



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 07:08 PM UTC

PDB ID : 6RUV / pdb_00006ruv
Title : Structure of the SCIN stabilized C3bBb convertase bound to Properdin and a the non-inhibitory nanobody hFPNb1
Authors : Pedersen, D.V.; Andersen, G.R.
Deposited on : 2019-05-29
Resolution : 6.15 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

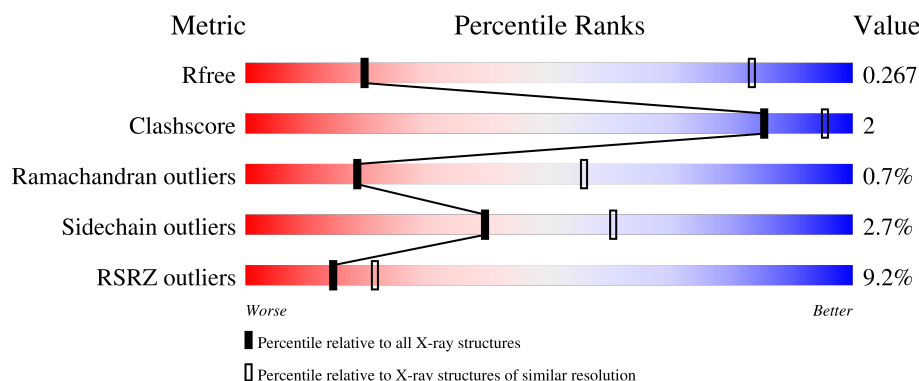
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 6.15 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}	180053	1147 (8.30-4.00)
Clashscore	190562	1008 (8.30-4.02)
Ramachandran outliers	187476	1036 (8.30-4.00)
Sidechain outliers	187428	1002 (8.30-4.00)
RSRZ outliers	180081	1140 (8.30-4.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	R	131	2% 89% 5% • 5%
1	S	131	8% 93% • 5%
2	U	170	8% 55% 7% 38%
2	X	170	6% 82% 13% • •
3	V	221	12% 81% 14% • •

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Mol	Chain	Length	Quality of chain
3	Y	221	
4	A	645	
4	G	645	
5	B	915	
5	H	915	
6	J	505	
6	L	505	
7	N	86	
7	Q	86	
8	C	2	
8	D	2	
8	F	2	
8	I	2	
8	K	2	
9	E	3	
9	M	3	
10	O	2	
10	P	2	
10	T	2	
10	W	2	
10	Z	2	
10	a	2	
10	b	2	
10	c	2	

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	NAG	Z	1	X	-	-	-
10	NAG	b	1	X	-	-	-
9	FUC	E	3	X	-	-	-
9	NAG	M	1	X	-	-	-
9	FUC	M	3	X	-	-	-

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 41916 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 Nanobody hFPNb1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	R	124	Total	C	N	O	S	0	0	0
			951	588	172	187	4			
1	S	124	Total	C	N	O	S	0	0	0
			951	588	172	187	4			

- Molecule 2 is a protein called Properdin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	U	105	Total	C	N	O	S	0	0	0
			800	492	143	153	12			
2	X	163	Total	C	N	O	S	0	0	0
			1228	746	227	234	21			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
U	192	GLU	-	expression tag	UNP P27918
U	193	ASN	-	expression tag	UNP P27918
U	194	LEU	-	expression tag	UNP P27918
U	195	TYR	-	expression tag	UNP P27918
U	196	PHE	-	expression tag	UNP P27918
U	197	GLN	-	expression tag	UNP P27918
X	192	GLU	-	expression tag	UNP P27918
X	193	ASN	-	expression tag	UNP P27918
X	194	LEU	-	expression tag	UNP P27918
X	195	TYR	-	expression tag	UNP P27918
X	196	PHE	-	expression tag	UNP P27918
X	197	GLN	-	expression tag	UNP P27918

