



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 25, 2021 – 01:45 PM JST

PDB ID : 7BSM  
Title : Mevo lectin complex with 2alpha-mannobiose  
Authors : Sivaji, N.; Suguna, K.; Surolia, A.; Vijayan, M.  
Deposited on : 2020-03-31  
Resolution : 2.80 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](mailto: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.

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

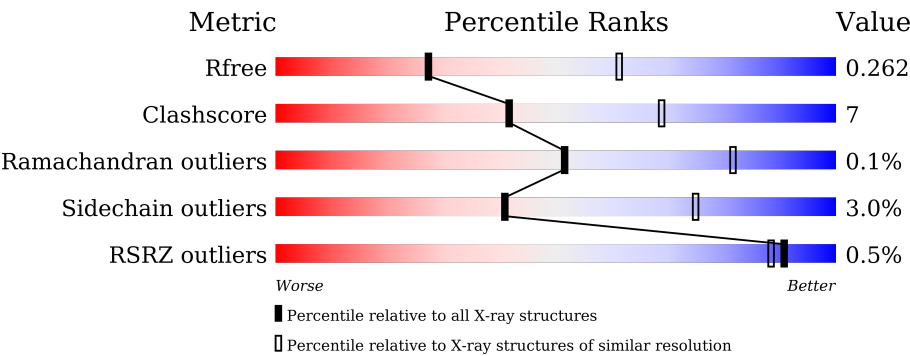
MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.16  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.16

# 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 2.80 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.













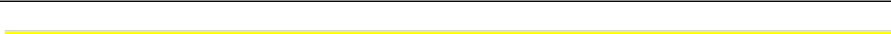


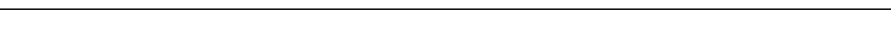
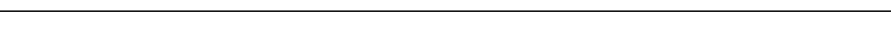
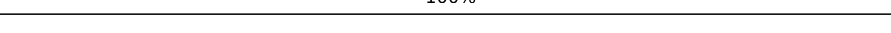
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	A	145	<div><div>%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>82%14%..</div></div>
1	B	145	<div><div>%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>84%10%5%</div></div>
1	C	145	<div><div></div><div><div></div><div></div><div></div><div></div><div></div></div><div>86%10%..</div></div>
1	D	145	<div><div></div><div><div></div><div></div><div></div><div></div><div></div></div><div>85%11%..</div></div>
1	E	145	<div><div></div><div><div></div><div></div><div></div><div></div><div></div></div><div>86%10%..</div></div>
1	F	145	<div><div>%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>87%9%..</div></div>

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Mol	Chain	Length	Quality of chain
1	G	145	 84% 10% . .
1	H	145	 86% 10% . .
1	I	145	 2% 76% 19% . .
1	J	145	 1% 82% 14% .
1	K	145	 88% 8% . .
1	L	145	 1% 88% 9% .
1	M	145	 1% 88% 7% . .
1	N	145	 86% 10% .
2	O	2	 50% 50%
2	P	2	 50% 50%
2	Q	2	 100%
2	R	2	 100%
2	S	2	 100%
2	T	2	 100%
2	U	2	 100%
2	V	2	 100%

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
2	MAN	O	1	-	-	-	X
2	MAN	P	2	-	-	X	-
2	MAN	T	1	-	-	-	X
2	MAN	U	1	-	-	-	X
3	MAN	H	201	-	-	-	X
3	MAN	I	202	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14852 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 lectin.

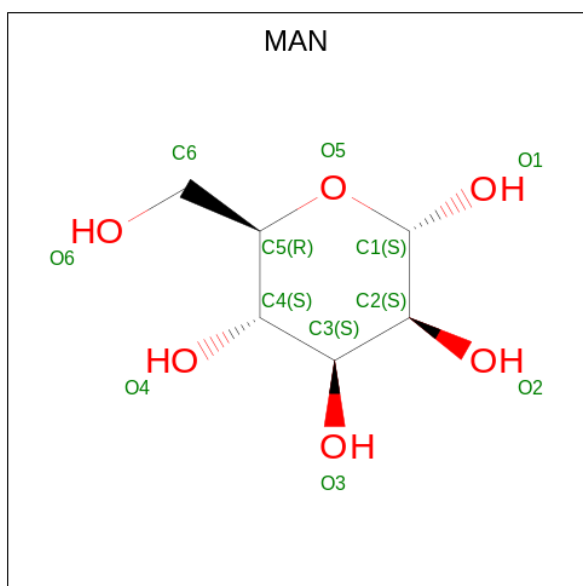
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	140	Total	C	N	O	S	0	0	0
			1065	678	173	211	3			
1	B	138	Total	C	N	O	S	0	0	0
			1011	642	166	201	2			
1	C	140	Total	C	N	O	S	0	0	0
			1038	664	171	200	3			
1	D	140	Total	C	N	O	S	0	0	0
			1051	671	171	206	3			
1	E	140	Total	C	N	O	S	0	0	0
			1058	674	172	209	3			
1	F	140	Total	C	N	O	S	0	0	0
			1040	669	168	200	3			
1	G	140	Total	C	N	O	S	0	0	0
			1044	666	168	207	3			
1	H	140	Total	C	N	O	S	0	0	0
			1065	679	174	209	3			
1	I	140	Total	C	N	O	S	0	0	0
			1036	657	169	207	3			
1	J	140	Total	C	N	O	S	0	0	0
			1028	657	171	198	2			
1	K	140	Total	C	N	O	S	0	0	0
			1043	666	170	204	3			
1	L	140	Total	C	N	O	S	0	0	0
			1050	670	172	205	3			
1	M	140	Total	C	N	O	S	0	0	0
			1049	672	171	203	3			
1	N	140	Total	C	N	O	S	0	0	0
			1050	670	172	205	3			

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	O	2	Total	C	O	0	0	0
			23	12	11			
2	P	2	Total	C	O	0	0	0
			23	12	11			
2	Q	2	Total	C	O	0	0	0
			23	12	11			
2	R	2	Total	C	O	0	0	0
			23	12	11			
2	S	2	Total	C	O	0	0	0
			23	12	11			
2	T	2	Total	C	O	0	0	0
			23	12	11			
2	U	2	Total	C	O	0	0	0
			23	12	11			
2	V	2	Total	C	O	0	0	0
			23	12	11			

- Molecule 3 is alpha-D-mannopyranose (three-letter code: MAN) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).



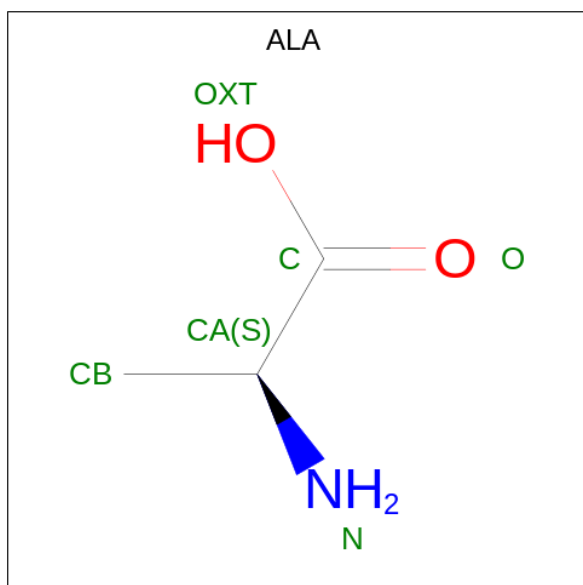
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	H	1	Total	C	O	0	0
			12	6	6		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	H	1	Total	C	O	0	0
			11	6	5		
3	I	1	Total	C	O	0	0
			12	6	6		

- Molecule 4 is ALANINE (three-letter code: ALA) (formula:  $C_3H_7NO_2$ ).

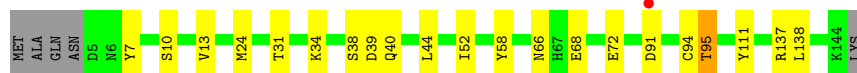
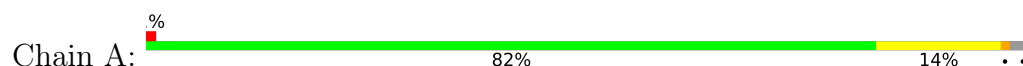


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	I	1	Total	C	N	O	0	0
			5	3	1	1		

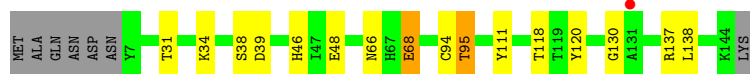
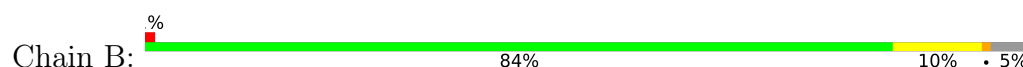
### 3 Residue-property plots [i](#)

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: lectin



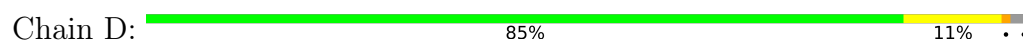
- Molecule 1: lectin



- Molecule 1: lectin



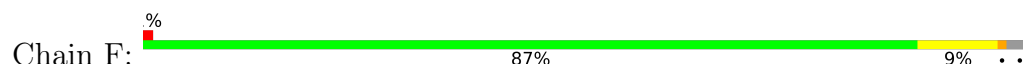
- Molecule 1: lectin



- Molecule 1: lectin

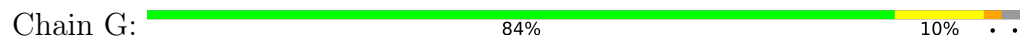


- Molecule 1: lectin

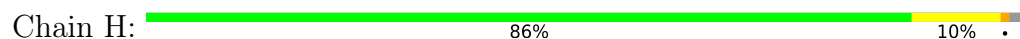




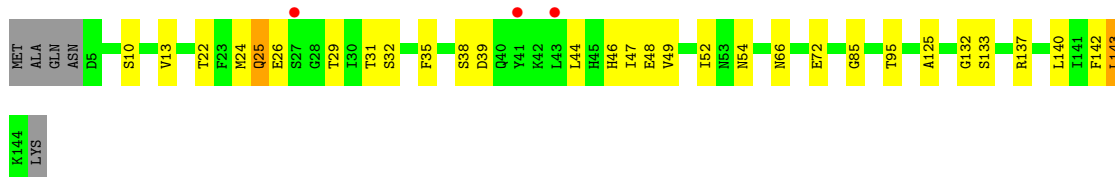
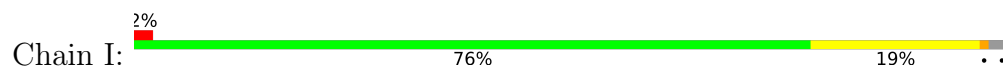
- Molecule 1: lectin



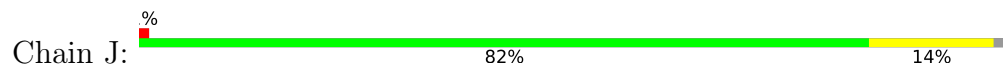
- Molecule 1: lectin



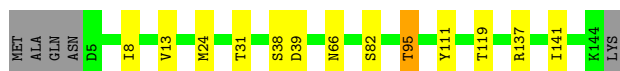
- Molecule 1: lectin



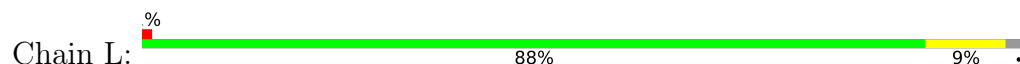
- Molecule 1: lectin



- Molecule 1: lectin

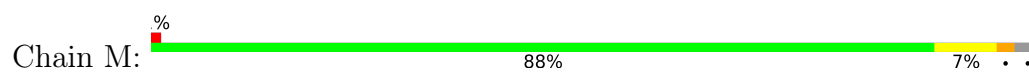


- Molecule 1: lectin

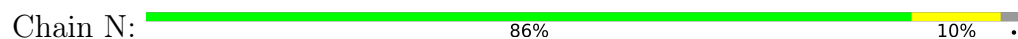


- Molecule 1: lectin





- Molecule 1: lectin



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



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



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



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



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



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



MAN1  
MAN2

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

Chain U:  100%

MAN1  
MAN2

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

Chain V:  100%

MAN1  
MAN2

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	170.36Å 170.36Å 192.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	96.25 – 2.80 85.18 – 2.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (96.25-2.80) 100.0 (85.18-2.80)	Depositor EDS
$R_{merge}$	0.22	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.76 (at 2.82Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, $R_{free}$	0.227 , 0.260 0.231 , 0.262	Depositor DCC
$R_{free}$ test set	3494 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	59.5	Xtriage
Anisotropy	0.596	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 42.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	14852	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.52% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: 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	0.81	0/1084	1.04	0/1462
1	B	0.80	0/1028	1.01	0/1390
1	C	0.77	0/1057	1.00	0/1429
1	D	0.83	0/1070	1.02	0/1445
1	E	0.76	0/1077	0.99	0/1454
1	F	0.76	0/1059	0.97	0/1430
1	G	0.82	0/1063	1.00	0/1438
1	H	0.76	0/1084	1.00	0/1461
1	I	0.75	0/1053	0.98	0/1423
1	J	0.85	0/1047	1.06	0/1417
1	K	0.80	0/1062	1.05	0/1436
1	L	0.75	0/1069	0.96	0/1444
1	M	0.82	0/1068	1.05	0/1441
1	N	0.82	0/1069	1.00	0/1444
All	All	0.79	0/14890	1.01	0/20114

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	1065	0	1044	19	0
1	B	1011	0	971	12	0
1	C	1038	0	1009	21	0
1	D	1051	0	1023	22	0
1	E	1058	0	1031	20	0
1	F	1040	0	1014	26	0
1	G	1044	0	1005	14	0
1	H	1065	0	1051	12	0
1	I	1036	0	998	20	0
1	J	1028	0	989	24	0
1	K	1043	0	1008	7	0
1	L	1050	0	1023	8	0
1	M	1049	0	1028	13	0
1	N	1050	0	1023	11	0
2	O	23	0	21	5	0
2	P	23	0	21	14	0
2	Q	23	0	21	0	0
2	R	23	0	21	0	0
2	S	23	0	21	2	0
2	T	23	0	21	2	0
2	U	23	0	21	0	0
2	V	23	0	21	0	0
3	H	23	0	21	2	0
3	I	12	0	12	2	0
4	I	5	0	4	0	0
All	All	14852	0	14422	206	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 7.

