



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 12:13 AM BST

PDB ID : 6MDT
Title : Crystal structure of the B41 SOSIP.664 Env trimer with PGT124 and 35O22 Fabs, in P63 space group
Authors : Kumar, S.; Sarkar, A.; Wilson, I.A.
Deposited on : 2018-09-05
Resolution : 3.82 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
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) : 2.13.1

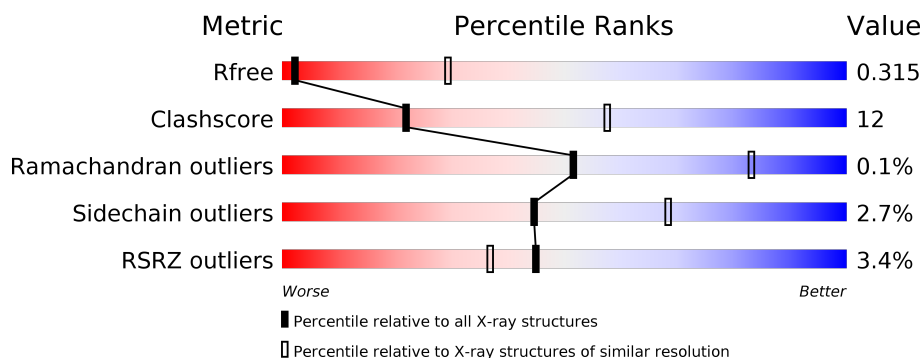
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.82 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.



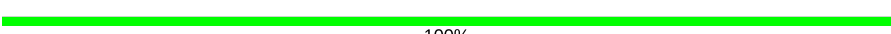




Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1231 (4.04-3.60)
Clashscore	141614	1031 (4.02-3.62)
Ramachandran outliers	138981	1261 (4.04-3.60)
Sidechain outliers	138945	1255 (4.04-3.60)
RSRZ outliers	127900	1139 (4.04-3.60)

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 on 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 $\leq 5\%$. 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	B	153	<div> <div>4%</div> <div> <div></div> <div>73%</div> <div>14%</div> <div>••</div> <div>11%</div> </div> </div>
2	G	482	<div> <div>%</div> <div> <div></div> <div>67%</div> <div>26%</div> <div>•</div> <div>6%</div> </div> </div>
3	D	243	<div> <div>9%</div> <div> <div></div> <div>79%</div> <div>20%</div> <div>•</div> </div> </div>
4	E	216	<div> <div>3%</div> <div> <div></div> <div>83%</div> <div>15%</div> <div>•</div> </div> </div>
5	H	236	<div> <div>3%</div> <div> <div></div> <div>67%</div> <div>30%</div> <div>••</div> </div> </div>
6	L	214	<div> <div></div> <div> <div></div> <div>77%</div> <div>21%</div> <div>••</div> </div> </div>

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Mol	Chain	Length	Quality of chain
7	A	5	
7	I	5	
7	K	5	
7	Q	5	
8	C	7	
9	F	2	
10	J	3	
10	M	3	
10	O	3	
10	S	3	
11	N	4	
11	P	4	
12	R	4	
13	T	9	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	BMA	M	3	-	-	-	X
10	BMA	S	3	-	-	-	X
14	NAG	G	633	-	-	-	X
7	NAG	A	1	-	-	-	X
7	NAG	A	2	-	-	-	X
7	MAN	A	4	-	-	-	X
9	NAG	F	2	-	-	-	X

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 12314 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 Transmembrane protein gp41.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	136	Total	C	N	O	S	0	0	0
			1077	688	181	201	7			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	605	CYS	THR	conflict	UNP B3UES2

- Molecule 2 is a protein called Surface protein gp120.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	455	Total	C	N	O	S	0	0	0
			3562	2237	628	671	26			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	501	CYS	ALA	conflict	UNP B3UF58

- Molecule 3 is a protein called 35O22 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	240	Total	C	N	O	S	0	0	0
			1813	1150	303	352	8			

- Molecule 4 is a protein called 35O22 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	213	Total	C	N	O	S	0	0	0
			1615	1012	267	328	8			

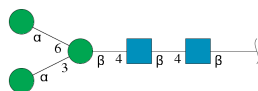
- Molecule 5 is a protein called PGT124 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	H	231	Total	C	N	O	S	0	0	0
			1754	1111	293	345	5			

- Molecule 6 is a protein called PGT124 Fab light chain.

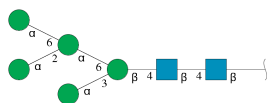
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	L	211	Total	C	N	O	S	0	0	0
			1601	1008	271	317	5			

- Molecule 7 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.



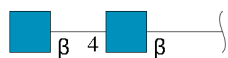
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	A	5	Total	C	N	O		0	0	0
			61	34	2	25				
7	I	5	Total	C	N	O		0	0	0
			61	34	2	25				
7	K	5	Total	C	N	O		0	0	0
			61	34	2	25				
7	Q	5	Total	C	N	O		0	0	0
			61	34	2	25				

- Molecule 8 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-[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
8	C	7	Total	C	N	O		0	0	0
			83	46	2	35				

- Molecule 9 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
9	F	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 10 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.



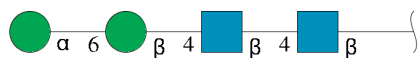
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	J	3	Total	C	N	O	0	0	0
			39	22	2	15			
10	M	3	Total	C	N	O	0	0	0
			39	22	2	15			
10	O	3	Total	C	N	O	0	0	0
			39	22	2	15			
10	S	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 11 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.



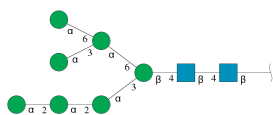
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	N	4	Total	C	N	O	0	0	0
			50	28	2	20			
11	P	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 12 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.



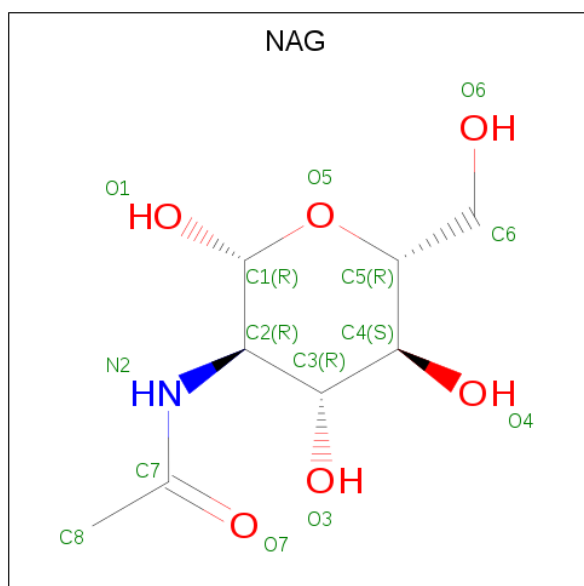
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
12	R	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 13 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	T	9	Total	C	N	O	0	0	0
			105	58	2	45			

- Molecule 14 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



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

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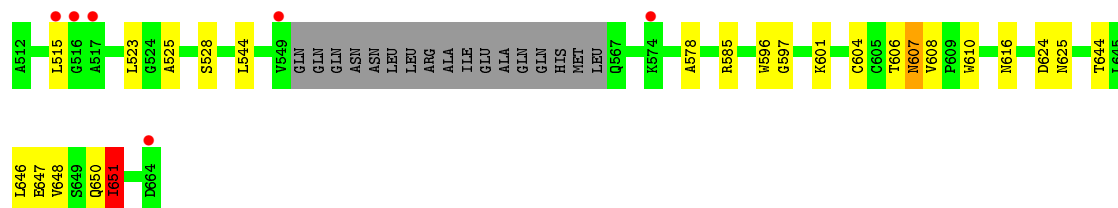
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
14	B	1	Total	C	N	O	0	0
			14	8	1	5		
14	B	1	Total	C	N	O	0	0
			14	8	1	5		
14	G	1	Total	C	N	O	0	0
			14	8	1	5		
14	G	1	Total	C	N	O	0	0
			14	8	1	5		
14	G	1	Total	C	N	O	0	0
			14	8	1	5		
14	G	1	Total	C	N	O	0	0
			14	8	1	5		
14	G	1	Total	C	N	O	0	0
			14	8	1	5		

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.

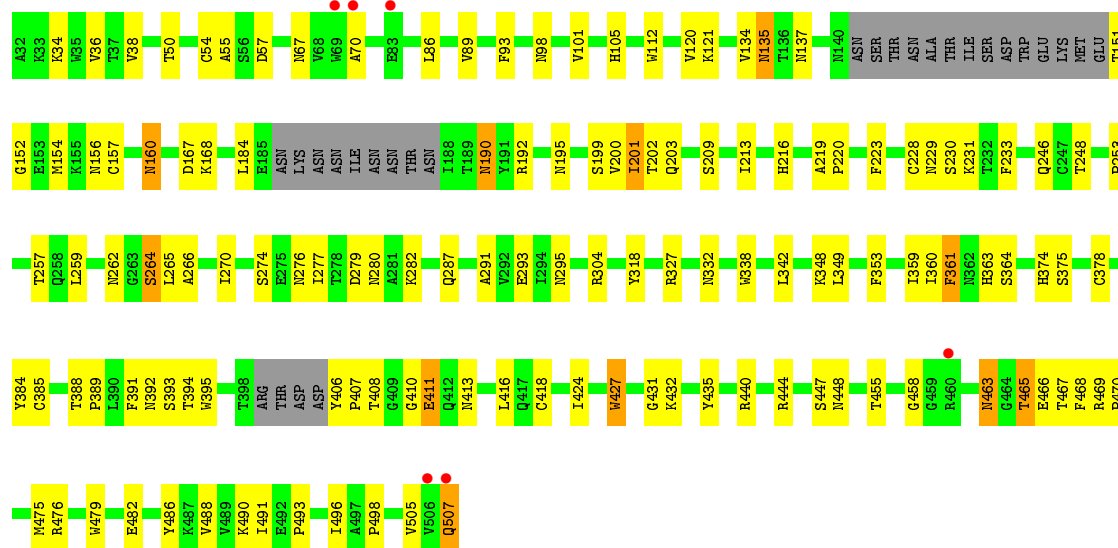
- Molecule 1: Transmembrane protein gp41

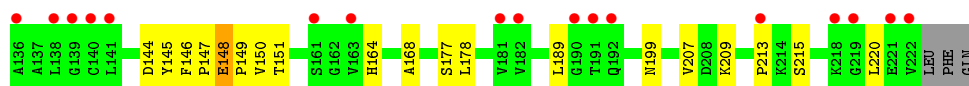
Chain B: 



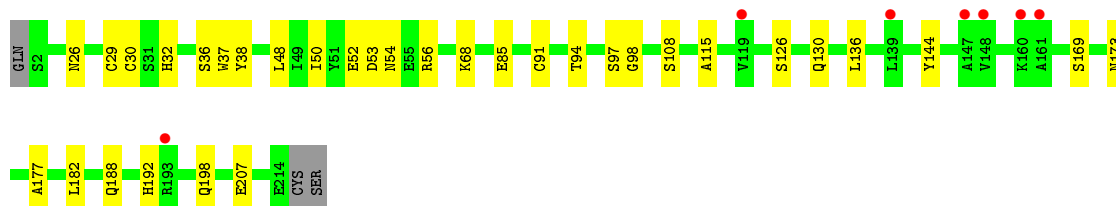
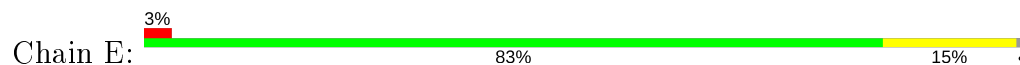
- Molecule 2: Surface protein gp120

Chain G: 

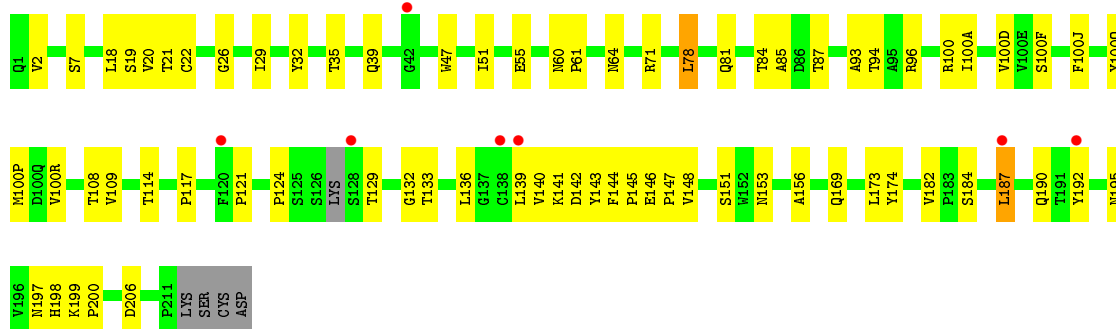




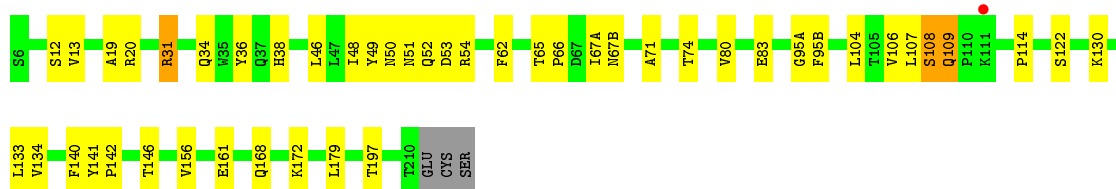
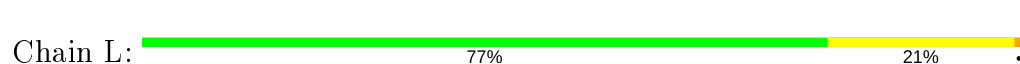
- Molecule 4: 35O22 Fab light chain



- Molecule 5: PGT124 Fab heavy chain



- Molecule 6: PGT124 Fab light chain



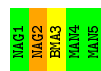
- Molecule 7: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 7: alpha-D-mannopyranose-(1-3)-[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

nose

Chain I: 

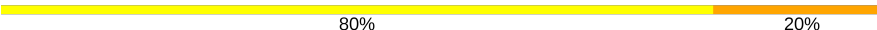


• Molecule 7: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K: 



• Molecule 7: 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 Q: 



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



• Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F: 



• Molecule 10: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J: 



• Molecule 10: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:  33% 67%



- Molecule 10: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:  33% 67%



- Molecule 10: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain S:  33% 67%



- Molecule 11: 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 N:  75% 25%



- Molecule 11: 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 P:  50% 50%



- Molecule 12: 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 R:  50% 50%



- Molecule 13: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain T:  33% 33% 33%

MA01
MA02
MA03
MA04
MA05
MA06
MA07
MA08
MA09

4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	129.34Å 129.34Å 313.07Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	41.96 – 3.82 41.96 – 3.82	Depositor EDS
% Data completeness (in resolution range)	99.9 (41.96-3.82) 99.9 (41.96-3.82)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.48 (at 3.76Å)	Xtriage
Refinement program	PHENIX (1.12_2829)	Depositor
R, R_{free}	0.294 , 0.311 0.300 , 0.315	Depositor DCC
R_{free} test set	1359 reflections (4.73%)	wwPDB-VP
Wilson B-factor (Å ²)	98.9	Xtriage
Anisotropy	0.359	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 18.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.35$, $\langle L^2 \rangle = 0.17$	Xtriage
Estimated twinning fraction	0.177 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	12314	wwPDB-VP
Average B, all atoms (Å ²)	124.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.88% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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, NAG, 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	B	0.27	0/1096	0.46	0/1487
2	G	0.29	0/3637	0.49	0/4946
3	D	0.24	0/1860	0.45	0/2533
4	E	0.24	0/1659	0.45	0/2269
5	H	0.28	0/1797	0.58	1/2453 (0.0%)
6	L	0.30	0/1644	0.52	4/2246 (0.2%)
All	All	0.27	0/11693	0.49	5/15934 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	85	ALA	N-CA-CB	8.14	121.50	110.10
6	L	109	GLN	N-CA-C	-6.07	94.60	111.00
6	L	108	SER	CA-C-O	5.19	131.00	120.10
6	L	108	SER	CA-C-N	-5.04	106.11	117.20
6	L	108	SER	CB-CA-C	-5.01	100.59	110.10

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	B	1077	0	1066	23	0
2	G	3562	0	3486	108	0
3	D	1813	0	1781	33	0
4	E	1615	0	1544	21	0
5	H	1754	0	1719	72	0
6	L	1601	0	1544	33	0
7	A	61	0	52	4	0
7	I	61	0	52	1	0
7	K	61	0	52	3	0
7	Q	61	0	52	3	0
8	C	83	0	70	7	0
9	F	28	0	25	0	0
10	J	39	0	34	2	0
10	M	39	0	34	3	0
10	O	39	0	34	2	0
10	S	39	0	34	1	0
11	N	50	0	43	0	0
11	P	50	0	43	1	0
12	R	50	0	43	5	0
13	T	105	0	86	11	0
14	B	42	0	39	1	0
14	G	84	0	78	1	0
All	All	12314	0	11911	286	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 12.