- Molecule 3 is a protein called Properdin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	V	215	Total	C	N	O	S	0	0	0
			1666	1030	313	301	22			
3	Y	215	Total	C	N	O	S	0	0	0
			1666	1030	313	301	22			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
V	255	GLY	-	expression tag	UNP P27918
V	470	GLU	-	expression tag	UNP P27918
V	471	ASN	-	expression tag	UNP P27918
V	472	LEU	-	expression tag	UNP P27918
V	473	TYR	-	expression tag	UNP P27918
V	474	PHE	-	expression tag	UNP P27918
V	475	GLN	-	expression tag	UNP P27918
Y	255	GLY	-	expression tag	UNP P27918
Y	470	GLU	-	expression tag	UNP P27918
Y	471	ASN	-	expression tag	UNP P27918
Y	472	LEU	-	expression tag	UNP P27918
Y	473	TYR	-	expression tag	UNP P27918
Y	474	PHE	-	expression tag	UNP P27918
Y	475	GLN	-	expression tag	UNP P27918

- Molecule 4 is a protein called Complement C3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	A	645	Total	C	N	O	S	0	0	0
			5025	3198	851	961	15			
4	G	645	Total	C	N	O	S	0	0	0
			5025	3198	851	961	15			

- Molecule 5 is a protein called Complement C3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	B	913	Total	C	N	O	S	0	0	0
			7293	4619	1228	1408	38			
5	H	913	Total	C	N	O	S	0	0	0
			7293	4619	1228	1408	38			

- Molecule 6 is a protein called Complement factor B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	J	505	Total	C	N	O	S	0	0	0
			4007	2546	689	752	20			
6	L	505	Total	C	N	O	S	0	0	0
			4007	2546	689	752	20			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	254	GLY	ASP	conflict	UNP P00751
J	674	ALA	SER	conflict	UNP P00751
L	254	GLY	ASP	conflict	UNP P00751
L	674	ALA	SER	conflict	UNP P00751

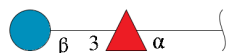
- Molecule 7 is a protein called Inhibitor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	N	84	Total	C	N	O	S	0	0	0
			683	432	111	138	2			
7	Q	84	Total	C	N	O	S	0	0	0
			683	432	111	138	2			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
N	0	GLY	ALA	conflict	UNP A0A0H2DUF0
Q	0	GLY	ALA	conflict	UNP A0A0H2DUF0

- Molecule 8 is an oligosaccharide called beta-D-glucopyranose-(1-3)-alpha-L-fucopyranose.



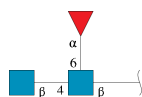
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
8	C	2	Total	C	O	0	0	0
			21	12	9			
8	D	2	Total	C	O	0	0	0
			21	12	9			
8	F	2	Total	C	O	0	0	0
			21	12	9			
8	I	2	Total	C	O	0	0	0
			21	12	9			

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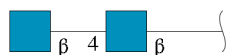
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
8	K	2	Total	C	O	0	0	0
			21	12	9			

- Molecule 9 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



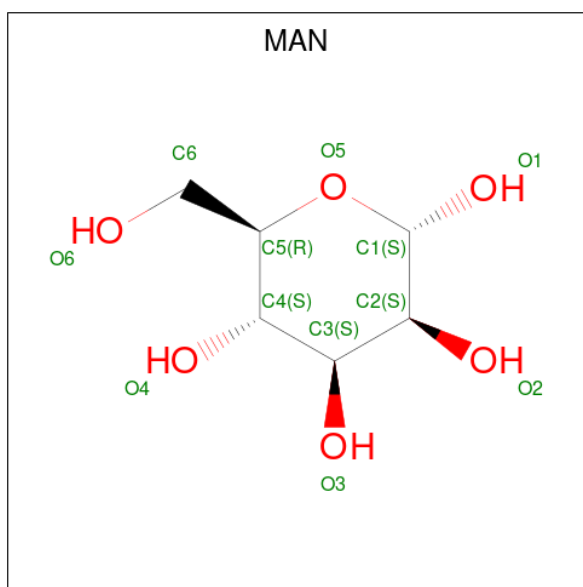
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	E	3	Total	C	N	O	0	0	0
			38	22	2	14			
9	M	3	Total	C	N	O	0	0	0
			38	22	2	14			

