Full wwPDB X-ray Structure Validation Report (i)

Oct 8, 2023 – 07:51 AM EDT

PDB ID	:	6E3L
Title	:	Interferon gamma signalling complex with IFNGR1 and IFNGR2
Authors	:	Jude, K.M.; Mendoza, J.L.; Garcia, K.C.
Deposited on	:	2018-07-14
Resolution	:	3.80 Å(reported)

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

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

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

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

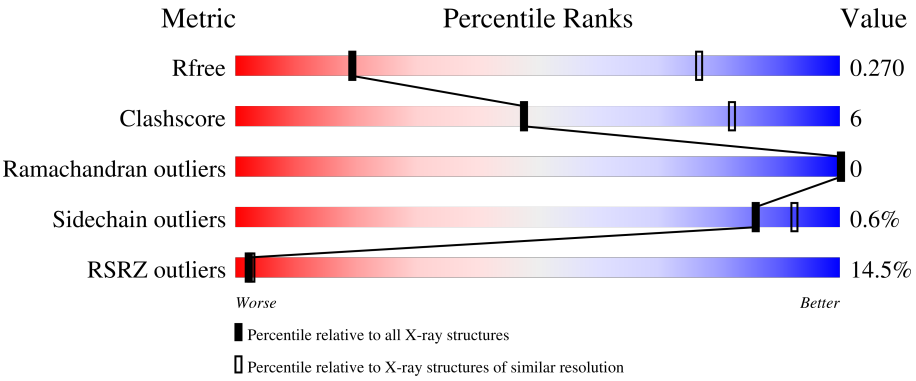
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.80 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	1212 (4.00-3.60)
Clashscore	141614	1288 (4.00-3.60)
Ramachandran outliers	138981	1243 (4.00-3.60)
Sidechain outliers	138945	1237 (4.00-3.60)
RSRZ outliers	127900	1121 (4.00-3.60)

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	148	3% 77% 7% 16%
1	B	148	5% 73% 12% 15%
2	C	242	% 74% 10% 16%
2	D	242	4% 70% 14% 17%
3	E	233	56% 70% 21% 9%

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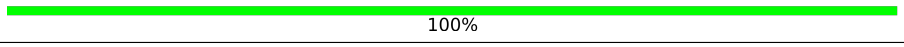
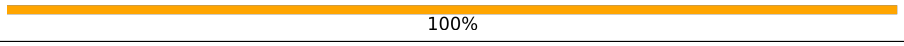
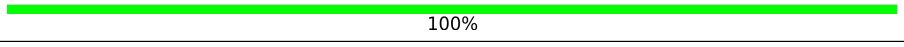
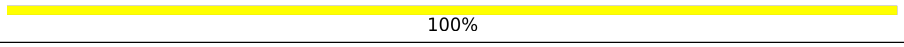
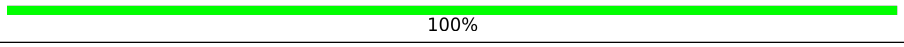
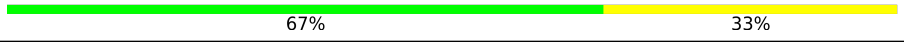
Mol	Chain	Length	Quality of chain
3	I	233	
4	F	2	
4	J	2	
4	M	2	
5	G	3	
5	H	3	
5	K	3	
6	L	6	

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
4	NAG	J	2	-	-	-	X
5	NAG	H	1	-	-	-	X
5	NAG	H	2	-	-	-	X
7	NAG	E	307	-	-	-	X
8	CYS	E	308	-	-	-	X
8	CYS	I	312	-	-	-	X

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 8976 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 Interferon gamma.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	125	Total	C	N	O	S	0	0	0
			1027	653	173	198	3			
1	B	126	Total	C	N	O	S	0	0	0
			1020	647	171	199	3			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP P01579
A	-2	PRO	-	expression tag	UNP P01579
A	-1	GLY	-	expression tag	UNP P01579
A	0	SER	-	expression tag	UNP P01579
A	134	ALA	-	expression tag	UNP P01579
A	135	ALA	-	expression tag	UNP P01579
A	136	ALA	-	expression tag	UNP P01579
A	137	HIS	-	expression tag	UNP P01579
A	138	HIS	-	expression tag	UNP P01579
A	139	HIS	-	expression tag	UNP P01579
A	140	HIS	-	expression tag	UNP P01579
A	141	HIS	-	expression tag	UNP P01579
A	142	HIS	-	expression tag	UNP P01579
A	143	HIS	-	expression tag	UNP P01579
A	144	HIS	-	expression tag	UNP P01579
B	-3	GLY	-	expression tag	UNP P01579
B	-2	PRO	-	expression tag	UNP P01579
B	-1	GLY	-	expression tag	UNP P01579
B	0	SER	-	expression tag	UNP P01579
B	134	ALA	-	expression tag	UNP P01579
B	135	ALA	-	expression tag	UNP P01579
B	136	ALA	-	expression tag	UNP P01579
B	137	HIS	-	expression tag	UNP P01579
B	138	HIS	-	expression tag	UNP P01579
B	139	HIS	-	expression tag	UNP P01579

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Chain	Residue	Modelled	Actual	Comment	Reference
B	140	HIS	-	expression tag	UNP P01579
B	141	HIS	-	expression tag	UNP P01579
B	142	HIS	-	expression tag	UNP P01579
B	143	HIS	-	expression tag	UNP P01579
B	144	HIS	-	expression tag	UNP P01579

- Molecule 2 is a protein called Interferon gamma receptor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	204	Total	C	N	O	S	0	0	0
			1618	1029	271	307	11			
2	D	202	Total	C	N	O	S	0	0	0
			1572	997	260	305	10			

There are 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	GLY	-	expression tag	UNP P15260
C	0	SER	-	expression tag	UNP P15260
C	149	ILE	THR	engineered mutation	UNP P15260
C	161	LYS	MET	engineered mutation	UNP P15260
C	167	LYS	GLN	engineered mutation	UNP P15260
C	174	ASN	LYS	engineered mutation	UNP P15260
C	182	ARG	GLN	engineered mutation	UNP P15260
C	205	ASN	HIS	engineered mutation	UNP P15260
C	230	ALA	-	expression tag	UNP P15260
C	231	ALA	-	expression tag	UNP P15260
C	232	ALA	-	expression tag	UNP P15260
C	233	HIS	-	expression tag	UNP P15260
C	234	HIS	-	expression tag	UNP P15260
C	235	HIS	-	expression tag	UNP P15260
C	236	HIS	-	expression tag	UNP P15260
C	237	HIS	-	expression tag	UNP P15260
C	238	HIS	-	expression tag	UNP P15260
C	239	HIS	-	expression tag	UNP P15260
C	240	HIS	-	expression tag	UNP P15260
D	-1	GLY	-	expression tag	UNP P15260
D	0	SER	-	expression tag	UNP P15260
D	149	ILE	THR	engineered mutation	UNP P15260
D	161	LYS	MET	engineered mutation	UNP P15260
D	167	LYS	GLN	engineered mutation	UNP P15260
D	174	ASN	LYS	engineered mutation	UNP P15260

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Chain	Residue	Modelled	Actual	Comment	Reference
D	182	ARG	GLN	engineered mutation	UNP P15260
D	205	ASN	HIS	engineered mutation	UNP P15260
D	230	ALA	-	expression tag	UNP P15260
D	231	ALA	-	expression tag	UNP P15260
D	232	ALA	-	expression tag	UNP P15260
D	233	HIS	-	expression tag	UNP P15260
D	234	HIS	-	expression tag	UNP P15260
D	235	HIS	-	expression tag	UNP P15260
D	236	HIS	-	expression tag	UNP P15260
D	237	HIS	-	expression tag	UNP P15260
D	238	HIS	-	expression tag	UNP P15260
D	239	HIS	-	expression tag	UNP P15260
D	240	HIS	-	expression tag	UNP P15260

- Molecule 3 is a protein called Interferon gamma receptor 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	213	Total	C	N	O	S	0	0	0
			1684	1082	281	312	9			
3	I	213	Total	C	N	O	S	0	0	0
			1698	1090	286	313	9			

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	26	GLY	-	expression tag	UNP P38484
E	27	SER	-	expression tag	UNP P38484
E	248	ALA	-	expression tag	UNP P38484
E	249	ALA	-	expression tag	UNP P38484
E	250	ALA	-	expression tag	UNP P38484
E	251	HIS	-	expression tag	UNP P38484
E	252	HIS	-	expression tag	UNP P38484
E	253	HIS	-	expression tag	UNP P38484
E	254	HIS	-	expression tag	UNP P38484
E	255	HIS	-	expression tag	UNP P38484
E	256	HIS	-	expression tag	UNP P38484
E	257	HIS	-	expression tag	UNP P38484
E	258	HIS	-	expression tag	UNP P38484
I	26	GLY	-	expression tag	UNP P38484
I	27	SER	-	expression tag	UNP P38484
I	248	ALA	-	expression tag	UNP P38484
I	249	ALA	-	expression tag	UNP P38484

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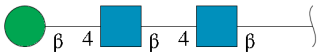
Chain	Residue	Modelled	Actual	Comment	Reference
I	250	ALA	-	expression tag	UNP P38484
I	251	HIS	-	expression tag	UNP P38484
I	252	HIS	-	expression tag	UNP P38484
I	253	HIS	-	expression tag	UNP P38484
I	254	HIS	-	expression tag	UNP P38484
I	255	HIS	-	expression tag	UNP P38484
I	256	HIS	-	expression tag	UNP P38484
I	257	HIS	-	expression tag	UNP P38484
I	258	HIS	-	expression tag	UNP P38484

- 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	F	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	J	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	M	2	Total	C	N	O	0	0	0
			28	16	2	10			

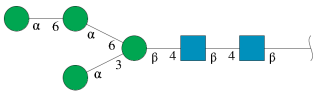
- Molecule 5 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	G	3	Total	C	N	O	0	0	0
			39	22	2	15			
5	H	3	Total	C	N	O	0	0	0
			39	22	2	15			
5	K	3	Total	C	N	O	0	0	0
			39	22	2	15			

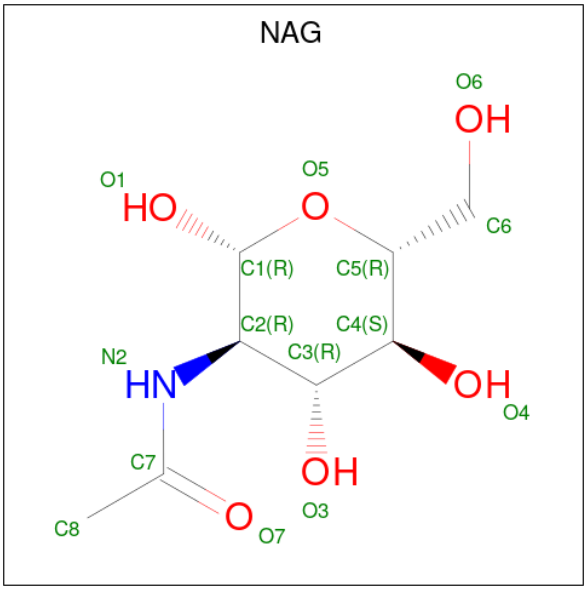
- Molecule 6 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-

beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



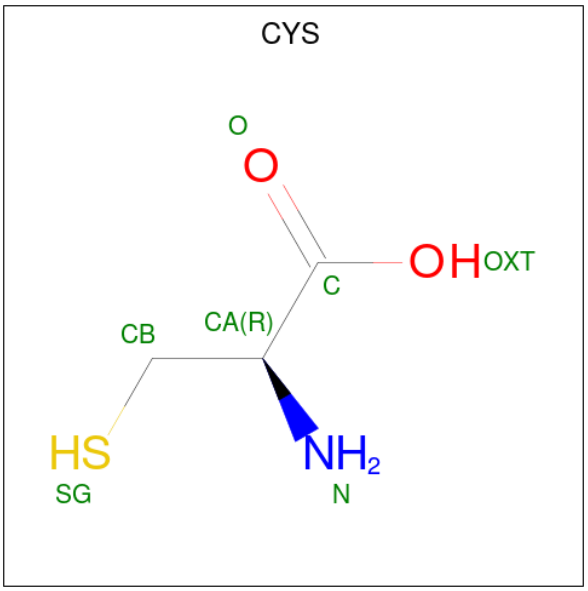
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	L	6	Total	C	N	O	0	0	0
			72	40	2	30			

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 8 is CYSTEINE (three-letter code: CYS) (formula: $C_3H_7NO_2S$).



