THR
1	C	259	GLY

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	851/908 (94%)	842 (99%)	9 (1%)	73	85
1	B	847/908 (93%)	833 (98%)	14 (2%)	60	78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	C	851/908 (94%)	838 (98%)	13 (2%)	65 80
1	D	851/908 (94%)	843 (99%)	8 (1%)	78 88
2	E	97/103 (94%)	96 (99%)	1 (1%)	76 86
2	F	97/103 (94%)	97 (100%)	0	100 100
2	G	96/103 (93%)	94 (98%)	2 (2%)	53 72
2	H	94/103 (91%)	92 (98%)	2 (2%)	53 72
All	All	3784/4044 (94%)	3735 (99%)	49 (1%)	69 82

5 of 49 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	138	THR
1	C	876	HIS
1	C	152	SER
1	C	526	VAL
1	D	445	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	778	HIS
2	E	41	HIS
1	C	458	ASN
1	D	108	HIS
1	D	292	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

30 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	$\#\|Z\| > 2$
3	NAG	I	1	3,1	14,14,15	0.47	0	17,19,21	0.47	0
3	NAG	I	2	3	14,14,15	0.73	0	17,19,21	0.90	1 (5%)
3	BMA	I	3	3	11,11,12	0.98	1 (9%)	15,15,17	1.17	1 (6%)
3	MAN	I	4	3	11,11,12	1.02	0	15,15,17	1.04	1 (6%)
4	NAG	J	1	4,1	14,14,15	0.32	0	17,19,21	0.74	1 (5%)
4	NAG	J	2	4	14,14,15	0.57	0	17,19,21	0.40	0
4	NAG	K	1	4,1	14,14,15	0.33	0	17,19,21	0.54	0
4	NAG	K	2	4	14,14,15	0.41	0	17,19,21	0.38	0
5	NAG	L	1	1,5	14,14,15	0.64	1 (7%)	17,19,21	0.89	1 (5%)
5	NAG	L	2	5	14,14,15	0.18	0	17,19,21	0.64	0
5	BMA	L	3	5	11,11,12	1.61	2 (18%)	15,15,17	1.31	2 (13%)
5	MAN	L	4	5	11,11,12	1.55	3 (27%)	15,15,17	1.23	1 (6%)
3	NAG	M	1	3,1	14,14,15	0.31	0	17,19,21	1.06	1 (5%)
3	NAG	M	2	3	14,14,15	0.58	1 (7%)	17,19,21	0.42	0
3	BMA	M	3	3	11,11,12	0.89	0	15,15,17	0.91	0
3	MAN	M	4	3	11,11,12	1.00	0	15,15,17	1.32	1 (6%)
4	NAG	N	1	4,1	14,14,15	0.22	0	17,19,21	0.96	1 (5%)
4	NAG	N	2	4	14,14,15	0.85	1 (7%)	17,19,21	0.47	0
4	NAG	O	1	4,1	14,14,15	0.65	1 (7%)	17,19,21	0.72	1 (5%)
4	NAG	O	2	4	14,14,15	0.68	0	17,19,21	0.40	0
6	NAG	P	1	1,6	14,14,15	0.30	0	17,19,21	0.63	0
6	NAG	P	2	6	14,14,15	0.49	0	17,19,21	0.82	1 (5%)
6	BMA	P	3	6	11,11,12	1.72	3 (27%)	15,15,17	2.10	6 (40%)
6	MAN	P	4	6	11,11,12	1.57	2 (18%)	15,15,17	1.27	2 (13%)
6	MAN	P	5	6	11,11,12	2.05	3 (27%)	15,15,17	1.65	1 (6%)
7	NAG	Q	1	1,7	14,14,15	0.76	1 (7%)	17,19,21	0.51	0
7	NAG	Q	2	7	14,14,15	0.30	0	17,19,21	0.63	0
7	BMA	Q	3	7	11,11,12	1.33	2 (18%)	15,15,17	1.14	0
4	NAG	R	1	4,1	14,14,15	0.62	0	17,19,21	0.75	1 (5%)
4	NAG	R	2	4	14,14,15	0.90	1 (7%)	17,19,21	0.73	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
3	NAG	I	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	I	2	3	-	1/6/23/26	0/1/1/1
3	BMA	I	3	3	-	1/2/19/22	0/1/1/1
3	MAN	I	4	3	-	0/2/19/22	0/1/1/1
4	NAG	J	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	J	2	4	-	4/6/23/26	0/1/1/1
4	NAG	K	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	K	2	4	-	2/6/23/26	0/1/1/1
5	NAG	L	1	1,5	-	1/6/23/26	0/1/1/1
5	NAG	L	2	5	-	2/6/23/26	0/1/1/1
5	BMA	L	3	5	-	0/2/19/22	0/1/1/1
5	MAN	L	4	5	-	2/2/19/22	1/1/1/1
3	NAG	M	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	M	2	3	-	2/6/23/26	0/1/1/1
3	BMA	M	3	3	-	2/2/19/22	0/1/1/1
3	MAN	M	4	3	-	2/2/19/22	0/1/1/1
4	NAG	N	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	N	2	4	-	2/6/23/26	0/1/1/1
4	NAG	O	1	4,1	-	3/6/23/26	0/1/1/1
4	NAG	O	2	4	-	2/6/23/26	0/1/1/1
6	NAG	P	1	1,6	-	4/6/23/26	0/1/1/1
6	NAG	P	2	6	-	1/6/23/26	0/1/1/1
6	BMA	P	3	6	-	1/2/19/22	0/1/1/1
6	MAN	P	4	6	-	2/2/19/22	0/1/1/1
6	MAN	P	5	6	-	1/2/19/22	0/1/1/1
7	NAG	Q	1	1,7	-	0/6/23/26	0/1/1/1
7	NAG	Q	2	7	-	1/6/23/26	0/1/1/1
7	BMA	Q	3	7	-	2/2/19/22	0/1/1/1
4	NAG	R	1	4,1	-	1/6/23/26	0/1/1/1
4	NAG	R	2	4	-	1/6/23/26	0/1/1/1

The worst 5 of 22 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	P	3	BMA	C1-C2	3.86	1.61	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	P	5	MAN	O5-C5	3.72	1.51	1.43
6	P	5	MAN	C2-C3	3.69	1.58	1.52
6	P	4	MAN	C1-C2	3.40	1.60	1.52
4	R	2	NAG	C1-C2	3.18	1.57	1.52

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	P	5	MAN	C1-O5-C5	4.91	118.85	112.19
6	P	3	BMA	C1-O5-C5	4.45	118.23	112.19
3	M	4	MAN	C1-O5-C5	4.03	117.66	112.19
5	L	4	MAN	C1-O5-C5	3.64	117.12	112.19
6	P	3	BMA	O5-C1-C2	3.08	115.53	110.77

There are no chirality outliers.

5 of 49 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	M	1	NAG	C3-C2-N2-C7
6	P	1	NAG	C1-C2-N2-C7
6	P	1	NAG	O5-C5-C6-O6
4	O	1	NAG	O5-C5-C6-O6
4	K	2	NAG	O5-C5-C6-O6

All (1) ring outliers are listed below:

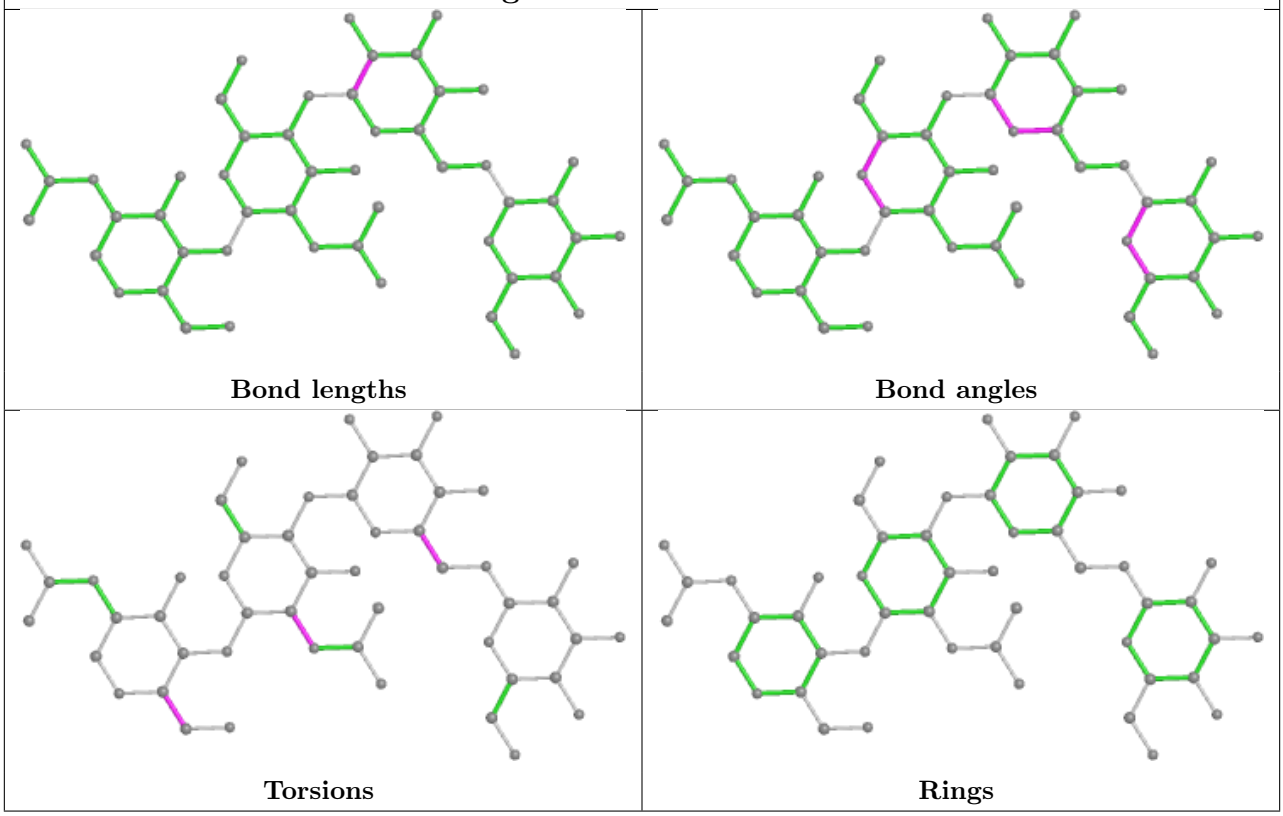
Mol	Chain	Res	Type	Atoms
5	L	4	MAN	C1-C2-C3-C4-C5-O5

8 monomers are involved in 14 short contacts:

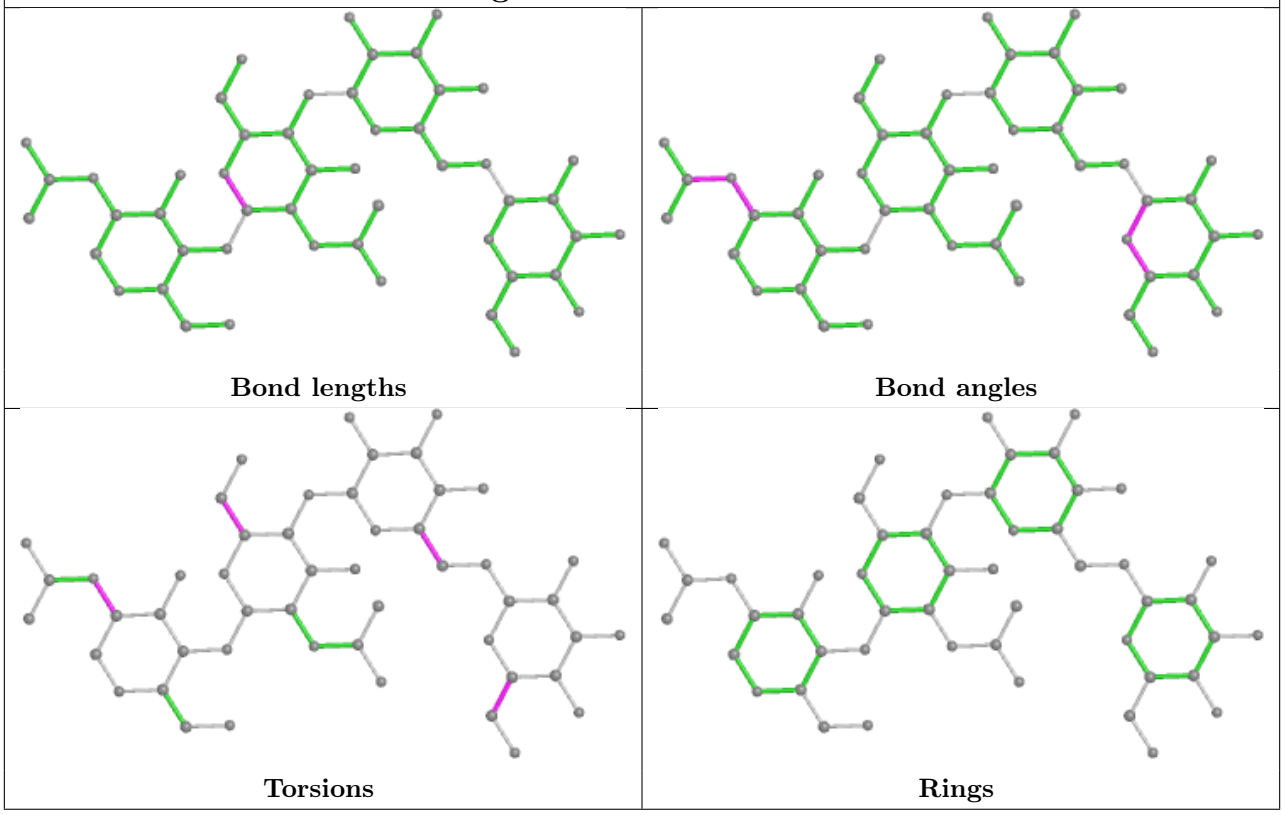
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	M	1	NAG	5	0
6	P	4	MAN	3	0
4	O	1	NAG	2	0
6	P	3	BMA	1	0
3	I	3	BMA	1	0
3	I	2	NAG	2	0
6	P	1	NAG	2	0
4	O	2	NAG	1	0