All (206) 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:O:1:MAN:H1	2:O:2:MAN:H5	1.32	1.11
1:E:85:GLY:C	1:E:95:THR:HG22	1.75	1.08
1:C:85:GLY:C	1:C:95:THR:HG22	1.72	1.07
1:F:133:SER:N	2:P:2:MAN:H62	1.68	1.07
1:J:85:GLY:C	1:J:95:THR:HG22	1.77	1.05
1:M:31:THR:HG23	1:N:120:TYR:OH	1.56	1.05
1:L:85:GLY:C	1:L:95:THR:HG22	1.84	0.97
1:B:130:GLY:HA3	1:B:137:ARG:NH1	1.78	0.97
1:F:37:TRP:HZ3	1:F:69:VAL:HG23	1.33	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:THR:CG2	1:A:52:ILE:HG22	1.99	0.92
1:J:7:TYR:CE2	1:J:24:MET:HE2	2.06	0.91
1:C:116:LEU:CD1	1:D:69:VAL:CG2	2.49	0.90
1:F:133:SER:N	2:P:2:MAN:C6	2.36	0.89
1:D:30:ILE:HD11	1:D:124:LEU:CD2	2.05	0.87
1:F:133:SER:H	2:P:2:MAN:C6	1.88	0.86
2:O:1:MAN:C1	2:O:2:MAN:H5	2.06	0.86
1:G:95:THR:HG22	1:G:111:TYR:O	1.76	0.85
1:A:95:THR:HG22	1:A:111:TYR:O	1.77	0.85
1:C:116:LEU:CD1	1:D:69:VAL:HG23	2.07	0.85
1:B:95:THR:HG22	1:B:111:TYR:O	1.77	0.85
1:F:95:THR:HG22	1:F:111:TYR:O	1.77	0.85
1:M:95:THR:HG22	1:M:111:TYR:O	1.78	0.83
2:O:1:MAN:H1	2:O:2:MAN:C5	2.08	0.83
1:K:95:THR:HG22	1:K:111:TYR:O	1.77	0.83
1:F:133:SER:H	2:P:2:MAN:H62	1.37	0.83
1:A:31:THR:HG23	1:A:52:ILE:CG2	2.09	0.83
1:F:37:TRP:CZ3	1:F:69:VAL:HG23	2.14	0.82
1:H:95:THR:HG22	1:H:111:TYR:O	1.77	0.82
1:D:95:THR:HG22	1:D:111:TYR:O	1.79	0.81
1:I:25:GLN:NE2	1:I:54:ASN:HD22	1.80	0.80
1:C:85:GLY:O	1:C:95:THR:HG22	1.80	0.79
1:I:25:GLN:NE2	1:I:54:ASN:ND2	2.30	0.78
1:M:31:THR:CG2	1:N:120:TYR:OH	2.32	0.78
1:F:134:ASP:H	2:P:2:MAN:C6	1.97	0.77
1:C:116:LEU:HD11	1:D:69:VAL:CG2	2.14	0.75
1:C:85:GLY:C	1:C:95:THR:CG2	2.53	0.75
1:A:31:THR:CG2	1:A:52:ILE:CG2	2.65	0.75
1:E:6:ASN:C	1:E:144:LYS:HD2	2.07	0.75
1:J:39:ASP:H	1:J:66:ASN:HD21	1.36	0.73
1:L:86:TYR:N	1:L:95:THR:HG22	2.03	0.73
1:D:39:ASP:H	1:D:66:ASN:HD21	1.36	0.73
1:L:39:ASP:H	1:L:66:ASN:HD21	1.36	0.73
1:A:31:THR:HG23	1:A:52:ILE:HG23	1.71	0.73
1:K:39:ASP:H	1:K:66:ASN:HD21	1.37	0.72
1:B:130:GLY:HA3	1:B:137:ARG:HH12	1.50	0.72
1:H:39:ASP:H	1:H:66:ASN:HD21	1.38	0.72
1:I:39:ASP:H	1:I:66:ASN:HD21	1.37	0.72
1:M:39:ASP:H	1:M:66:ASN:HD21	1.37	0.72
1:C:39:ASP:H	1:C:66:ASN:HD21	1.37	0.72
1:N:39:ASP:H	1:N:66:ASN:HD21	1.36	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:25:GLN:HE21	1:I:54:ASN:HD22	1.36	0.72
1:F:39:ASP:H	1:F:66:ASN:HD21	1.37	0.71
1:C:116:LEU:HD12	1:D:69:VAL:CG2	2.18	0.71
1:G:39:ASP:H	1:G:66:ASN:HD21	1.38	0.71
1:E:125:ALA:HB2	1:E:143:LEU:HD13	1.70	0.71
1:G:25:GLN:HE22	1:G:54:ASN:HD22	1.39	0.71
1:E:39:ASP:H	1:E:66:ASN:HD21	1.37	0.71
1:A:39:ASP:H	1:A:66:ASN:HD21	1.37	0.71
1:B:39:ASP:H	1:B:66:ASN:HD21	1.38	0.71
1:J:16:VAL:O	1:J:16:VAL:HG12	1.92	0.70
1:I:10:SER:HB2	1:N:72:GLU:OE1	1.92	0.70
1:E:67:HIS:HE1	1:J:40:GLN:OE1	1.76	0.69
1:D:30:ILE:HD11	1:D:124:LEU:HD21	1.75	0.68
1:A:40:GLN:HG3	1:M:67:HIS:CE1	2.28	0.67
1:J:85:GLY:O	1:J:95:THR:HG22	1.94	0.67
1:E:85:GLY:O	1:E:95:THR:HG22	1.96	0.66
1:F:133:SER:HB2	2:P:2:MAN:H61	1.77	0.66
1:J:7:TYR:CD2	1:J:24:MET:CE	2.78	0.66
1:E:5:ASP:O	1:E:144:LYS:NZ	2.27	0.65
1:C:116:LEU:HD12	1:D:69:VAL:HG23	1.76	0.64
1:J:7:TYR:CD2	1:J:24:MET:HE2	2.34	0.63
1:C:118:THR:HG22	1:D:105:LYS:HD2	1.81	0.62
1:F:45:HIS:ND1	1:F:134:ASP:OD1	2.33	0.62
1:C:116:LEU:HG	1:D:69:VAL:HG23	1.82	0.61
1:D:30:ILE:HD11	1:D:124:LEU:CG	2.30	0.61
1:F:132:GLY:C	2:P:2:MAN:H62	2.21	0.61
1:F:72:GLU:OE1	1:G:10:SER:HB2	2.01	0.61
1:C:116:LEU:CG	1:D:69:VAL:HG23	2.31	0.60
1:E:67:HIS:HE1	1:J:40:GLN:CD	2.04	0.60
1:N:125:ALA:HB2	1:N:143:LEU:CD1	2.32	0.59
1:I:22:THR:CG2	1:I:24:MET:CE	2.80	0.59
1:C:116:LEU:HD11	1:D:69:VAL:HG21	1.83	0.59
1:E:86:TYR:N	1:E:95:THR:HG22	2.16	0.59
1:H:10:SER:HB2	1:I:72:GLU:OE1	2.04	0.58
1:C:86:TYR:N	1:C:95:THR:HG22	2.18	0.56
1:F:45:HIS:CE1	1:F:134:ASP:OD1	2.59	0.56
1:H:136:ASP:OD2	3:H:202:MAN:O4	2.21	0.56
1:J:86:TYR:N	1:J:95:THR:HG22	2.21	0.56
1:G:40:GLN:OE1	1:H:39:ASP:OD2	2.24	0.55
1:J:7:TYR:CE2	1:J:24:MET:CE	2.86	0.55
1:L:125:ALA:HB2	1:L:143:LEU:CD1	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:16:VAL:O	1:F:16:VAL:HG12	2.05	0.55
1:F:132:GLY:CA	2:P:2:MAN:H62	2.37	0.54
1:E:85:GLY:C	1:E:95:THR:CG2	2.63	0.54
1:B:118:THR:HG22	1:G:105:LYS:HD2	1.90	0.54
1:A:40:GLN:CG	1:M:67:HIS:CE1	2.90	0.54
1:E:67:HIS:CE1	1:J:40:GLN:OE1	2.59	0.54
1:F:95:THR:CG2	1:F:111:TYR:O	2.55	0.54
1:A:72:GLU:OE1	1:E:10:SER:HB2	2.08	0.53
1:D:30:ILE:HD11	1:D:124:LEU:HG	1.90	0.53
1:M:31:THR:HG23	1:N:120:TYR:HH	1.71	0.53
1:B:95:THR:CG2	1:B:111:TYR:O	2.55	0.52
1:D:77:GLU:OE2	1:D:105:LYS:HE2	2.09	0.52
1:J:7:TYR:CZ	1:J:24:MET:HE2	2.44	0.52
1:N:125:ALA:HB2	1:N:143:LEU:HD13	1.90	0.52
1:J:16:VAL:O	1:J:16:VAL:CG1	2.57	0.52
1:I:132:GLY:HA3	3:I:202:MAN:O3	2.10	0.51
1:I:44:LEU:HD23	1:I:47:ILE:HD11	1.92	0.51
1:E:67:HIS:CE1	1:J:40:GLN:CD	2.84	0.51
1:M:95:THR:CG2	1:M:111:TYR:O	2.54	0.51
1:J:7:TYR:CD2	1:J:24:MET:HE1	2.45	0.51
1:B:94:CYS:SG	1:B:138:LEU:HB3	2.52	0.50
1:D:95:THR:CG2	1:D:111:TYR:O	2.57	0.50
1:H:77:GLU:O	1:H:123:LYS:HE2	2.11	0.50
1:K:24:MET:SD	1:K:141:ILE:HD13	2.52	0.50
1:E:95:THR:HG23	1:E:111:TYR:O	2.11	0.50
1:H:95:THR:CG2	1:H:111:TYR:O	2.55	0.50
1:B:34:LYS:HD3	1:B:68:GLU:OE2	2.12	0.50
1:C:12:GLU:OE2	1:C:137:ARG:HD2	2.12	0.49
1:I:22:THR:CG2	1:I:24:MET:HE2	2.42	0.49
1:J:85:GLY:C	1:J:95:THR:CG2	2.66	0.49
1:A:40:GLN:CG	1:M:67:HIS:HE1	2.25	0.49
1:A:13:VAL:O	1:A:137:ARG:HA	2.13	0.49
1:C:72:GLU:OE1	1:F:10:SER:HB2	2.12	0.49
1:M:25:GLN:HG3	1:M:26:GLU:O	2.13	0.49
1:A:34:LYS:HD3	1:A:68:GLU:HG3	1.95	0.48
1:F:134:ASP:H	2:P:2:MAN:H61	1.77	0.48
1:J:95:THR:HG23	1:J:111:TYR:O	2.12	0.48
1:H:13:VAL:O	1:H:137:ARG:HA	2.14	0.48
1:J:13:VAL:O	1:J:137:ARG:HA	2.13	0.48
1:I:13:VAL:O	1:I:137:ARG:HA	2.14	0.48
1:H:133:SER:HB2	3:H:201:MAN:H1	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:13:VAL:O	1:L:137:ARG:HA	2.14	0.48
1:K:13:VAL:O	1:K:137:ARG:HA	2.13	0.48
1:H:36:ASN:HD21	1:L:88:LYS:HE3	1.79	0.48
1:N:13:VAL:O	1:N:137:ARG:HA	2.14	0.48
1:E:125:ALA:CB	1:E:143:LEU:HD13	2.43	0.48
1:K:82:SER:HG	1:K:119:THR:HG1	1.62	0.47
1:M:13:VAL:O	1:M:137:ARG:HA	2.14	0.47
1:G:95:THR:CG2	1:G:111:TYR:O	2.57	0.47
2:T:1:MAN:H1	2:T:2:MAN:C5	2.45	0.47
1:E:6:ASN:HA	1:E:144:LYS:HD3	1.97	0.47
1:I:25:GLN:HE22	1:I:54:ASN:ND2	2.10	0.47
1:K:95:THR:CG2	1:K:111:TYR:O	2.57	0.47
1:D:134:ASP:H	2:O:2:MAN:H62	1.79	0.47
1:G:13:VAL:O	1:G:137:ARG:HA	2.15	0.47
1:G:77:GLU:OE2	1:G:105:LYS:HE2	2.14	0.47
1:I:140:LEU:HB2	1:I:142:PHE:HE1	1.80	0.47
1:C:116:LEU:HD12	1:D:69:VAL:HG22	1.96	0.46
1:N:93:ARG:NH1	1:N:134:ASP:OD2	2.49	0.46
1:J:45:HIS:HA	1:J:134:ASP:HA	1.97	0.46
1:F:133:SER:CB	2:P:2:MAN:H61	2.42	0.45
1:A:95:THR:CG2	1:A:111:TYR:O	2.55	0.45
1:L:125:ALA:HB2	1:L:143:LEU:HD12	1.98	0.45
2:S:1:MAN:H1	2:S:2:MAN:O5	2.15	0.45
1:L:85:GLY:O	1:L:95:THR:HG22	2.14	0.45
1:B:120:TYR:OH	1:G:31:THR:HB	2.18	0.44
1:I:35:PHE:CD1	1:I:47:ILE:HG12	2.52	0.44
1:A:7:TYR:CD1	1:A:24:MET:HE1	2.51	0.44
1:B:130:GLY:CA	1:B:137:ARG:NH1	2.66	0.44
1:G:125:ALA:HB2	1:G:143:LEU:CD1	2.48	0.44
1:I:22:THR:HG22	1:I:24:MET:CE	2.47	0.44
1:J:7:TYR:CG	1:J:24:MET:HE1	2.53	0.44
1:F:45:HIS:HA	1:F:134:ASP:HA	1.99	0.43
1:A:31:THR:HG22	1:A:52:ILE:HG22	1.96	0.43
1:E:7:TYR:N	1:E:144:LYS:HD2	2.32	0.43
1:F:37:TRP:CZ3	1:F:69:VAL:CG2	2.94	0.43
1:F:134:ASP:N	2:P:2:MAN:H61	2.34	0.43
1:I:29:THR:H	1:I:52:ILE:HG22	1.82	0.43
1:F:133:SER:N	2:P:2:MAN:H61	2.28	0.43
1:A:91:ASP:OD2	1:N:40:GLN:O	2.36	0.42
2:O:1:MAN:C2	2:O:2:MAN:H5	2.49	0.42
1:G:45:HIS:HA	1:G:134:ASP:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:13:VAL:O	1:D:137:ARG:HA	2.19	0.42
1:I:85:GLY:C	1:I:95:THR:OG1	2.58	0.42
2:T:1:MAN:H1	2:T:2:MAN:H5	2.01	0.42
1:C:118:THR:CG2	1:D:105:LYS:HD2	2.49	0.42
1:E:6:ASN:C	1:E:144:LYS:CD	2.82	0.42
1:F:133:SER:CA	2:P:2:MAN:H61	2.50	0.42
1:G:25:GLN:NE2	1:G:54:ASN:HD22	2.13	0.42
1:C:40:GLN:HG3	2:S:1:MAN:H3	2.02	0.42
3:I:202:MAN:HO3	3:I:202:MAN:C6	2.33	0.42
1:H:29:THR:CG2	1:H:143:LEU:HD11	2.50	0.41
1:F:134:ASP:N	2:P:2:MAN:C6	2.75	0.41
1:A:94:CYS:SG	1:A:138:LEU:HB3	2.60	0.41
1:M:38:SER:HA	1:M:66:ASN:ND2	2.35	0.41
1:A:38:SER:HA	1:A:66:ASN:ND2	2.36	0.41
1:A:58:TYR:N	1:A:58:TYR:CD1	2.89	0.41
1:J:7:TYR:CG	1:J:24:MET:CE	3.03	0.41
1:B:38:SER:HA	1:B:66:ASN:ND2	2.36	0.41
1:C:13:VAL:O	1:C:137:ARG:HA	2.21	0.41
1:J:82:SER:OG	1:J:119:THR:OG1	2.35	0.41
1:G:38:SER:HA	1:G:66:ASN:ND2	2.36	0.41
1:I:38:SER:HA	1:I:66:ASN:ND2	2.36	0.41
1:C:29:THR:H	1:C:52:ILE:HG22	1.86	0.41
1:N:38:SER:HA	1:N:66:ASN:ND2	2.36	0.41
1:H:29:THR:H	1:H:52:ILE:HG22	1.86	0.41
1:I:46:HIS:CE1	1:I:48:GLU:HG3	2.56	0.41
1:D:38:SER:HA	1:D:66:ASN:ND2	2.35	0.40
1:J:58:TYR:CD1	1:J:58:TYR:N	2.89	0.40
1:K:38:SER:HA	1:K:66:ASN:ND2	2.36	0.40
1:E:38:SER:HA	1:E:66:ASN:ND2	2.36	0.40
1:M:25:GLN:HG2	1:M:28:GLY:HA3	2.04	0.40
1:B:46:HIS:CE1	1:B:48:GLU:HG3	2.57	0.40
1:E:6:ASN:HA	1:E:144:LYS:CD	2.52	0.40
1:I:125:ALA:HB2	1:I:143:LEU:HD13	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	138/145 (95%)	131 (95%)	7 (5%)	0	100	100
1	B	136/145 (94%)	131 (96%)	5 (4%)	0	100	100
1	C	138/145 (95%)	134 (97%)	4 (3%)	0	100	100
1	D	138/145 (95%)	132 (96%)	6 (4%)	0	100	100
1	E	138/145 (95%)	132 (96%)	6 (4%)	0	100	100
1	F	138/145 (95%)	131 (95%)	7 (5%)	0	100	100
1	G	138/145 (95%)	134 (97%)	4 (3%)	0	100	100
1	H	138/145 (95%)	130 (94%)	8 (6%)	0	100	100
1	I	138/145 (95%)	131 (95%)	7 (5%)	0	100	100
1	J	138/145 (95%)	134 (97%)	4 (3%)	0	100	100
1	K	138/145 (95%)	134 (97%)	4 (3%)	0	100	100
1	L	138/145 (95%)	131 (95%)	6 (4%)	1 (1%)	22	53
1	M	138/145 (95%)	133 (96%)	5 (4%)	0	100	100
1	N	138/145 (95%)	133 (96%)	5 (4%)	0	100	100
All	All	1930/2030 (95%)	1851 (96%)	78 (4%)	1 (0%)	51	81