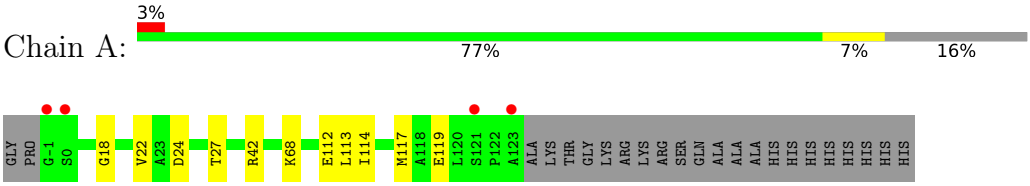
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	E	1	Total	C	N	O	S	0	0
			7	3	1	2	1		
8	I	1	Total	C	N	O	S	0	0
			7	3	1	2	1		

3 Residue-property plots

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: Interferon gamma

Chain A:

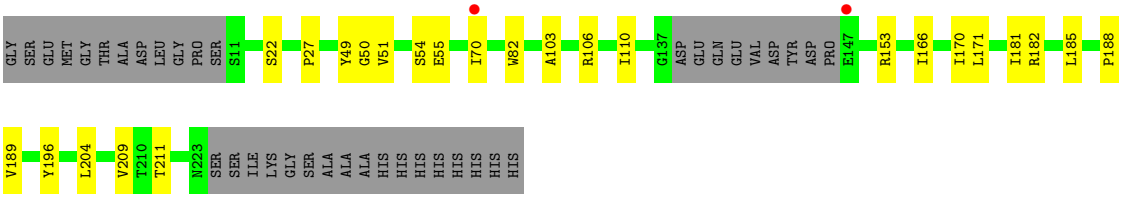


• Molecule 1: Interferon gamma

Chain B:

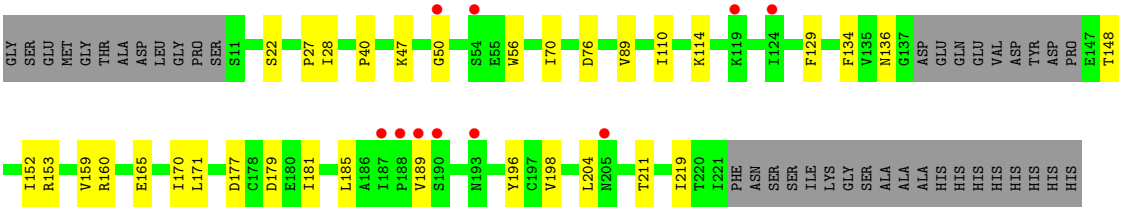
• Molecule 2: Interferon gamma receptor 1

Chain C:



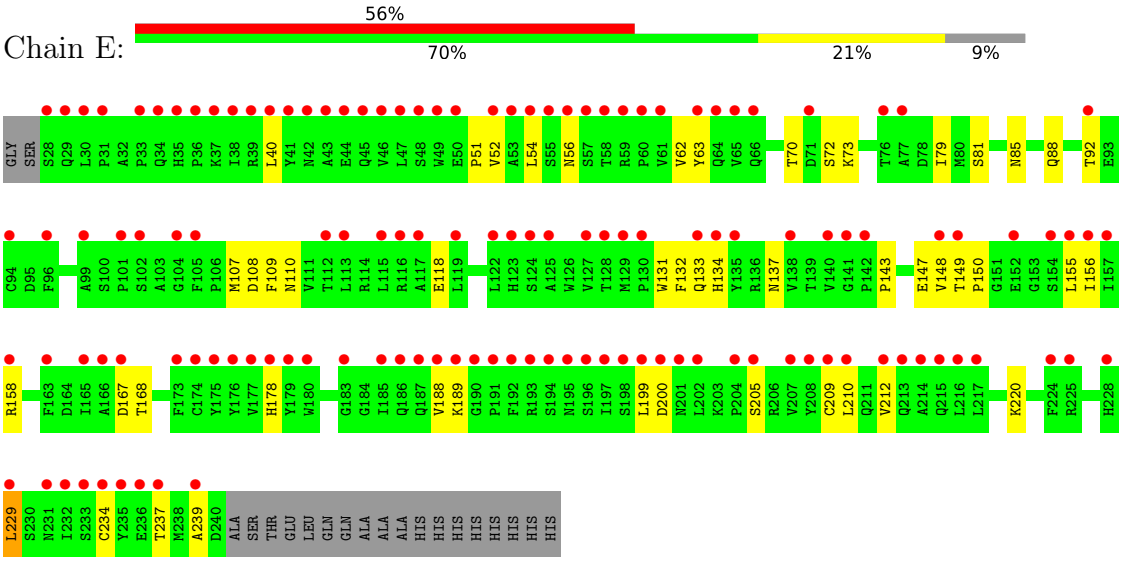
• Molecule 2: Interferon gamma receptor 1

Chain D:



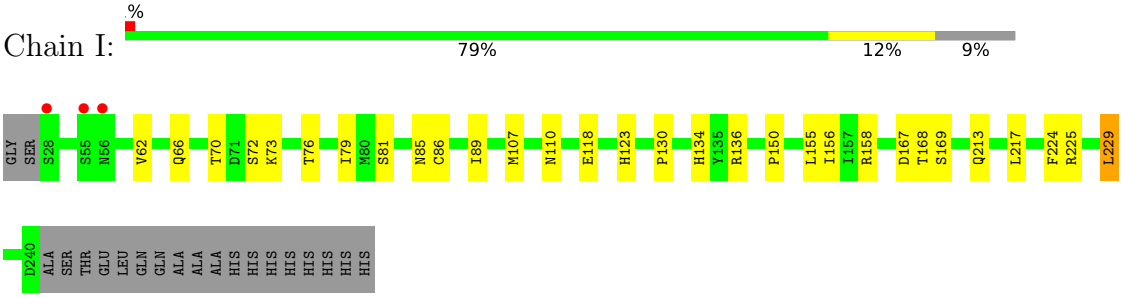
• Molecule 3: Interferon gamma receptor 2

Chain E:



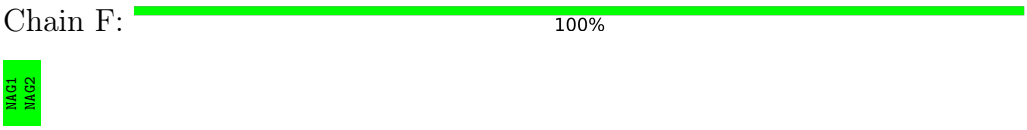
• Molecule 3: Interferon gamma receptor 2

Chain I:



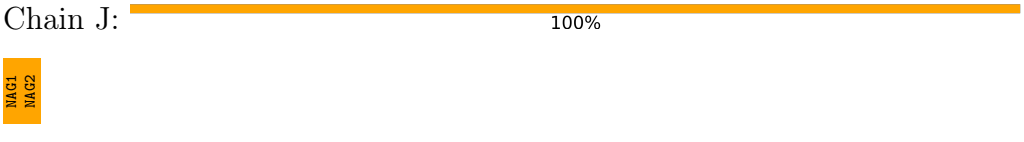
• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:



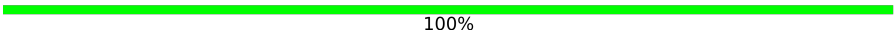
• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:



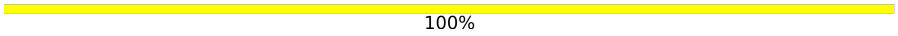
• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:



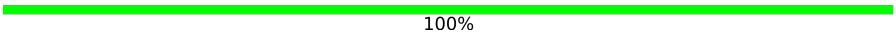
• Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:



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

Chain H:



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

Chain K:

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

Chain L:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	78.69Å 150.21Å 212.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.74 – 3.80 48.74 – 3.80	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.74-3.80) 88.6 (48.74-3.80)	Depositor EDS
R_{merge}	0.27	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.71 (at 3.77Å)	Xtriage
Refinement program	PHENIX 1.14_3211	Depositor
R, R_{free}	0.248 , 0.272 0.248 , 0.270	Depositor DCC
R_{free} test set	1693 reflections (6.61%)	wwPDB-VP
Wilson B-factor (Å^2)	133.4	Xtriage
Anisotropy	0.540	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 149.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	8976	wwPDB-VP
Average B, all atoms (Å^2)	216.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.48% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, BMA, MAN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.26	0/1045	0.39	0/1399
1	B	0.28	0/1038	0.42	0/1394
2	C	0.26	0/1654	0.48	0/2250
2	D	0.28	0/1607	0.50	0/2194
3	E	0.32	0/1735	0.58	0/2372
3	I	0.28	0/1749	0.51	0/2388
All	All	0.28	0/8828	0.50	0/11997

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	1027	0	1021	10	0
1	B	1020	0	993	16	0
2	C	1618	0	1573	17	0
2	D	1572	0	1490	19	0
3	E	1684	0	1605	42	0
3	I	1698	0	1634	23	0
4	F	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	J	28	0	25	1	0
4	M	28	0	25	0	0
5	G	39	0	34	1	0
5	H	39	0	34	0	0
5	K	39	0	34	2	0
6	L	72	0	61	2	0
7	A	14	0	13	0	0
7	B	14	0	13	0	0
7	D	14	0	13	0	0
7	E	28	0	26	2	0
8	E	7	0	3	0	0
8	I	7	0	3	0	0
All	All	8976	0	8625	107	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 6.