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

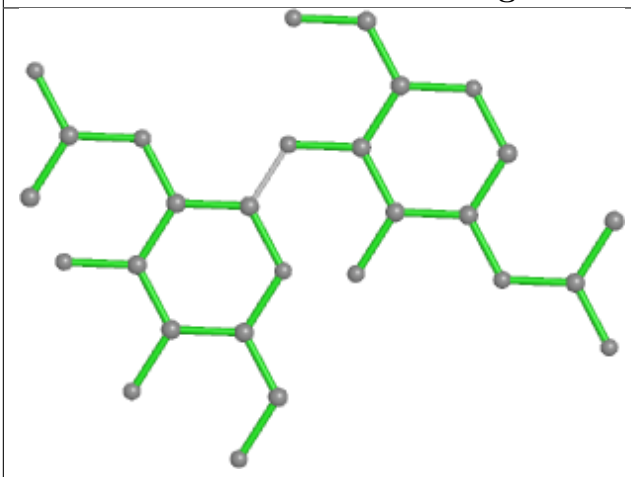
Oligosaccharide Chain I



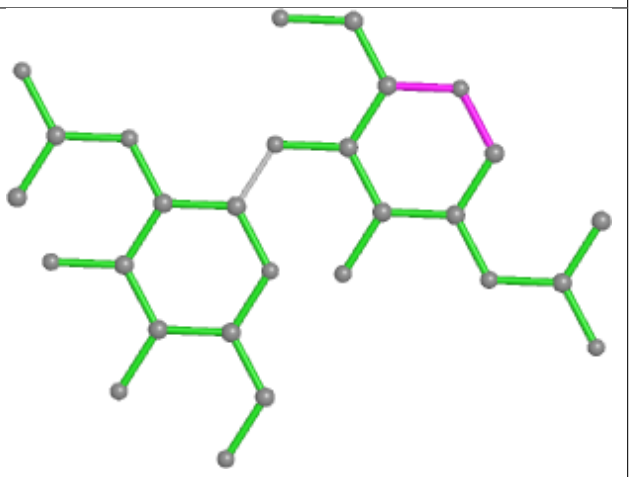
Oligosaccharide Chain M



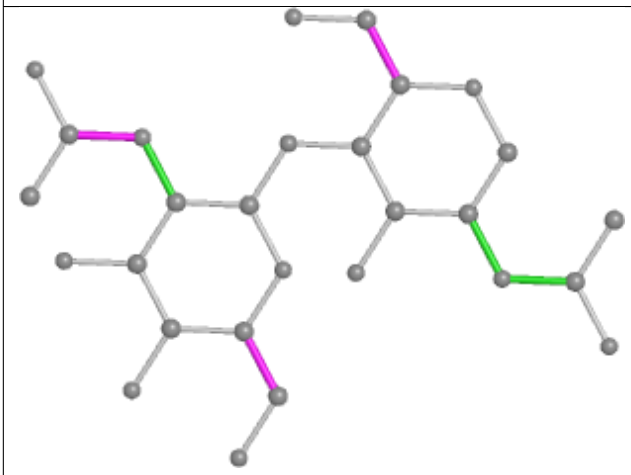
Oligosaccharide Chain J



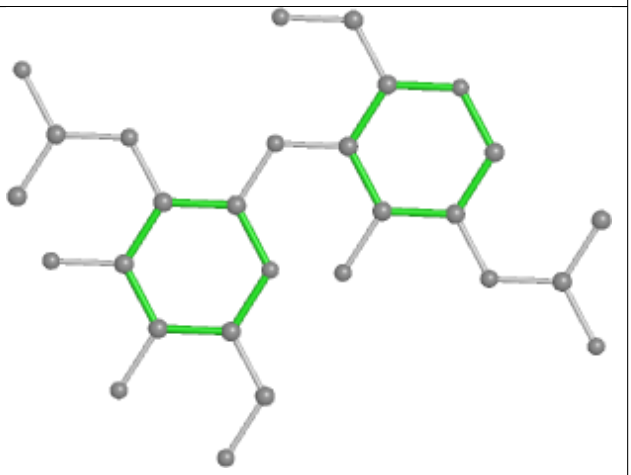
Bond lengths



Bond angles

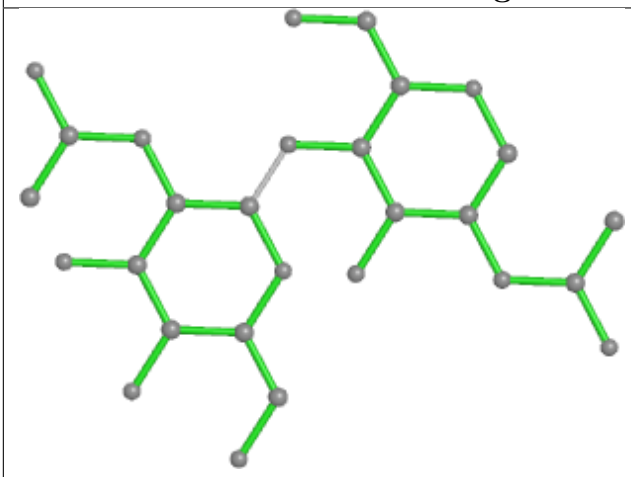


Torsions

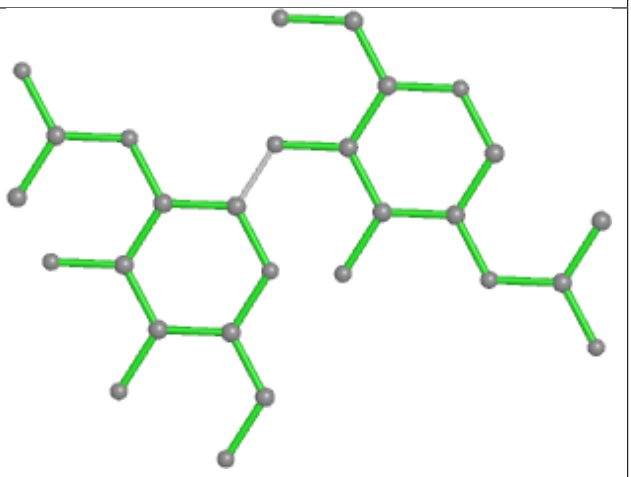


Rings

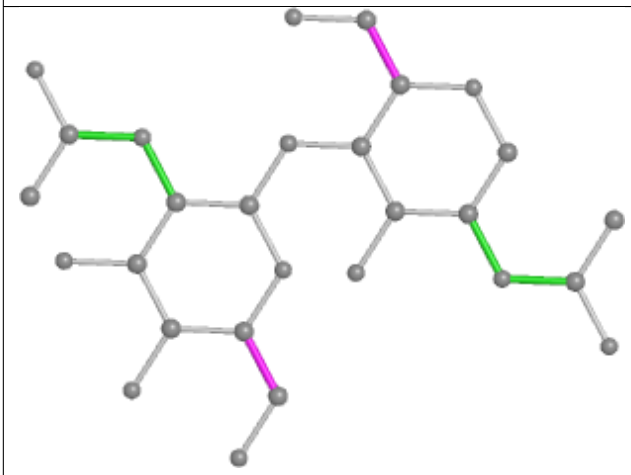
Oligosaccharide Chain K



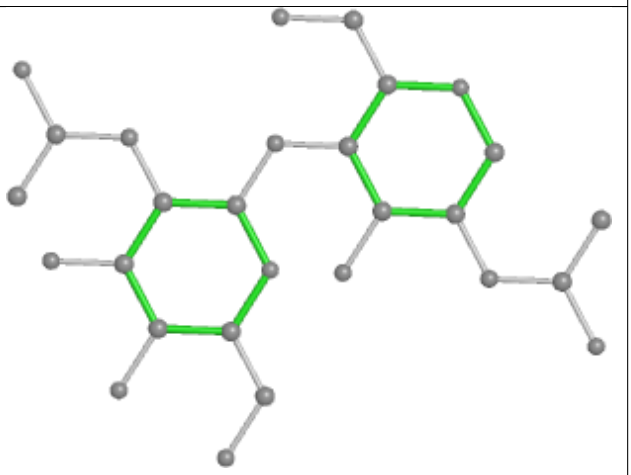
Bond lengths



Bond angles

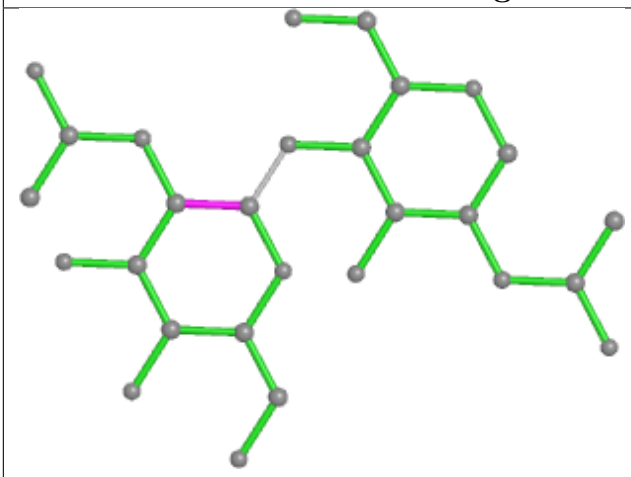


Torsions

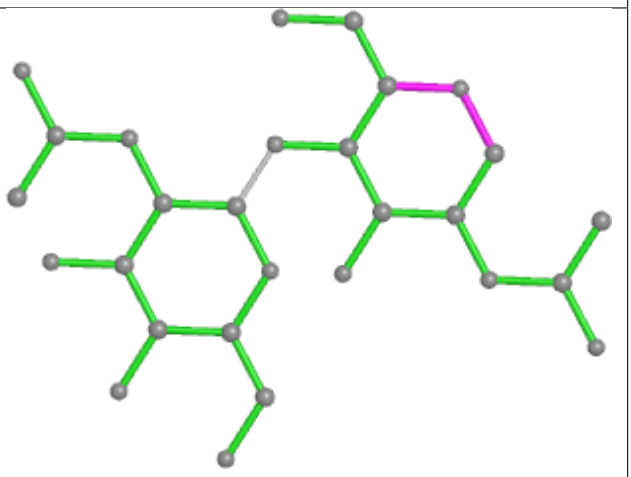


Rings