- Molecule 10 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
10	O	2	Total	C	N	O	0	0	0
			28	16	2	10			
10	P	2	Total	C	N	O	0	0	0
			28	16	2	10			
10	T	2	Total	C	N	O	0	0	0
			28	16	2	10			
10	W	2	Total	C	N	O	0	0	0
			28	16	2	10			
10	Z	2	Total	C	N	O	0	0	0
			28	16	2	10			
10	a	2	Total	C	N	O	0	0	0
			28	16	2	10			
10	b	2	Total	C	N	O	0	0	0
			28	16	2	10			
10	c	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 11 is alpha-D-mannopyranose (CCD ID: MAN) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	U	1	Total	C	O	0	0
			11	6	5		
11	U	1	Total	C	O	0	0
			11	6	5		
11	V	1	Total	C	O	0	0
			11	6	5		
11	V	1	Total	C	O	0	0
			11	6	5		
11	V	1	Total	C	O	0	0
			11	6	5		
11	V	1	Total	C	O	0	0
			11	6	5		
11	V	1	Total	C	O	0	0
			11	6	5		
11	X	1	Total	C	O	0	0
			11	6	5		
11	X	1	Total	C	O	0	0
			11	6	5		
11	X	1	Total	C	O	0	0
			11	6	5		
11	X	1	Total	C	O	0	0
			11	6	5		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	Y	1	Total	C	O	0	0
			11	6	5		
11	Y	1	Total	C	O	0	0
			11	6	5		
11	Y	1	Total	C	O	0	0
			11	6	5		
11	Y	1	Total	C	O	0	0
			11	6	5		
11	Y	1	Total	C	O	0	0
			11	6	5		
11	Y	1	Total	C	O	0	0
			11	6	5		

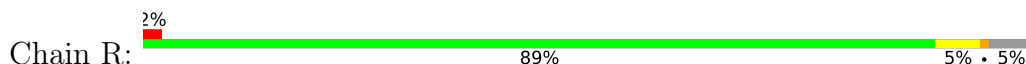
- Molecule 12 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	J	1	Total	Mg	0	0
			1	1		
12	L	1	Total	Mg	0	0
			1	1		

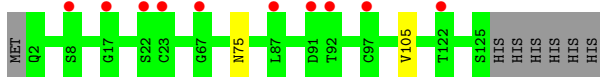
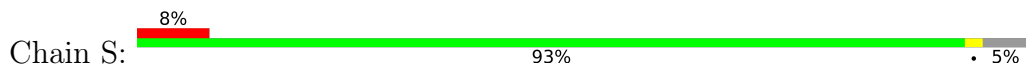
3 Residue-property plots [i](#)

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.

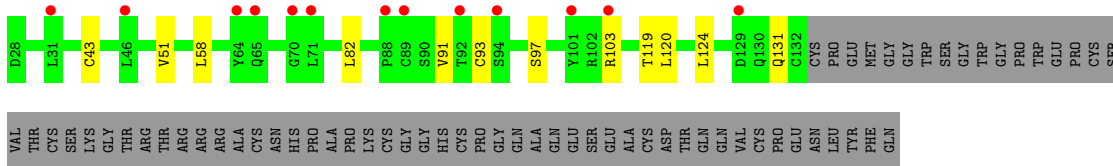
- Molecule 1: Nanobody hFPNb1



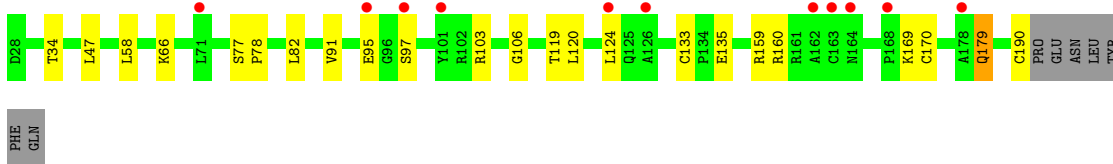
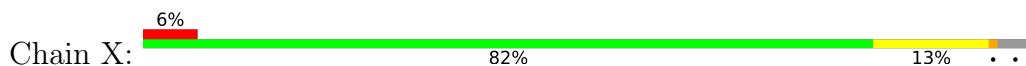
- Molecule 1: Nanobody hFPNb1