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	26	GLU

### 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	A	113/119 (95%)	110 (97%)	3 (3%)	44	78
1	B	103/119 (87%)	100 (97%)	3 (3%)	42	76
1	C	106/119 (89%)	104 (98%)	2 (2%)	57	85
1	D	109/119 (92%)	104 (95%)	5 (5%)	27	60
1	E	111/119 (93%)	109 (98%)	2 (2%)	59	86
1	F	105/119 (88%)	103 (98%)	2 (2%)	57	85
1	G	108/119 (91%)	105 (97%)	3 (3%)	43	77
1	H	113/119 (95%)	110 (97%)	3 (3%)	44	78
1	I	107/119 (90%)	100 (94%)	7 (6%)	17	44
1	J	103/119 (87%)	99 (96%)	4 (4%)	32	66
1	K	107/119 (90%)	104 (97%)	3 (3%)	43	77
1	L	109/119 (92%)	107 (98%)	2 (2%)	59	86
1	M	108/119 (91%)	104 (96%)	4 (4%)	34	68
1	N	109/119 (92%)	106 (97%)	3 (3%)	43	77
All	All	1511/1666 (91%)	1465 (97%)	46 (3%)	41	75

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	SER
1	A	44	LEU
1	A	95	THR
1	B	31	THR
1	B	68	GLU
1	B	95	THR
1	C	31	THR
1	C	137	ARG
1	D	68	GLU
1	D	78	THR
1	D	95	THR
1	D	114	GLU
1	D	133	SER
1	E	31	THR
1	E	143	LEU
1	F	31	THR
1	F	95	THR

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Mol	Chain	Res	Type
1	G	25	GLN
1	G	31	THR
1	G	95	THR
1	H	31	THR
1	H	95	THR
1	H	123	LYS
1	I	25	GLN
1	I	26	GLU
1	I	31	THR
1	I	32	SER
1	I	49	VAL
1	I	133	SER
1	I	143	LEU
1	J	10	SER
1	J	11	THR
1	J	31	THR
1	J	32	SER
1	K	8	ILE
1	K	31	THR
1	K	95	THR
1	L	24	MET
1	L	31	THR
1	M	16	VAL
1	M	25	GLN
1	M	31	THR
1	M	95	THR
1	N	25	GLN
1	N	31	THR
1	N	133	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	66	ASN
1	B	46	HIS
1	B	66	ASN
1	C	25	GLN
1	C	46	HIS
1	C	66	ASN
1	D	25	GLN
1	D	66	ASN
1	E	25	GLN

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Mol	Chain	Res	Type
1	E	66	ASN
1	E	67	HIS
1	F	25	GLN
1	F	46	HIS
1	F	66	ASN
1	G	25	GLN
1	G	56	ASN
1	G	66	ASN
1	H	25	GLN
1	H	56	ASN
1	H	66	ASN
1	I	25	GLN
1	I	46	HIS
1	I	66	ASN
1	J	46	HIS
1	J	66	ASN
1	K	25	GLN
1	K	56	ASN
1	K	66	ASN
1	L	66	ASN
1	M	46	HIS
1	M	66	ASN
1	M	67	HIS
1	N	46	HIS
1	N	66	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

16 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$
2	MAN	O	1	2	12,12,12	0.50	0	17,17,17	0.80	1 (5%)
2	MAN	O	2	2	11,11,12	0.30	0	15,15,17	0.86	0
2	MAN	P	1	2	12,12,12	0.94	1 (8%)	16,17,17	1.81	4 (25%)
2	MAN	P	2	2	11,11,12	1.75	4 (36%)	15,15,17	1.41	1 (6%)
2	MAN	Q	1	2	12,12,12	1.25	2 (16%)	17,17,17	1.33	3 (17%)
2	MAN	Q	2	2	11,11,12	1.72	4 (36%)	15,15,17	0.87	0
2	MAN	R	1	2	12,12,12	1.09	0	17,17,17	1.64	5 (29%)
2	MAN	R	2	2	11,11,12	1.61	2 (18%)	15,15,17	1.25	1 (6%)
2	MAN	S	1	2	12,12,12	1.64	2 (16%)	17,17,17	1.35	3 (17%)
2	MAN	S	2	2	11,11,12	1.75	3 (27%)	15,15,17	1.11	1 (6%)
2	MAN	T	1	2	12,12,12	1.96	5 (41%)	17,17,17	2.03	8 (47%)
2	MAN	T	2	2	11,11,12	4.24	6 (54%)	15,15,17	2.27	4 (26%)
2	MAN	U	1	2	12,12,12	0.51	0	17,17,17	0.81	1 (5%)
2	MAN	U	2	2	11,11,12	0.29	0	15,15,17	0.87	1 (6%)
2	MAN	V	1	2	12,12,12	0.76	0	17,17,17	0.98	1 (5%)
2	MAN	V	2	2	11,11,12	1.59	3 (27%)	15,15,17	1.64	2 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MAN	O	1	2	-	1/2/22/22	0/1/1/1
2	MAN	O	2	2	-	2/2/19/22	0/1/1/1
2	MAN	P	2	2	-	1/2/19/22	0/1/1/1
2	MAN	Q	1	2	-	1/2/22/22	0/1/1/1
2	MAN	Q	2	2	-	0/2/19/22	0/1/1/1
2	MAN	R	1	2	-	1/2/22/22	0/1/1/1
2	MAN	R	2	2	-	0/2/19/22	0/1/1/1
2	MAN	S	1	2	-	2/2/22/22	0/1/1/1
2	MAN	S	2	2	-	0/2/19/22	0/1/1/1
2	MAN	T	1	2	-	0/2/22/22	0/1/1/1
2	MAN	T	2	2	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MAN	U	1	2	-	2/2/22/22	0/1/1/1
2	MAN	U	2	2	-	2/2/19/22	0/1/1/1
2	MAN	V	1	2	-	0/2/22/22	0/1/1/1
2	MAN	V	2	2	-	0/2/19/22	0/1/1/1