All (107) 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)
2:D:27:PRO:HG2	2:D:70:ILE:HG13	1.74	0.69
2:D:28:ILE:HD11	5:G:1:NAG:H82	1.77	0.66
2:C:170:ILE:HD11	2:C:185:LEU:HD13	1.81	0.64
2:D:171:LEU:HD21	3:E:168:THR:HB	1.80	0.63
3:I:79:ILE:HG13	3:I:85:ASN:HB2	1.81	0.63
3:E:131:TRP:HZ3	3:E:133:GLN:HG3	1.63	0.62
3:E:149:THR:HB	3:E:156:ILE:HD11	1.82	0.62
1:B:84:SER:HB3	3:E:133:GLN:HE22	1.66	0.60
3:E:54:LEU:HD23	7:E:307:NAG:HN2	1.67	0.60
1:B:79:VAL:HG11	3:E:108:ASP:HB3	1.83	0.58
2:D:110:ILE:HD12	2:D:204:LEU:HD11	1.84	0.58
3:E:62:VAL:HG21	3:E:88:GLN:OE1	2.03	0.58
3:E:189:LYS:NZ	3:E:200:ASP:OD1	2.36	0.58
3:E:62:VAL:HG23	3:E:118:GLU:HG3	1.86	0.58
2:C:110:ILE:HB	2:C:211:THR:HG22	1.86	0.57
1:A:22:VAL:HG12	2:C:49:TYR:HE2	1.68	0.57
1:B:78:ASN:HA	1:B:82:PHE:HD2	1.70	0.57
3:E:205:SER:OG	3:E:239:ALA:HA	2.04	0.57
2:D:22:SER:HB2	2:D:27:PRO:HB3	1.88	0.56
2:C:27:PRO:HG2	2:C:70:ILE:HG13	1.88	0.56
2:C:51:VAL:O	2:C:54:SER:OG	2.25	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:188:PRO:HB2	3:I:156:ILE:HD12	1.89	0.54
3:E:54:LEU:CD2	7:E:307:NAG:HN2	2.20	0.54
1:A:119:GLU:HB3	1:B:42:ARG:HH12	1.72	0.54
2:C:204:LEU:HD22	2:C:209:VAL:HB	1.89	0.53
2:D:110:ILE:HB	2:D:211:THR:HG22	1.90	0.53
1:B:9:GLU:HA	1:B:12:LYS:HB2	1.90	0.53
3:I:150:PRO:HA	3:I:155:LEU:HD23	1.90	0.53
1:B:72:THR:HG23	3:E:109:PHE:HE2	1.75	0.52
1:A:42:ARG:HH12	1:B:119:GLU:HB3	1.73	0.52
1:A:113:LEU:HD21	1:B:73:ILE:HD13	1.93	0.51
2:C:55:GLU:N	2:C:55:GLU:OE1	2.44	0.51
2:C:171:LEU:HD21	3:I:168:THR:HB	1.92	0.51
1:B:68:LYS:NZ	3:E:81:SER:O	2.43	0.50
1:A:18:GLY:O	2:C:82:TRP:NE1	2.38	0.50
3:I:70:THR:OG1	3:I:110:ASN:HB3	2.12	0.50
2:D:170:ILE:HD11	2:D:185:LEU:HD13	1.94	0.50
3:I:79:ILE:CG1	3:I:85:ASN:HB2	2.42	0.50
3:I:86:CYS:HA	3:I:89:ILE:HD13	1.93	0.50
2:D:153:ARG:NH2	3:E:167:ASP:HA	2.27	0.49
3:E:209:CYS:HA	3:E:234:CYS:HA	1.94	0.49
3:E:40:LEU:HD12	3:E:137:ASN:HB2	1.94	0.49
1:B:27:THR:CG2	2:D:50:GLY:HA2	2.43	0.49
2:C:153:ARG:NH2	3:I:167:ASP:HA	2.28	0.49
3:E:143:PRO:HG2	3:E:212:VAL:HG12	1.94	0.48
3:E:148:VAL:HG21	3:E:210:LEU:HD21	1.95	0.47
1:B:83:ASN:ND2	3:E:220:LYS:HG2	2.29	0.47
3:E:150:PRO:HA	3:E:155:LEU:HD23	1.95	0.47
1:B:16:ASN:HB3	1:B:19:HIS:HD2	1.80	0.47
3:I:118:GLU:HA	3:I:123:HIS:HA	1.97	0.47
3:E:149:THR:O	3:E:156:ILE:HG12	2.14	0.47
3:E:178:HIS:HD2	3:E:229:LEU:HD21	1.80	0.47
3:E:107:MET:HG2	3:E:134:HIS:CD2	2.50	0.47
3:E:79:ILE:HG13	3:E:85:ASN:HB2	1.97	0.46
2:D:159:VAL:HG22	2:D:198:VAL:HG22	1.97	0.46
1:B:83:ASN:HA	3:E:220:LYS:HD3	1.98	0.46
3:I:213:GLN:HB2	3:I:229:LEU:HG	1.97	0.46
3:E:56:ASN:N	3:E:56:ASN:OD1	2.36	0.46
3:I:217:LEU:HD23	3:I:224:PHE:HB3	1.96	0.46
3:E:178:HIS:CD2	3:E:229:LEU:HD21	2.51	0.46
3:I:62:VAL:HG11	5:K:2:NAG:C8	2.46	0.46
3:E:72:SER:OG	3:E:73:LYS:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:178:HIS:ND1	3:E:188:VAL:HG22	2.31	0.45
3:I:66:GLN:HG2	3:I:76:THR:HA	1.97	0.45
1:A:68:LYS:HE3	3:I:81:SER:O	2.17	0.45
3:E:79:ILE:HD12	3:E:79:ILE:H	1.81	0.45
3:I:62:VAL:HG11	5:K:2:NAG:H82	1.98	0.45
1:A:117:MET:HE3	1:A:117:MET:HB3	1.85	0.45
2:D:189:VAL:HG12	2:D:196:TYR:CZ	2.52	0.45
1:A:27:THR:CG2	2:C:50:GLY:HA2	2.47	0.45
2:D:76:ASP:OD1	2:D:148:THR:OG1	2.34	0.45
3:I:118:GLU:HB3	3:I:123:HIS:HB3	1.98	0.44
1:B:72:THR:HG23	3:E:109:PHE:CE2	2.52	0.44
3:E:147:GLU:HB2	3:E:158:ARG:HG3	1.99	0.44
2:D:40:PRO:HB3	2:D:89:VAL:HG12	2.00	0.44
2:D:114:LYS:HB2	2:D:129:PHE:HB2	2.00	0.43
3:E:79:ILE:HD11	3:E:85:ASN:HB2	2.00	0.43
1:A:114:ILE:H	1:A:114:ILE:HD12	1.84	0.43
3:E:51:PRO:HB3	3:E:92:THR:HG21	1.99	0.43
3:I:72:SER:OG	3:I:73:LYS:N	2.51	0.43
1:A:112:GLU:OE1	1:B:30:LEU:HG	2.19	0.43
2:C:166:ILE:HG12	3:I:158:ARG:NH2	2.34	0.43
2:D:160:ARG:HA	2:D:165:GLU:HA	2.00	0.42
2:C:181:ILE:HG13	2:C:182:ARG:HG2	2.01	0.42
3:E:205:SER:N	3:E:237:THR:OG1	2.52	0.42
3:I:107:MET:HG2	3:I:134:HIS:CD2	2.54	0.42
4:J:1:NAG:O3	4:J:2:NAG:O5	2.36	0.42
2:D:47:LYS:HB2	2:D:56:TRP:CE3	2.54	0.42
1:B:114:ILE:H	1:B:114:ILE:HD12	1.84	0.42
3:E:88:GLN:NE2	3:E:118:GLU:OE1	2.50	0.42
3:I:217:LEU:HD23	3:I:217:LEU:HA	1.85	0.41
2:C:22:SER:HA	2:C:27:PRO:HA	2.01	0.41
2:C:189:VAL:HG12	2:C:196:TYR:CZ	2.55	0.41
3:I:167:ASP:OD1	3:I:169:SER:OG	2.28	0.41
3:E:40:LEU:HD11	3:E:132:PHE:CD1	2.55	0.41
2:C:103:ALA:HB3	2:C:106:ARG:HB3	2.02	0.41
3:E:70:THR:OG1	3:E:110:ASN:HB3	2.20	0.41
6:L:3:BMA:H61	6:L:4:MAN:H2	1.75	0.41
3:E:62:VAL:HG22	3:E:118:GLU:O	2.21	0.41
3:E:199:LEU:HD23	3:E:199:LEU:HA	1.98	0.41
3:I:136:ARG:O	3:I:225:ARG:HD3	2.21	0.41
3:E:79:ILE:CD1	3:E:85:ASN:HB2	2.51	0.41
2:D:219:ILE:HD12	2:D:219:ILE:HA	1.99	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:52:VAL:HG23	3:E:63:TYR:HE2	1.86	0.40
2:D:134:PHE:CE2	2:D:152:ILE:HD11	2.56	0.40
2:D:179:ASP:OD1	2:D:181:ILE:HG22	2.21	0.40
3:I:130:PRO:HB2	6:L:1:NAG:H61	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	123/148 (83%)	121 (98%)	2 (2%)	0	100	100
1	B	124/148 (84%)	123 (99%)	1 (1%)	0	100	100
2	C	200/242 (83%)	195 (98%)	5 (2%)	0	100	100
2	D	198/242 (82%)	193 (98%)	5 (2%)	0	100	100
3	E	211/233 (91%)	203 (96%)	8 (4%)	0	100	100
3	I	211/233 (91%)	204 (97%)	7 (3%)	0	100	100
All	All	1067/1246 (86%)	1039 (97%)	28 (3%)	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	115/132 (87%)	114 (99%)	1 (1%)	78 88
1	B	112/132 (85%)	111 (99%)	1 (1%)	78 88
2	C	184/218 (84%)	184 (100%)	0	100 100
2	D	176/218 (81%)	174 (99%)	2 (1%)	73 85
3	E	185/203 (91%)	184 (100%)	1 (0%)	88 94
3	I	188/203 (93%)	187 (100%)	1 (0%)	88 94
All	All	960/1106 (87%)	954 (99%)	6 (1%)	86 92

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	ASP
1	B	24	ASP
2	D	136	ASN
2	D	177	ASP
3	E	229	LEU
3	I	229	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	19	HIS

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)

21 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	$\#\|Z\| > 2$
4	NAG	F	1	4,2	14,14,15	0.46	0	17,19,21	0.69	0
4	NAG	F	2	4	14,14,15	0.44	0	17,19,21	0.58	0
5	NAG	G	1	5,2	14,14,15	0.58	0	17,19,21	0.63	0
5	NAG	G	2	5	14,14,15	0.62	0	17,19,21	0.93	1 (5%)
5	BMA	G	3	5	11,11,12	1.11	1 (9%)	15,15,17	0.98	1 (6%)
5	NAG	H	1	3,5	14,14,15	0.61	0	17,19,21	0.67	0
5	NAG	H	2	5	14,14,15	0.27	0	17,19,21	0.45	0
5	BMA	H	3	5	11,11,12	0.54	0	15,15,17	0.67	0
4	NAG	J	1	4,3	14,14,15	0.45	0	17,19,21	0.80	1 (5%)
4	NAG	J	2	4	14,14,15	0.45	0	17,19,21	0.71	1 (5%)
5	NAG	K	1	3,5	14,14,15	0.34	0	17,19,21	0.60	0
5	NAG	K	2	5	14,14,15	0.28	0	17,19,21	0.50	0
5	BMA	K	3	5	11,11,12	0.58	0	15,15,17	0.67	0
6	NAG	L	1	3,6	14,14,15	1.11	1 (7%)	17,19,21	1.64	3 (17%)
6	NAG	L	2	6	14,14,15	0.28	0	17,19,21	0.58	0
6	BMA	L	3	6	11,11,12	0.68	0	15,15,17	1.12	1 (6%)
6	MAN	L	4	6	11,11,12	0.64	0	15,15,17	1.01	2 (13%)
6	MAN	L	5	6	11,11,12	1.20	1 (9%)	15,15,17	1.02	1 (6%)
6	MAN	L	6	6	11,11,12	0.78	1 (9%)	15,15,17	1.29	2 (13%)
4	NAG	M	1	4,3	14,14,15	0.37	0	17,19,21	0.61	0
4	NAG	M	2	4	14,14,15	0.25	0	17,19,21	0.49	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
4	NAG	F	1	4,2	-	0/6/23/26	0/1/1/1
4	NAG	F	2	4	-	0/6/23/26	0/1/1/1
5	NAG	G	1	5,2	-	0/6/23/26	0/1/1/1
5	NAG	G	2	5	-	1/6/23/26	0/1/1/1
5	BMA	G	3	5	-	2/2/19/22	0/1/1/1
5	NAG	H	1	3,5	-	2/6/23/26	0/1/1/1
5	NAG	H	2	5	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	BMA	H	3	5	-	0/2/19/22	0/1/1/1
4	NAG	J	1	4,3	-	2/6/23/26	0/1/1/1
4	NAG	J	2	4	-	0/6/23/26	0/1/1/1
5	NAG	K	1	3,5	-	2/6/23/26	0/1/1/1
5	NAG	K	2	5	-	2/6/23/26	0/1/1/1
5	BMA	K	3	5	-	0/2/19/22	0/1/1/1
6	NAG	L	1	3,6	-	1/6/23/26	0/1/1/1
6	NAG	L	2	6	-	0/6/23/26	0/1/1/1
6	BMA	L	3	6	-	0/2/19/22	0/1/1/1
6	MAN	L	4	6	-	2/2/19/22	0/1/1/1
6	MAN	L	5	6	-	0/2/19/22	0/1/1/1
6	MAN	L	6	6	-	2/2/19/22	0/1/1/1
4	NAG	M	1	4,3	-	0/6/23/26	0/1/1/1
4	NAG	M	2	4	-	2/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	L	1	NAG	O5-C1	-3.64	1.37	1.43
5	G	3	BMA	C1-C2	2.99	1.59	1.52
6	L	5	MAN	O5-C5	2.52	1.48	1.43
6	L	6	MAN	C1-C2	2.26	1.57	1.52