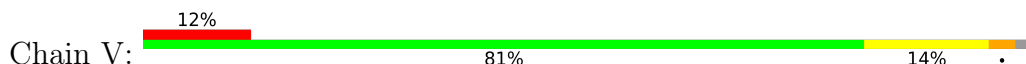
- Molecule 2: Properdin

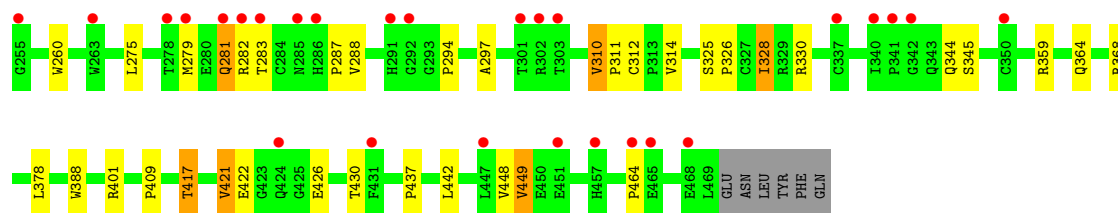


- Molecule 2: Properdin

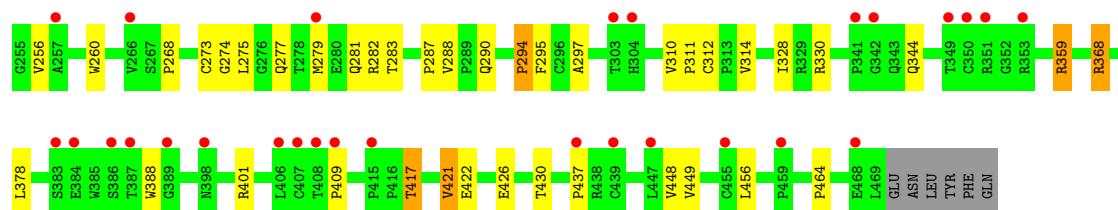
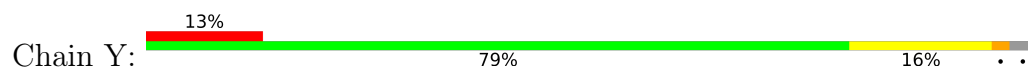


- Molecule 3: Properdin

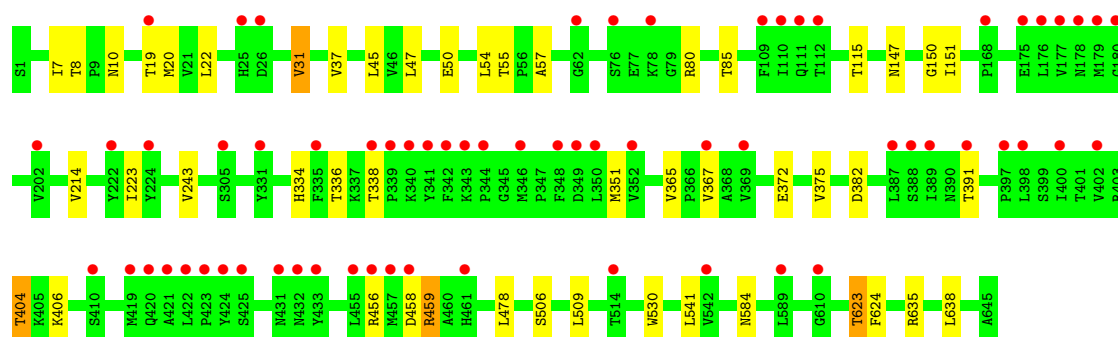
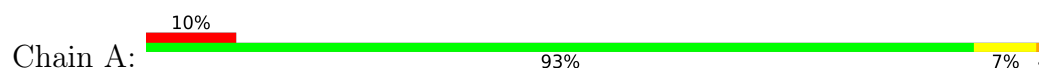