All (286) 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:G:413:ASN:HD21	12:R:1:NAG:C1	1.51	1.24
5:H:29:ILE:HB	5:H:71:ARG:HD2	1.20	1.18
2:G:413:ASN:ND2	12:R:1:NAG:C1	2.09	1.15
5:H:29:ILE:HD13	5:H:71:ARG:HE	1.20	1.01
5:H:94:THR:HG22	5:H:100(R):VAL:HB	1.43	0.99
2:G:332:ASN:HD21	13:T:1:NAG:C1	1.79	0.95
2:G:266:ALA:H	2:G:287:GLN:HE21	0.96	0.95
3:D:54:SER:HB2	8:C:5:MAN:H62	1.50	0.94
5:H:29:ILE:CB	5:H:71:ARG:HD2	1.98	0.94
2:G:389:PRO:HB3	7:Q:1:NAG:H62	1.47	0.93
5:H:29:ILE:HB	5:H:71:ARG:CD	1.98	0.92
6:L:20:ARG:HG2	6:L:74:THR:HG22	1.52	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:L:80:VAL:HG12	6:L:109:GLN:NE2	1.86	0.89
2:G:266:ALA:N	2:G:287:GLN:HE21	1.71	0.88
2:G:332:ASN:ND2	13:T:1:NAG:C1	2.40	0.84
2:G:266:ALA:H	2:G:287:GLN:NE2	1.76	0.83
5:H:100(D):VAL:HG22	13:T:1:NAG:H5	1.57	0.83
3:D:126:PRO:HB2	3:D:215:SER:HB2	1.60	0.82
2:G:295:ASN:HD22	10:M:1:NAG:H83	1.44	0.82
2:G:264:SER:OG	2:G:482:GLU:OE1	1.97	0.81
3:D:97:LEU:HD21	7:A:1:NAG:H82	1.63	0.80
5:H:94:THR:CG2	5:H:100(R):VAL:HB	2.12	0.79
2:G:360:ILE:HG21	2:G:395:TRP:HD1	1.47	0.77
2:G:134:VAL:HG21	2:G:154:MET:HG3	1.67	0.77
5:H:35:THR:HG21	5:H:100(P):MET:CE	2.15	0.77
2:G:38:VAL:HG12	2:G:496:ILE:HG22	1.69	0.74
5:H:100(D):VAL:CG2	13:T:1:NAG:H5	2.17	0.74
5:H:29:ILE:HD13	5:H:71:ARG:NE	2.00	0.74
2:G:55:ALA:HB3	2:G:216:HIS:HB2	1.70	0.73
2:G:135:ASN:N	2:G:135:ASN:OD1	2.22	0.73
2:G:427:TRP:HD1	2:G:475:MET:HG2	1.55	0.71
5:H:29:ILE:CD1	5:H:71:ARG:HE	2.00	0.70
5:H:20:VAL:HG12	5:H:21:THR:N	2.06	0.70
3:D:168:ALA:HA	3:D:178:LEU:HB3	1.72	0.70
5:H:148:VAL:HG22	5:H:198:HIS:HD2	1.56	0.69
5:H:199:LYS:HB2	5:H:200:PRO:HD3	1.74	0.69
2:G:121:LYS:HA	2:G:202:THR:HA	1.76	0.68
2:G:360:ILE:HG12	2:G:394:THR:HA	1.76	0.68
2:G:363:HIS:CD2	2:G:364:SER:HB3	2.29	0.67
6:L:80:VAL:HG12	6:L:109:GLN:HE21	1.57	0.67
4:E:136:LEU:HD12	4:E:182:LEU:HD23	1.77	0.66
5:H:142:ASP:HB2	5:H:173:LEU:HB2	1.78	0.66
3:D:150:VAL:HG11	3:D:178:LEU:HD21	1.78	0.66
2:G:219:ALA:O	2:G:246:GLN:NE2	2.29	0.66
6:L:141:TYR:HB3	6:L:142:PRO:HD3	1.78	0.66
5:H:35:THR:HG21	5:H:100(P):MET:HE2	1.77	0.66
7:I:2:NAG:H3	7:I:2:NAG:H83	1.77	0.66
5:H:132:GLY:O	5:H:184:SER:N	2.28	0.65
3:D:146:PHE:HB3	3:D:147:PRO:HD3	1.79	0.65
2:G:264:SER:O	2:G:287:GLN:NE2	2.29	0.65
5:H:195:ASN:ND2	5:H:206:ASP:OD2	2.30	0.65
4:E:50:ILE:HG23	4:E:53:ASP:O	1.96	0.65
2:G:202:THR:HB	2:G:432:LYS:HE2	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:197:ASN:OD1	5:H:198:HIS:N	2.31	0.64
5:H:84:THR:HA	5:H:109:VAL:HB	1.81	0.63
1:B:616:ASN:HD22	14:B:701:NAG:C7	2.11	0.63
5:H:87:THR:HG23	5:H:87:THR:O	1.99	0.62
4:E:115:ALA:HB3	4:E:144:TYR:H	1.65	0.62
1:B:578:ALA:HB1	2:G:220:PRO:HB3	1.82	0.62
6:L:54:ARG:NH2	6:L:62:PHE:O	2.29	0.62
2:G:137:ASN:HB3	6:L:95(A):GLY:HA2	1.82	0.61
3:D:128:SER:HB2	3:D:220:LEU:HB2	1.82	0.61
2:G:304:ARG:HB3	2:G:440:ARG:HH11	1.64	0.61
2:G:201:ILE:HD11	2:G:435:TYR:HB2	1.83	0.61
5:H:22:CYS:HB3	5:H:78:LEU:HG	1.82	0.61
2:G:266:ALA:N	2:G:287:GLN:NE2	2.42	0.60
2:G:359:ILE:HG23	2:G:465:THR:HG21	1.83	0.60
4:E:26:ASN:HA	4:E:29:CYS:HB2	1.83	0.60
2:G:270:ILE:HG13	2:G:348:LYS:HG3	1.82	0.60
2:G:389:PRO:HD2	2:G:416:LEU:HD22	1.83	0.60
1:B:585:ARG:NH2	2:G:491:ILE:O	2.34	0.59
1:B:608:VAL:N	1:B:650:GLN:OE1	2.36	0.59
2:G:392:ASN:HD21	7:Q:1:NAG:H83	1.68	0.59
6:L:83:GLU:HB2	6:L:106:VAL:HG23	1.85	0.59
2:G:262:ASN:HD21	7:K:1:NAG:C1	2.16	0.58
2:G:361:PHE:HB3	2:G:468:PHE:HB2	1.84	0.58
5:H:20:VAL:CG1	5:H:21:THR:N	2.66	0.58
6:L:83:GLU:HG3	6:L:104:LEU:O	2.02	0.58
5:H:169:GLN:HG3	6:L:161:GLU:HG3	1.86	0.58
2:G:393:SER:HA	2:G:406:TYR:HD2	1.68	0.58
3:D:148:GLU:N	3:D:149:PRO:HD2	2.19	0.58
2:G:280:ASN:HD22	2:G:458:GLY:HA2	1.68	0.58
1:B:607:ASN:N	1:B:607:ASN:OD1	2.37	0.57
2:G:57:ASP:OD1	2:G:57:ASP:N	2.37	0.57
5:H:100(D):VAL:HG22	13:T:1:NAG:C5	2.32	0.57
6:L:66:PRO:HB2	13:T:5:MAN:O3	2.04	0.57
5:H:124:PRO:HG3	5:H:136:LEU:HB3	1.85	0.57
2:G:407:PRO:HG2	2:G:410:GLY:HA3	1.87	0.57
5:H:141:LYS:HG2	5:H:142:ASP:H	1.70	0.57
5:H:35:THR:HG21	5:H:100(P):MET:HE3	1.86	0.57
3:D:66:ARG:NH2	3:D:86:ASP:OD2	2.38	0.56
4:E:29:CYS:SG	4:E:30:CYS:N	2.78	0.56
2:G:463:ASN:HD22	2:G:463:ASN:H	1.52	0.56
1:B:528:SER:OG	8:C:1:NAG:O7	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:190:ASN:N	2:G:190:ASN:OD1	2.38	0.56
1:B:610:TRP:HE3	2:G:36:VAL:HG12	1.69	0.56
1:B:523:LEU:HD11	2:G:491:ILE:HD11	1.88	0.56
5:H:84:THR:O	5:H:87:THR:HG22	2.05	0.56
2:G:360:ILE:HG21	2:G:395:TRP:CD1	2.35	0.56
1:B:607:ASN:OD1	1:B:650:GLN:NE2	2.39	0.56
3:D:168:ALA:HB2	3:D:178:LEU:HD23	1.87	0.55
2:G:413:ASN:HD22	12:R:1:NAG:C1	2.15	0.55
3:D:1:GLU:HG3	7:A:2:NAG:O7	2.06	0.55
1:B:610:TRP:HB3	2:G:34:LYS:HB2	1.89	0.55
5:H:19:SER:O	5:H:20:VAL:HG23	2.07	0.54
5:H:20:VAL:CG1	5:H:21:THR:H	2.20	0.54
5:H:94:THR:HG23	5:H:94:THR:O	2.07	0.54
3:D:119:PRO:HB3	3:D:145:TYR:HB3	1.90	0.54
6:L:12:SER:HB3	6:L:107:LEU:HD11	1.88	0.54
5:H:141:LYS:HZ1	6:L:130:LYS:HD2	1.72	0.54
2:G:447:SER:OG	7:K:1:NAG:N2	2.36	0.53
12:R:2:NAG:H83	12:R:2:NAG:H3	1.90	0.53
4:E:29:CYS:HB3	4:E:32:HIS:CE1	2.44	0.53
2:G:200:VAL:HG23	2:G:432:LYS:HG3	1.91	0.53
8:C:3:BMA:H2	8:C:7:MAN:H5	1.91	0.53
5:H:144:PHE:H	5:H:145:PRO:HD2	1.74	0.53
5:H:29:ILE:CG2	5:H:71:ARG:HD2	2.38	0.53
3:D:87:THR:HG23	3:D:110:THR:HA	1.89	0.53
5:H:20:VAL:HG12	5:H:21:THR:H	1.71	0.53
5:H:184:SER:HA	5:H:187:LEU:HB2	1.90	0.52
4:E:54:ASN:OD1	4:E:54:ASN:N	2.39	0.52
3:D:151:THR:OG1	3:D:199:ASN:O	2.25	0.52
5:H:129:THR:OG1	5:H:133:THR:OG1	2.00	0.52
1:B:644:THR:O	1:B:648:VAL:HG12	2.09	0.52
3:D:99:ASP:OD1	3:D:100:GLY:N	2.41	0.52
2:G:455:THR:N	2:G:469:ARG:O	2.42	0.52
3:D:47:TRP:CZ2	3:D:49:GLY:HA2	2.45	0.52
2:G:463:ASN:ND2	2:G:463:ASN:O	2.43	0.52
3:D:31:PHE:HA	8:C:1:NAG:O6	2.09	0.52
2:G:151:THR:OG1	2:G:152:GLY:N	2.42	0.52
5:H:87:THR:OG1	5:H:108:THR:HA	2.10	0.51
3:D:2:GLY:N	7:A:2:NAG:H82	2.26	0.51
4:E:37:TRP:HB2	4:E:50:ILE:HB	1.92	0.51
1:B:610:TRP:CE3	2:G:36:VAL:HG12	2.45	0.51
6:L:34:GLN:HG3	6:L:49:TYR:HA	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:T:4:MAN:O4	13:T:4:MAN:O6	2.29	0.51
2:G:444:ARG:NH2	12:R:2:NAG:O7	2.44	0.51
1:B:544:LEU:HD21	2:G:493:PRO:HG3	1.93	0.51
8:C:4:MAN:HO4	8:C:6:MAN:H3	1.76	0.51
2:G:167:ASP:OD1	2:G:168:LYS:N	2.44	0.51
2:G:199:SER:OG	2:G:431:GLY:O	2.26	0.51
6:L:107:LEU:O	6:L:108:SER:OG	2.22	0.51
6:L:46:LEU:O	6:L:46:LEU:HD12	2.10	0.51
6:L:48:ILE:HG12	6:L:54:ARG:HG2	1.93	0.51
2:G:112:TRP:CD2	2:G:427:TRP:HH2	2.29	0.50
5:H:87:THR:O	5:H:87:THR:CG2	2.59	0.50
6:L:50:ASN:HB3	6:L:53:ASP:HB2	1.93	0.50
5:H:114:THR:HG23	5:H:145:PRO:HG3	1.94	0.50
2:G:363:HIS:HD2	2:G:364:SER:HB3	1.74	0.50
2:G:411:GLU:O	7:Q:2:NAG:H81	2.12	0.50
2:G:86:LEU:HB3	2:G:89:VAL:HG21	1.93	0.50
5:H:100(D):VAL:HA	13:T:2:NAG:O7	2.12	0.50
6:L:13:VAL:HG11	6:L:19:ALA:HB2	1.93	0.50
6:L:51:ASN:HB3	6:L:52:GLN:OE1	2.12	0.50
2:G:203:GLN:HG3	2:G:435:TYR:HD2	1.77	0.49
2:G:349:LEU:O	2:G:353:PHE:HB2	2.12	0.49
5:H:19:SER:O	5:H:20:VAL:CG2	2.61	0.49
2:G:93:PHE:CD2	2:G:228:CYS:HB2	2.48	0.49
2:G:112:TRP:CG	2:G:427:TRP:HH2	2.31	0.49
5:H:61:PRO:HA	5:H:64:ASN:HB2	1.95	0.49
3:D:30:ASN:O	8:C:1:NAG:O6	2.31	0.49
4:E:30:CYS:HB3	4:E:68:LYS:HD2	1.93	0.49
2:G:388:THR:HB	2:G:389:PRO:HD3	1.94	0.49
1:B:515:LEU:H	1:B:515:LEU:HD23	1.78	0.48
1:B:625:ASN:HD22	7:A:1:NAG:C1	2.26	0.48
2:G:391:PHE:CE2	2:G:470:PRO:HG3	2.48	0.48
2:G:120:VAL:O	2:G:203:GLN:N	2.42	0.48
2:G:93:PHE:CE2	2:G:228:CYS:HB2	2.48	0.48
5:H:7:SER:O	5:H:20:VAL:HG13	2.13	0.48
5:H:100(A):ILE:HG23	5:H:100(J):PHE:HB3	1.95	0.48
5:H:143:TYR:O	5:H:174:TYR:N	2.35	0.48
6:L:168:GLN:HG2	6:L:172:LYS:O	2.13	0.48
6:L:67(A):ILE:HG22	13:T:5:MAN:H2	1.95	0.48
4:E:198:GLN:HG2	4:E:207:GLU:HG3	1.95	0.48
2:G:98:ASN:ND2	2:G:486:TYR:O	2.47	0.48
1:B:610:TRP:CE3	2:G:498:PRO:HB3	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:60:ASN:O	5:H:64:ASN:N	2.47	0.48
5:H:100(D):VAL:HG12	5:H:100(F):SER:H	1.78	0.48
2:G:265:LEU:HD11	2:G:291:ALA:HB2	1.96	0.48
5:H:144:PHE:N	5:H:145:PRO:HD2	2.29	0.48
4:E:36:SER:OG	4:E:91:CYS:HB3	2.14	0.48
2:G:105:HIS:CG	2:G:476:ARG:HG2	2.48	0.48
5:H:139:LEU:HD23	5:H:140:VAL:N	2.29	0.47
3:D:94:LYS:HB3	3:D:102:LEU:HB2	1.96	0.47
11:P:3:BMA:O2	11:P:4:MAN:C1	2.63	0.47
2:G:293:GLU:OE2	10:S:1:NAG:H61	2.15	0.47
2:G:276:ASN:HB3	2:G:282:LYS:HG3	1.96	0.47
5:H:121:PRO:O	6:L:122:SER:HB3	2.15	0.47
6:L:36:TYR:CE1	6:L:46:LEU:HB3	2.50	0.47
2:G:216:HIS:ND1	2:G:248:THR:O	2.45	0.47
2:G:67:ASN:OD1	2:G:209:SER:OG	2.31	0.47
5:H:143:TYR:CZ	5:H:148:VAL:HG21	2.50	0.47
2:G:230:SER:HB2	2:G:233:PHE:HB2	1.96	0.47
5:H:35:THR:OG1	5:H:47:TRP:NE1	2.44	0.47
7:K:3:BMA:H2	7:K:4:MAN:H5	1.97	0.47
2:G:223:PHE:CE2	2:G:490:LYS:HB3	2.50	0.46
4:E:50:ILE:HD13	4:E:56:ARG:HA	1.98	0.46
2:G:156:ASN:OD1	2:G:157:CYS:N	2.49	0.46
4:E:188:GLN:O	4:E:192:HIS:ND1	2.48	0.46
10:O:2:NAG:O7	10:O:2:NAG:O3	2.30	0.46
3:D:114:ALA:HB3	3:D:146:PHE:CZ	2.51	0.46
3:D:47:TRP:CH2	4:E:98:GLY:HA3	2.51	0.46
3:D:207:VAL:HG12	3:D:209:LYS:HG2	1.97	0.46
10:O:2:NAG:H4	10:O:3:BMA:H2	1.73	0.45
5:H:146:GLU:N	5:H:147:PRO:HD2	2.32	0.45
2:G:279:ASP:HB3	2:G:282:LYS:HG2	1.97	0.45
5:H:94:THR:CG2	5:H:94:THR:O	2.64	0.45
5:H:2:VAL:HA	5:H:26:GLY:HA3	1.98	0.45
3:D:56:ASP:OD1	3:D:57:LYS:N	2.49	0.45
6:L:67(A):ILE:HG13	6:L:67(B):ASN:H	1.82	0.45
2:G:280:ASN:ND2	2:G:458:GLY:HA2	2.32	0.45
2:G:363:HIS:HA	2:G:470:PRO:HD2	1.99	0.45
5:H:143:TYR:CE1	5:H:174:TYR:HB2	2.52	0.45
5:H:18:LEU:O	5:H:81:GLN:HA	2.16	0.45
6:L:31:ARG:NH1	6:L:51:ASN:ND2	2.65	0.45
2:G:274:SER:HB3	2:G:277:ILE:HG12	1.98	0.44
2:G:203:GLN:HE22	2:G:318:TYR:HD2	1.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:100:ARG:HH12	13:T:5:MAN:C6	2.31	0.44
3:D:116:THR:HG23	3:D:147:PRO:HG2	2.00	0.44
4:E:38:TYR:CZ	4:E:48:LEU:HD13	2.52	0.44
5:H:182:VAL:HG21	5:H:192:TYR:HE2	1.82	0.44
10:M:1:NAG:H61	10:M:2:NAG:C7	2.48	0.44
1:B:525:ALA:HB1	1:B:528:SER:HB2	1.98	0.44
3:D:189:LEU:HD22	3:D:213:PRO:HB2	1.99	0.44
3:D:94:LYS:HG2	3:D:95:GLY:N	2.31	0.44
2:G:384:TYR:OH	2:G:424:ILE:HD13	2.17	0.44
2:G:192:ARG:NH2	14:G:611:NAG:O5	2.50	0.44
2:G:385:CYS:HA	2:G:418:CYS:HA	2.00	0.44
5:H:117:PRO:HB3	5:H:143:TYR:HD2	1.83	0.44
5:H:51:ILE:HD11	5:H:55:GLU:HA	1.99	0.44
5:H:142:ASP:OD1	5:H:142:ASP:N	2.51	0.43
3:D:144:ASP:H	3:D:177:SER:HG	1.66	0.43
4:E:85:GLU:HG3	4:E:108:SER:HA	2.00	0.43
6:L:31:ARG:HH12	6:L:51:ASN:ND2	2.16	0.43
2:G:332:ASN:HB3	10:M:1:NAG:H81	2.00	0.43
2:G:195:ASN:HD21	2:G:201:ILE:HD12	1.82	0.43
2:G:229:ASN:CG	10:J:1:NAG:H62	2.39	0.43
6:L:156:VAL:HG11	6:L:179:LEU:HD11	2.00	0.43
2:G:160:ASN:N	2:G:160:ASN:OD1	2.51	0.43
1:B:610:TRP:CD2	2:G:498:PRO:HB3	2.53	0.43
4:E:169:SER:O	4:E:177:ALA:N	2.44	0.43
1:B:596:TRP:CE2	1:B:646:LEU:HD23	2.54	0.43
2:G:55:ALA:N	2:G:216:HIS:O	2.52	0.43
2:G:363:HIS:CE1	2:G:388:THR:HG23	2.54	0.43
1:B:606:THR:HG21	1:B:646:LEU:HD11	2.00	0.42
2:G:363:HIS:HE1	2:G:388:THR:HG23	1.84	0.42
5:H:117:PRO:HB3	5:H:143:TYR:CD2	2.54	0.42
5:H:29:ILE:HB	5:H:71:ARG:NE	2.32	0.42
5:H:153:ASN:HB2	5:H:156:ALA:HB3	2.01	0.42
4:E:126:SER:O	4:E:130:GLN:HG3	2.19	0.42
2:G:101:VAL:HG13	2:G:479:TRP:HB2	2.00	0.42
2:G:359:ILE:HG12	2:G:465:THR:HB	2.01	0.42
2:G:359:ILE:HG13	2:G:466:GLU:O	2.20	0.42
5:H:96:ARG:HD2	5:H:100(O):TYR:OH	2.20	0.42
6:L:141:TYR:CB	6:L:142:PRO:HD3	2.48	0.42
2:G:338:TRP:HE1	2:G:342:LEU:HD12	1.84	0.42
2:G:70:ALA:HB3	2:G:213:ILE:HG22	2.02	0.42
2:G:50:THR:HG22	2:G:488:VAL:HG21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:229:ASN:ND2	10:J:1:NAG:H62	2.35	0.42
6:L:114:PRO:HB3	6:L:140:PHE:HB3	2.02	0.42
1:B:597:GLY:N	1:B:651:ILE:HG12	2.35	0.42
2:G:184:LEU:HG	2:G:190:ASN:HB2	2.02	0.42
2:G:304:ARG:HB3	2:G:440:ARG:NH1	2.34	0.42
6:L:133:LEU:HB2	6:L:179:LEU:HB3	2.02	0.42
3:D:56:ASP:OD2	8:C:4:MAN:O4	2.38	0.41
1:B:607:ASN:H	1:B:650:GLN:CD	2.24	0.41
4:E:94:THR:OG1	4:E:97:SER:HB3	2.19	0.41
2:G:505:VAL:O	2:G:507:GLN:HG3	2.21	0.41
3:D:63:PHE:HB3	3:D:67:VAL:CG2	2.49	0.41
2:G:496:ILE:H	2:G:496:ILE:HG13	1.63	0.41
13:T:5:MAN:H2	13:T:6:MAN:H2	1.87	0.41
3:D:148:GLU:N	3:D:149:PRO:CD	2.83	0.41
2:G:121:LYS:HB3	2:G:121:LYS:HE2	1.88	0.41
5:H:93:ALA:HB1	5:H:100(P):MET:HB3	2.01	0.41
6:L:146:THR:OG1	6:L:197:THR:HB	2.21	0.41
3:D:28:ARG:HG2	3:D:72(H):PHE:O	2.20	0.41
4:E:37:TRP:HD1	4:E:50:ILE:HG21	1.85	0.41
5:H:182:VAL:HG11	5:H:192:TYR:CE2	2.56	0.41
5:H:151:SER:OG	5:H:195:ASN:HB2	2.20	0.40
4:E:52:GLU:O	4:E:53:ASP:HB2	2.22	0.40
2:G:231:LYS:HD3	2:G:231:LYS:HA	1.90	0.40
5:H:39:GLN:OE1	6:L:38:HIS:NE2	2.54	0.40
2:G:257:THR:OG1	2:G:375:SER:OG	2.30	0.40
6:L:65:THR:OG1	6:L:71:ALA:HA	2.21	0.40
1:B:601:LYS:HE2	1:B:604:CYS:HB3	2.03	0.40
3:D:100(E):LEU:HD12	3:D:100(F):PRO:HD2	2.03	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	B	132/153 (86%)	120 (91%)	11 (8%)	1 (1%)	19	56
2	G	447/482 (93%)	411 (92%)	36 (8%)	0	100	100
3	D	238/243 (98%)	229 (96%)	9 (4%)	0	100	100
4	E	211/216 (98%)	197 (93%)	14 (7%)	0	100	100
5	H	227/236 (96%)	215 (95%)	12 (5%)	0	100	100
6	L	209/214 (98%)	191 (91%)	18 (9%)	0	100	100
All	All	1464/1544 (95%)	1363 (93%)	100 (7%)	1 (0%)	51	83