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	T	2	MAN	C2-C3	11.04	1.68	1.52
2	T	2	MAN	O2-C2	4.90	1.53	1.43
2	T	2	MAN	O5-C1	4.22	1.50	1.43
2	S	1	MAN	C4-C5	-3.63	1.45	1.53
2	S	1	MAN	O5-C5	-3.52	1.35	1.44
2	T	2	MAN	C1-C2	3.51	1.60	1.52
2	P	2	MAN	C2-C3	-3.34	1.47	1.52
2	Q	2	MAN	O5-C1	-3.33	1.38	1.43
2	T	1	MAN	O5-C1	3.11	1.50	1.42
2	V	2	MAN	O5-C1	-3.11	1.38	1.43
2	T	2	MAN	O5-C5	3.11	1.49	1.43
2	R	2	MAN	O5-C1	-3.04	1.38	1.43
2	T	1	MAN	C1-C2	2.98	1.59	1.52
2	R	2	MAN	O5-C5	-2.94	1.37	1.43
2	S	2	MAN	C4-C5	-2.93	1.46	1.53
2	S	2	MAN	O5-C5	-2.87	1.37	1.43
2	S	2	MAN	O5-C1	-2.87	1.39	1.43
2	V	2	MAN	O5-C5	-2.77	1.37	1.43
2	T	2	MAN	O3-C3	2.71	1.49	1.43
2	T	1	MAN	C4-C3	2.69	1.59	1.52
2	P	2	MAN	O5-C5	-2.65	1.38	1.43
2	Q	2	MAN	C2-C3	-2.61	1.48	1.52
2	T	1	MAN	C4-C5	2.60	1.58	1.53
2	V	2	MAN	C4-C5	-2.37	1.48	1.53
2	T	1	MAN	O2-C2	2.27	1.48	1.43
2	Q	1	MAN	C4-C3	-2.26	1.46	1.52
2	P	2	MAN	O5-C1	-2.25	1.40	1.43
2	P	1	MAN	C4-C5	-2.23	1.48	1.53
2	Q	2	MAN	C4-C5	-2.21	1.48	1.53
2	P	2	MAN	O4-C4	-2.19	1.37	1.43
2	Q	1	MAN	O5-C5	-2.10	1.39	1.44
2	Q	2	MAN	O5-C5	-2.05	1.39	1.43

All (36) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	V	2	MAN	O5-C5-C6	-4.67	99.88	107.20
2	T	2	MAN	C1-O5-C5	4.39	118.14	112.19
2	P	1	MAN	C3-C4-C5	-3.97	103.15	110.24
2	T	2	MAN	O2-C2-C3	3.82	117.79	110.14
2	T	2	MAN	O5-C5-C6	-3.79	101.27	107.20
2	P	2	MAN	O5-C5-C6	-3.67	101.46	107.20
2	T	2	MAN	O3-C3-C2	3.58	116.84	109.99
2	T	1	MAN	O5-C5-C6	3.51	115.16	106.44
2	P	1	MAN	C4-C3-C2	-3.39	104.91	110.82
2	R	1	MAN	C1-O5-C5	-3.32	107.40	113.66
2	T	1	MAN	O5-C5-C4	-3.27	103.75	109.69
2	P	1	MAN	O5-C5-C6	3.14	114.24	106.44
2	R	2	MAN	O5-C5-C6	-3.11	102.32	107.20
2	S	1	MAN	O1-C1-O5	-3.05	101.22	110.38
2	Q	1	MAN	C4-C3-C2	-2.97	105.63	110.82
2	R	1	MAN	C4-C3-C2	-2.85	105.85	110.82
2	T	1	MAN	O2-C2-C1	2.78	115.60	109.16
2	T	1	MAN	O3-C3-C2	-2.72	104.06	110.35
2	R	1	MAN	O5-C5-C6	2.69	113.13	106.44
2	P	1	MAN	O5-C5-C4	-2.54	105.09	109.69
2	V	2	MAN	C1-C2-C3	2.53	112.78	109.67
2	T	1	MAN	O2-C2-C3	-2.47	104.65	110.35
2	T	1	MAN	O5-C1-C2	2.42	114.61	110.28
2	Q	1	MAN	C3-C4-C5	-2.38	106.00	110.24
2	T	1	MAN	C6-C5-C4	2.38	118.57	113.00
2	R	1	MAN	C3-C4-C5	-2.36	106.02	110.24
2	R	1	MAN	O5-C5-C4	-2.34	105.45	109.69
2	Q	1	MAN	C1-C2-C3	-2.31	105.52	110.31
2	U	1	MAN	C1-O5-C5	-2.31	109.30	113.66
2	S	2	MAN	O4-C4-C3	-2.25	105.16	110.35
2	S	1	MAN	O5-C1-C2	2.24	114.28	110.28
2	V	1	MAN	C1-C2-C3	-2.24	105.67	110.31
2	O	1	MAN	C1-O5-C5	-2.18	109.56	113.66
2	S	1	MAN	O5-C5-C4	-2.05	105.98	109.69
2	U	2	MAN	C1-O5-C5	-2.04	109.42	112.19
2	T	1	MAN	C3-C4-C5	-2.04	106.59	110.24

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	S	1	MAN	C4-C5-C6-O6
2	T	2	MAN	O5-C5-C6-O6

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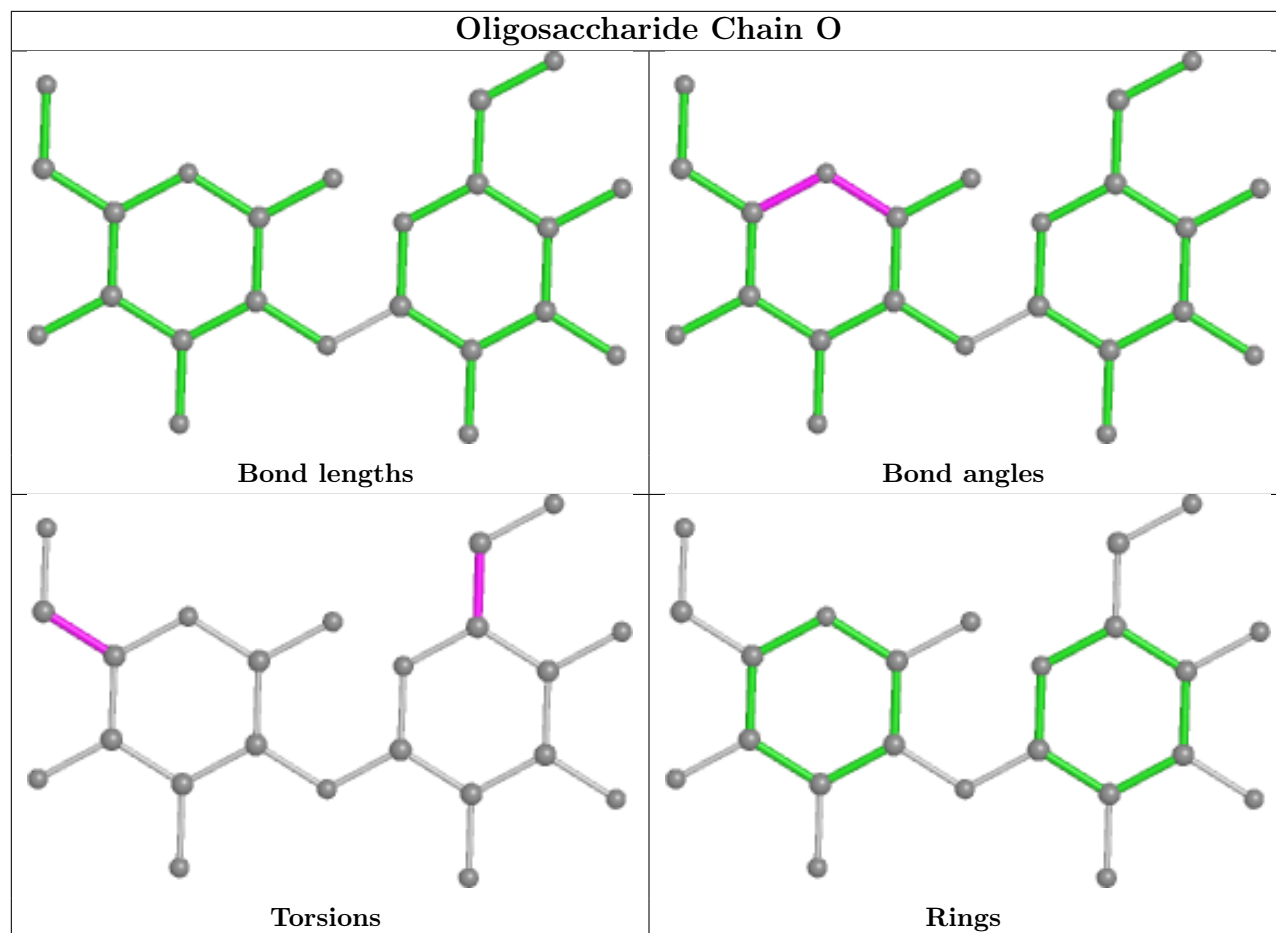
Mol	Chain	Res	Type	Atoms
2	Q	1	MAN	O5-C5-C6-O6
2	O	2	MAN	O5-C5-C6-O6
2	S	1	MAN	O5-C5-C6-O6
2	P	2	MAN	O5-C5-C6-O6
2	T	2	MAN	C4-C5-C6-O6
2	U	2	MAN	O5-C5-C6-O6
2	U	2	MAN	C4-C5-C6-O6
2	U	1	MAN	C4-C5-C6-O6
2	O	1	MAN	O5-C5-C6-O6
2	R	1	MAN	O5-C5-C6-O6
2	U	1	MAN	O5-C5-C6-O6
2	O	2	MAN	C4-C5-C6-O6

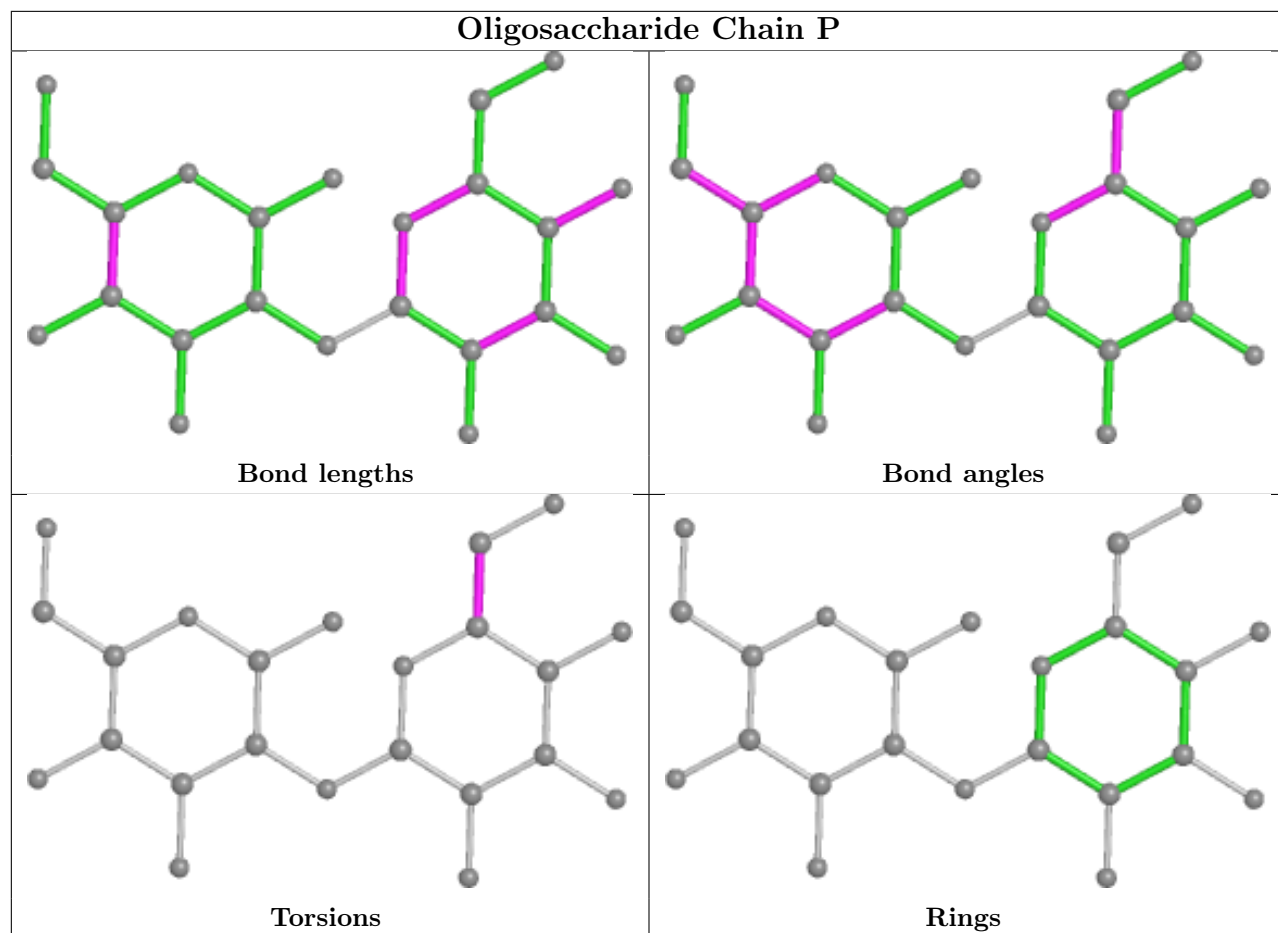
There are no ring outliers.