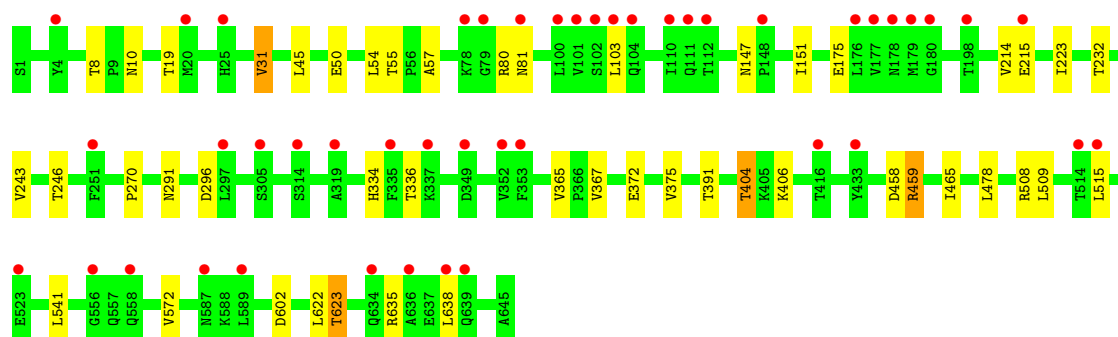
• Molecule 3: Properdin



• Molecule 4: Complement C3

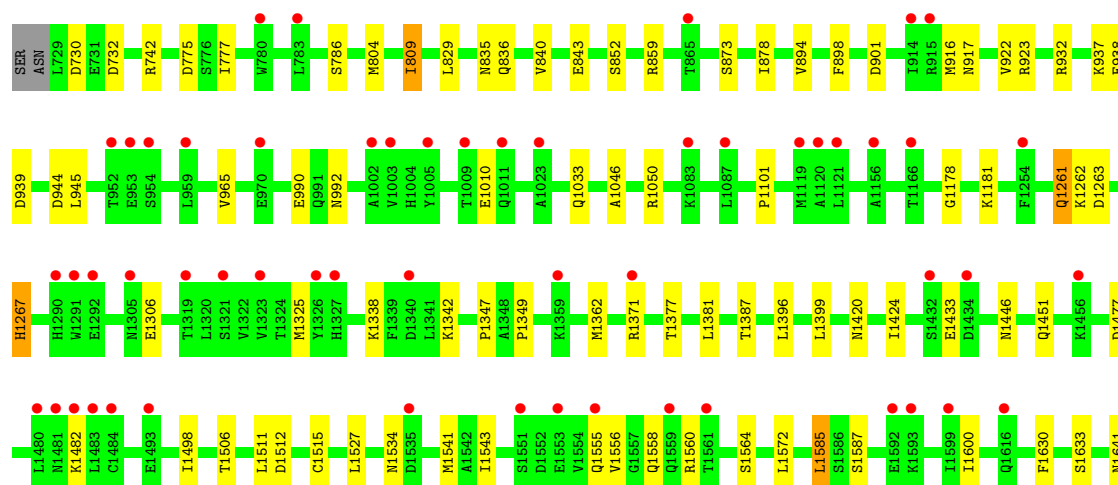


• Molecule 4: Complement C3

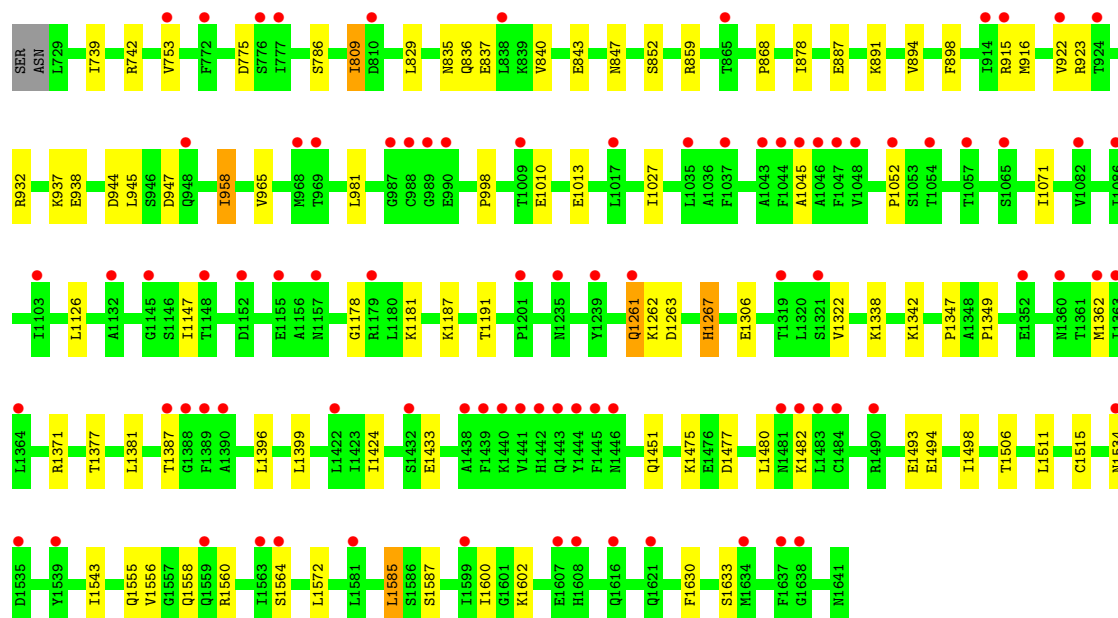
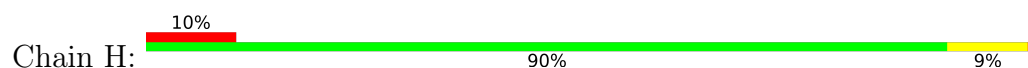