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	651	ILE

5.3.2 Protein sidechains ⓘ

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	B	115/130 (88%)	111 (96%)	4 (4%)	36	63
2	G	401/427 (94%)	381 (95%)	20 (5%)	24	55
3	D	203/206 (98%)	201 (99%)	2 (1%)	76	86
4	E	186/189 (98%)	185 (100%)	1 (0%)	88	94
5	H	199/204 (98%)	195 (98%)	4 (2%)	55	75
6	L	177/180 (98%)	174 (98%)	3 (2%)	60	78
All	All	1281/1336 (96%)	1247 (97%)	34 (3%)	44	68

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	607	ASN
1	B	624	ASP
1	B	647	GLU
1	B	651	ILE

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Mol	Chain	Res	Type
2	G	54	CYS
2	G	135	ASN
2	G	160	ASN
2	G	190	ASN
2	G	201	ILE
2	G	253	PRO
2	G	259	LEU
2	G	264	SER
2	G	327	ARG
2	G	361	PHE
2	G	374	HIS
2	G	378	CYS
2	G	408	THR
2	G	411	GLU
2	G	427	TRP
2	G	448	ASN
2	G	463	ASN
2	G	465	THR
2	G	467	THR
2	G	507	GLN
3	D	148	GLU
3	D	164	HIS
4	E	173	ASN
5	H	32	TYR
5	H	78	LEU
5	H	187	LEU
5	H	190	GLN
6	L	31	ARG
6	L	95(B)	PHE
6	L	134	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
2	G	258	GLN
2	G	262	ASN
2	G	287	GLN
2	G	363	HIS
2	G	413	ASN
2	G	463	ASN
6	L	51	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

62 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	$\# Z > 2$
7	NAG	A	1	1,7	14,14,15	0.58	0	17,19,21	0.65	0
7	NAG	A	2	3,7	14,14,15	0.26	0	17,19,21	1.08	1 (5%)
7	BMA	A	3	7	11,11,12	0.61	0	15,15,17	1.76	3 (20%)
7	MAN	A	4	7	11,11,12	0.56	0	15,15,17	0.88	1 (6%)
7	MAN	A	5	7	11,11,12	0.46	0	15,15,17	0.73	0
8	NAG	C	1	8,2	14,14,15	0.55	0	17,19,21	0.43	0
8	NAG	C	2	8	14,14,15	0.37	0	17,19,21	0.49	0
8	BMA	C	3	8	11,11,12	0.26	0	15,15,17	1.34	3 (20%)
8	MAN	C	4	8	11,11,12	0.92	1 (9%)	15,15,17	2.61	5 (33%)
8	MAN	C	5	8	11,11,12	0.54	0	15,15,17	1.30	2 (13%)
8	MAN	C	6	8	11,11,12	0.29	0	15,15,17	0.84	1 (6%)
8	MAN	C	7	8	11,11,12	0.25	0	15,15,17	0.97	1 (6%)
9	NAG	F	1	9,2	14,14,15	0.20	0	17,19,21	0.48	0
9	NAG	F	2	9	14,14,15	0.33	0	17,19,21	0.47	0
7	NAG	I	1	2,7	14,14,15	0.29	0	17,19,21	0.47	0
7	NAG	I	2	7	14,14,15	1.14	1 (7%)	17,19,21	1.32	1 (5%)
7	BMA	I	3	7	11,11,12	0.37	0	15,15,17	1.26	1 (6%)
7	MAN	I	4	7	11,11,12	0.44	0	15,15,17	0.87	0
7	MAN	I	5	7	11,11,12	0.36	0	15,15,17	0.77	0
10	NAG	J	1	10,2	14,14,15	0.94	1 (7%)	17,19,21	1.80	5 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	NAG	J	2	10	14,14,15	1.02	1 (7%)	17,19,21	0.83	1 (5%)
10	BMA	J	3	10	11,11,12	0.40	0	15,15,17	0.77	0
7	NAG	K	1	7	14,14,15	1.12	1 (7%)	17,19,21	0.51	0
7	NAG	K	2	7	14,14,15	0.14	0	17,19,21	0.47	0
7	BMA	K	3	7	11,11,12	0.44	0	15,15,17	1.12	1 (6%)
7	MAN	K	4	7	11,11,12	0.58	0	15,15,17	0.93	1 (6%)
7	MAN	K	5	7	11,11,12	0.43	0	15,15,17	0.81	1 (6%)
10	NAG	M	1	10,2	14,14,15	0.72	1 (7%)	17,19,21	0.55	0
10	NAG	M	2	10	14,14,15	0.41	0	17,19,21	1.34	2 (11%)
10	BMA	M	3	10	11,11,12	0.38	0	15,15,17	0.82	0
11	NAG	N	1	11,2	14,14,15	0.29	0	17,19,21	0.53	0
11	NAG	N	2	11	14,14,15	0.38	0	17,19,21	0.55	0
11	BMA	N	3	11	11,11,12	0.72	0	15,15,17	1.20	0
11	MAN	N	4	11	11,11,12	0.81	0	15,15,17	1.38	3 (20%)
10	NAG	O	1	10,2	14,14,15	0.43	0	17,19,21	0.55	0
10	NAG	O	2	10	14,14,15	0.53	0	17,19,21	0.47	0
10	BMA	O	3	10	11,11,12	0.64	0	15,15,17	0.79	0
11	NAG	P	1	11,2	14,14,15	0.34	0	17,19,21	0.63	0
11	NAG	P	2	11	14,14,15	0.53	0	17,19,21	0.64	0
11	BMA	P	3	11	11,11,12	0.25	0	15,15,17	0.76	0
11	MAN	P	4	11	11,11,12	0.24	0	15,15,17	0.57	0
7	NAG	Q	1	2,7	14,14,15	0.31	0	17,19,21	0.48	0
7	NAG	Q	2	2,7	14,14,15	0.54	0	17,19,21	0.93	1 (5%)
7	BMA	Q	3	7	11,11,12	0.56	0	15,15,17	1.11	1 (6%)
7	MAN	Q	4	7	11,11,12	0.31	0	15,15,17	0.88	1 (6%)
7	MAN	Q	5	7	11,11,12	0.32	0	15,15,17	0.87	1 (6%)
12	NAG	R	1	12	14,14,15	0.64	1 (7%)	17,19,21	0.58	0
12	NAG	R	2	12	14,14,15	0.53	0	17,19,21	1.42	2 (11%)
12	BMA	R	3	12	11,11,12	0.32	0	15,15,17	0.75	0
12	MAN	R	4	12	11,11,12	0.61	0	15,15,17	0.66	0
10	NAG	S	1	10,2	14,14,15	0.33	0	17,19,21	0.51	0
10	NAG	S	2	10	14,14,15	0.37	0	17,19,21	0.60	0
10	BMA	S	3	10	11,11,12	0.41	0	15,15,17	0.85	1 (6%)
13	NAG	T	1	13	14,14,15	0.49	0	17,19,21	0.59	0
13	NAG	T	2	13	14,14,15	0.91	1 (7%)	17,19,21	0.95	1 (5%)
13	BMA	T	3	13	11,11,12	0.85	0	15,15,17	2.89	5 (33%)
13	MAN	T	4	13	11,11,12	0.36	0	15,15,17	1.70	3 (20%)
13	MAN	T	5	13,6	11,11,12	0.49	0	15,15,17	1.76	3 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	MAN	T	6	13	11,11,12	0.24	0	15,15,17	0.75	0
13	MAN	T	7	13	11,11,12	0.32	0	15,15,17	0.92	0
13	MAN	T	8	13	11,11,12	0.36	0	15,15,17	0.69	0
13	MAN	T	9	13	11,11,12	0.43	0	15,15,17	0.85	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
7	NAG	A	1	1,7	-	0/6/23/26	0/1/1/1
7	NAG	A	2	3,7	-	2/6/23/26	0/1/1/1
7	BMA	A	3	7	-	1/2/19/22	0/1/1/1
7	MAN	A	4	7	-	0/2/19/22	0/1/1/1
7	MAN	A	5	7	-	2/2/19/22	0/1/1/1
8	NAG	C	1	8,2	-	2/6/23/26	0/1/1/1
8	NAG	C	2	8	-	0/6/23/26	0/1/1/1
8	BMA	C	3	8	-	2/2/19/22	0/1/1/1
8	MAN	C	4	8	-	2/2/19/22	0/1/1/1
8	MAN	C	5	8	-	2/2/19/22	0/1/1/1
8	MAN	C	6	8	-	2/2/19/22	0/1/1/1
8	MAN	C	7	8	-	2/2/19/22	0/1/1/1
9	NAG	F	1	9,2	-	0/6/23/26	0/1/1/1
9	NAG	F	2	9	-	2/6/23/26	0/1/1/1
7	NAG	I	1	2,7	-	1/6/23/26	0/1/1/1
7	NAG	I	2	7	-	4/6/23/26	0/1/1/1
7	BMA	I	3	7	-	2/2/19/22	0/1/1/1
7	MAN	I	4	7	-	0/2/19/22	0/1/1/1
7	MAN	I	5	7	-	2/2/19/22	0/1/1/1
10	NAG	J	1	10,2	-	3/6/23/26	0/1/1/1
10	NAG	J	2	10	-	2/6/23/26	0/1/1/1
10	BMA	J	3	10	-	0/2/19/22	0/1/1/1
7	NAG	K	1	7	-	1/6/23/26	0/1/1/1
7	NAG	K	2	7	-	0/6/23/26	0/1/1/1
7	BMA	K	3	7	-	2/2/19/22	0/1/1/1
7	MAN	K	4	7	-	0/2/19/22	0/1/1/1
7	MAN	K	5	7	-	0/2/19/22	0/1/1/1
10	NAG	M	1	10,2	-	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	NAG	M	2	10	-	2/6/23/26	0/1/1/1
10	BMA	M	3	10	-	0/2/19/22	0/1/1/1
11	NAG	N	1	11,2	-	2/6/23/26	0/1/1/1
11	NAG	N	2	11	-	4/6/23/26	0/1/1/1
11	BMA	N	3	11	-	1/2/19/22	0/1/1/1
11	MAN	N	4	11	-	1/2/19/22	0/1/1/1
10	NAG	O	1	10,2	-	1/6/23/26	0/1/1/1
10	NAG	O	2	10	-	3/6/23/26	0/1/1/1
10	BMA	O	3	10	-	1/2/19/22	0/1/1/1
11	NAG	P	1	11,2	-	4/6/23/26	0/1/1/1
11	NAG	P	2	11	-	2/6/23/26	0/1/1/1
11	BMA	P	3	11	-	1/2/19/22	0/1/1/1
11	MAN	P	4	11	-	0/2/19/22	0/1/1/1
7	NAG	Q	1	2,7	-	4/6/23/26	0/1/1/1
7	NAG	Q	2	2,7	-	0/6/23/26	0/1/1/1
7	BMA	Q	3	7	-	2/2/19/22	0/1/1/1
7	MAN	Q	4	7	-	0/2/19/22	0/1/1/1
7	MAN	Q	5	7	-	0/2/19/22	0/1/1/1
12	NAG	R	1	12	-	2/6/23/26	0/1/1/1
12	NAG	R	2	12	-	5/6/23/26	0/1/1/1
12	BMA	R	3	12	-	0/2/19/22	0/1/1/1
12	MAN	R	4	12	-	1/2/19/22	0/1/1/1
10	NAG	S	1	10,2	-	2/6/23/26	0/1/1/1
10	NAG	S	2	10	-	0/6/23/26	0/1/1/1
10	BMA	S	3	10	-	0/2/19/22	0/1/1/1
13	NAG	T	1	13	-	2/6/23/26	0/1/1/1
13	NAG	T	2	13	-	1/6/23/26	0/1/1/1
13	BMA	T	3	13	-	1/2/19/22	0/1/1/1
13	MAN	T	4	13	-	2/2/19/22	0/1/1/1
13	MAN	T	5	13,6	-	0/2/19/22	0/1/1/1
13	MAN	T	6	13	-	0/2/19/22	0/1/1/1
13	MAN	T	7	13	-	2/2/19/22	0/1/1/1
13	MAN	T	8	13	-	2/2/19/22	0/1/1/1
13	MAN	T	9	13	-	0/2/19/22	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	K	1	NAG	O5-C1	-4.08	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	I	2	NAG	C1-C2	3.89	1.58	1.52
10	J	2	NAG	O5-C1	-3.60	1.38	1.43
10	J	1	NAG	O5-C1	-2.71	1.39	1.43
13	T	2	NAG	O5-C1	-2.56	1.39	1.43
8	C	4	MAN	O2-C2	2.24	1.48	1.43
12	R	1	NAG	C1-C2	2.11	1.55	1.52
10	M	1	NAG	O5-C1	-2.10	1.40	1.43