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	L	1	NAG	C1-O5-C5	-3.92	106.88	112.19
6	L	6	MAN	C1-O5-C5	3.85	117.41	112.19
6	L	1	NAG	C2-N2-C7	3.63	128.07	122.90
5	G	2	NAG	C1-O5-C5	2.80	115.98	112.19
6	L	4	MAN	C1-O5-C5	2.51	115.59	112.19
6	L	6	MAN	O2-C2-C3	-2.28	105.58	110.14
5	G	3	BMA	C1-O5-C5	2.27	115.27	112.19
4	J	1	NAG	C1-O5-C5	2.24	115.22	112.19
4	J	2	NAG	C1-O5-C5	2.14	115.09	112.19
6	L	4	MAN	O2-C2-C3	-2.13	105.87	110.14
6	L	3	BMA	O2-C2-C3	-2.12	105.89	110.14
6	L	1	NAG	O4-C4-C5	-2.12	104.03	109.30
6	L	5	MAN	O2-C2-C3	-2.05	106.04	110.14

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	L	1	NAG	C3-C2-N2-C7
5	K	1	NAG	O5-C5-C6-O6
5	H	1	NAG	O5-C5-C6-O6
5	K	1	NAG	C4-C5-C6-O6
5	H	1	NAG	C4-C5-C6-O6
5	G	3	BMA	O5-C5-C6-O6
4	J	1	NAG	C4-C5-C6-O6
6	L	4	MAN	O5-C5-C6-O6
4	J	1	NAG	O5-C5-C6-O6
6	L	6	MAN	O5-C5-C6-O6
5	G	3	BMA	C4-C5-C6-O6
6	L	4	MAN	C4-C5-C6-O6
4	M	2	NAG	C4-C5-C6-O6
5	G	2	NAG	C1-C2-N2-C7
4	M	2	NAG	O5-C5-C6-O6
5	H	2	NAG	C4-C5-C6-O6
5	K	2	NAG	C4-C5-C6-O6
5	H	2	NAG	O5-C5-C6-O6
5	K	2	NAG	O5-C5-C6-O6
6	L	6	MAN	C4-C5-C6-O6

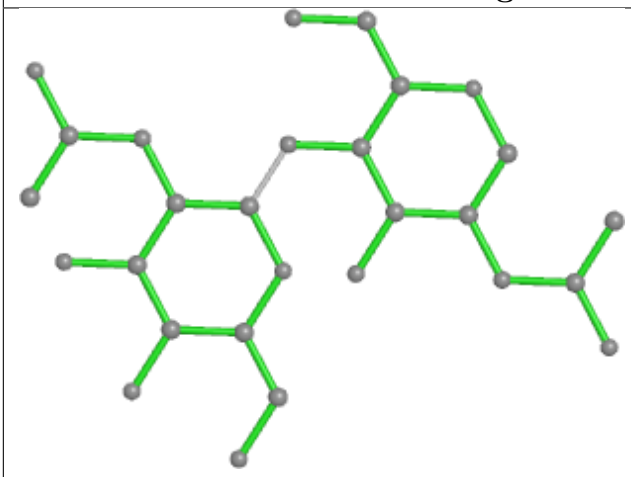
There are no ring outliers.

7 monomers are involved in 6 short contacts:

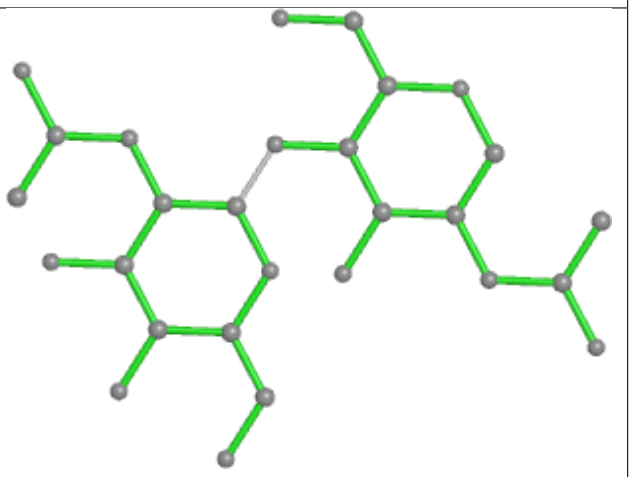
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	L	4	MAN	1	0
5	K	2	NAG	2	0
6	L	3	BMA	1	0
6	L	1	NAG	1	0
4	J	2	NAG	1	0
4	J	1	NAG	1	0
5	G	1	NAG	1	0