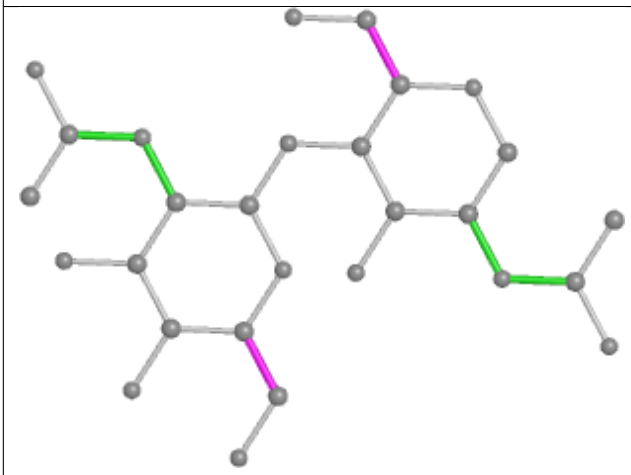
Oligosaccharide Chain N



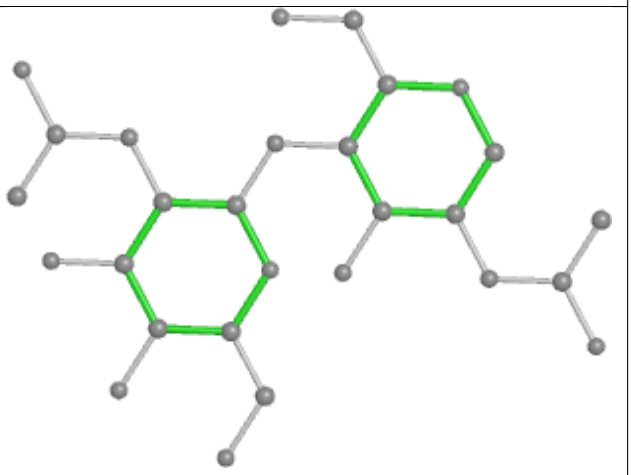
Bond lengths



Bond angles

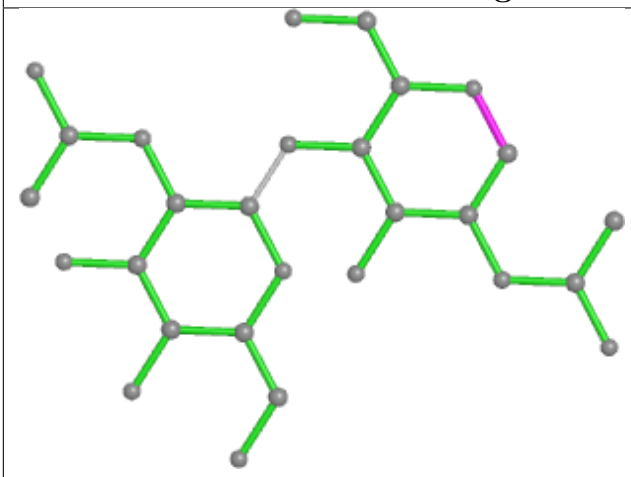


Torsions

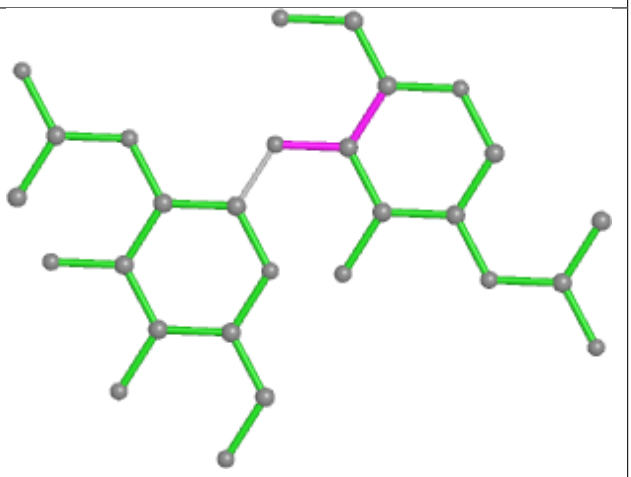


Rings

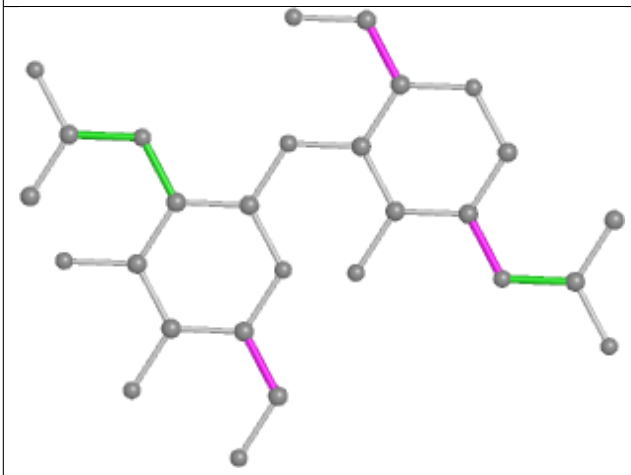
Oligosaccharide Chain O



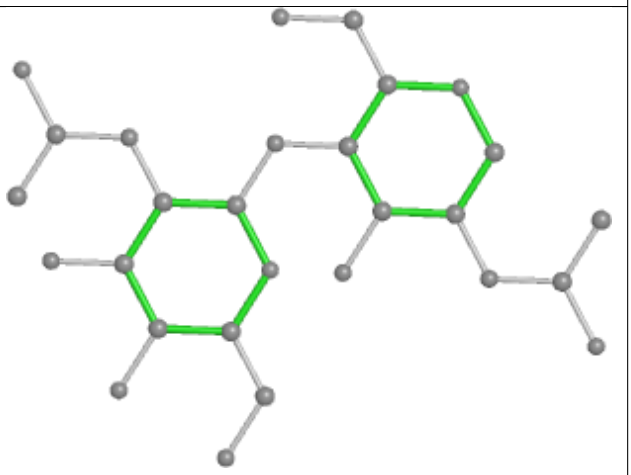
Bond lengths



Bond angles

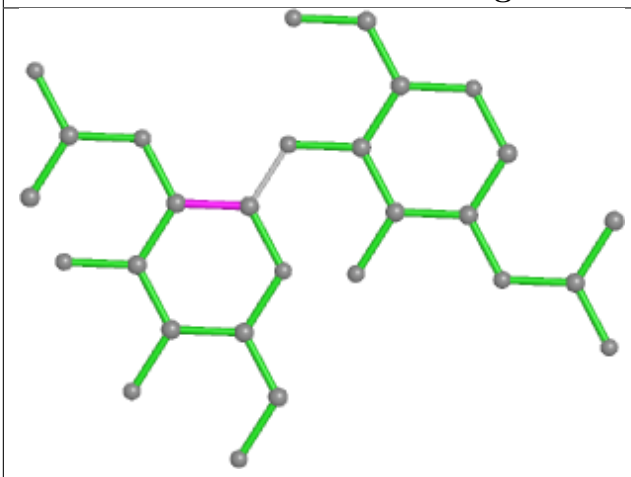


Torsions

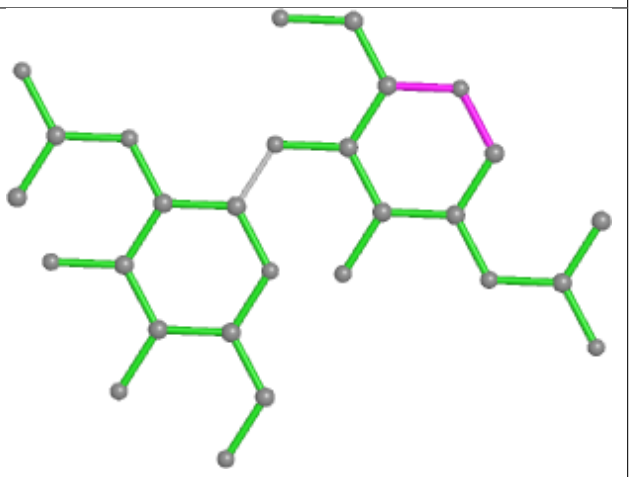


Rings

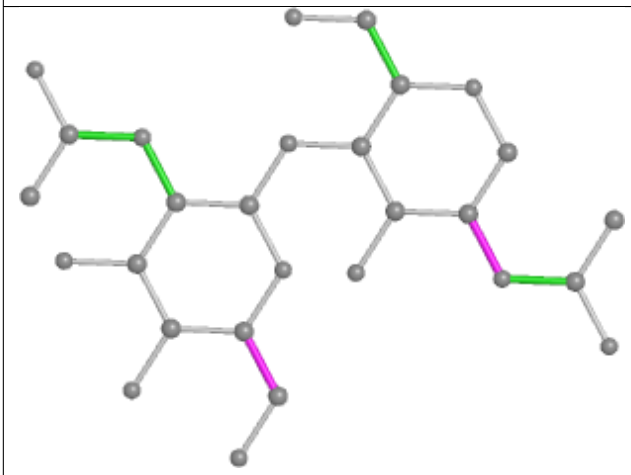
Oligosaccharide Chain R



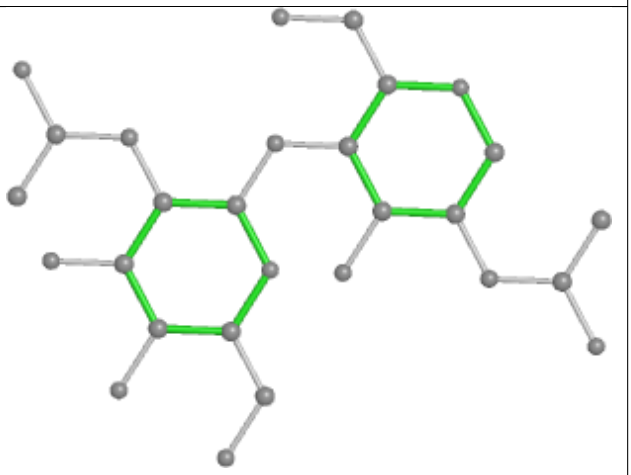
Bond lengths



Bond angles

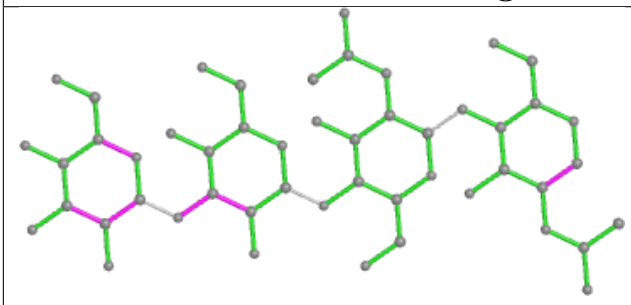


Torsions