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	T	3	BMA	O5-C1-C2	7.65	122.57	110.77
8	C	4	MAN	C1-C2-C3	-6.21	102.04	109.67
13	T	3	BMA	O3-C3-C2	-5.11	100.21	109.99
8	C	4	MAN	O2-C2-C3	4.97	120.10	110.14
10	J	1	NAG	C1-O5-C5	-4.47	106.13	112.19
12	R	2	NAG	C2-N2-C7	4.46	129.26	122.90
13	T	4	MAN	C1-C2-C3	4.21	114.84	109.67
10	M	2	NAG	C1-O5-C5	4.10	117.75	112.19
7	I	2	NAG	C2-N2-C7	4.03	128.65	122.90
13	T	5	MAN	O2-C2-C1	-3.99	100.99	109.15
7	A	3	BMA	O5-C1-C2	-3.83	104.86	110.77
8	C	4	MAN	O2-C2-C1	3.59	116.50	109.15
13	T	3	BMA	O5-C5-C4	-3.57	102.14	110.83
7	I	3	BMA	O5-C5-C6	3.56	112.78	107.20
13	T	5	MAN	O3-C3-C2	-3.30	103.67	109.99
8	C	4	MAN	C6-C5-C4	-3.24	105.42	113.00
10	J	1	NAG	C2-N2-C7	3.08	127.29	122.90
7	K	3	BMA	O3-C3-C2	-3.03	104.19	109.99
13	T	5	MAN	O5-C1-C2	-2.99	106.16	110.77
7	A	3	BMA	C1-O5-C5	-2.89	108.27	112.19
7	Q	2	NAG	C2-N2-C7	2.81	126.90	122.90
8	C	7	MAN	O5-C1-C2	-2.79	106.46	110.77
13	T	3	BMA	C1-O5-C5	-2.74	108.47	112.19
13	T	4	MAN	O5-C1-C2	-2.70	106.61	110.77
13	T	3	BMA	O2-C2-C1	2.60	114.47	109.15
8	C	3	BMA	O5-C1-C2	-2.57	106.80	110.77
11	N	4	MAN	O5-C5-C6	2.53	111.18	107.20
11	N	4	MAN	C1-C2-C3	2.53	112.77	109.67
8	C	5	MAN	O5-C1-C2	-2.52	106.88	110.77
10	J	1	NAG	O4-C4-C5	-2.50	103.10	109.30
7	K	5	MAN	O5-C1-C2	-2.49	106.93	110.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	R	2	NAG	C1-C2-N2	2.45	114.68	110.49
7	A	2	NAG	C2-N2-C7	2.44	126.38	122.90
10	J	2	NAG	C1-O5-C5	2.38	115.42	112.19
7	Q	3	BMA	O5-C5-C6	-2.36	103.51	107.20
7	Q	5	MAN	O5-C1-C2	-2.31	107.21	110.77
13	T	4	MAN	O2-C2-C1	-2.28	104.48	109.15
8	C	6	MAN	O5-C1-C2	-2.28	107.25	110.77
10	M	2	NAG	C2-N2-C7	2.26	126.12	122.90
10	S	3	BMA	O5-C5-C6	2.24	110.72	107.20
8	C	3	BMA	C1-O5-C5	-2.23	109.17	112.19
10	J	1	NAG	C1-C2-N2	2.23	114.29	110.49
8	C	5	MAN	O5-C5-C6	2.22	110.68	107.20
7	A	3	BMA	C1-C2-C3	-2.21	106.95	109.67
13	T	2	NAG	C3-C4-C5	-2.19	106.33	110.24
11	N	4	MAN	C1-O5-C5	2.16	115.12	112.19
7	K	4	MAN	O5-C1-C2	-2.14	107.47	110.77
8	C	3	BMA	C3-C4-C5	-2.12	106.47	110.24
7	Q	4	MAN	O5-C1-C2	-2.08	107.56	110.77
8	C	4	MAN	O4-C4-C5	-2.05	104.20	109.30
10	J	1	NAG	C3-C4-C5	2.05	113.90	110.24
7	A	4	MAN	O5-C1-C2	-2.05	107.61	110.77

There are no chirality outliers.

All (88) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	J	1	NAG	C4-C5-C6-O6
11	P	1	NAG	O5-C5-C6-O6
7	K	3	BMA	C4-C5-C6-O6
8	C	4	MAN	C4-C5-C6-O6
8	C	1	NAG	O5-C5-C6-O6
7	Q	3	BMA	O5-C5-C6-O6
8	C	7	MAN	O5-C5-C6-O6
10	S	1	NAG	O5-C5-C6-O6
13	T	4	MAN	O5-C5-C6-O6
8	C	6	MAN	O5-C5-C6-O6
10	J	1	NAG	O5-C5-C6-O6
11	P	2	NAG	O5-C5-C6-O6
10	M	1	NAG	O5-C5-C6-O6
13	T	8	MAN	O5-C5-C6-O6
7	Q	3	BMA	C4-C5-C6-O6
8	C	4	MAN	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
7	I	3	BMA	O5-C5-C6-O6
7	K	3	BMA	O5-C5-C6-O6
7	I	5	MAN	O5-C5-C6-O6
10	O	2	NAG	C1-C2-N2-C7
11	P	1	NAG	C1-C2-N2-C7
10	J	1	NAG	C1-C2-N2-C7
8	C	1	NAG	C4-C5-C6-O6
11	P	1	NAG	C4-C5-C6-O6
10	M	1	NAG	C4-C5-C6-O6
13	T	8	MAN	C4-C5-C6-O6
12	R	2	NAG	C8-C7-N2-C2
12	R	2	NAG	O7-C7-N2-C2
10	M	1	NAG	C8-C7-N2-C2
10	M	1	NAG	O7-C7-N2-C2
13	T	1	NAG	C8-C7-N2-C2
13	T	1	NAG	O7-C7-N2-C2
7	Q	1	NAG	C8-C7-N2-C2
7	Q	1	NAG	O7-C7-N2-C2
11	N	2	NAG	C8-C7-N2-C2
11	N	2	NAG	O7-C7-N2-C2
12	R	1	NAG	C8-C7-N2-C2
12	R	1	NAG	O7-C7-N2-C2
7	I	2	NAG	C8-C7-N2-C2
7	I	2	NAG	O7-C7-N2-C2
8	C	5	MAN	O5-C5-C6-O6
11	N	4	MAN	O5-C5-C6-O6
11	N	2	NAG	C4-C5-C6-O6
7	I	3	BMA	C4-C5-C6-O6
7	A	2	NAG	C1-C2-N2-C7
11	N	1	NAG	C4-C5-C6-O6
10	J	2	NAG	O5-C5-C6-O6
9	F	2	NAG	C4-C5-C6-O6
11	P	2	NAG	C4-C5-C6-O6
8	C	5	MAN	C4-C5-C6-O6
10	S	1	NAG	C4-C5-C6-O6
7	Q	1	NAG	C4-C5-C6-O6
11	N	2	NAG	O5-C5-C6-O6
8	C	6	MAN	C4-C5-C6-O6
12	R	2	NAG	C4-C5-C6-O6
13	T	7	MAN	O5-C5-C6-O6
7	A	2	NAG	O5-C5-C6-O6
9	F	2	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
8	C	7	MAN	C4-C5-C6-O6
8	C	3	BMA	C4-C5-C6-O6
13	T	2	NAG	O5-C5-C6-O6
11	N	1	NAG	O5-C5-C6-O6
7	I	5	MAN	C4-C5-C6-O6
7	A	3	BMA	O5-C5-C6-O6
11	P	3	BMA	O5-C5-C6-O6
7	Q	1	NAG	O5-C5-C6-O6
7	I	2	NAG	O5-C5-C6-O6
11	N	3	BMA	O5-C5-C6-O6
10	O	2	NAG	O5-C5-C6-O6
10	O	3	BMA	O5-C5-C6-O6
10	O	1	NAG	O5-C5-C6-O6
12	R	4	MAN	O5-C5-C6-O6
10	M	2	NAG	O5-C5-C6-O6
12	R	2	NAG	O5-C5-C6-O6
10	M	2	NAG	C3-C2-N2-C7
7	I	1	NAG	C4-C5-C6-O6
10	J	2	NAG	C4-C5-C6-O6
13	T	7	MAN	C4-C5-C6-O6
13	T	4	MAN	C4-C5-C6-O6
13	T	3	BMA	C4-C5-C6-O6
8	C	3	BMA	O5-C5-C6-O6
7	K	1	NAG	C1-C2-N2-C7
10	O	2	NAG	C3-C2-N2-C7
11	P	1	NAG	C3-C2-N2-C7
7	I	2	NAG	C3-C2-N2-C7
7	A	5	MAN	C4-C5-C6-O6
12	R	2	NAG	C3-C2-N2-C7
7	A	5	MAN	O5-C5-C6-O6

There are no ring outliers.

29 monomers are involved in 43 short contacts:

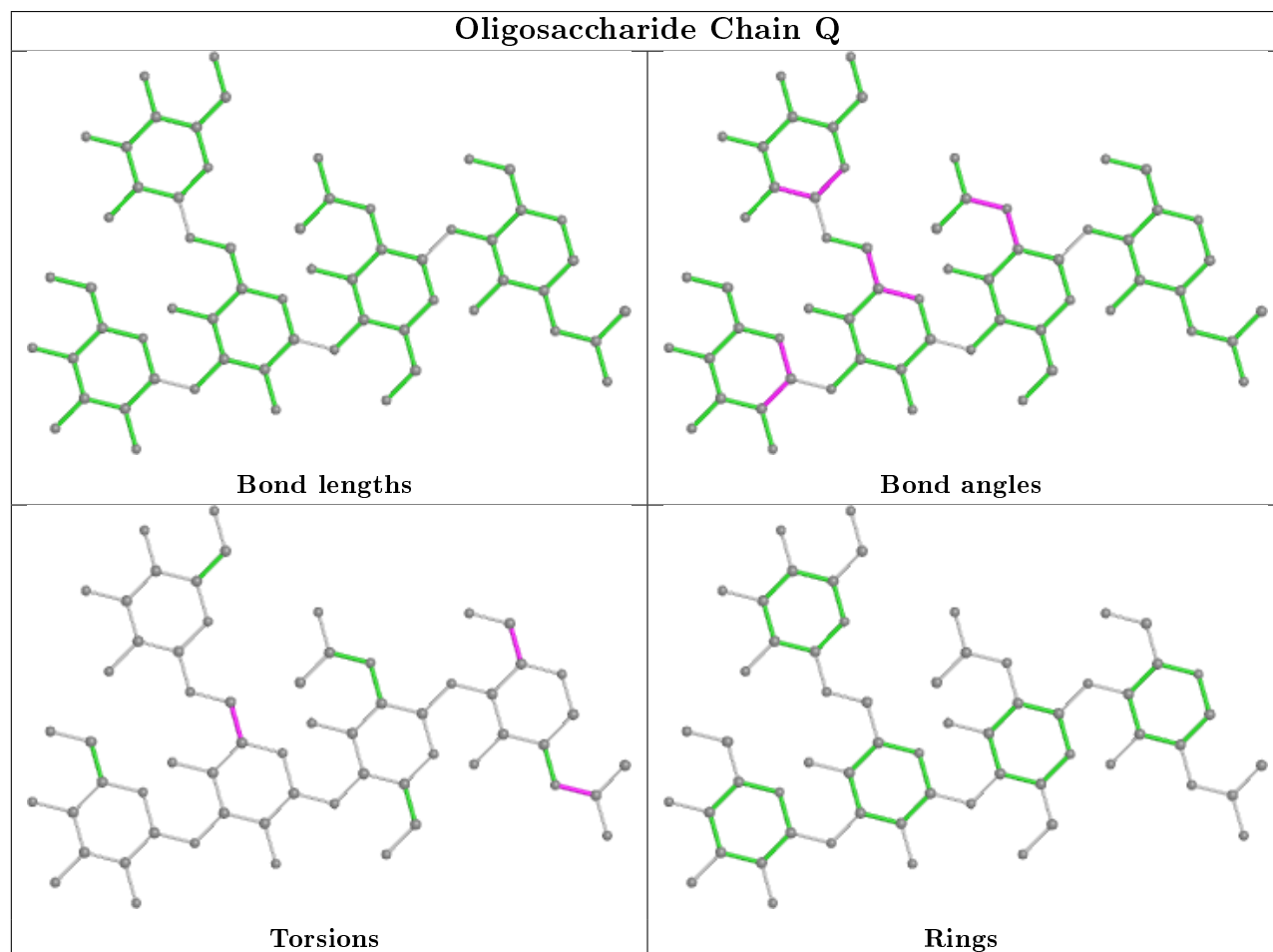
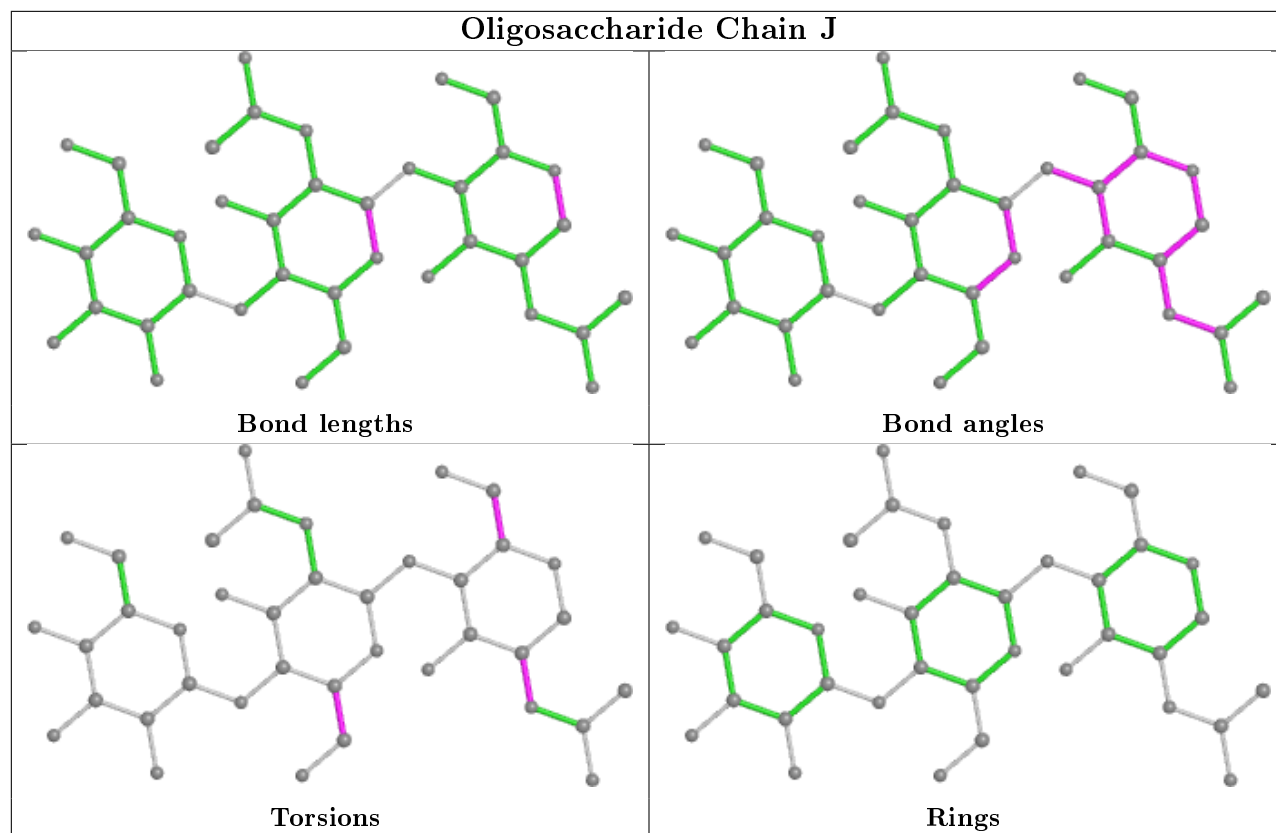
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	C	3	BMA	1	0
8	C	6	MAN	1	0
10	O	2	NAG	2	0
12	R	2	NAG	2	0
8	C	4	MAN	2	0
10	O	3	BMA	1	0
7	A	1	NAG	2	0

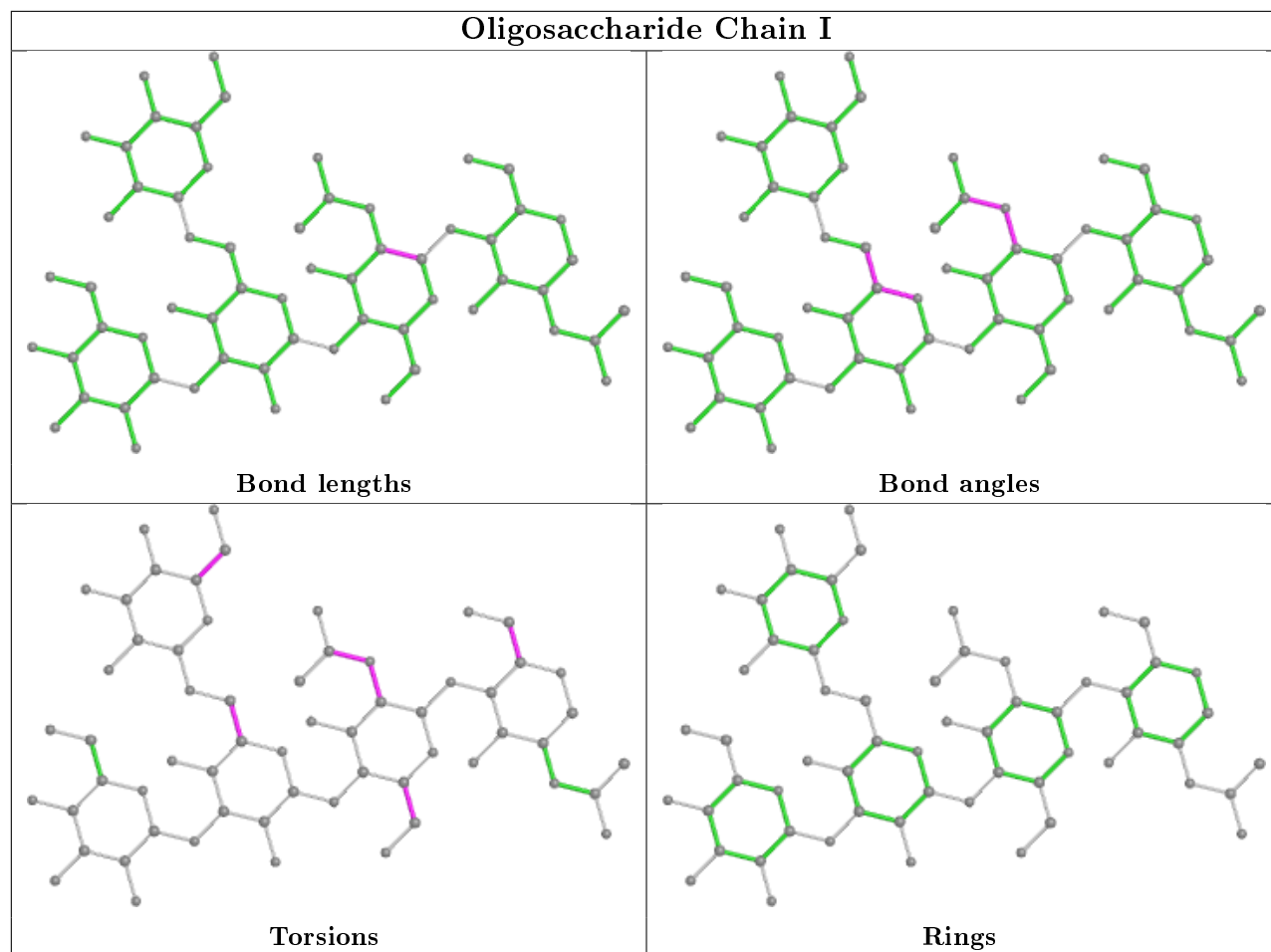
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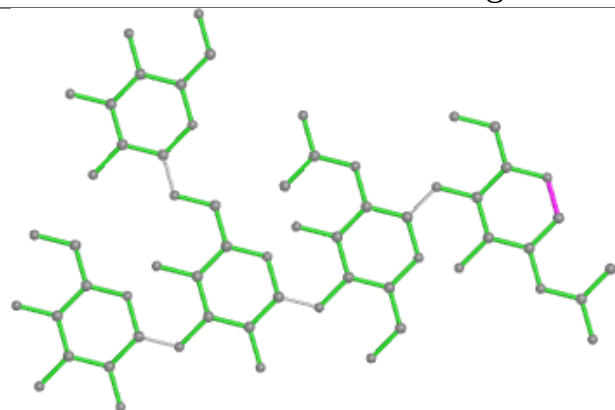
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	P	4	MAN	1	0
10	M	1	NAG	3	0
10	S	1	NAG	1	0
10	M	2	NAG	1	0
7	K	3	BMA	1	0
8	C	1	NAG	3	0
13	T	1	NAG	5	0
7	Q	1	NAG	2	0
11	P	3	BMA	1	0
7	K	1	NAG	2	0
10	J	1	NAG	2	0
8	C	7	MAN	1	0
7	K	4	MAN	1	0
13	T	2	NAG	1	0
13	T	4	MAN	1	0
13	T	5	MAN	4	0
12	R	1	NAG	3	0
7	Q	2	NAG	1	0
8	C	5	MAN	1	0
13	T	6	MAN	1	0
7	I	2	NAG	1	0
7	A	2	NAG	2	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.