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

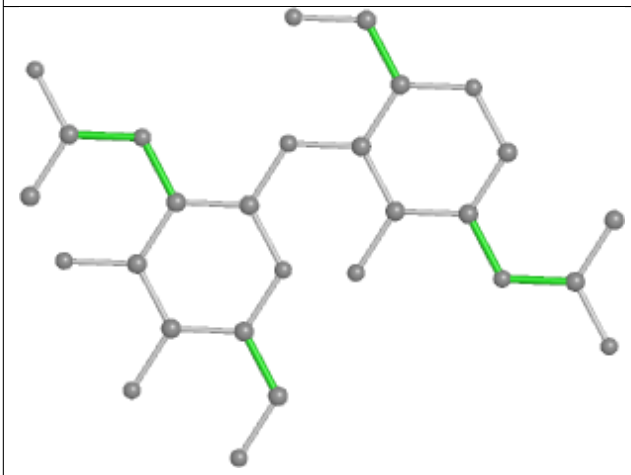
Oligosaccharide Chain F



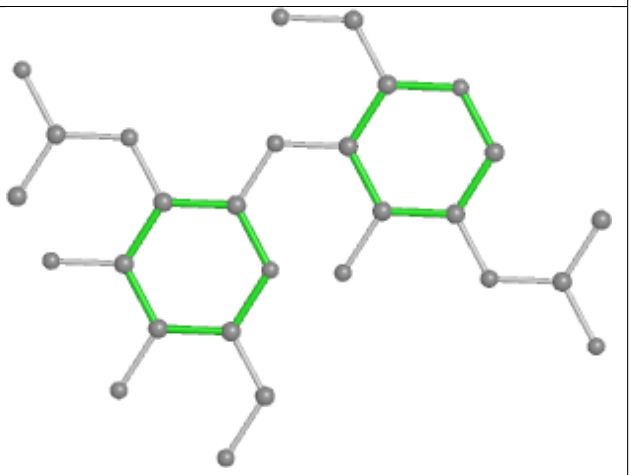
Bond lengths



Bond angles

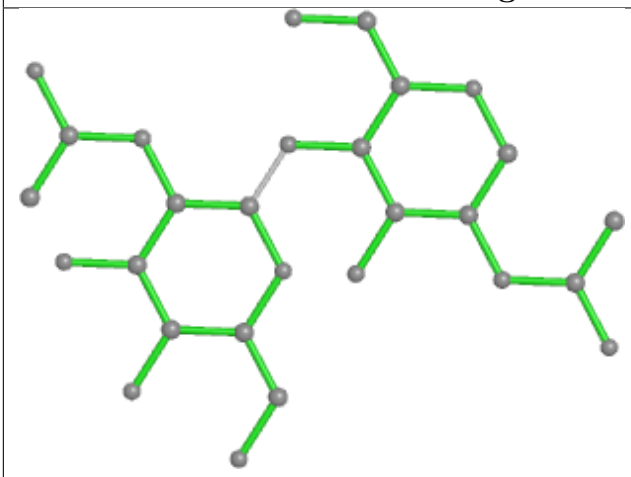


Torsions

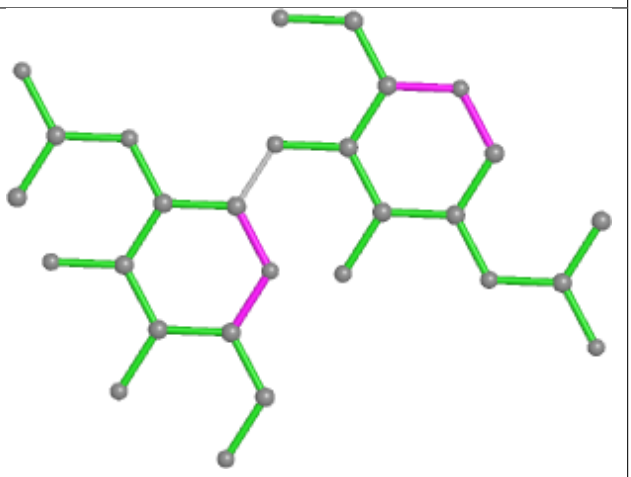


Rings

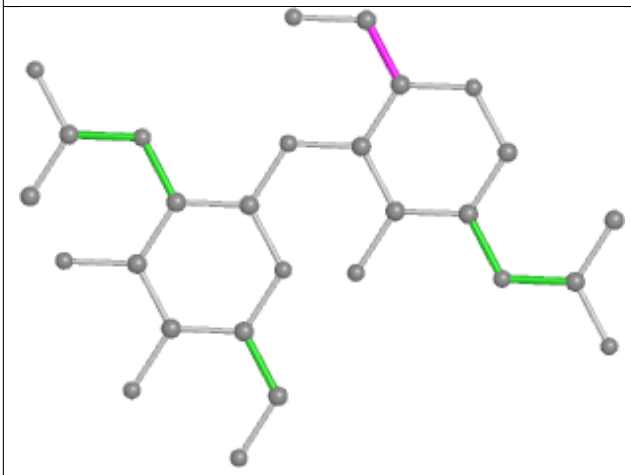
Oligosaccharide Chain J



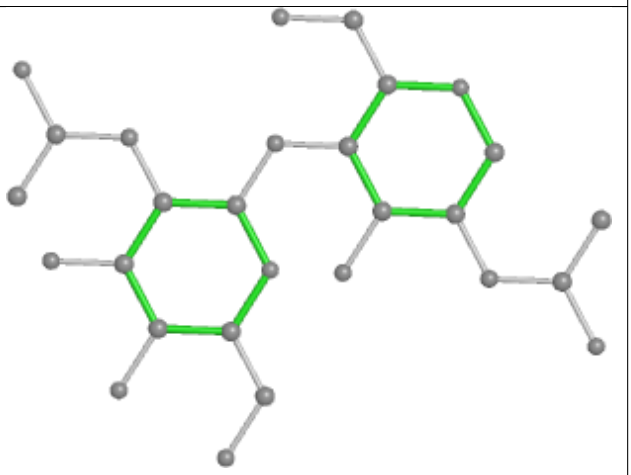
Bond lengths



Bond angles

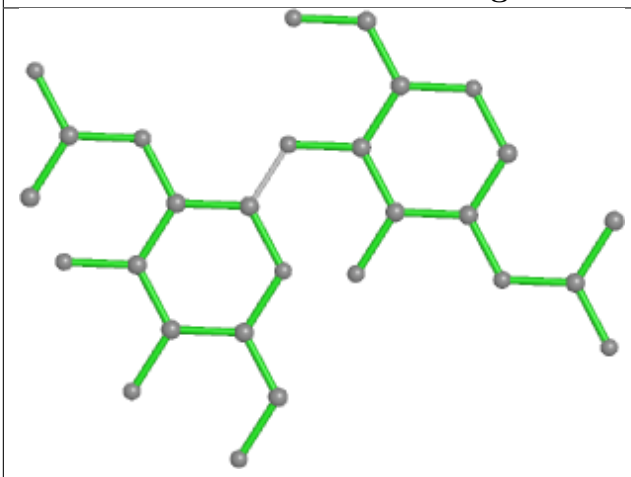


Torsions

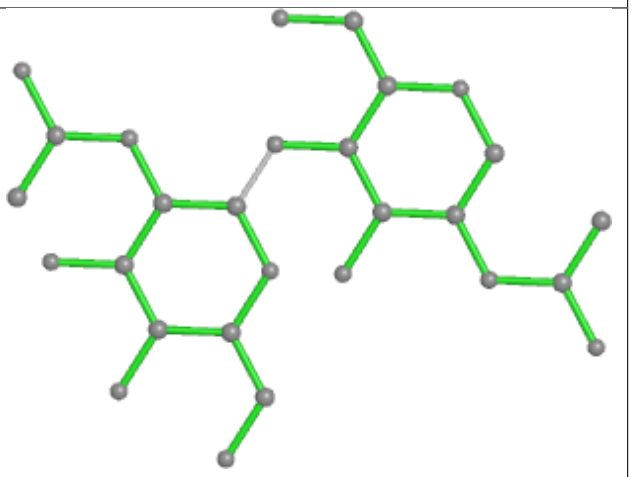


Rings

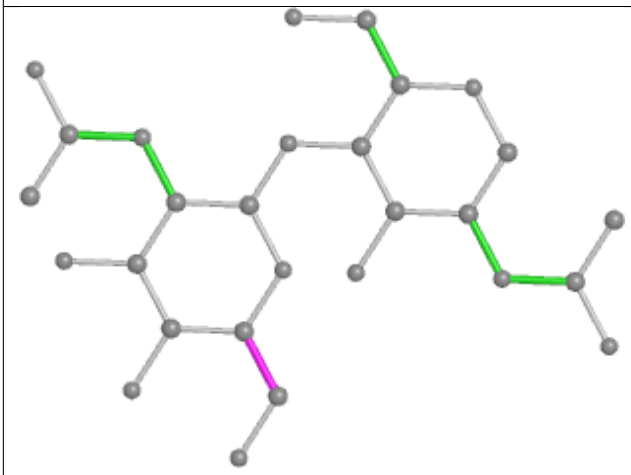
Oligosaccharide Chain M



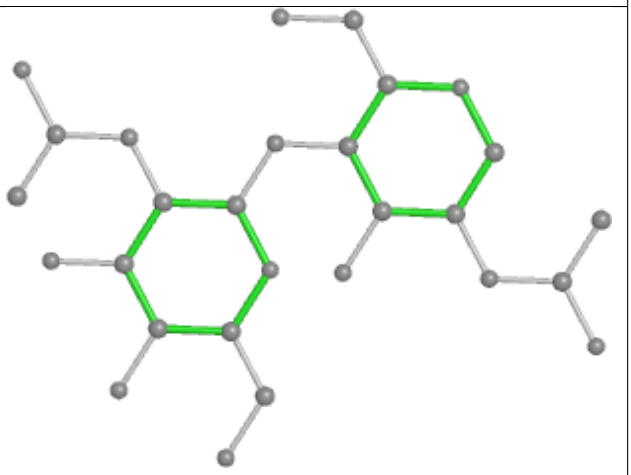
Bond lengths



Bond angles

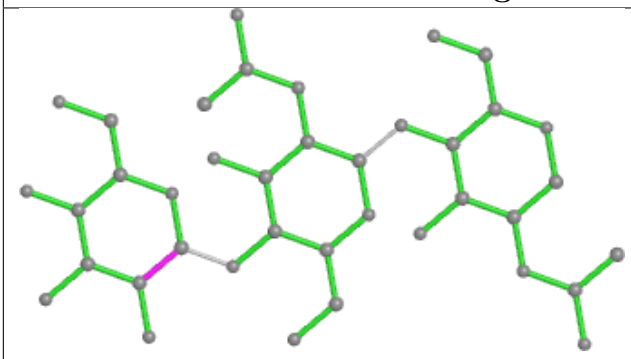


Torsions

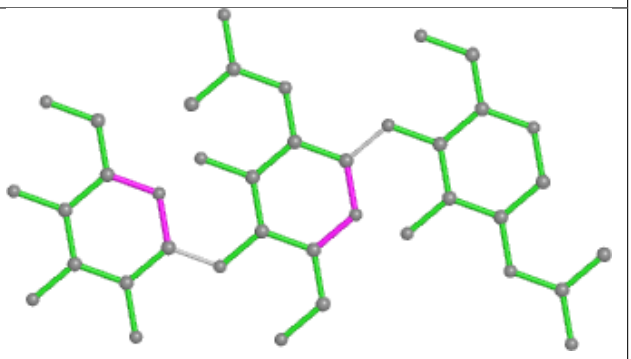


Rings

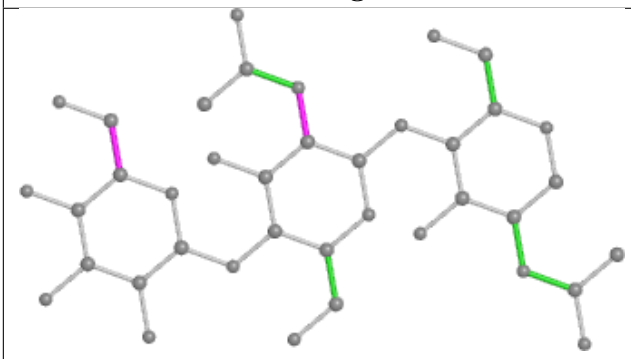
Oligosaccharide Chain G



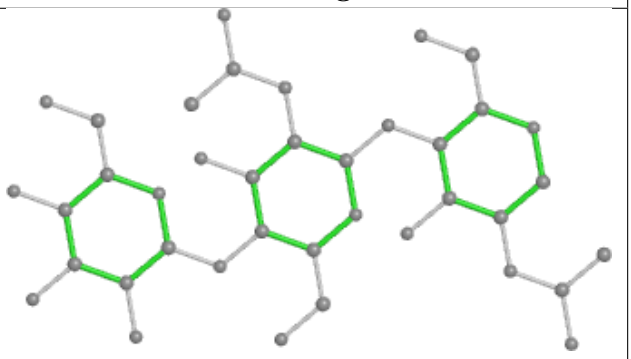
Bond lengths



Bond angles

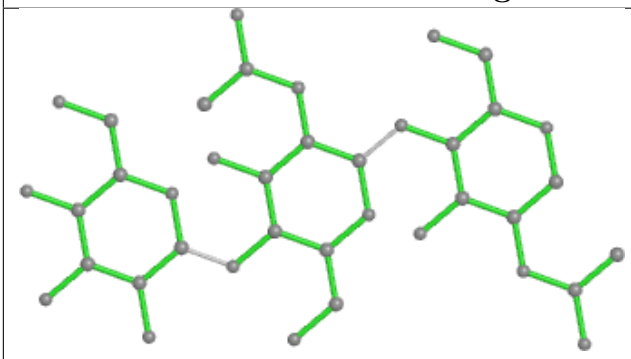


Torsions

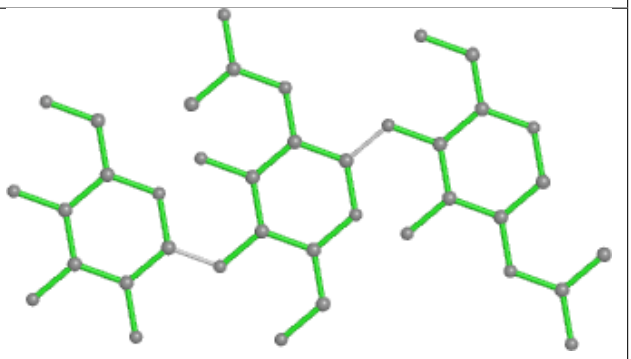


Rings

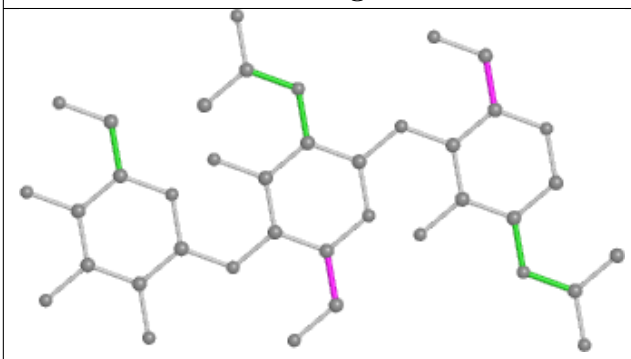
Oligosaccharide Chain H



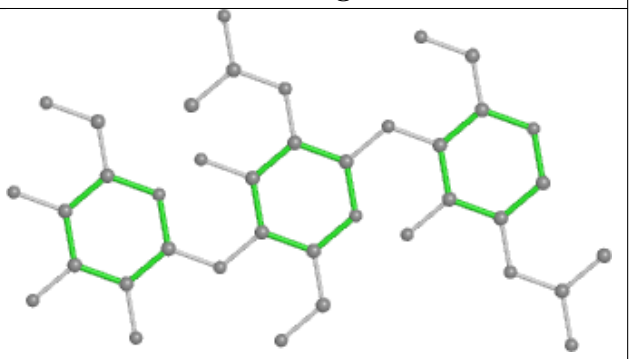
Bond lengths



Bond angles

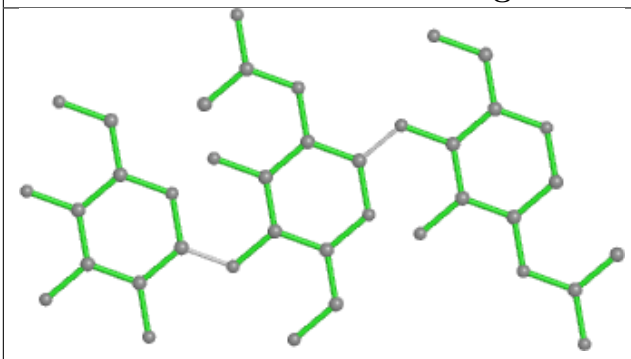


Torsions

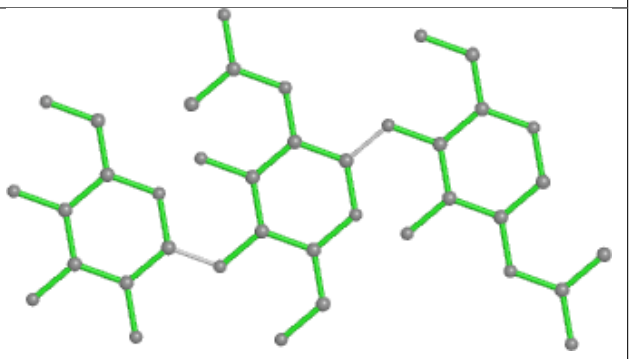


Rings

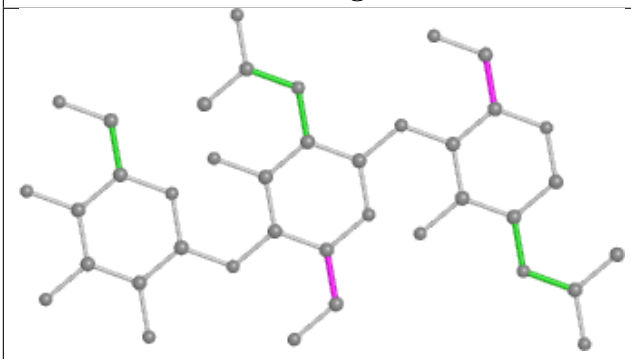
Oligosaccharide Chain K



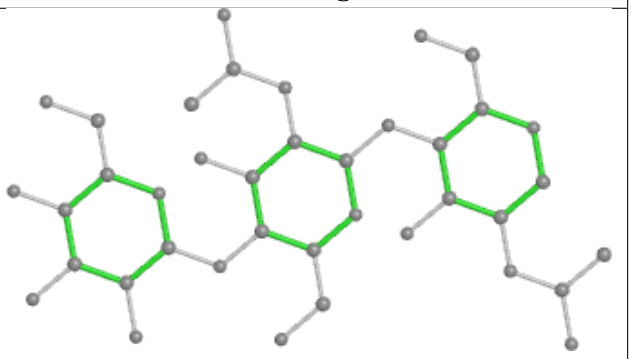
Bond lengths



Bond angles

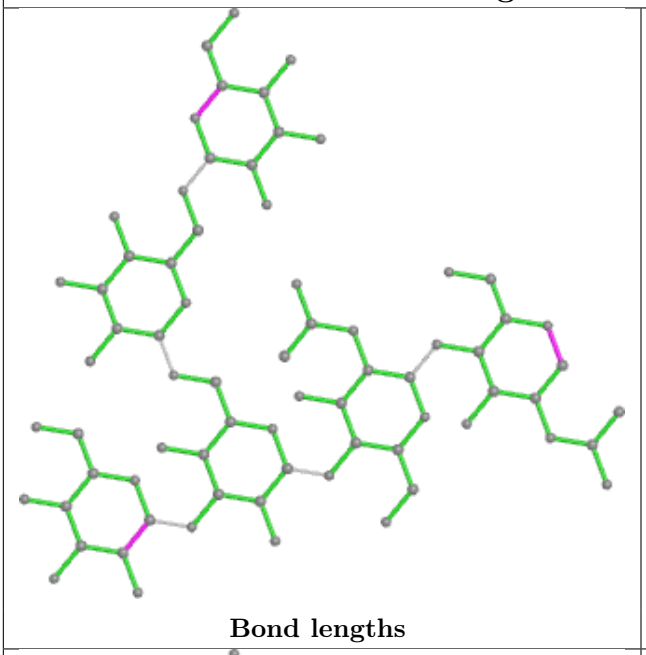


Torsions

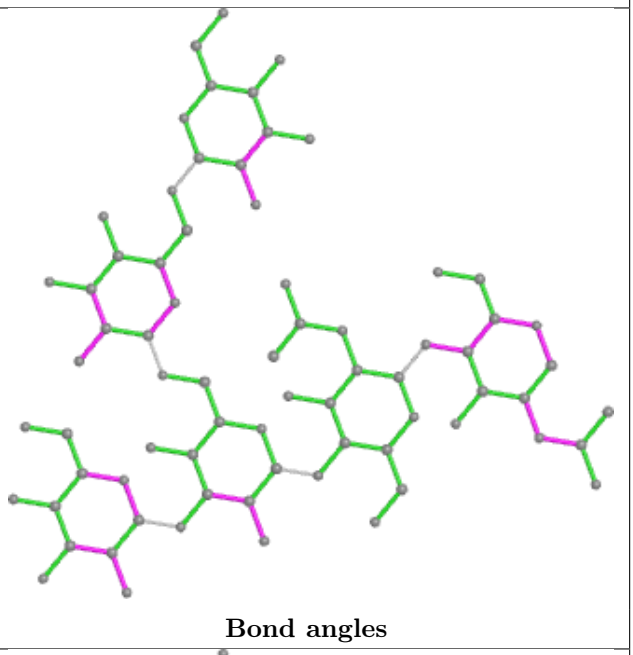


Rings

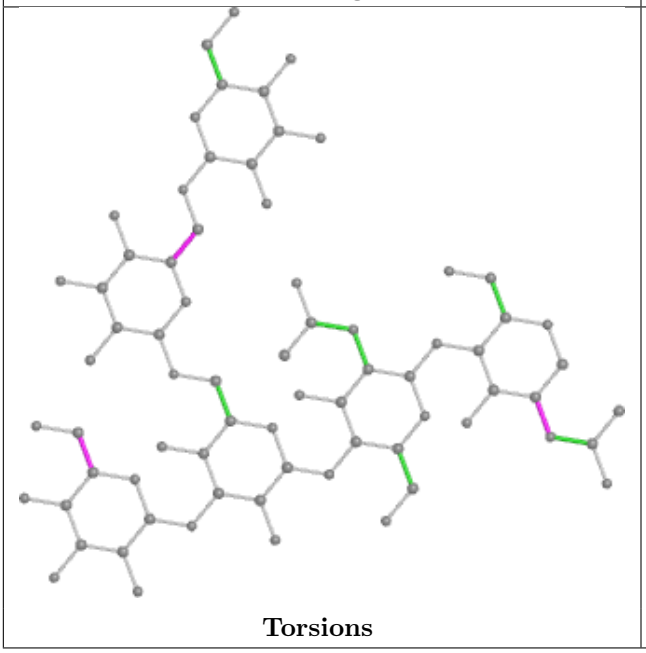
Oligosaccharide Chain L



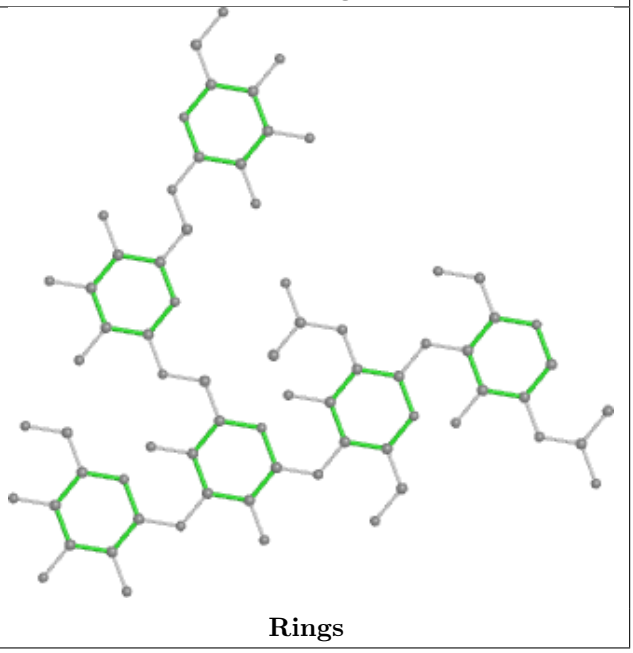
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry

7 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	CYS	I	312	3	5,6,6	1.54	2 (40%)	5,7,7	2.30	3 (60%)
7	NAG	A	201	1	14,14,15	0.38	0	17,19,21	0.72	0
7	NAG	E	304	3	14,14,15	0.90	1 (7%)	17,19,21	0.71	0
8	CYS	E	308	3	5,6,6	1.27	0	5,7,7	1.66	2 (40%)