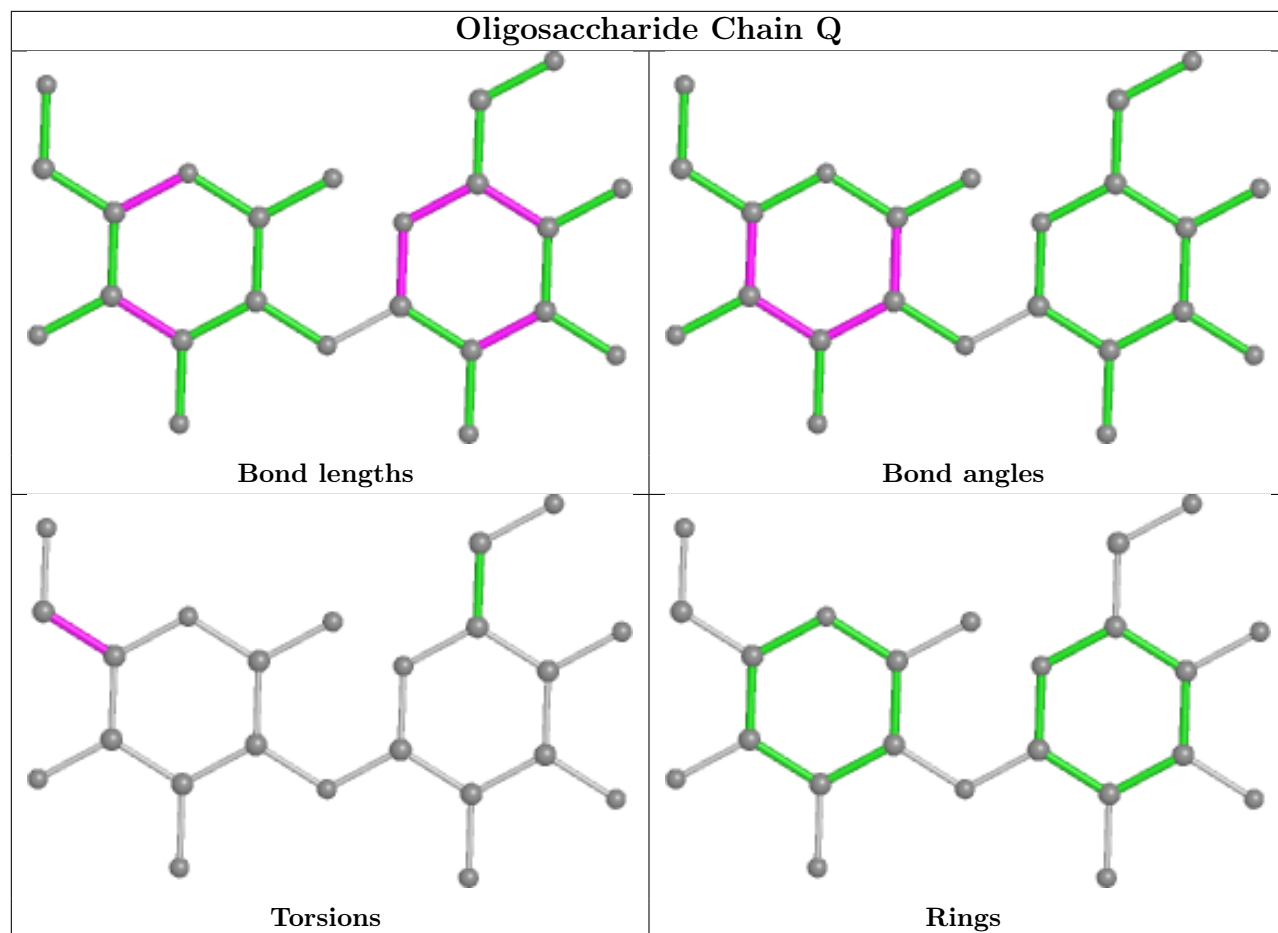
7 monomers are involved in 23 short contacts:

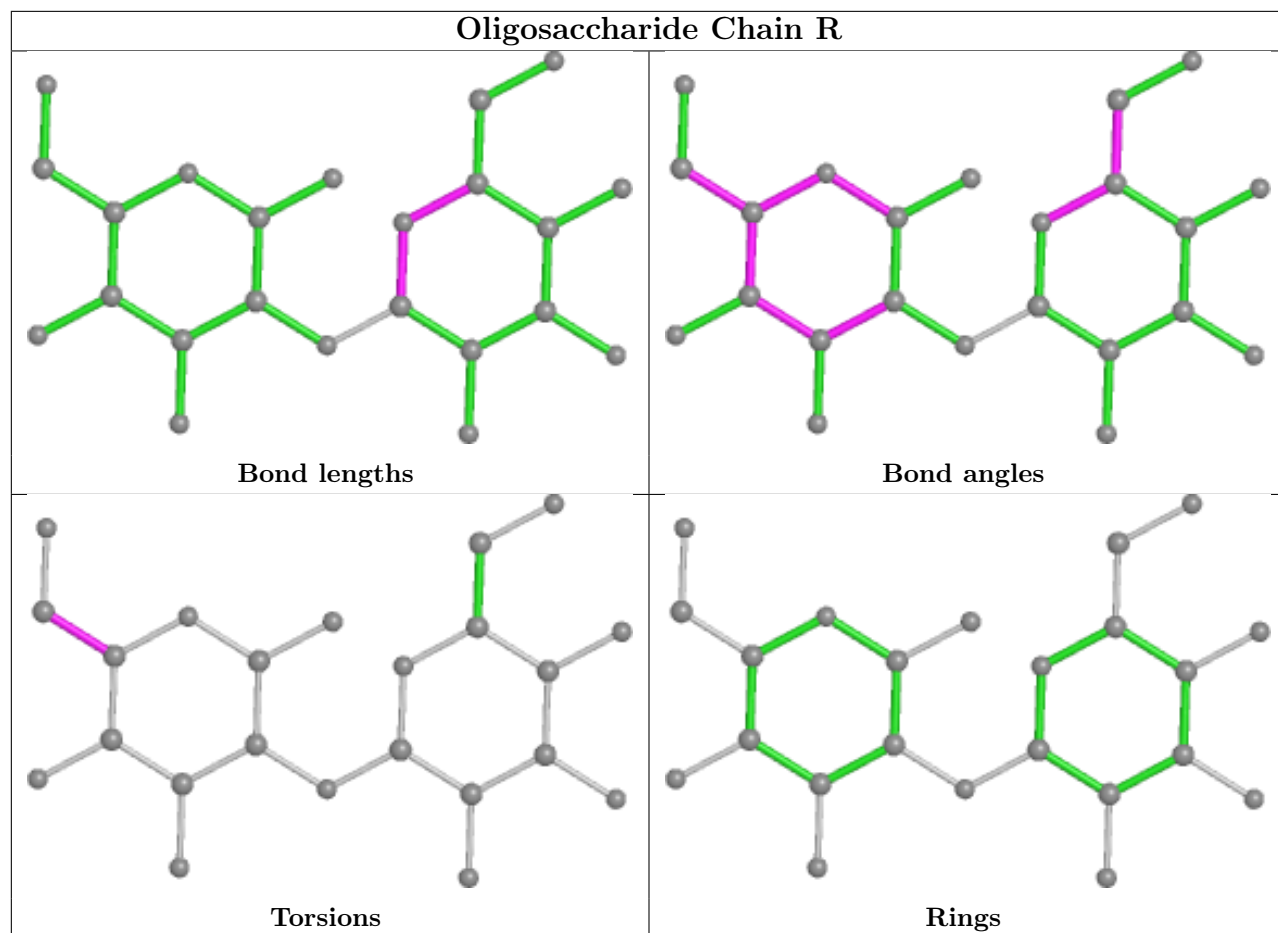
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	P	2	MAN	14	0
2	O	1	MAN	4	0
2	S	1	MAN	2	0
2	T	1	MAN	2	0
2	T	2	MAN	2	0
2	O	2	MAN	5	0
2	S	2	MAN	1	0

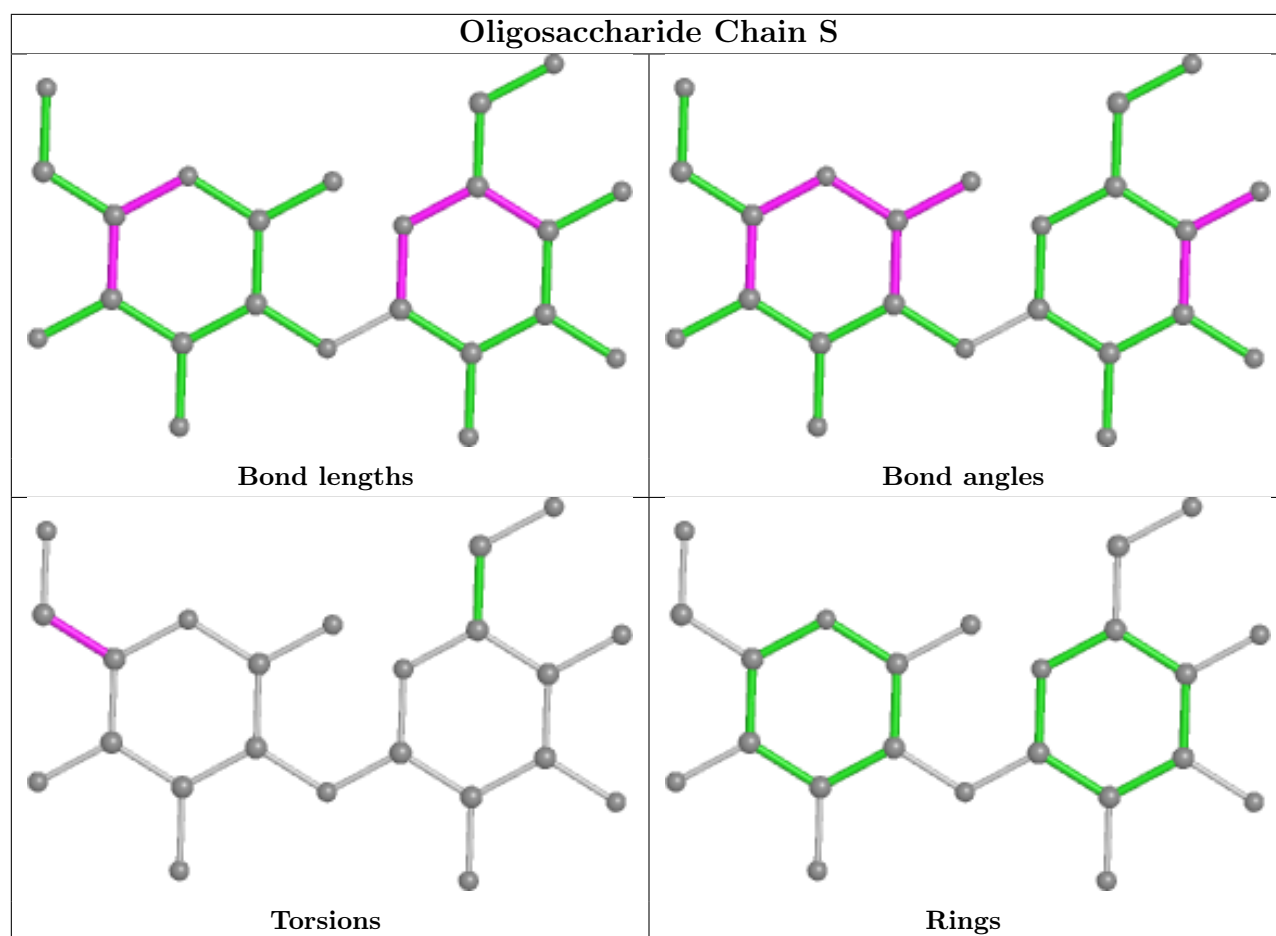
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