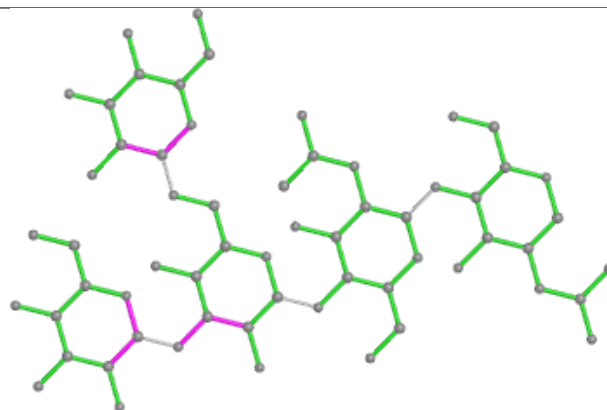




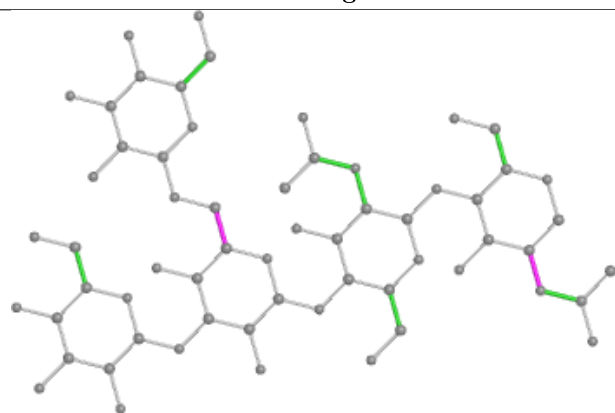
Oligosaccharide Chain K



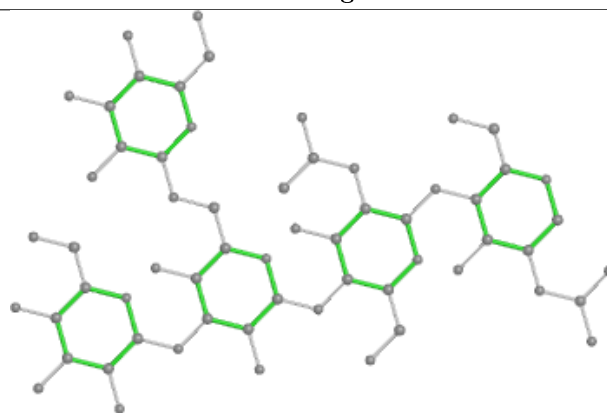
Bond lengths



Bond angles

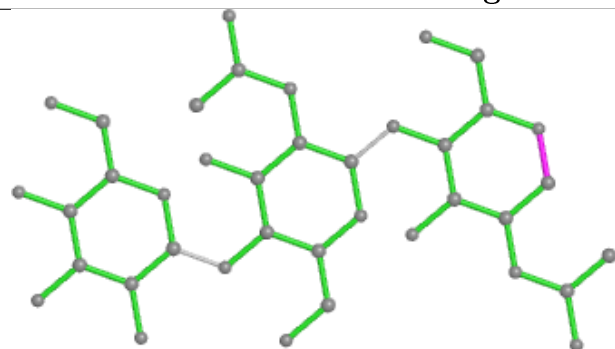


Torsions

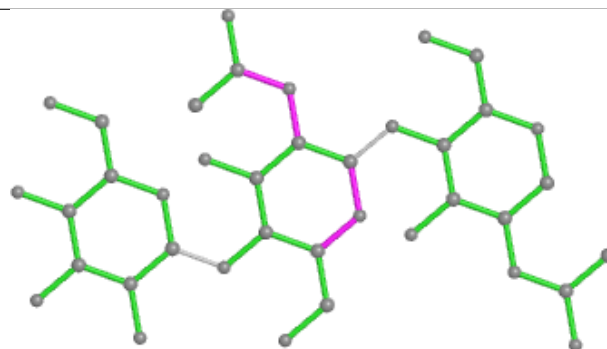


Rings

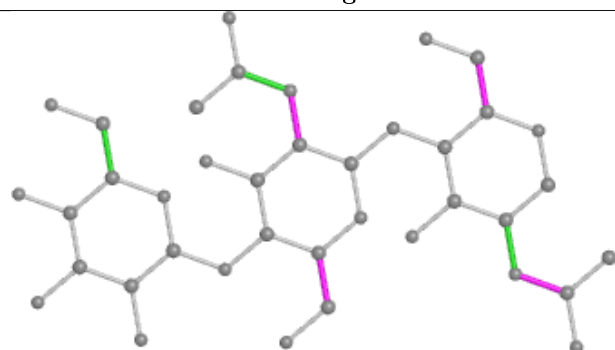
Oligosaccharide Chain M



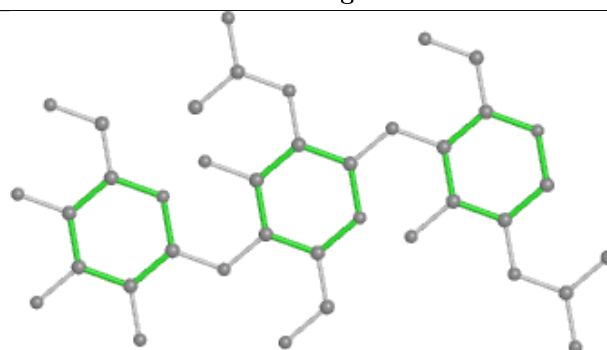
Bond lengths



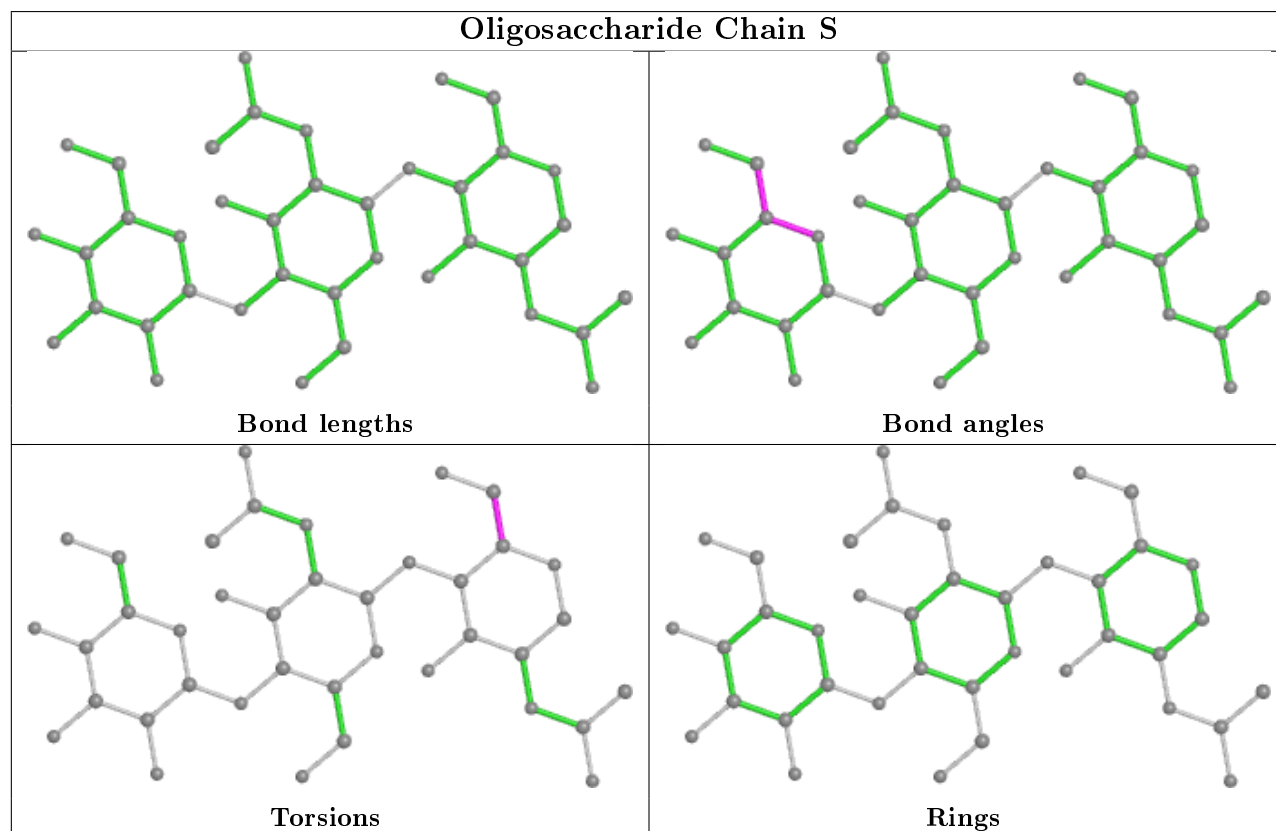
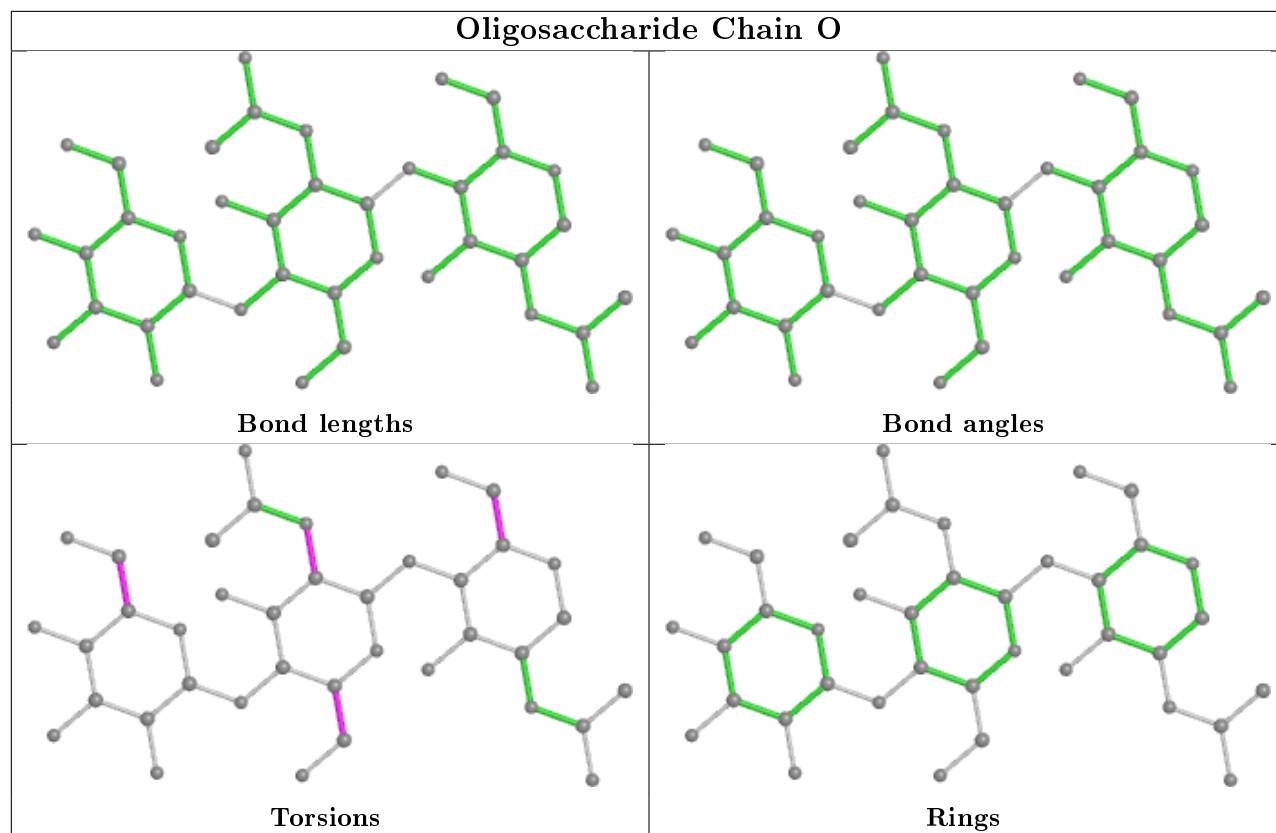
Bond angles

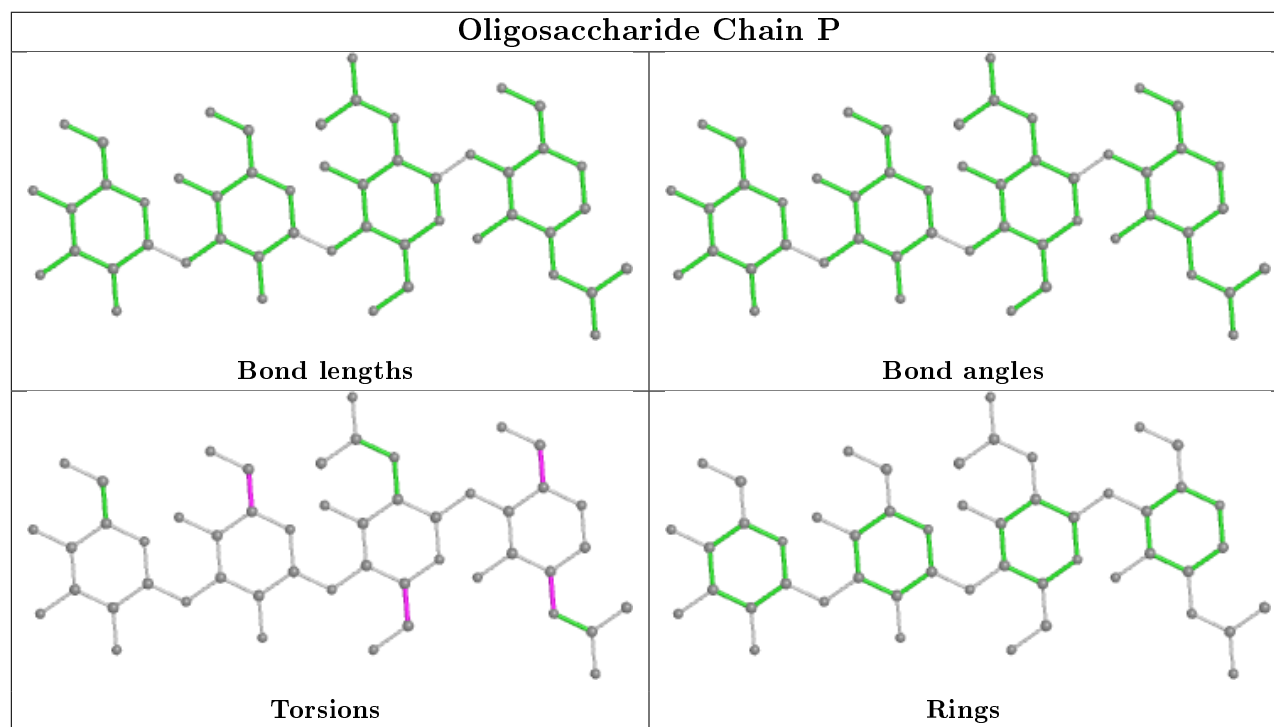
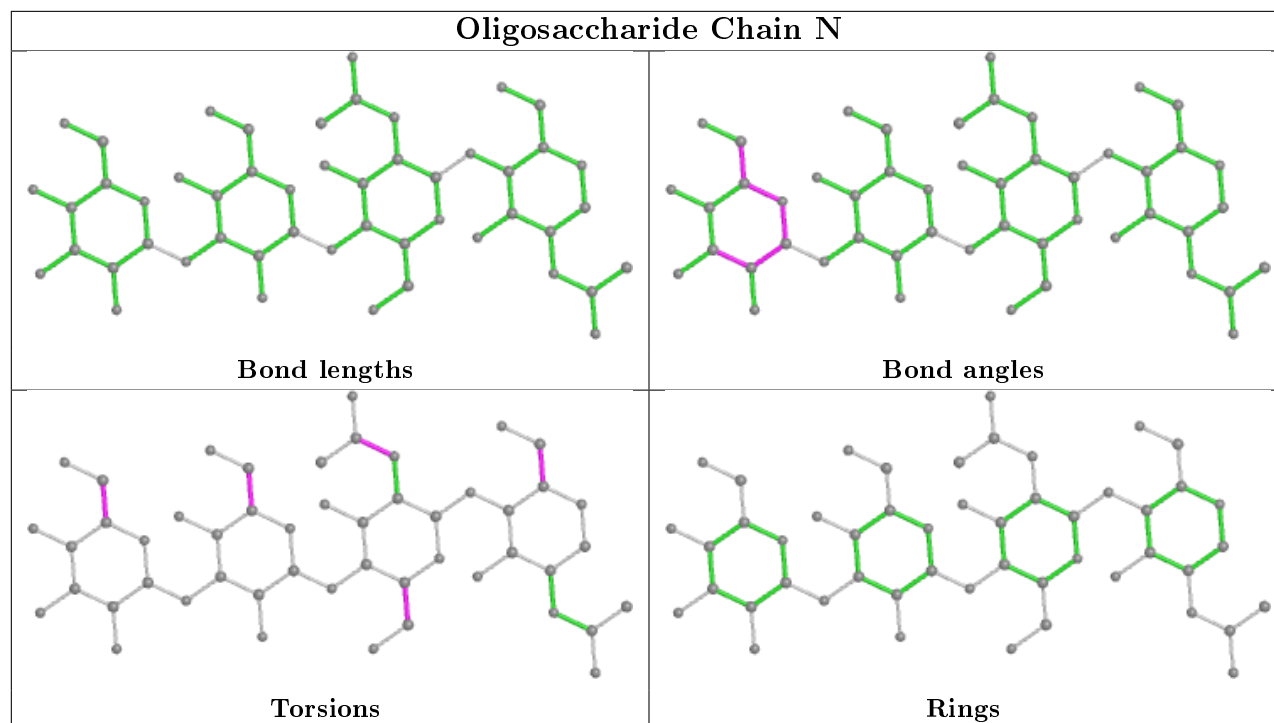