7	NAG	E	307	3	14,14,15	0.52	0	17,19,21	0.76	0
7	NAG	D	304	2	14,14,15	0.47	0	17,19,21	0.54	0
7	NAG	B	201	1	14,14,15	0.34	0	17,19,21	0.43	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	CYS	I	312	3	-	2/6/6/6	-
7	NAG	A	201	1	-	1/6/23/26	0/1/1/1
7	NAG	E	304	3	-	0/6/23/26	0/1/1/1
8	CYS	E	308	3	-	2/6/6/6	-
7	NAG	E	307	3	-	0/6/23/26	0/1/1/1
7	NAG	D	304	2	-	2/6/23/26	0/1/1/1
7	NAG	B	201	1	-	1/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	E	304	NAG	O5-C1	-2.93	1.39	1.43
8	I	312	CYS	OXT-C	-2.12	1.23	1.30
8	I	312	CYS	CB-CA	2.03	1.55	1.53

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	I	312	CYS	CB-CA-C	3.43	113.31	109.89
8	E	308	CYS	OXT-C-O	-2.94	117.41	124.09
8	I	312	CYS	OXT-C-O	-2.81	117.72	124.09
8	I	312	CYS	OXT-C-CA	2.35	121.37	113.38
8	E	308	CYS	OXT-C-CA	2.25	121.04	113.38

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	E	308	CYS	C-CA-CB-SG
7	A	201	NAG	C1-C2-N2-C7
8	I	312	CYS	C-CA-CB-SG
7	D	304	NAG	C1-C2-N2-C7
7	B	201	NAG	C4-C5-C6-O6
8	I	312	CYS	OXT-C-CA-N
8	E	308	CYS	OXT-C-CA-N
7	D	304	NAG	C3-C2-N2-C7

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	E	307	NAG	2	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	125/148 (84%)	0.28	4 (3%) 47 38	115, 159, 201, 230	0
1	B	126/148 (85%)	0.51	7 (5%) 24 20	122, 178, 235, 267	0
2	C	204/242 (84%)	-0.09	2 (0%) 82 76	128, 170, 224, 256	0
2	D	202/242 (83%)	0.14	10 (4%) 28 25	136, 218, 344, 355	0
3	E	213/233 (91%)	3.01	131 (61%) 0 0	266, 360, 421, 438	0
3	I	213/233 (91%)	0.02	3 (1%) 75 68	97, 140, 201, 271	0
All	All	1083/1246 (86%)	0.70	157 (14%) 2 2	97, 181, 383, 438	0

All (157) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	E	198	SER	13.1
3	E	53	ALA	10.9
3	E	197	ILE	10.6
3	E	155	LEU	10.4
3	E	56	ASN	8.9
3	E	36	PRO	8.9
3	E	38	ILE	8.5
3	E	157	ILE	8.4
3	E	194	SER	8.0
3	E	54	LEU	7.8
3	E	59	ARG	7.5
1	B	-1	GLY	7.1
3	E	57	SER	7.0
3	E	134	HIS	7.0
3	E	65	VAL	6.9
3	E	48	SER	6.6
3	E	217	LEU	6.6
3	E	39	ARG	6.0
3	E	60	PRO	6.0