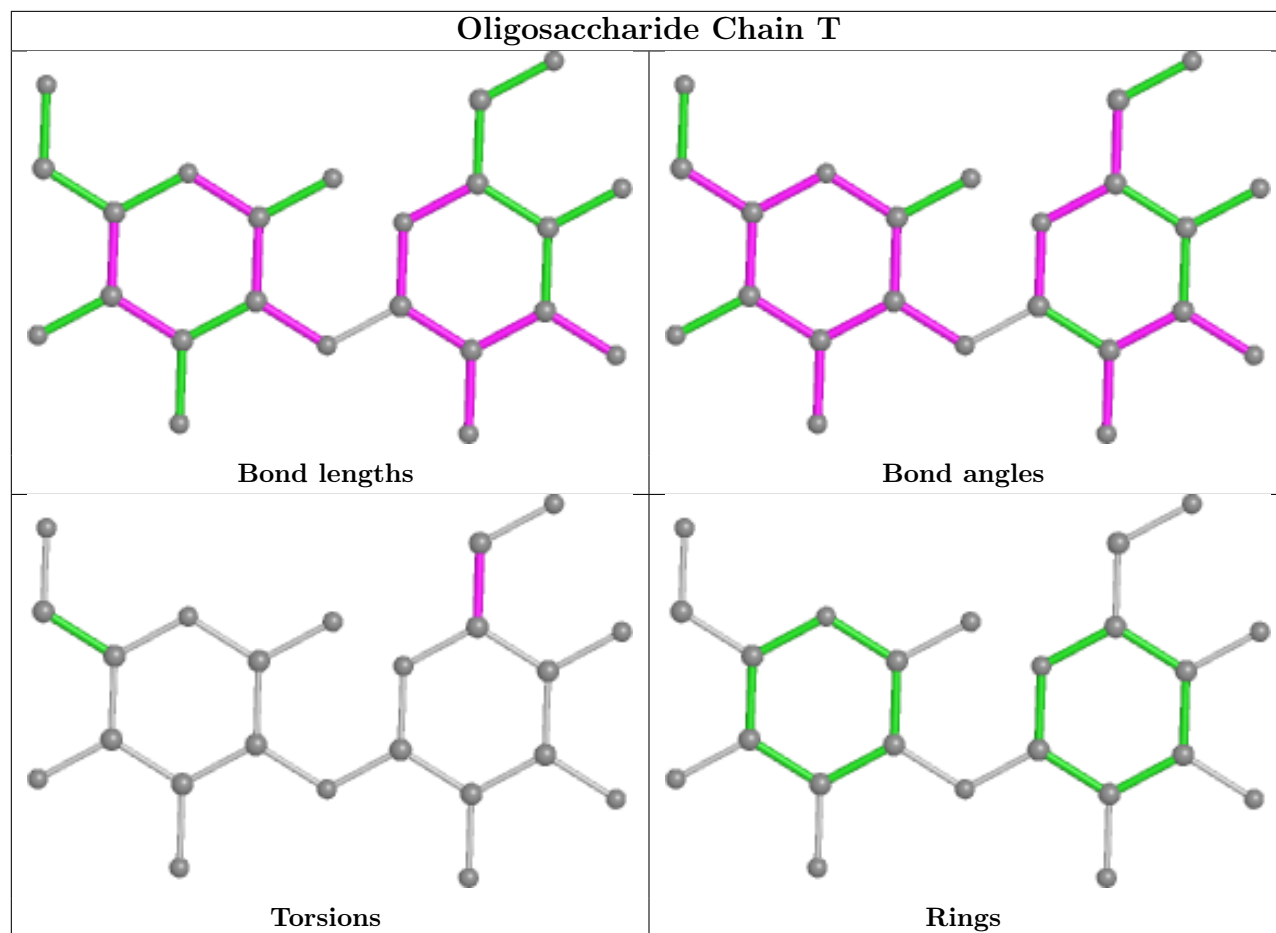




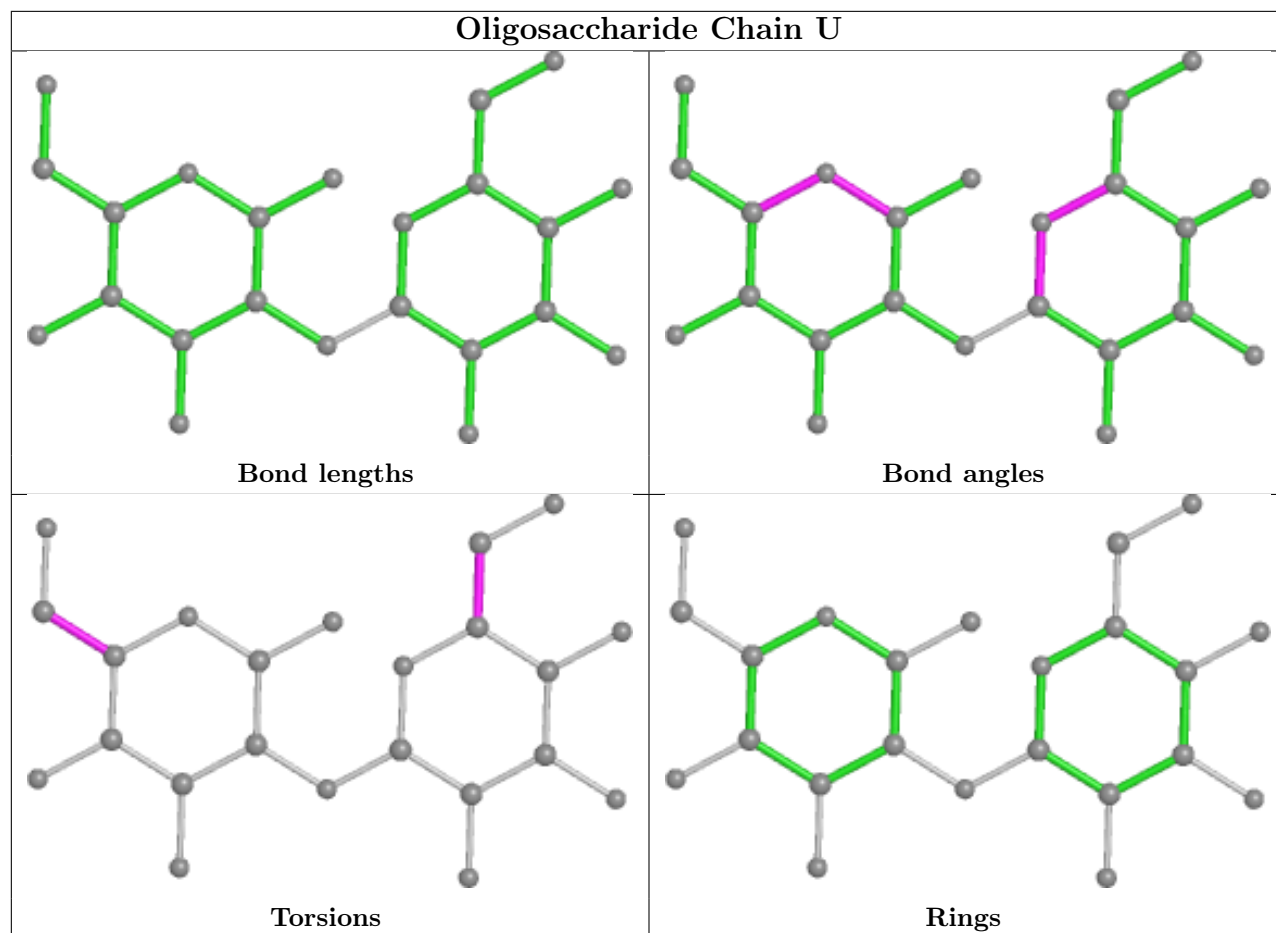


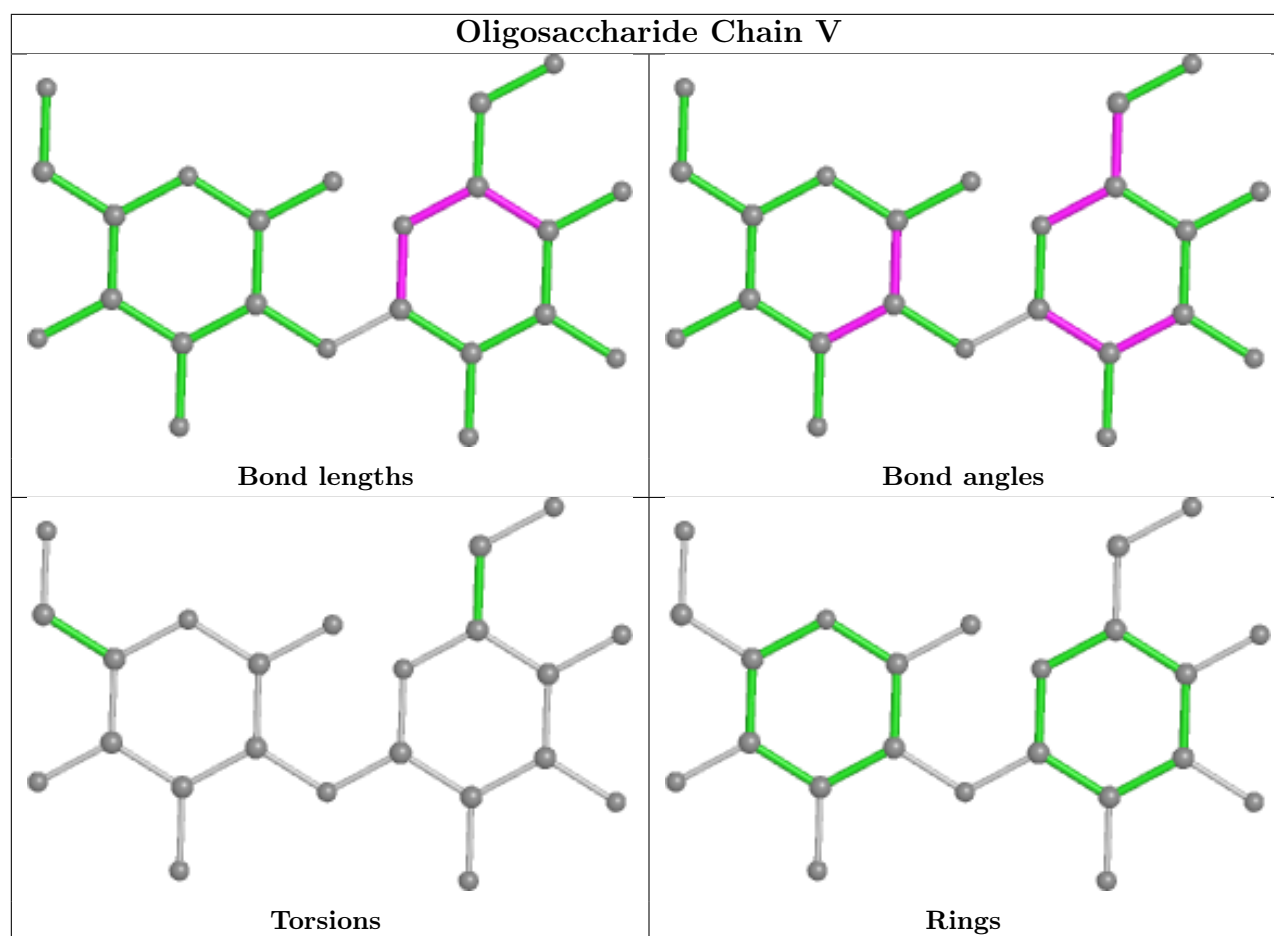












## 5.6 Ligand geometry [i](#)

4 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	$\# Z  > 2$
3	MAN	H	202	-	11,11,12	3.06	5 (45%)	15,15,17	2.01	8 (53%)
3	MAN	H	201	-	12,12,12	3.40	8 (66%)	17,17,17	1.97	6 (35%)
4	ALA	I	201	-	3,4,5	0.94	0	2,4,6	1.82	1 (50%)
3	MAN	I	202	-	12,12,12	1.11	2 (16%)	17,17,17	1.22	1 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MAN	H	202	-	-	0/2/19/22	0/1/1/1
3	MAN	H	201	-	-	2/2/22/22	0/1/1/1
4	ALA	I	201	-	-	0/0/2/4	-
3	MAN	I	202	-	-	2/2/22/22	0/1/1/1