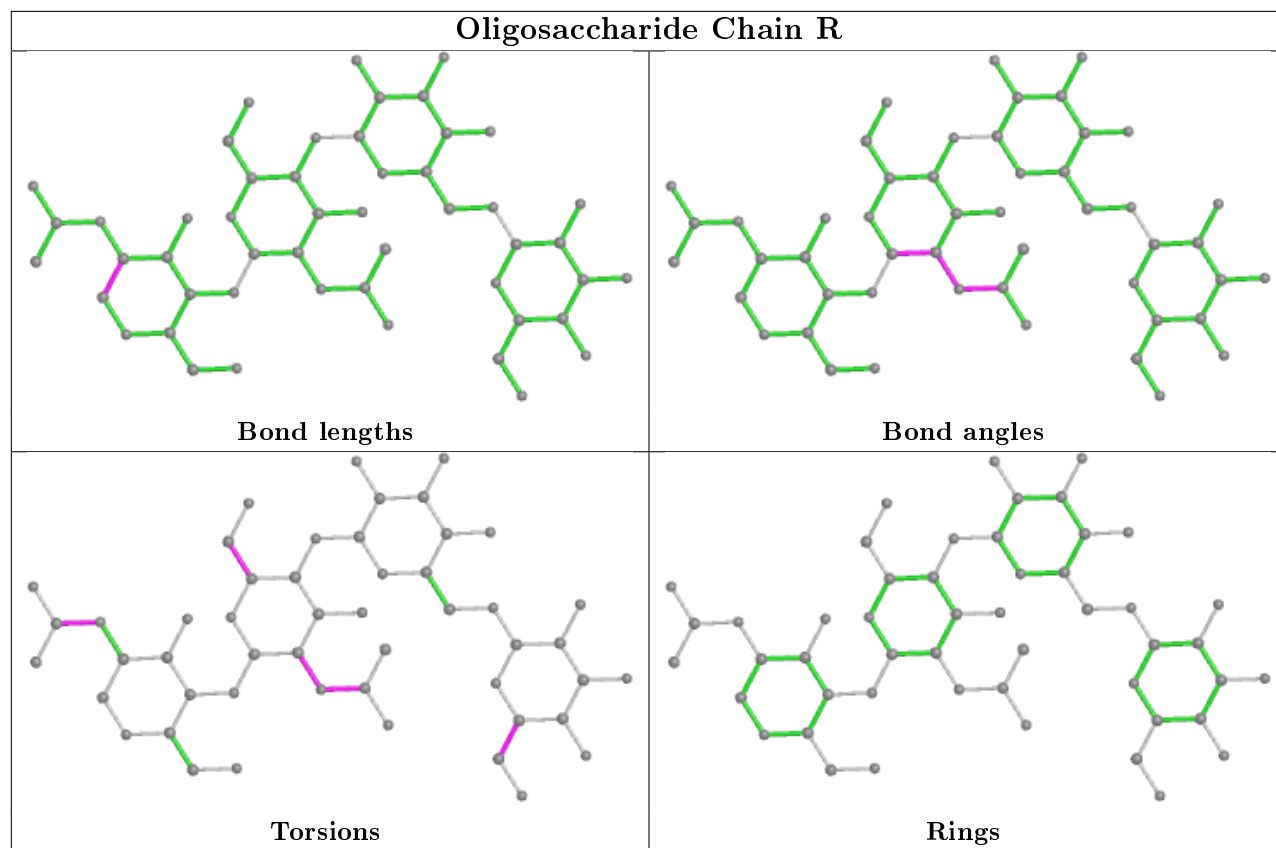
Torsions

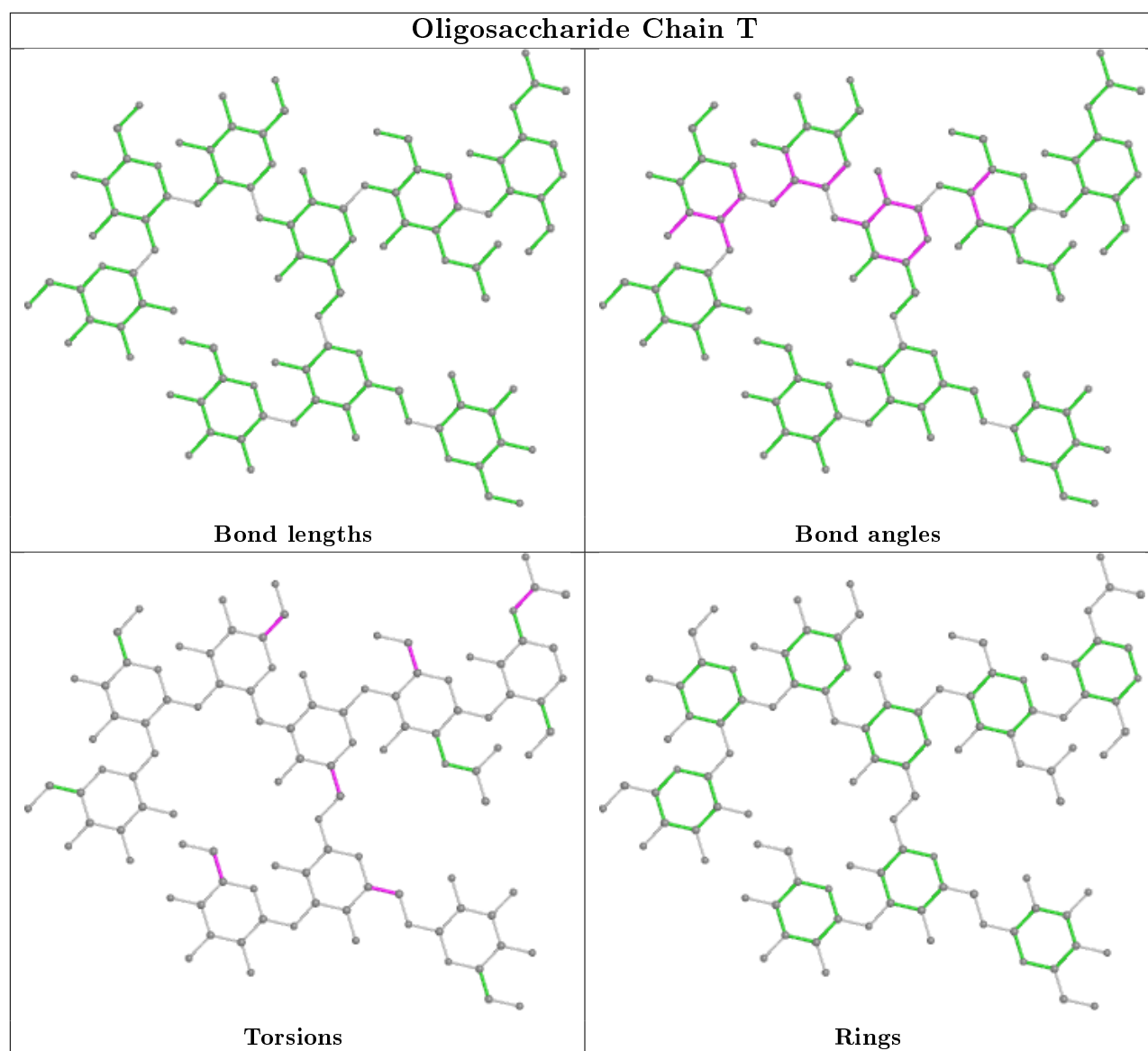


Rings









5.6 Ligand geometry ⓘ

9 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	$\# Z > 2$
14	NAG	G	625	2	14,14,15	0.26	0	17,19,21	0.34	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	NAG	B	701	1	14,14,15	0.22	0	17,19,21	0.40	0
14	NAG	G	646	2	14,14,15	0.53	0	17,19,21	0.61	1 (5%)
14	NAG	G	633	2	14,14,15	0.28	0	17,19,21	0.54	0
14	NAG	G	610	2	14,14,15	0.36	0	17,19,21	0.46	0
14	NAG	G	611	2	14,14,15	0.53	0	17,19,21	0.91	1 (5%)
14	NAG	B	707	1	14,14,15	0.51	0	17,19,21	0.41	0
14	NAG	G	654	2	14,14,15	0.27	0	17,19,21	0.65	0
14	NAG	B	708	1	14,14,15	0.34	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
14	NAG	G	625	2	-	0/6/23/26	0/1/1/1
14	NAG	B	701	1	-	0/6/23/26	0/1/1/1
14	NAG	G	646	2	-	2/6/23/26	0/1/1/1
14	NAG	G	633	2	-	2/6/23/26	0/1/1/1
14	NAG	G	610	2	-	4/6/23/26	0/1/1/1
14	NAG	G	611	2	-	0/6/23/26	0/1/1/1
14	NAG	B	707	1	-	0/6/23/26	0/1/1/1
14	NAG	G	654	2	-	2/6/23/26	0/1/1/1
14	NAG	B	708	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	G	611	NAG	C1-O5-C5	3.43	116.84	112.19
14	G	646	NAG	C1-O5-C5	2.02	114.93	112.19

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	G	654	NAG	O5-C5-C6-O6
14	G	610	NAG	C8-C7-N2-C2
14	G	610	NAG	O7-C7-N2-C2
14	G	610	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
14	G	654	NAG	C4-C5-C6-O6
14	G	610	NAG	C4-C5-C6-O6
14	G	633	NAG	C4-C5-C6-O6
14	G	633	NAG	O5-C5-C6-O6
14	G	646	NAG	O5-C5-C6-O6
14	G	646	NAG	C4-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	B	701	NAG	1	0
14	G	611	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, 95th 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	B	136/153 (88%)	0.14	6 (4%) 34 29	46, 87, 150, 168	0
2	G	455/482 (94%)	0.02	6 (1%) 77 70	47, 107, 175, 214	0
3	D	240/243 (98%)	0.30	23 (9%) 8 7	62, 150, 289, 309	0
4	E	213/216 (98%)	-0.14	7 (3%) 46 37	80, 144, 226, 242	0
5	H	231/236 (97%)	-0.01	7 (3%) 50 39	56, 129, 176, 198	0
6	L	211/214 (98%)	-0.25	1 (0%) 91 86	53, 115, 143, 156	0
All	All	1486/1544 (96%)	0.01	50 (3%) 45 37	46, 117, 219, 309	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	132	SER	8.4
3	D	190	GLY	7.5
2	G	506	VAL	6.6
5	H	42	GLY	6.5
2	G	69	TRP	6.2
3	D	218	LYS	5.6
3	D	131	THR	5.5
3	D	133	GLY	5.2
5	H	187	LEU	4.6
3	D	130	SER	4.5
3	D	191	THR	4.4
4	E	148	VAL	4.2
3	D	138	LEU	4.1
3	D	139	GLY	4.1
5	H	128	SER	3.8
3	D	163	VAL	3.8
2	G	70	ALA	3.8
3	D	182	VAL	3.8
2	G	460	ARG	3.6

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Mol	Chain	Res	Type	RSRZ
5	H	138	CYS	3.6
3	D	213	PRO	3.5
4	E	161	ALA	3.5
3	D	140	CYS	3.4
1	B	517	ALA	3.3
3	D	222	VAL	3.3
2	G	83	GLU	3.3
4	E	119	VAL	3.1
5	H	192	TYR	3.0
4	E	139	LEU	2.9
5	H	120	PHE	2.8
1	B	664	ASP	2.8
3	D	192	GLN	2.8
4	E	160	LYS	2.8
4	E	193	ARG	2.7
3	D	181	VAL	2.5
3	D	219	GLY	2.5
3	D	141	LEU	2.5
2	G	507	GLN	2.4
3	D	161	SER	2.4
3	D	221	GLU	2.3
5	H	139	LEU	2.3
4	E	147	ALA	2.3
1	B	549	VAL	2.3
1	B	574	LYS	2.3
3	D	136	ALA	2.2
3	D	124	LEU	2.2
3	D	134	GLY	2.1
1	B	515	LEU	2.1
6	L	111	LYS	2.1
1	B	516	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th 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.

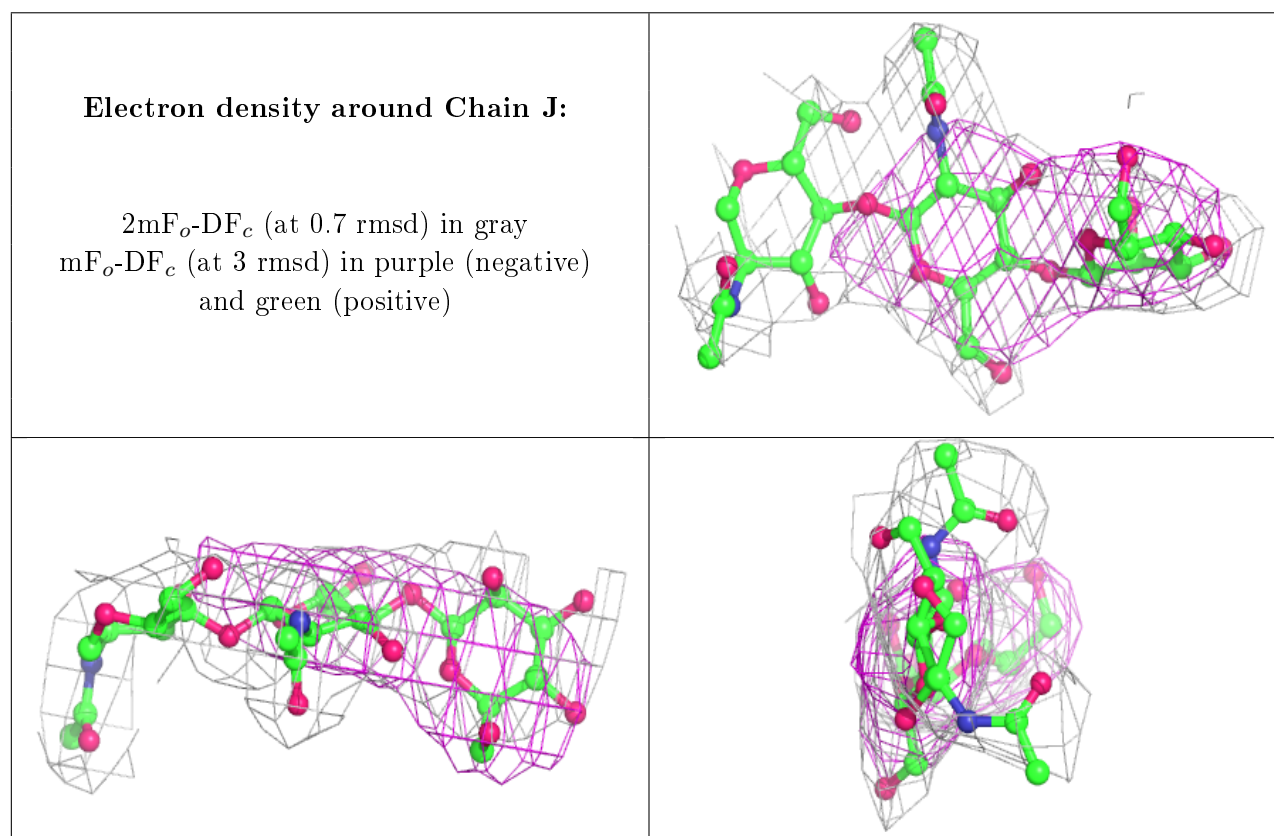
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
8	MAN	C	6	11/12	0.53	0.36	118,118,118,118	0
10	BMA	S	3	11/12	0.58	0.64	118,118,118,118	0
7	BMA	Q	3	11/12	0.59	0.20	118,118,118,118	0
8	MAN	C	4	11/12	0.60	0.18	118,118,118,118	0
13	MAN	T	9	11/12	0.60	0.38	76,76,76,76	0
7	NAG	A	2	14/15	0.62	0.56	118,118,118,118	0
7	MAN	A	5	11/12	0.67	0.33	76,76,76,76	0
10	BMA	O	3	11/12	0.70	0.32	39,39,39,39	0
7	MAN	A	4	11/12	0.70	0.57	42,42,42,42	0
10	NAG	M	1	14/15	0.71	0.22	118,118,118,118	0
10	NAG	S	2	14/15	0.71	0.22	118,118,118,118	0
10	BMA	M	3	11/12	0.71	0.42	118,118,118,118	0
8	MAN	C	5	11/12	0.73	0.33	118,118,118,118	0
12	NAG	R	2	14/15	0.74	0.37	118,118,118,118	0
7	MAN	I	4	11/12	0.74	0.29	37,37,37,37	0
11	MAN	P	4	11/12	0.75	0.30	76,76,76,76	0
11	BMA	N	3	11/12	0.75	0.30	76,76,76,76	0
9	NAG	F	2	14/15	0.75	0.44	118,118,118,118	0
7	MAN	Q	4	11/12	0.77	0.32	118,118,118,118	0
7	NAG	A	1	14/15	0.78	0.59	118,118,118,118	0
7	MAN	K	5	11/12	0.78	0.26	76,76,76,76	0
8	MAN	C	7	11/12	0.78	0.29	118,118,118,118	0
11	MAN	N	4	11/12	0.78	0.22	42,42,42,42	0
11	BMA	P	3	11/12	0.79	0.24	76,76,76,76	0
10	NAG	S	1	14/15	0.79	0.18	118,118,118,118	0
9	NAG	F	1	14/15	0.80	0.38	118,118,118,118	0
7	MAN	K	4	11/12	0.81	0.16	42,42,42,42	0
10	NAG	O	1	14/15	0.81	0.18	118,118,118,118	0
13	MAN	T	5	11/12	0.82	0.17	76,76,76,76	0
7	BMA	A	3	11/12	0.82	0.54	118,118,118,118	0
7	NAG	I	2	14/15	0.82	0.17	76,76,76,76	0
12	BMA	R	3	11/12	0.82	0.18	118,118,118,118	0
7	BMA	I	3	11/12	0.82	0.20	76,76,76,76	0
7	MAN	Q	5	11/12	0.82	0.19	118,118,118,118	0
10	NAG	O	2	14/15	0.82	0.33	118,118,118,118	0
11	NAG	P	2	14/15	0.83	0.22	118,118,118,118	0
13	MAN	T	7	11/12	0.83	0.23	76,76,76,76	0
7	NAG	I	1	14/15	0.83	0.25	118,118,118,118	0
7	BMA	K	3	11/12	0.83	0.12	118,118,118,118	0
7	NAG	K	1	14/15	0.83	0.27	118,118,118,118	0
12	NAG	R	1	14/15	0.83	0.25	118,118,118,118	0
10	NAG	M	2	14/15	0.84	0.40	118,118,118,118	0
13	NAG	T	1	14/15	0.84	0.32	118,118,118,118	0

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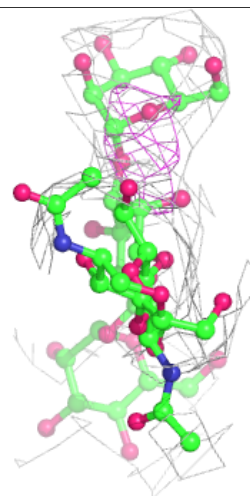
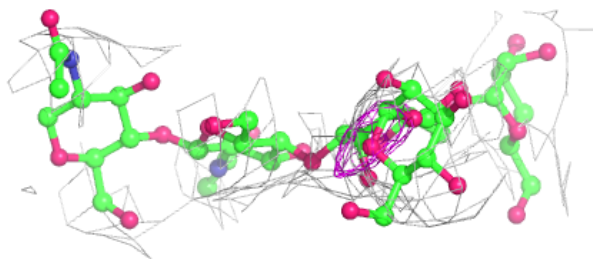
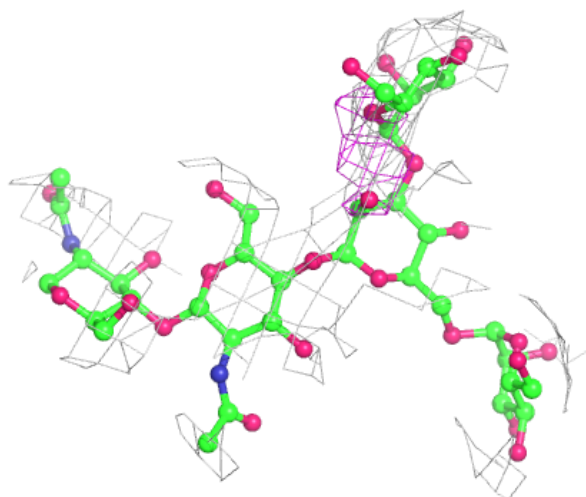
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
7	NAG	K	2	14/15	0.85	0.19	118,118,118,118	0
7	NAG	Q	2	14/15	0.85	0.15	118,118,118,118	0
13	MAN	T	6	11/12	0.86	0.23	76,76,76,76	0
12	MAN	R	4	11/12	0.86	0.19	37,37,37,37	0
10	NAG	J	1	14/15	0.87	0.24	118,118,118,118	0
11	NAG	N	2	14/15	0.87	0.17	76,76,76,76	0
8	NAG	C	2	14/15	0.87	0.25	118,118,118,118	0
10	BMA	J	3	11/12	0.88	0.32	46,46,46,46	0
7	MAN	I	5	11/12	0.88	0.32	76,76,76,76	0
8	BMA	C	3	11/12	0.88	0.19	118,118,118,118	0
13	MAN	T	8	11/12	0.89	0.24	76,76,76,76	0
8	NAG	C	1	14/15	0.90	0.23	118,118,118,118	0
13	BMA	T	3	11/12	0.90	0.16	76,76,76,76	0
11	NAG	N	1	14/15	0.90	0.23	118,118,118,118	0
7	NAG	Q	1	14/15	0.91	0.16	118,118,118,118	0
11	NAG	P	1	14/15	0.91	0.16	118,118,118,118	0
13	MAN	T	4	11/12	0.93	0.17	76,76,76,76	0
10	NAG	J	2	14/15	0.93	0.27	46,46,46,46	0
13	NAG	T	2	14/15	0.96	0.21	118,118,118,118	0

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



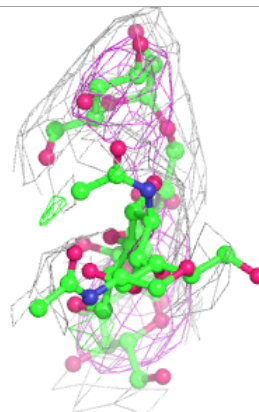
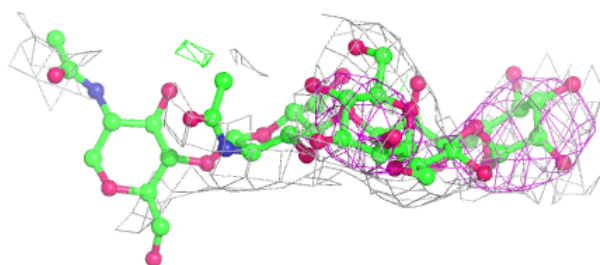
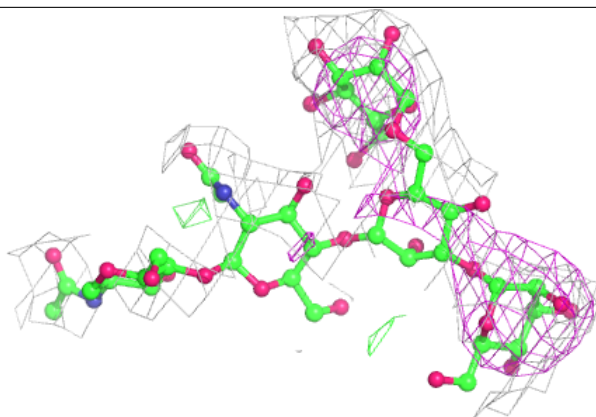
Electron density around Chain Q:

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



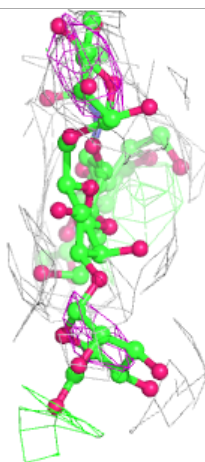
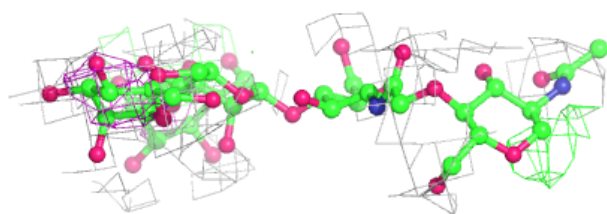
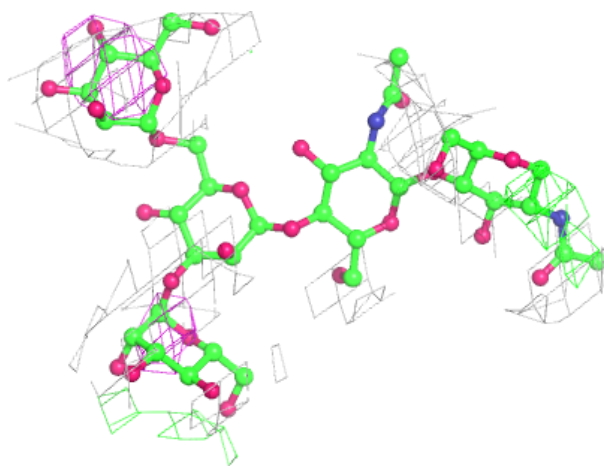
Electron density around Chain I:

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



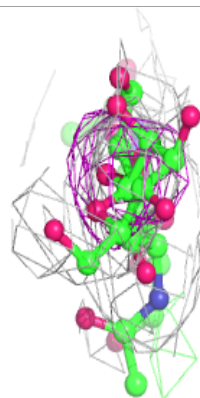
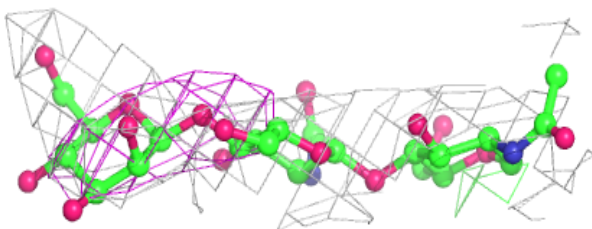
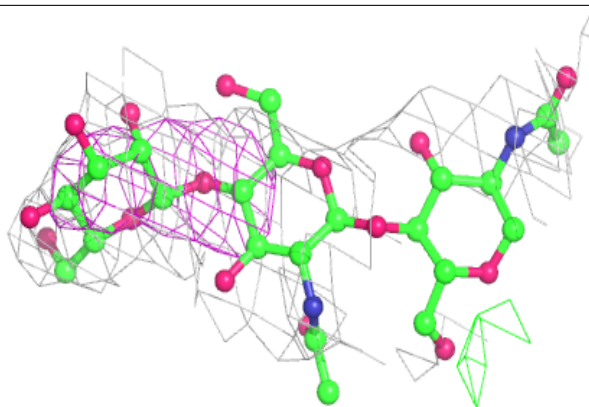
Electron density around Chain K:

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

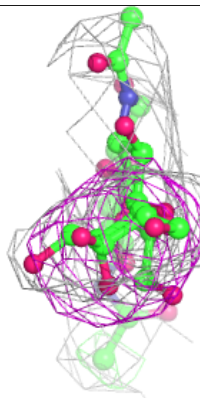
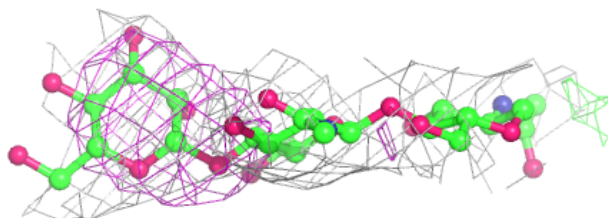
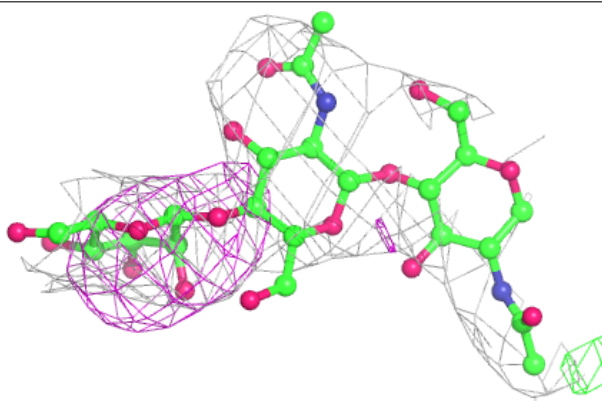


Electron density around Chain M:

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

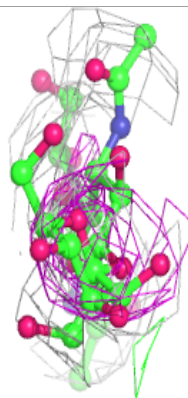
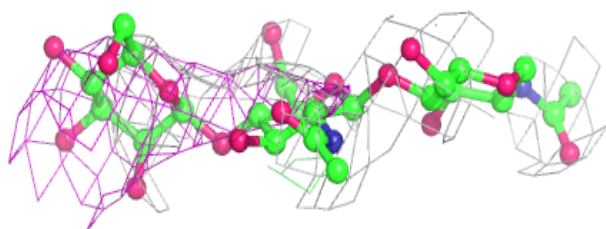
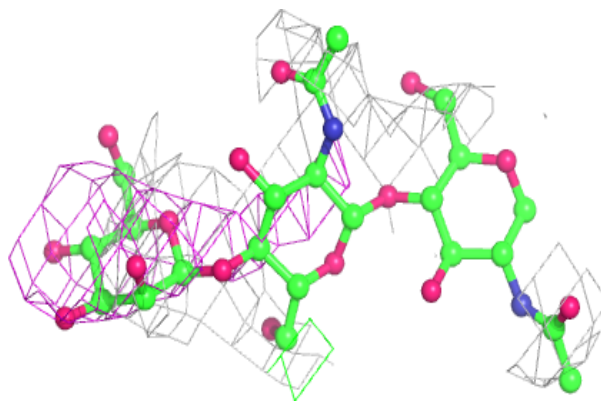
**Electron density around Chain O:**

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

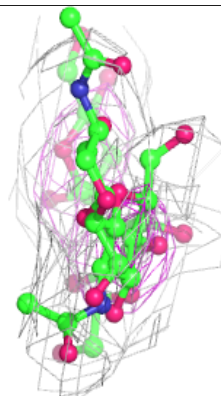
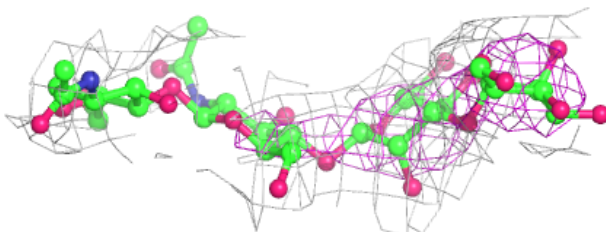
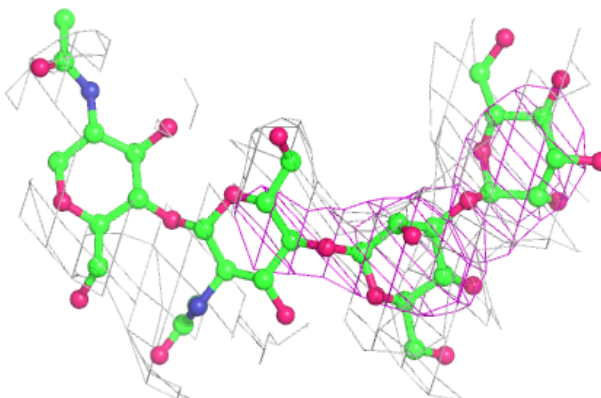


Electron density around Chain S:

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

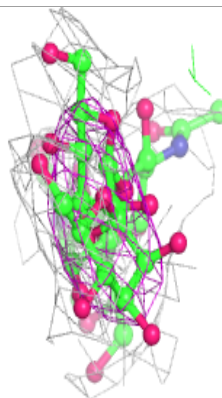
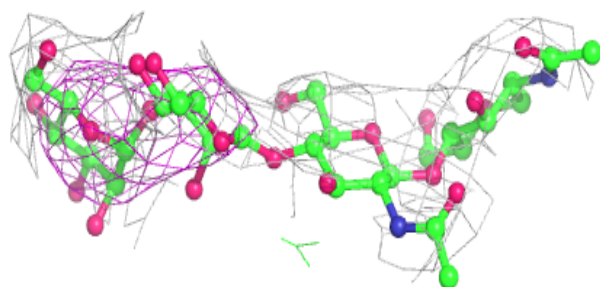
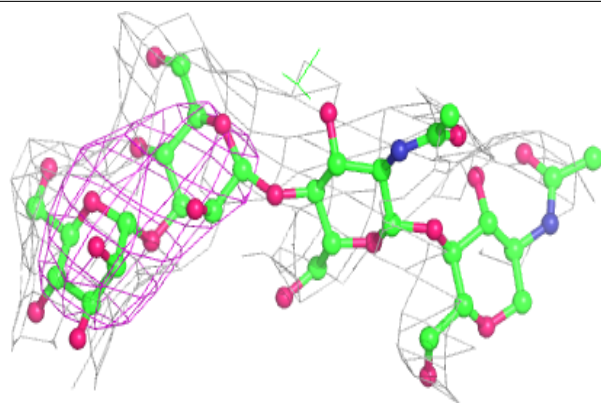
**Electron density around Chain N:**

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

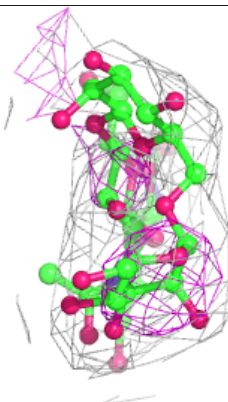
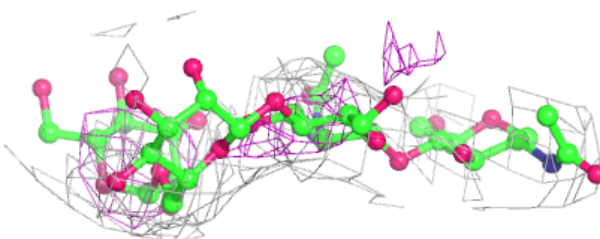
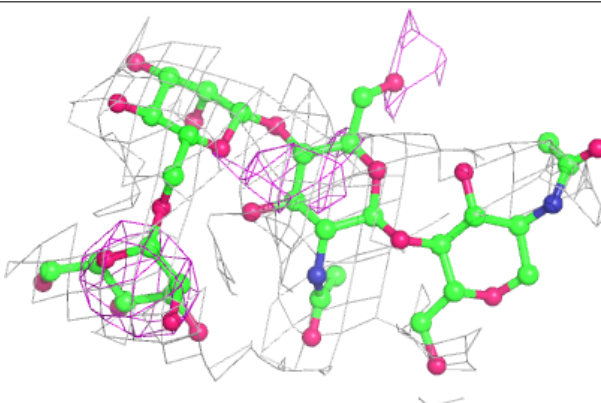


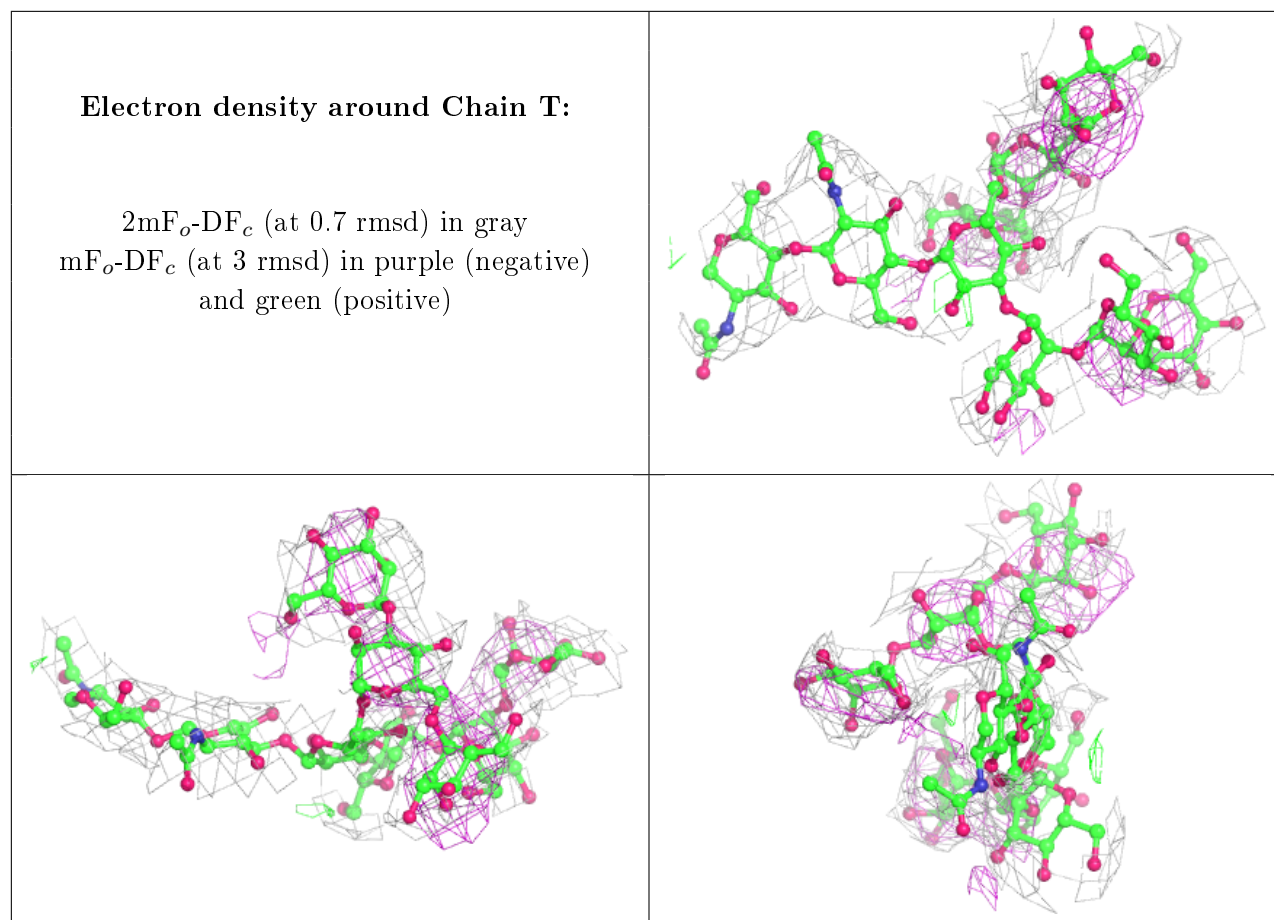
Electron density around Chain P:

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

**Electron density around Chain R:**

$2mF_o-DF_c$ (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, 95th 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
14	NAG	G	633	14/15	0.75	0.41	118,118,118,118	0
14	NAG	B	701	14/15	0.76	0.26	118,118,118,118	0
14	NAG	B	707	14/15	0.78	0.25	37,37,37,37	0
14	NAG	G	611	14/15	0.81	0.46	118,118,118,118	0
14	NAG	G	610	14/15	0.81	0.36	118,118,118,118	0
14	NAG	G	646	14/15	0.84	0.40	118,118,118,118	0
14	NAG	G	625	14/15	0.85	0.27	118,118,118,118	0
14	NAG	G	654	14/15	0.85	0.20	42,42,42,42	0
14	NAG	B	708	14/15	0.93	0.15	37,37,37,37	0

6.5 Other polymers

There are no such residues in this entry.