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Mol	Chain	Res	Type	RSRZ
3	E	96	PHE	6.0
3	E	235	TYR	5.9
3	E	33	PRO	5.9
1	B	0	SER	5.8
3	E	191	PRO	5.8
3	E	188	VAL	5.8
3	E	156	ILE	5.8
3	E	196	SER	5.7
1	B	2	ASP	5.6
3	E	64	GLN	5.4
3	E	77	ALA	5.4
3	E	200	ASP	5.2
3	E	199	LEU	5.2
3	E	45	GLN	5.2
3	E	102	SER	5.1
3	E	58	THR	5.1
3	E	148	VAL	4.9
3	E	40	LEU	4.8
3	E	236	GLU	4.8
3	E	140	VAL	4.8
3	E	44	GLU	4.8
3	E	189	LYS	4.7
3	E	210	LEU	4.7
3	E	190	GLY	4.7
3	E	47	LEU	4.6
3	E	129	MET	4.6
3	E	55	SER	4.6
3	E	37	LYS	4.5
3	E	43	ALA	4.4
3	E	49	TRP	4.4
3	E	216	LEU	4.4
3	E	154	SER	4.3
3	E	141	GLY	4.3
1	B	1	GLN	4.2
3	E	115	LEU	4.2
1	B	124	ALA	4.1
3	E	178	HIS	4.1
3	E	42	ASN	4.0
3	E	174	CYS	4.0
3	E	113	LEU	4.0
2	D	189	VAL	3.9
3	E	99	ALA	3.9

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Mol	Chain	Res	Type	RSRZ
3	E	66	GLN	3.9
3	E	232	ILE	3.9
3	E	192	PHE	3.9
3	E	166	ALA	3.9
3	E	176	TYR	3.8
3	E	187	GLN	3.8
3	E	112	THR	3.8
3	E	119	LEU	3.7
3	E	177	VAL	3.7
3	E	215	GLN	3.7
3	E	209	CYS	3.6
3	E	214	ALA	3.6
3	E	233	SER	3.6
1	A	-1	GLY	3.6
3	E	30	LEU	3.6
2	D	190	SER	3.5
3	E	125	ALA	3.5
3	E	142	PRO	3.5
3	E	173	PHE	3.5
3	E	46	VAL	3.5
3	E	201	ASN	3.4
3	E	61	VAL	3.4
3	E	135	TYR	3.3
3	E	116	ARG	3.3
3	E	29	GLN	3.3
2	D	119	LYS	3.3
3	E	213	GLN	3.3
3	E	35	HIS	3.3
3	I	55	SER	3.3
3	E	228	HIS	3.2
3	E	202	LEU	3.1
3	E	234	CYS	3.1
3	E	101	PRO	3.1
1	A	0	SER	3.1
2	D	50	GLY	3.0
3	E	122	LEU	3.0
3	E	130	PRO	3.0
3	E	237	THR	3.0
3	E	52	VAL	3.0
3	E	94	CYS	2.9
2	D	205	ASN	2.9
3	E	195	ASN	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	3	PRO	2.9
3	E	92	THR	2.9
3	E	28	SER	2.9
3	E	105	PHE	2.9
3	E	179	TYR	2.9
3	E	41	TYR	2.9
3	E	207	VAL	2.8
2	D	193	ASN	2.8
3	E	127	VAL	2.7
3	E	204	PRO	2.7
3	E	175	TYR	2.7
1	B	17	ALA	2.7
3	E	180	TRP	2.7
3	E	124	SER	2.7
3	E	152	GLU	2.7
3	E	31	PRO	2.7
3	E	34	GLN	2.7
3	E	212	VAL	2.7
3	E	149	THR	2.6
3	E	117	ALA	2.6
3	E	239	ALA	2.6
3	E	225	ARG	2.6
3	I	56	ASN	2.6
3	E	208	TYR	2.6
3	E	50	GLU	2.6
3	E	128	THR	2.6
3	E	133	GLN	2.6
3	E	193	ARG	2.5
3	E	158	ARG	2.4
3	E	104	GLY	2.4
3	E	123	HIS	2.4
3	E	224	PHE	2.4
3	E	167	ASP	2.4
3	E	229	LEU	2.4
3	E	138	VAL	2.4
2	D	54	SER	2.3
2	D	188	PRO	2.3
3	E	76	THR	2.3
3	E	186	GLN	2.3
1	A	121	SER	2.3
3	E	185	ILE	2.3
3	E	71	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
3	E	163	PHE	2.3
3	E	63	TYR	2.2
3	E	183	GLY	2.2
2	D	187	ILE	2.2
2	C	70	ILE	2.2
3	E	165	ILE	2.2
2	C	147	GLU	2.1
1	A	123	ALA	2.1
3	E	205	SER	2.1
3	E	231	ASN	2.1
3	I	28	SER	2.1
2	D	124	ILE	2.1

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	H	2	14/15	0.08	0.48	394,394,394,394	0
5	BMA	H	3	11/12	0.23	0.37	382,382,382,382	0
5	NAG	H	1	14/15	0.32	0.54	398,398,398,398	0
6	MAN	L	5	11/12	0.68	0.23	260,260,260,260	0
4	NAG	J	2	14/15	0.75	0.46	333,333,333,333	0
4	NAG	F	2	14/15	0.77	0.29	223,223,223,223	0
4	NAG	J	1	14/15	0.78	0.38	338,338,338,338	0
5	BMA	G	3	11/12	0.79	0.20	244,244,244,244	0
6	MAN	L	6	11/12	0.80	0.20	264,264,264,264	0
6	BMA	L	3	11/12	0.81	0.14	240,240,240,240	0
4	NAG	M	2	14/15	0.83	0.26	178,178,178,178	0
5	NAG	K	2	14/15	0.84	0.23	228,228,228,228	0
5	NAG	K	1	14/15	0.85	0.16	210,210,210,210	0
6	NAG	L	1	14/15	0.86	0.29	168,168,168,168	0
5	BMA	K	3	11/12	0.87	0.17	252,252,252,252	0
6	MAN	L	4	11/12	0.89	0.12	261,261,261,261	0

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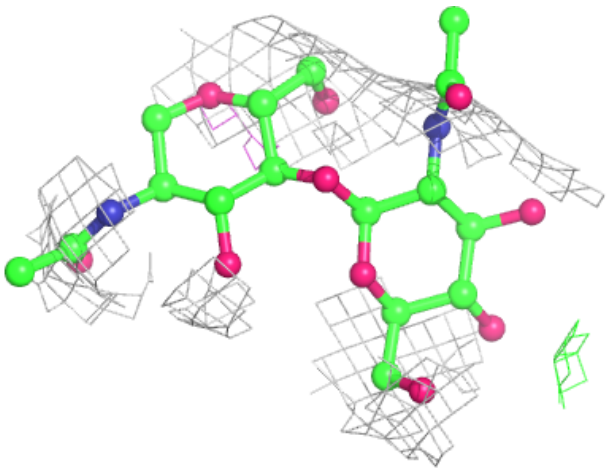
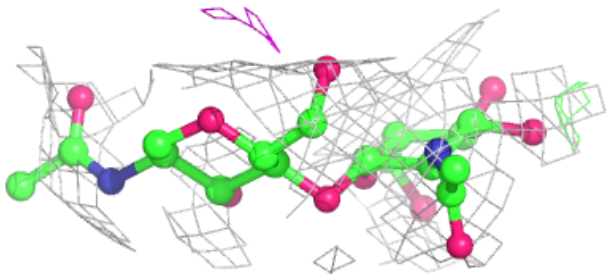
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	NAG	L	2	14/15	0.89	0.18	187,187,187,187	0
5	NAG	G	2	14/15	0.89	0.22	239,239,239,239	0
4	NAG	F	1	14/15	0.90	0.21	183,183,183,183	0
5	NAG	G	1	14/15	0.93	0.28	218,218,218,218	0
4	NAG	M	1	14/15	0.95	0.24	145,145,145,145	0

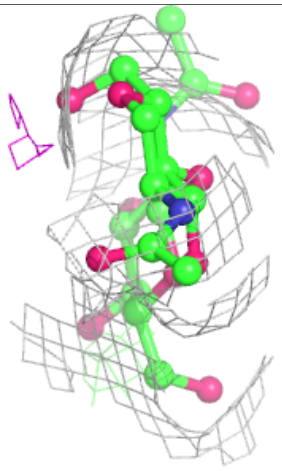
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain F:

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

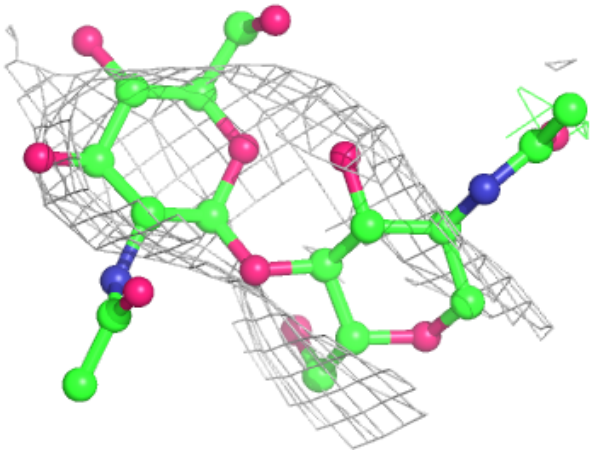


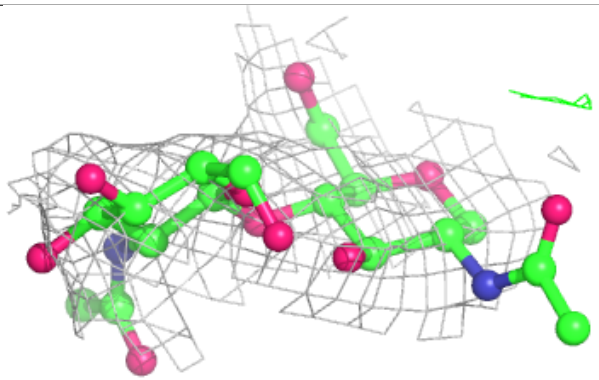


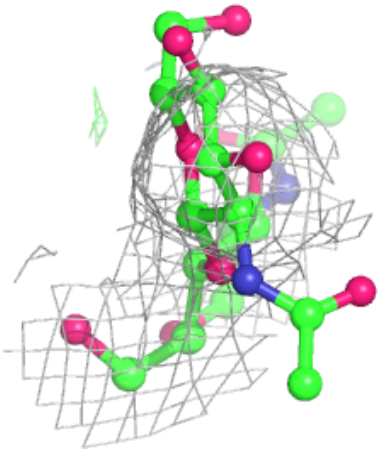


Electron density around Chain J:

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

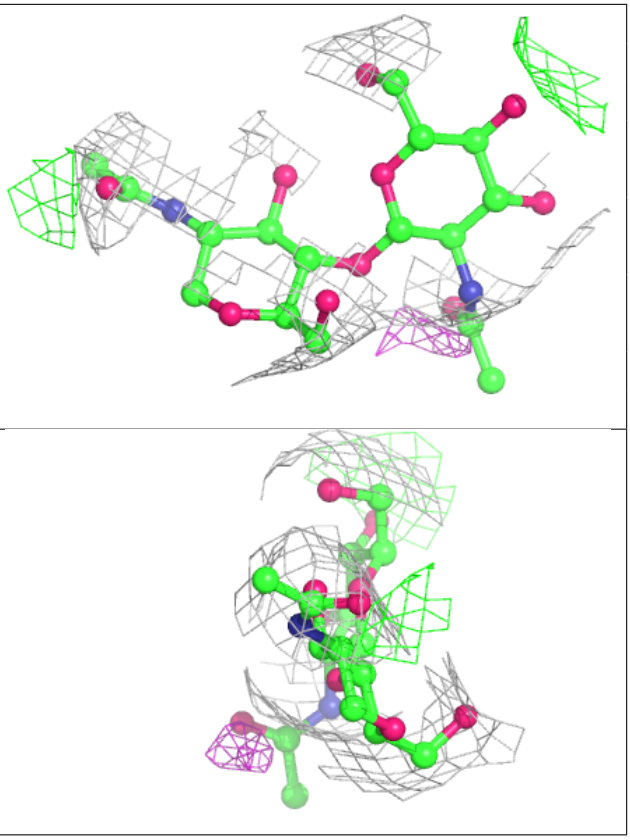






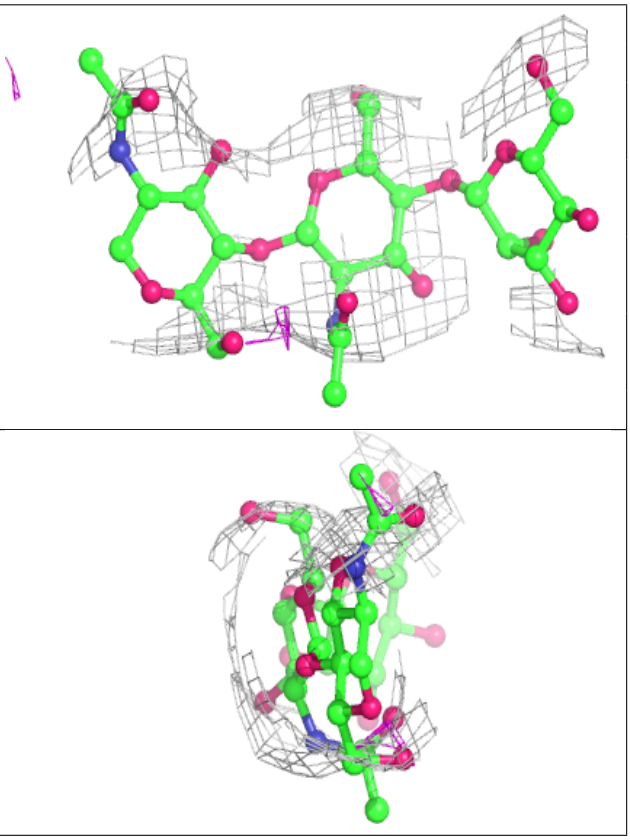
Electron density around Chain M:

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



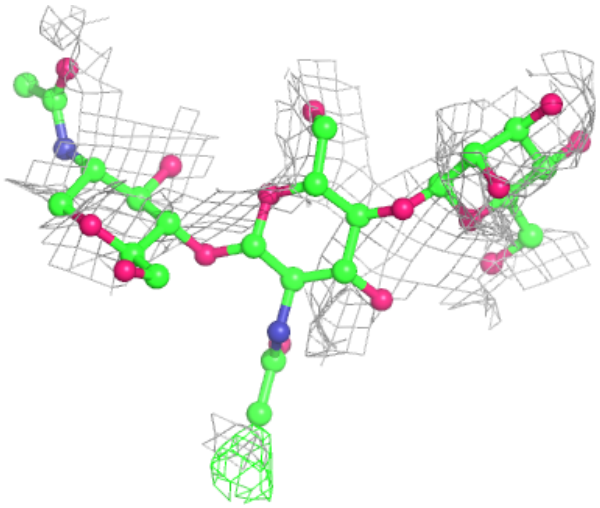
Electron density around Chain G:

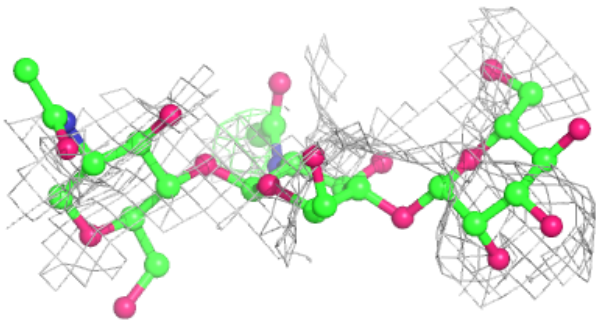
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

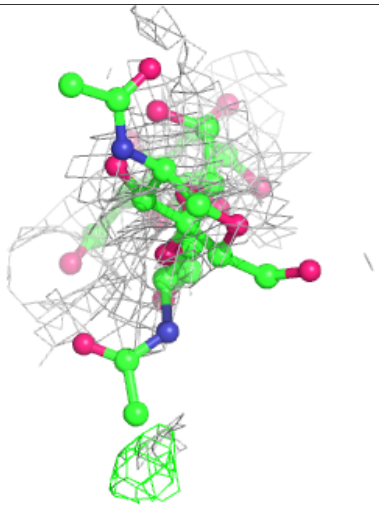


Electron density around Chain H:

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

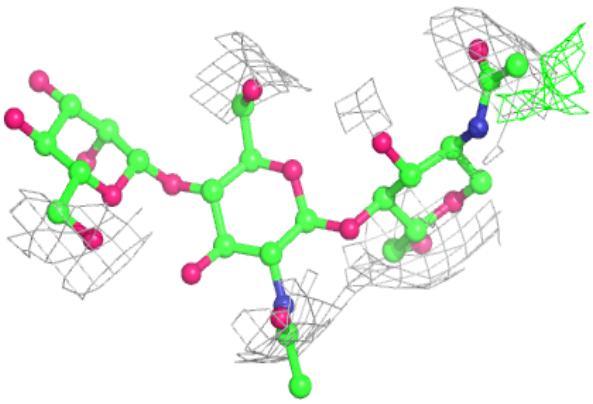


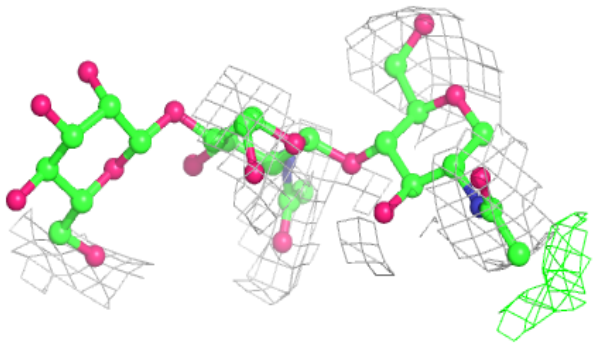


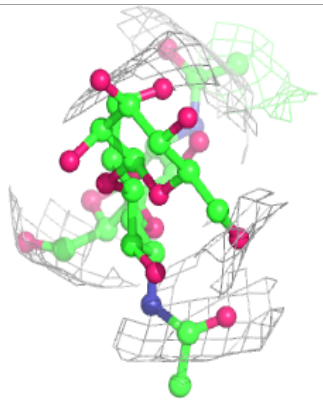


Electron density around Chain K:

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

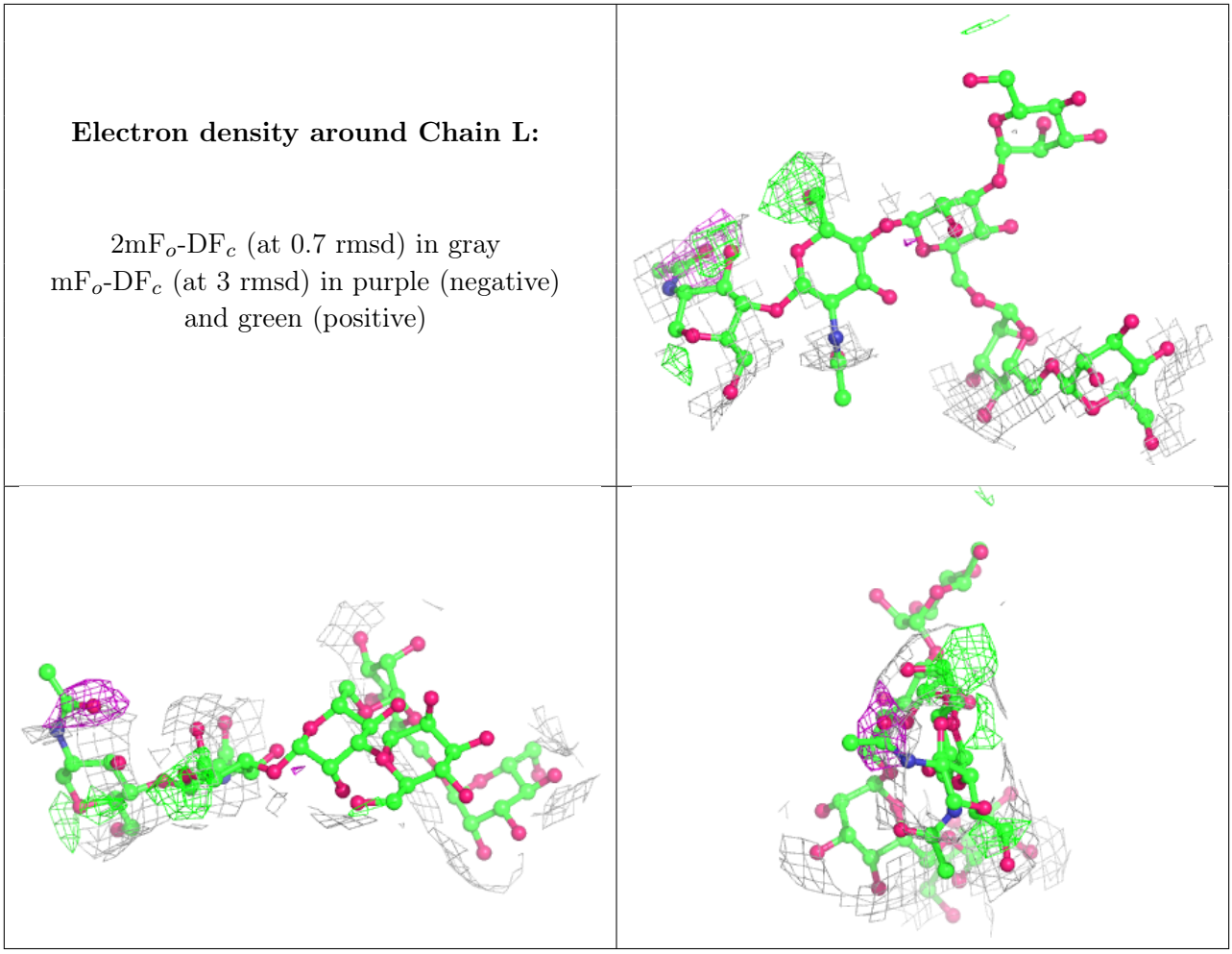






Electron density around Chain L:

$2mF_o$-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	CYS	E	308	7/7	-0.42	1.15	301,301,301,311	0
7	NAG	E	307	14/15	0.35	1.14	415,415,415,415	0
8	CYS	I	312	7/7	0.74	0.42	187,187,187,197	0
7	NAG	A	201	14/15	0.75	0.22	233,233,233,233	0
7	NAG	B	201	14/15	0.81	0.22	221,221,221,221	0
7	NAG	E	304	14/15	0.83	0.23	338,338,338,338	0
7	NAG	D	304	14/15	0.87	0.19	247,247,247,247	0

6.5 Other polymers (i)

There are no such residues in this entry.