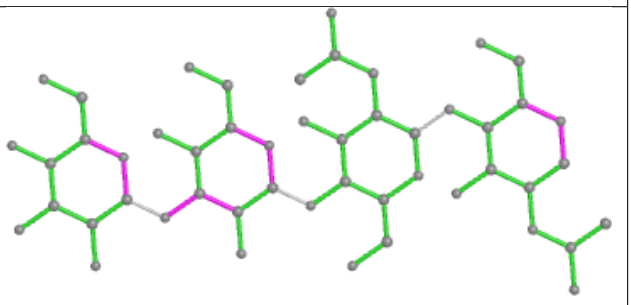


Rings

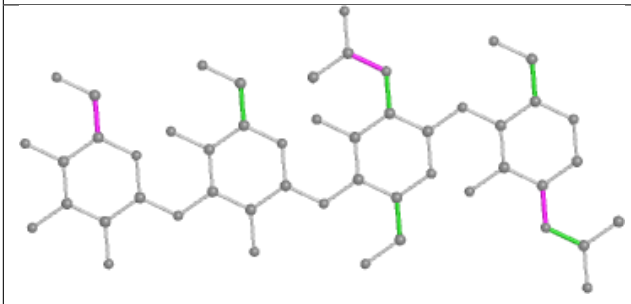
Oligosaccharide Chain L



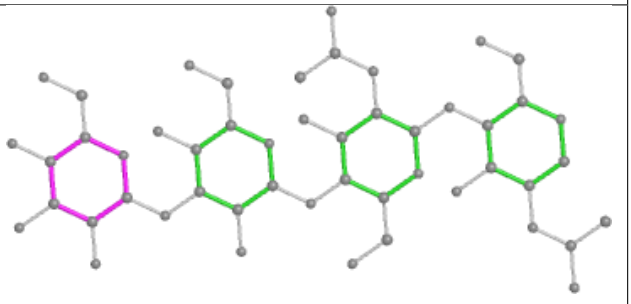
Bond lengths



Bond angles

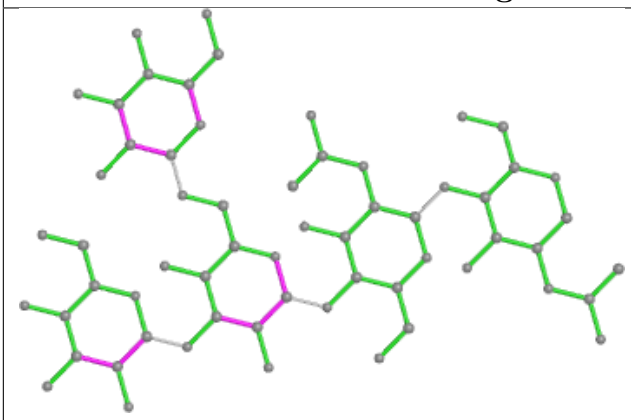


Torsions

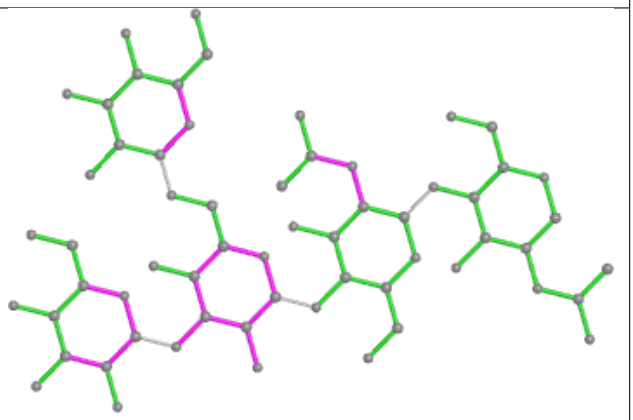


Rings

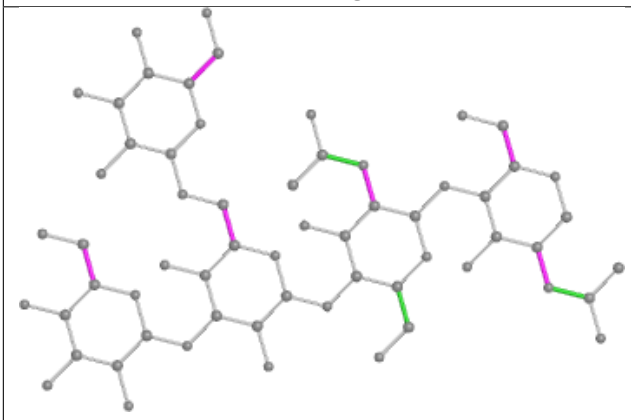
Oligosaccharide Chain P



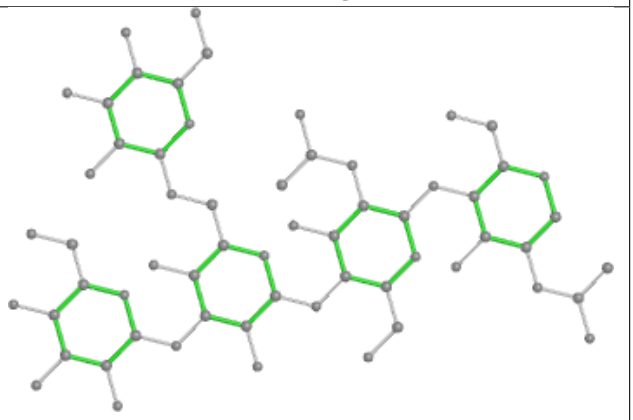
Bond lengths



Bond angles

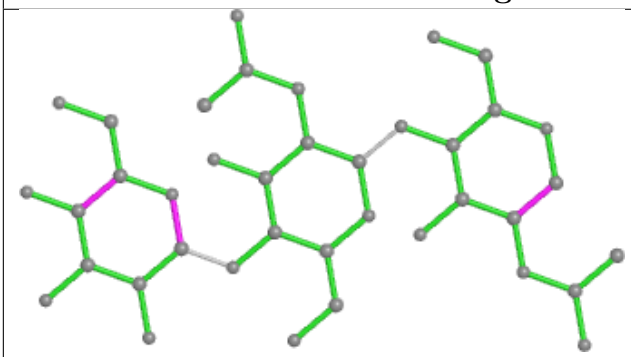


Torsions

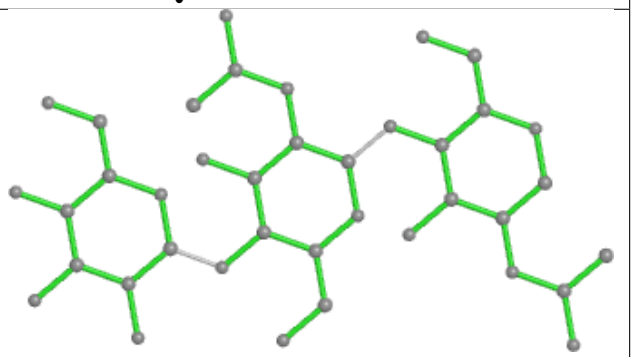


Rings

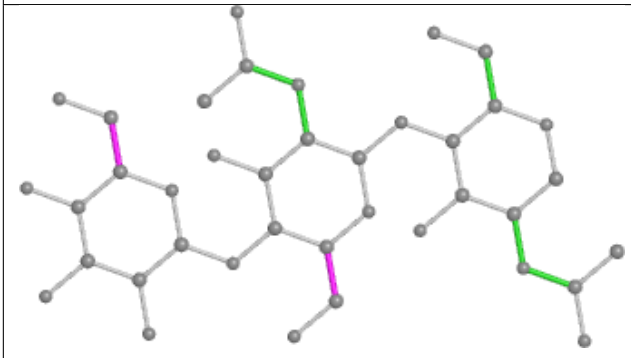
Oligosaccharide Chain Q



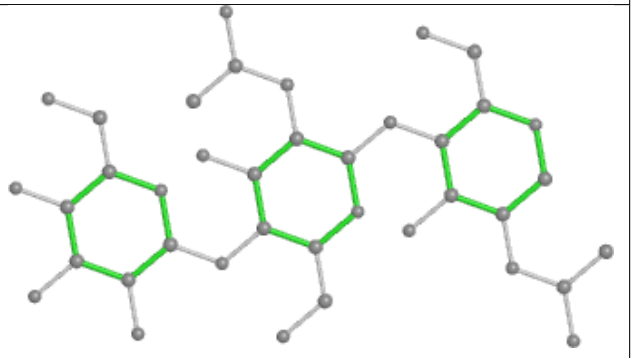
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry (i)