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	202	MAN	C1-C2	7.22	1.68	1.52
3	H	201	MAN	O5-C1	6.45	1.59	1.42
3	H	201	MAN	O1-C1	5.13	1.56	1.39
3	H	202	MAN	O5-C1	4.73	1.51	1.43
3	H	201	MAN	C4-C5	4.49	1.62	1.53
3	H	201	MAN	C4-C3	4.18	1.63	1.52
3	H	201	MAN	O2-C2	4.00	1.52	1.43
3	H	202	MAN	C4-C5	3.28	1.59	1.53
3	H	202	MAN	O3-C3	2.79	1.49	1.43
3	H	201	MAN	C1-C2	2.51	1.58	1.52
3	H	202	MAN	C2-C3	2.17	1.55	1.52
3	I	202	MAN	C3-C2	-2.15	1.46	1.52
3	H	201	MAN	C6-C5	2.14	1.59	1.51
3	H	201	MAN	O3-C3	2.13	1.48	1.43
3	I	202	MAN	O1-C1	2.08	1.46	1.39

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	201	MAN	C6-C5-C4	3.32	120.78	113.00
3	H	201	MAN	O3-C3-C4	3.17	117.68	110.35
3	H	201	MAN	O1-C1-O5	3.15	119.85	110.38
3	H	202	MAN	C1-C2-C3	3.10	113.47	109.67
3	H	202	MAN	O5-C5-C6	3.05	111.98	107.20
3	H	201	MAN	C1-C2-C3	-2.96	104.18	110.31
3	H	201	MAN	O2-C2-C1	2.82	115.70	109.16
3	H	202	MAN	O2-C2-C1	2.66	114.59	109.15
4	I	201	ALA	O-C-CA	-2.52	116.30	124.28
3	I	202	MAN	O5-C1-C2	-2.52	105.79	110.28
3	H	202	MAN	O2-C2-C3	-2.51	105.10	110.14
3	H	202	MAN	O4-C4-C3	-2.37	104.86	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	202	MAN	C2-C3-C4	-2.24	107.02	110.89
3	H	202	MAN	O3-C3-C2	2.22	114.25	109.99
3	H	201	MAN	C4-C3-C2	-2.07	107.21	110.82
3	H	202	MAN	C3-C4-C5	-2.03	106.62	110.24

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	H	201	MAN	C4-C5-C6-O6
3	I	202	MAN	O5-C5-C6-O6
3	H	201	MAN	O5-C5-C6-O6
3	I	202	MAN	C4-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	202	MAN	1	0
3	H	201	MAN	1	0
3	I	202	MAN	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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	140/145 (96%)	0.11	1 (0%) 87 84	37, 52, 78, 95	0
1	B	138/145 (95%)	0.15	1 (0%) 87 84	44, 67, 89, 102	0
1	C	140/145 (96%)	0.22	0 100 100	38, 53, 76, 85	0
1	D	140/145 (96%)	0.18	0 100 100	35, 51, 72, 91	0
1	E	140/145 (96%)	0.25	0 100 100	38, 57, 86, 120	0
1	F	140/145 (96%)	0.31	1 (0%) 87 84	39, 60, 85, 111	0
1	G	140/145 (96%)	0.16	0 100 100	39, 56, 73, 102	0
1	H	140/145 (96%)	0.19	0 100 100	41, 56, 75, 102	0
1	I	140/145 (96%)	0.25	3 (2%) 63 54	30, 68, 91, 112	0
1	J	140/145 (96%)	0.16	1 (0%) 87 84	33, 47, 70, 112	0
1	K	140/145 (96%)	0.16	0 100 100	39, 52, 73, 98	0
1	L	140/145 (96%)	0.29	1 (0%) 87 84	30, 59, 81, 98	0
1	M	140/145 (96%)	0.24	1 (0%) 87 84	33, 53, 82, 93	0
1	N	140/145 (96%)	0.15	0 100 100	40, 54, 76, 89	0
All	All	1958/2030 (96%)	0.20	9 (0%) 91 88	30, 56, 82, 120	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	143	LEU	3.8
1	J	27	SER	3.6
1	F	143	LEU	3.1
1	I	27	SER	2.6
1	I	41	TYR	2.6
1	A	91	ASP	2.2
1	B	131	ALA	2.2
1	M	143	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	I	43	LEU	2.0

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

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

## 6.3 Carbohydrates [i](#)

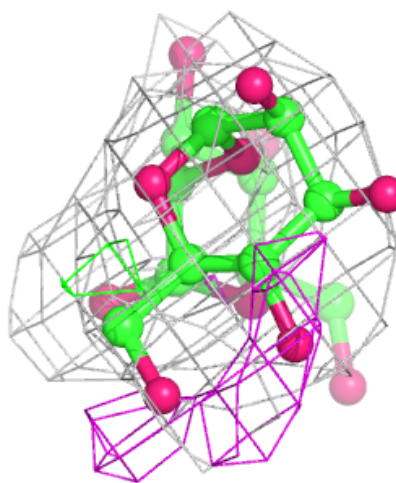
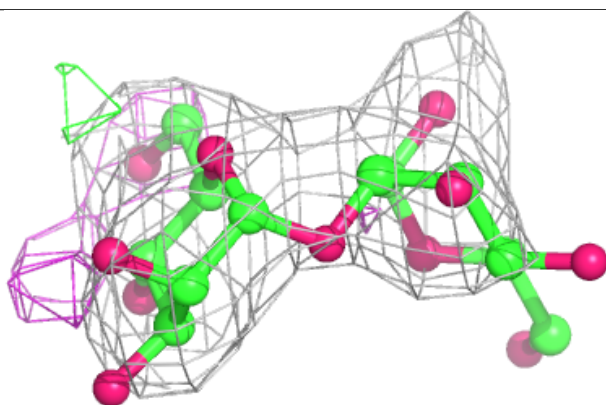
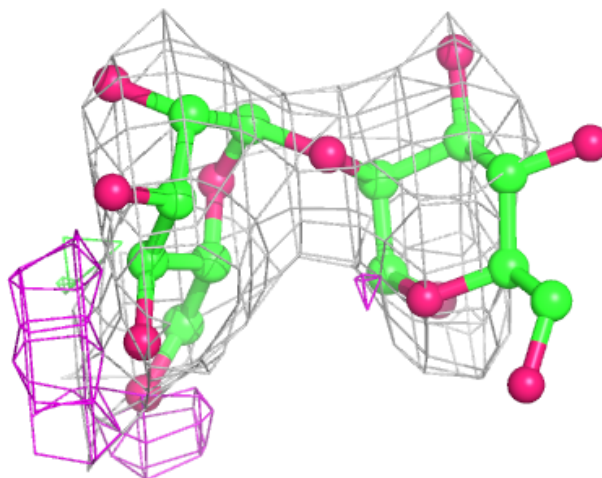
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	MAN	O	1	12/12	0.66	0.50	77,107,117,123	0
2	MAN	T	1	12/12	0.75	0.45	97,132,137,138	0
2	MAN	T	2	11/12	0.76	0.34	68,90,109,114	0
2	MAN	U	1	12/12	0.78	0.50	91,113,125,126	0
2	MAN	P	2	11/12	0.82	0.26	76,97,105,109	0
2	MAN	U	2	11/12	0.82	0.40	55,73,81,100	0
2	MAN	P	1	12/12	0.83	0.48	82,123,131,136	0
2	MAN	O	2	11/12	0.84	0.33	62,81,99,106	0
2	MAN	V	1	12/12	0.86	0.38	78,95,110,111	0
2	MAN	R	1	12/12	0.88	0.44	69,91,101,103	0
2	MAN	V	2	11/12	0.88	0.21	48,68,82,84	0
2	MAN	S	1	12/12	0.88	0.40	59,78,91,106	0
2	MAN	R	2	11/12	0.90	0.45	62,76,83,86	0
2	MAN	Q	1	12/12	0.91	0.31	65,93,98,102	0
2	MAN	S	2	11/12	0.92	0.35	50,67,75,75	0
2	MAN	Q	2	11/12	0.93	0.20	52,65,71,73	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.

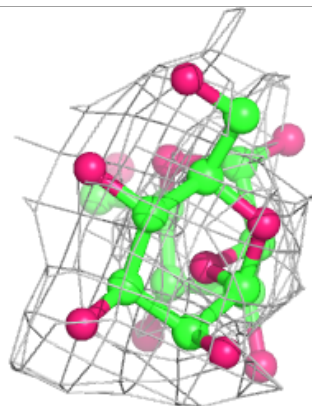
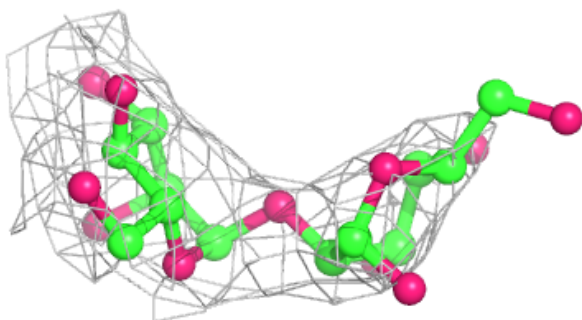
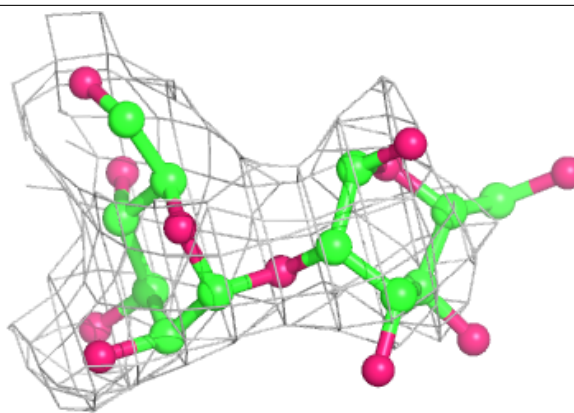
**Electron density around Chain O:**

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



**Electron density around Chain P:**

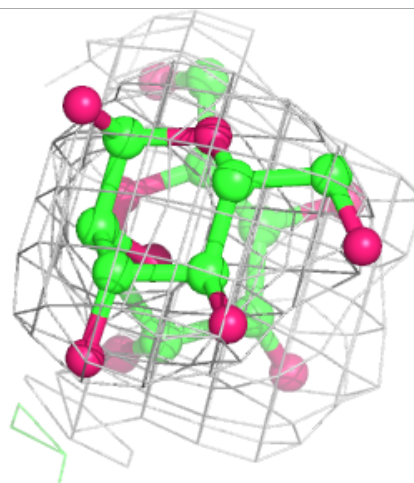
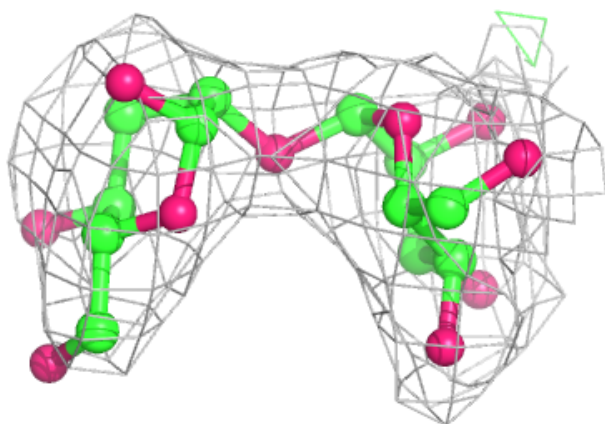
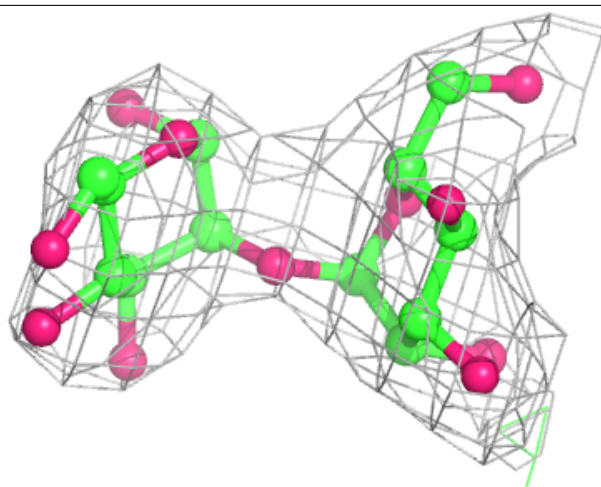
$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