10 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	$\#\|Z\| > 2$
8	NAG	B	1103	1	14,14,15	0.20	0	17,19,21	0.51	0
8	NAG	D	1101	1	14,14,15	0.44	0	17,19,21	0.65	1 (5%)
8	NAG	A	1103	1	14,14,15	0.60	1 (7%)	17,19,21	0.50	0
8	NAG	B	1101	1	14,14,15	0.82	1 (7%)	17,19,21	0.62	0
8	NAG	A	1101	1	14,14,15	0.57	0	17,19,21	0.52	0
8	NAG	C	1102	1	14,14,15	0.47	0	17,19,21	0.47	0
8	NAG	C	1101	1	14,14,15	0.65	0	17,19,21	0.76	0
8	NAG	D	1102	1	14,14,15	0.60	1 (7%)	17,19,21	0.62	0
8	NAG	A	1102	1	14,14,15	0.64	0	17,19,21	0.60	0
8	NAG	B	1102	1	14,14,15	0.48	0	17,19,21	0.51	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
8	NAG	B	1103	1	-	2/6/23/26	0/1/1/1
8	NAG	D	1101	1	-	3/6/23/26	0/1/1/1
8	NAG	A	1103	1	-	1/6/23/26	0/1/1/1
8	NAG	B	1101	1	-	1/6/23/26	0/1/1/1
8	NAG	A	1101	1	-	4/6/23/26	0/1/1/1
8	NAG	C	1102	1	-	1/6/23/26	0/1/1/1
8	NAG	C	1101	1	-	2/6/23/26	0/1/1/1
8	NAG	D	1102	1	-	2/6/23/26	0/1/1/1
8	NAG	A	1102	1	-	2/6/23/26	0/1/1/1
8	NAG	B	1102	1	-	2/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	1101	NAG	O5-C1	2.35	1.47	1.43
8	A	1103	NAG	C1-C2	2.04	1.55	1.52
8	D	1102	NAG	C1-C2	2.03	1.55	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	D	1101	NAG	C1-O5-C5	2.22	115.20	112.19

There are no chirality outliers.

5 of 20 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	B	1102	NAG	C4-C5-C6-O6
8	A	1101	NAG	O5-C5-C6-O6
8	B	1102	NAG	O5-C5-C6-O6
8	A	1101	NAG	C4-C5-C6-O6
8	A	1101	NAG	C8-C7-N2-C2

There are no ring outliers.

7 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	1103	NAG	1	0
8	D	1101	NAG	1	0
8	A	1103	NAG	1	0
8	B	1101	NAG	1	0
8	A	1101	NAG	2	0
8	C	1101	NAG	1	0
8	D	1102	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	939/1007 (93%)	0.93	191 (20%)	1	1	136, 195, 266, 306	0
1	B	935/1007 (92%)	1.17	232 (24%)	0	0	156, 213, 258, 322	0
1	C	939/1007 (93%)	1.05	210 (22%)	0	1	109, 198, 254, 299	0
1	D	939/1007 (93%)	1.11	233 (24%)	0	0	123, 224, 290, 319	0
2	E	108/114 (94%)	2.23	45 (41%)	0	0	227, 296, 318, 335	0
2	F	108/114 (94%)	2.44	53 (49%)	0	0	277, 350, 369, 379	0
2	G	107/114 (93%)	1.72	46 (42%)	0	0	221, 264, 284, 289	0
2	H	105/114 (92%)	2.67	50 (47%)	0	0	295, 346, 370, 382	0
All	All	4180/4484 (93%)	1.19	1060 (25%)	0	0	109, 213, 315, 382	0

The worst 5 of 1060 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	76	PRO	14.0
1	B	243	GLN	13.0
2	E	115	PHE	13.0
2	H	70	SER	12.2
1	C	52	SER	11.7

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

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

6.3 Carbohydrates

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

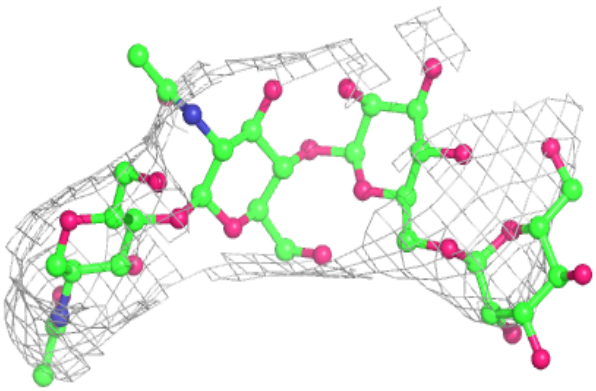
median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

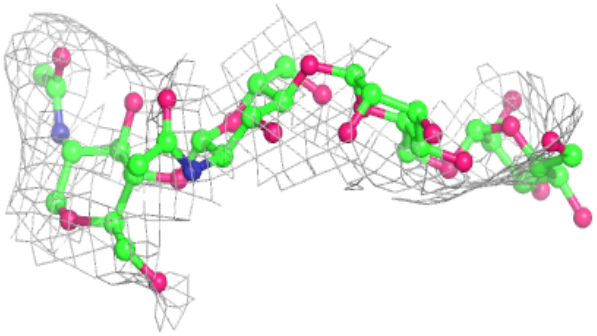
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	NAG	N	2	14/15	0.50	0.42	226,226,226,226	0
4	NAG	K	1	14/15	0.59	0.45	225,225,225,225	0
5	MAN	L	4	11/12	0.62	0.36	257,257,257,257	0
6	MAN	P	4	11/12	0.67	0.23	222,222,222,222	0
7	NAG	Q	1	14/15	0.72	0.29	199,199,199,199	0
3	NAG	I	1	14/15	0.73	0.28	199,199,199,199	0
3	MAN	I	4	11/12	0.74	0.57	246,246,246,246	0
4	NAG	R	2	14/15	0.75	0.28	253,253,253,253	0
4	NAG	N	1	14/15	0.77	0.25	233,233,233,233	0
6	MAN	P	5	11/12	0.77	0.33	229,229,229,229	0
3	BMA	I	3	11/12	0.77	0.27	230,230,230,230	0
3	MAN	M	4	11/12	0.78	0.32	251,251,251,251	0
5	NAG	L	2	14/15	0.78	0.31	191,191,191,191	0
6	NAG	P	1	14/15	0.79	0.37	224,224,224,224	0
4	NAG	O	2	14/15	0.79	0.51	228,228,228,228	0
4	NAG	J	1	14/15	0.81	0.49	211,211,211,211	0
7	BMA	Q	3	11/12	0.81	0.32	234,234,234,234	0
3	NAG	M	1	14/15	0.82	0.20	210,210,210,210	0
3	BMA	M	3	11/12	0.82	0.31	230,230,230,230	0
4	NAG	J	2	14/15	0.82	0.65	239,239,239,239	0
3	NAG	I	2	14/15	0.84	0.33	224,224,224,224	0
6	NAG	P	2	14/15	0.85	0.40	234,234,234,234	0
4	NAG	R	1	14/15	0.86	0.51	255,255,255,255	0
6	BMA	P	3	11/12	0.88	0.22	233,233,233,233	0
5	NAG	L	1	14/15	0.89	0.25	199,199,199,199	0
4	NAG	O	1	14/15	0.89	0.27	202,202,202,202	0
7	NAG	Q	2	14/15	0.90	0.49	221,221,221,221	0
4	NAG	K	2	14/15	0.90	0.32	246,246,246,246	0
5	BMA	L	3	11/12	0.91	0.17	234,234,234,234	0
3	NAG	M	2	14/15	0.93	0.22	212,212,212,212	0

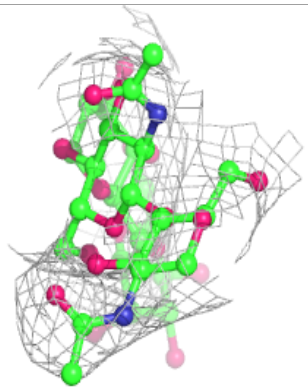
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain I:

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

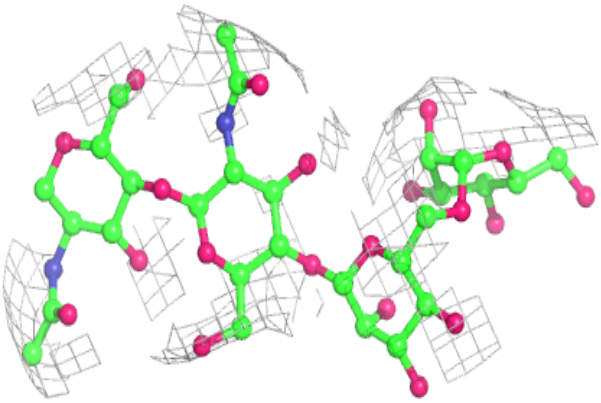


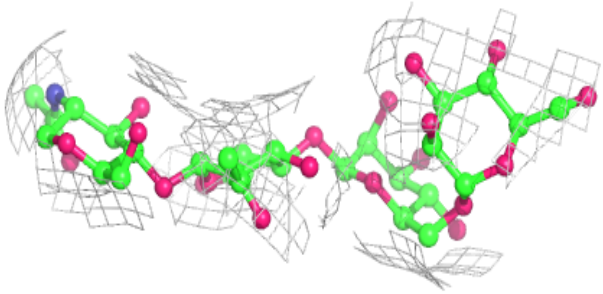


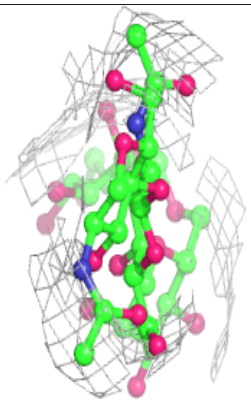


Electron density around Chain M:

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

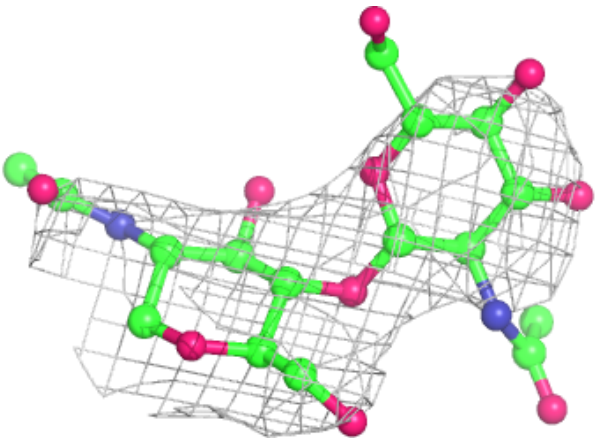


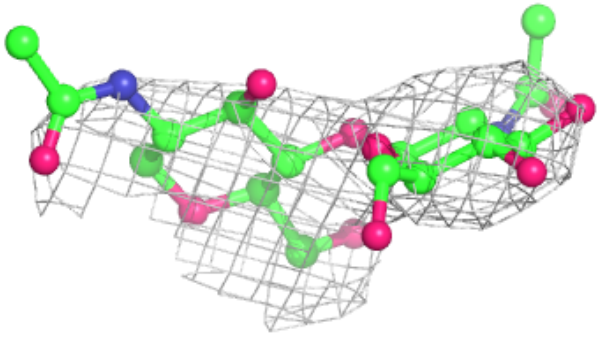


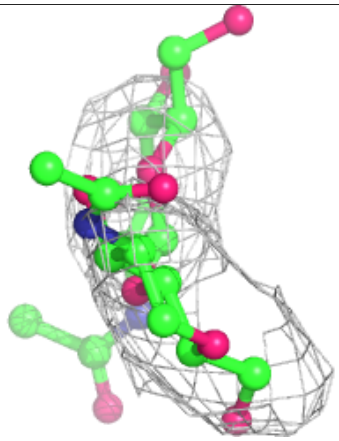


Electron density around Chain J:

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

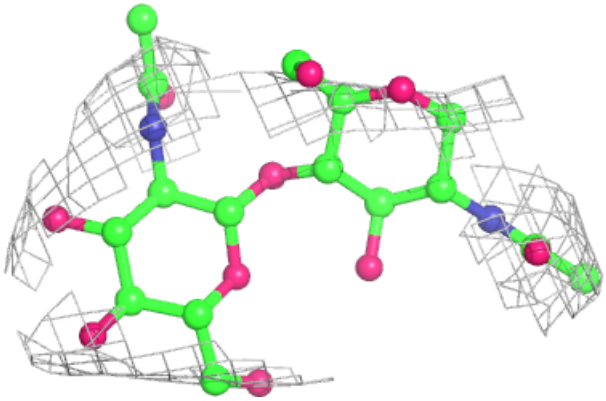


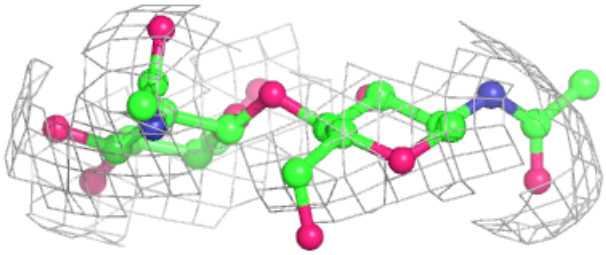


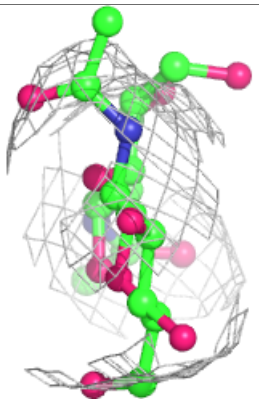


Electron density around Chain K:

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

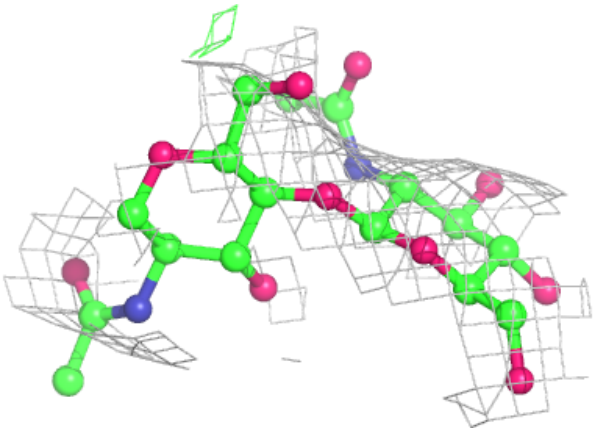


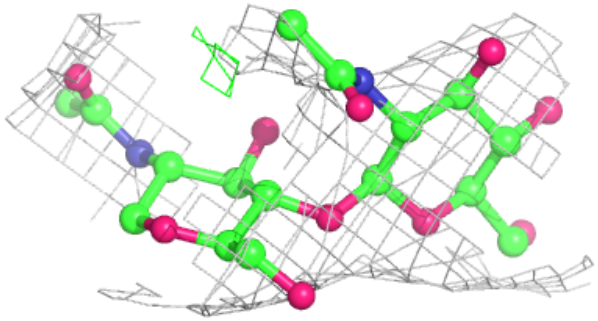


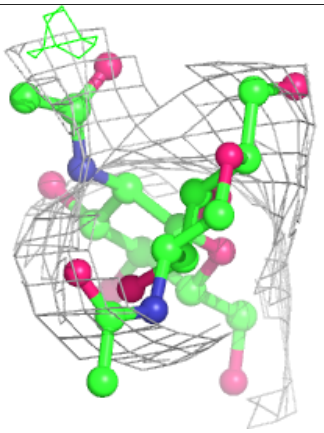


Electron density around Chain N:

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

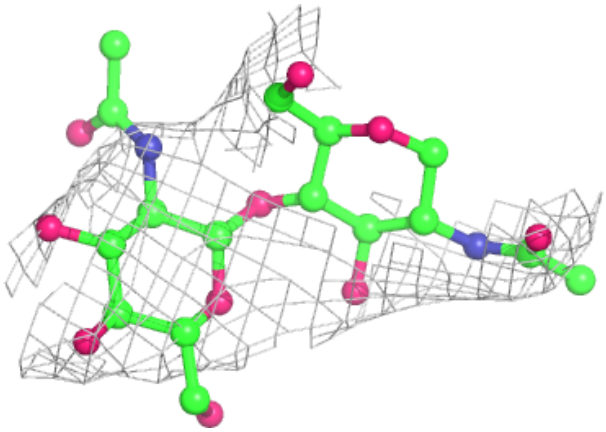


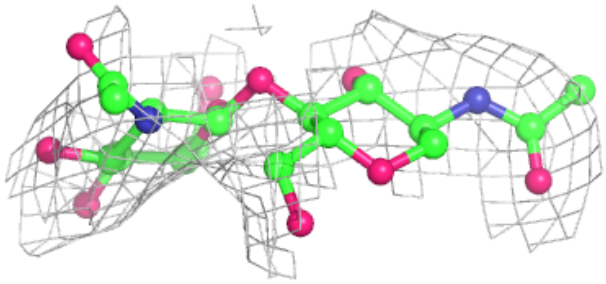


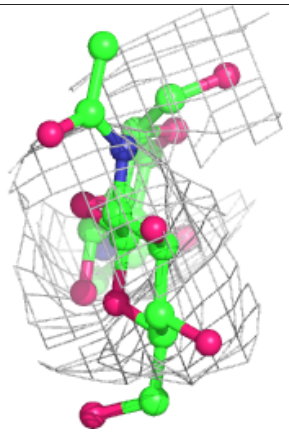


Electron density around Chain O:

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

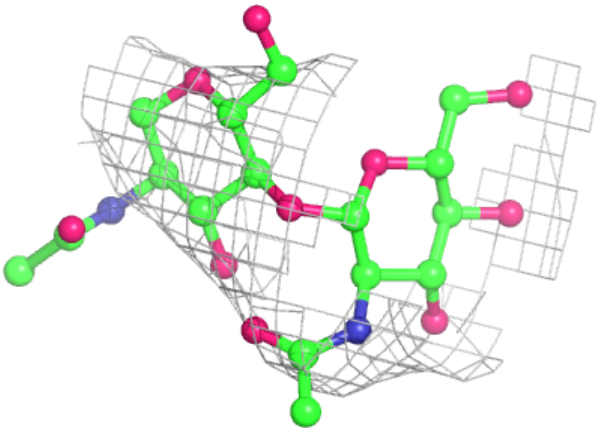


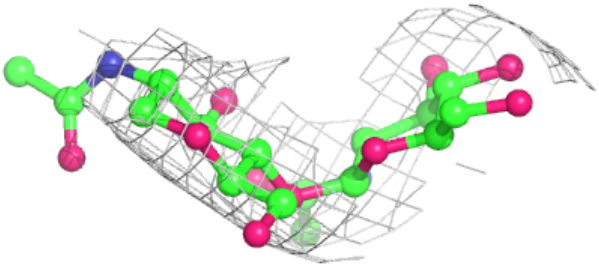


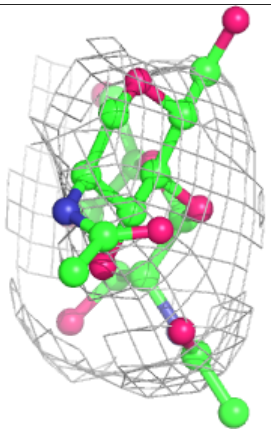


Electron density around Chain R:

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

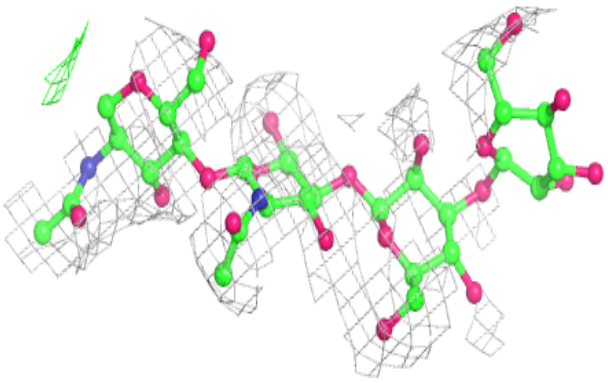


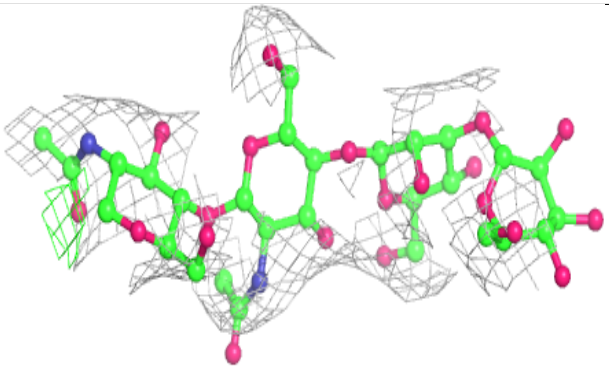


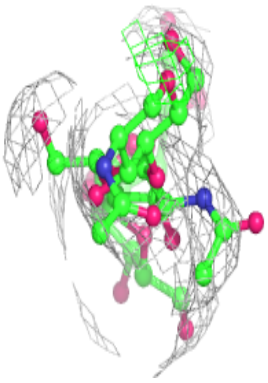


Electron density around Chain L:

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

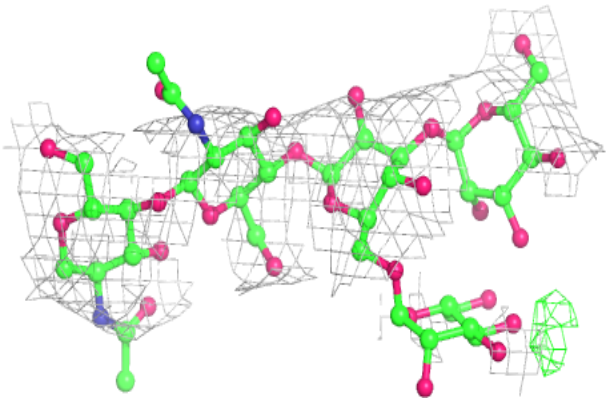


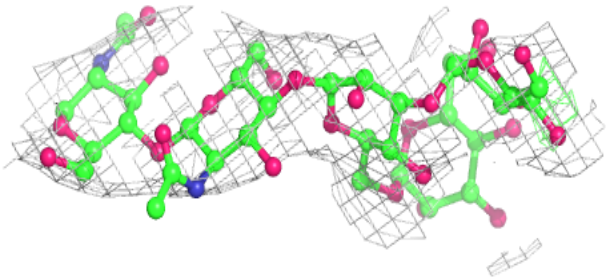


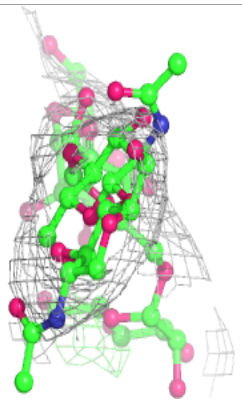


Electron density around Chain P:

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

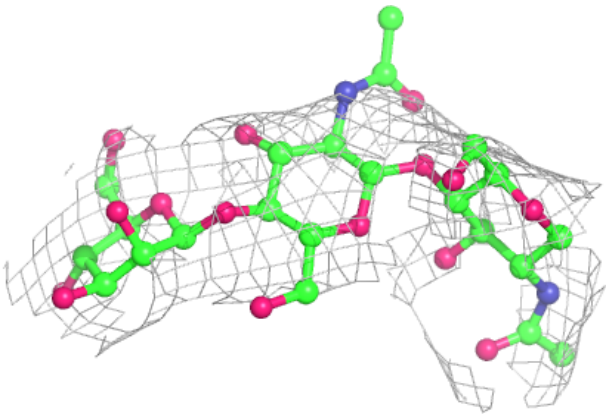


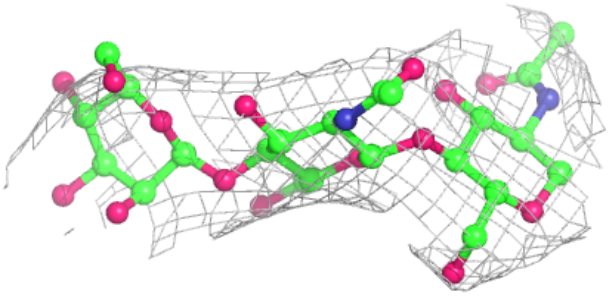


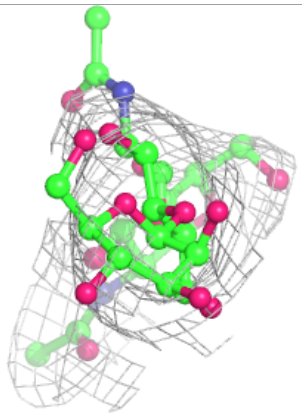


Electron density around Chain Q:

$2mF_o$-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
8	NAG	C	1101	14/15	0.47	0.54	175,175,175,175	0
8	NAG	A	1102	14/15	0.54	0.87	254,254,254,254	0
8	NAG	B	1102	14/15	0.61	0.43	235,235,235,235	0
8	NAG	A	1103	14/15	0.63	0.70	204,204,204,204	0
8	NAG	D	1101	14/15	0.70	0.76	246,246,246,246	0
8	NAG	B	1103	14/15	0.73	0.68	234,234,234,234	0
8	NAG	B	1101	14/15	0.78	0.29	264,264,264,264	0
8	NAG	C	1102	14/15	0.84	0.26	220,220,220,220	0
8	NAG	A	1101	14/15	0.91	0.28	209,209,209,209	0
8	NAG	D	1102	14/15	0.92	0.27	234,234,234,234	0

6.5 Other polymers

There are no such residues in this entry.