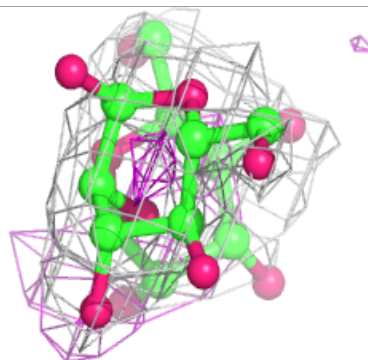
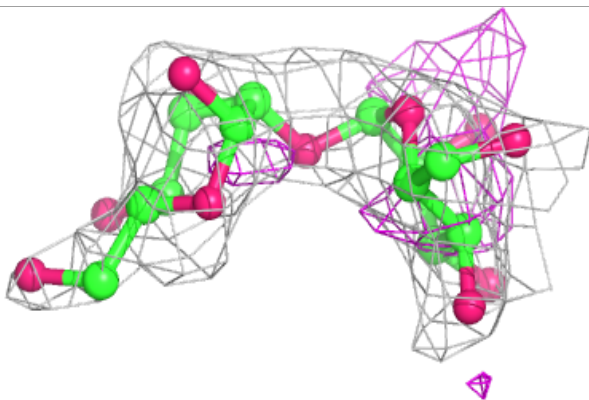
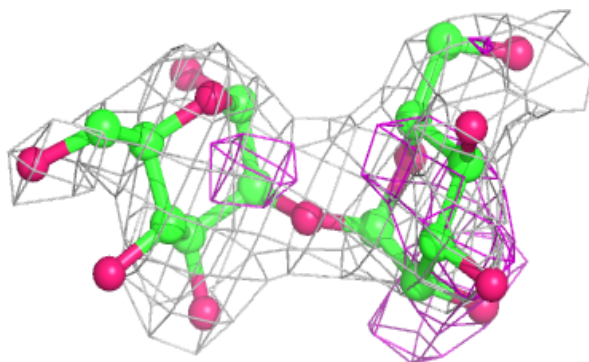
**Electron density around Chain Q:**

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



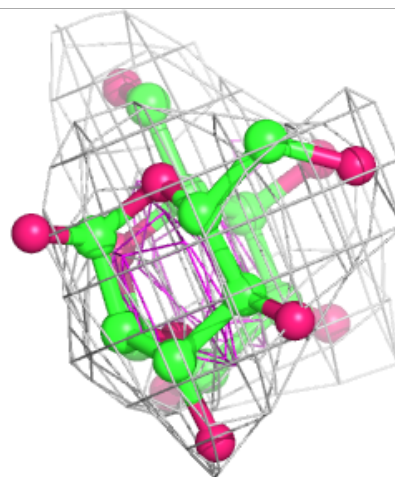
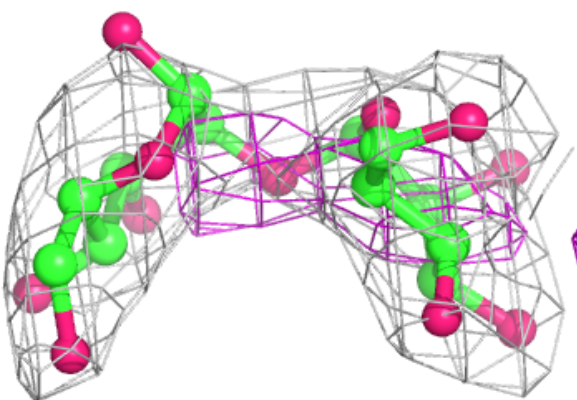
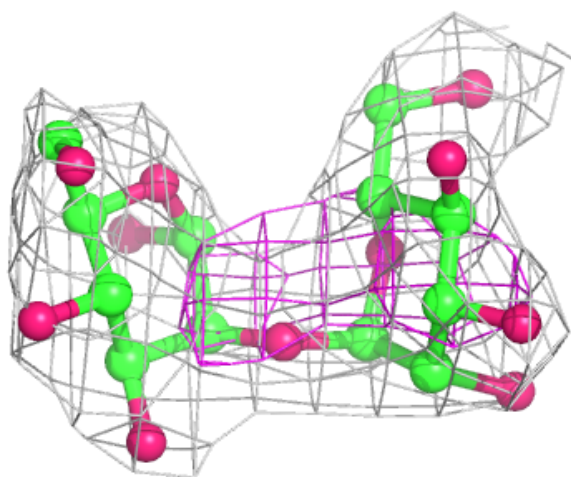
**Electron density around Chain R:**

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



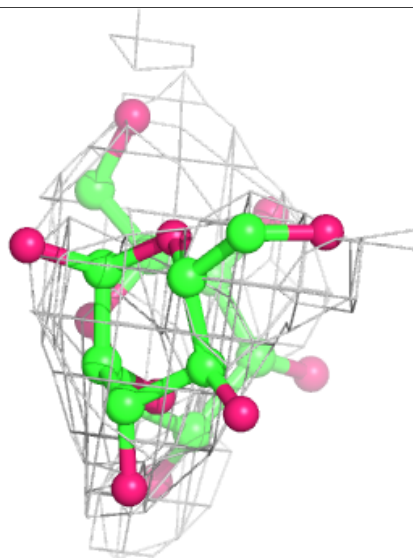
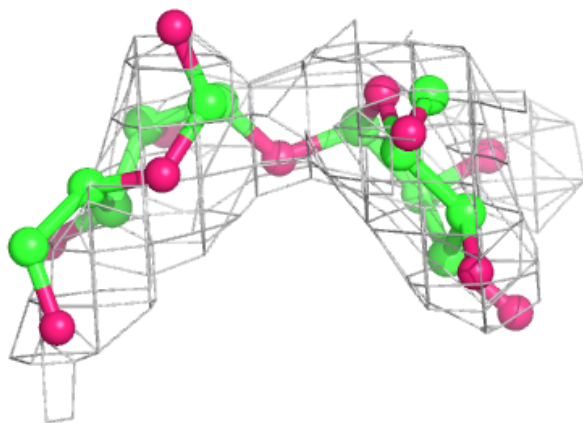
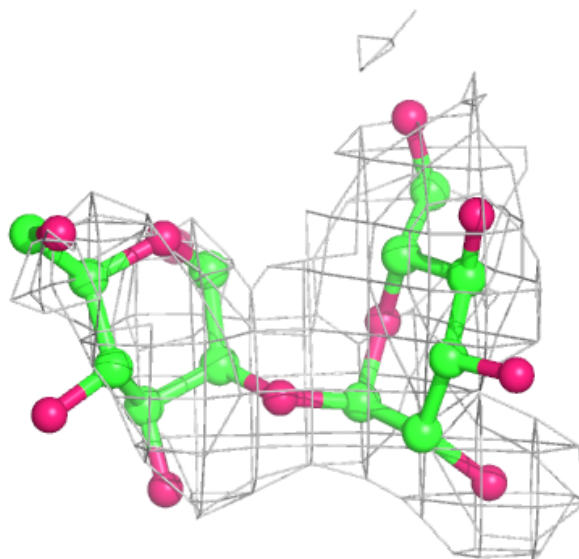
**Electron density around Chain S:**

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



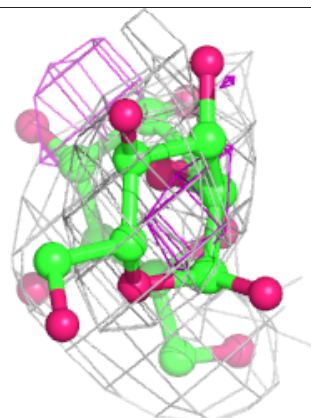
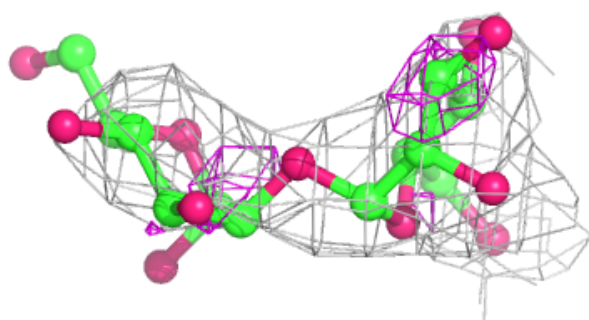
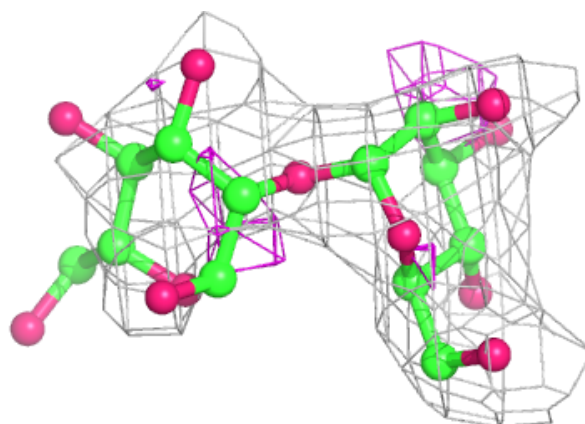
**Electron density around Chain T:**

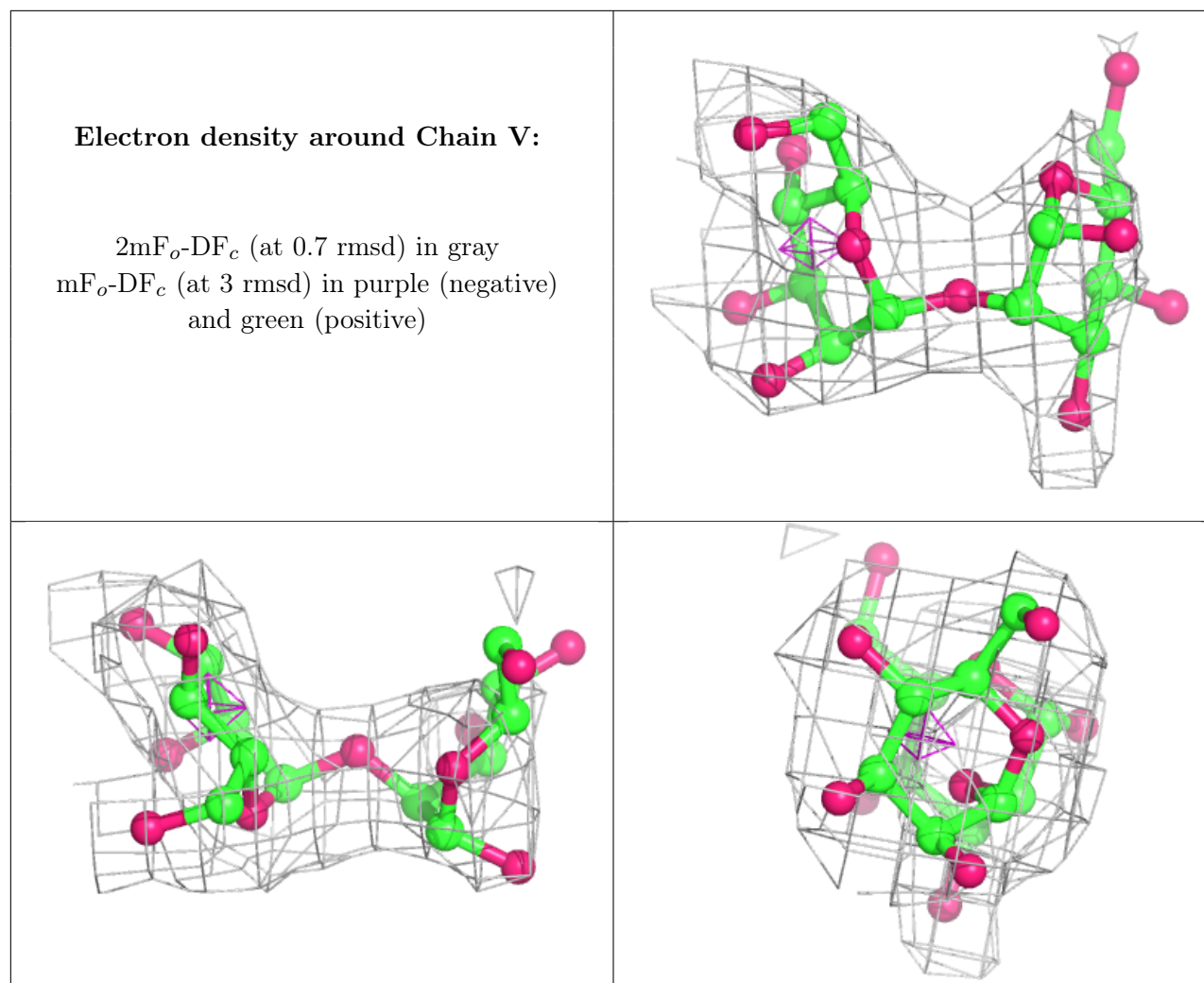
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around Chain U:**

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





## 6.4 Ligands [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<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
3	MAN	I	202	12/12	0.59	0.41	72,95,108,110	0
4	ALA	I	201	5/6	0.70	0.29	73,82,96,100	0
3	MAN	H	201	12/12	0.78	0.49	86,97,110,110	0
3	MAN	H	202	11/12	0.94	0.37	56,82,99,108	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.