• Molecule 5: Complement C3

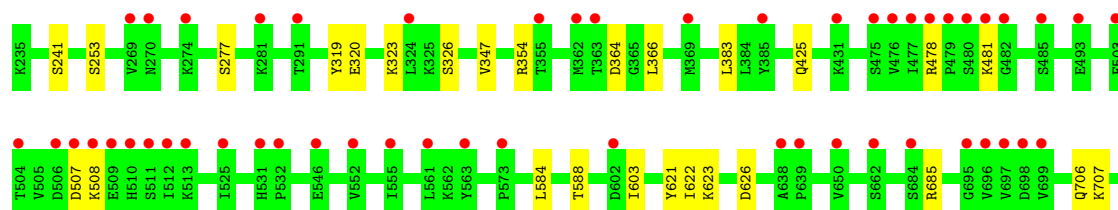




• Molecule 5: Complement C3

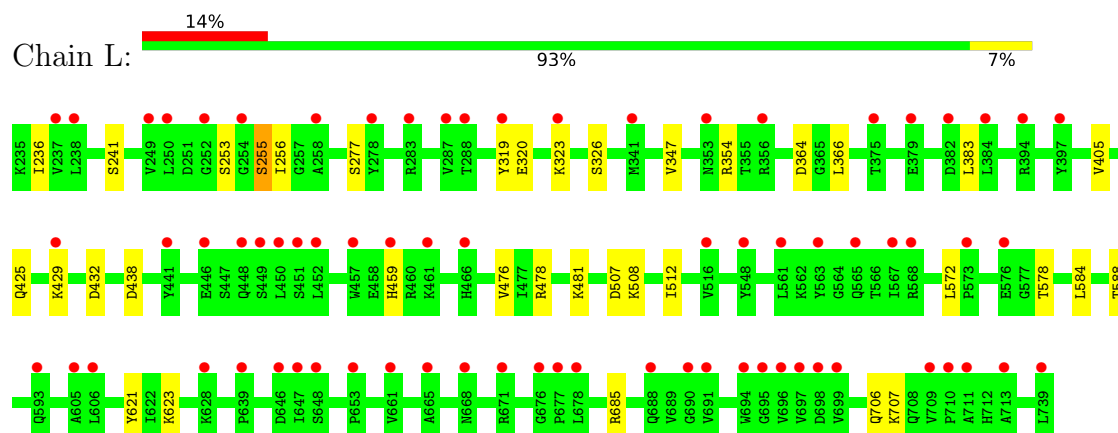


• Molecule 6: Complement factor B

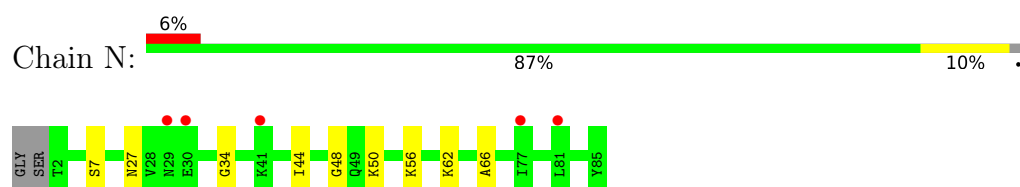




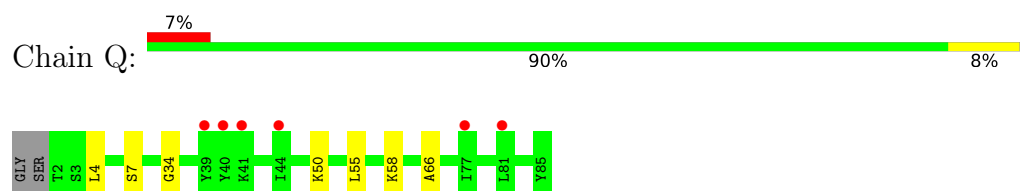
- Molecule 6: Complement factor B



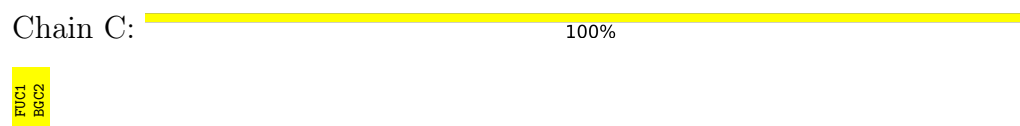
- Molecule 7: Inhibitor



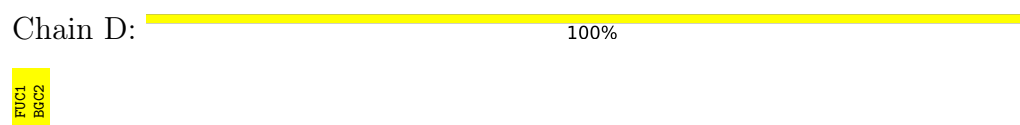
- Molecule 7: Inhibitor



- Molecule 8: beta-D-glucopyranose-(1-3)-alpha-L-fucopyranose



- Molecule 8: beta-D-glucopyranose-(1-3)-alpha-L-fucopyranose



- Molecule 8: beta-D-glucopyranose-(1-3)-alpha-L-fucopyranose



FUC1
BGC2

- Molecule 8: beta-D-glucopyranose-(1-3)-alpha-L-fucopyranose

Chain I:  100%

FUC1
BGC2

- Molecule 8: beta-D-glucopyranose-(1-3)-alpha-L-fucopyranose

Chain K:  100%

FUC1
BGC2

- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:  33% 67%

NAG1
NAG2
FUC3

- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:  100%

NAG1
NAG2
FUC3

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

Chain O:  100%

NAG1
NAG2

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

Chain P:  50% 50%

NAG1
NAG2

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

Chain T:  100%

MAG1
MAG2

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

Chain W:  50% 50%

MAG1
MAG2

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

Chain Z:  100%

MAG1
MAG2

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

Chain a:  50% 50%

MAG1
MAG2

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

Chain b:  100%

MAG1
MAG2

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

Chain c:  50% 50%

MAG1
MAG2

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	123.99Å 354.03Å 367.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.82 – 6.15 49.82 – 6.15	Depositor EDS
% Data completeness (in resolution range)	99.6 (49.82-6.15) 99.5 (49.82-6.15)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.10 (at 6.15Å)	Xtriage
Refinement program	PHENIX (1.14_3260: ???)	Depositor
R, R_{free}	0.242 , 0.271 0.243 , 0.267	Depositor DCC
R_{free} test set	1990 reflections (5.16%)	wwPDB-VP
Wilson B-factor (Å ²)	436.1	Xtriage
Anisotropy	0.347	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 876.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	0.030 for -h,l,k	Xtriage
F_o, F_c correlation	0.82	EDS
Total number of atoms	41916	wwPDB-VP
Average B, all atoms (Å ²)	499.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.85% 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: NAG, FUC, BGC, MAN, MG

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	R	0.22	0/967	0.49	0/1305
1	S	0.21	0/967	0.47	0/1305
2	U	0.21	0/819	0.54	0/1109
2	X	0.23	0/1261	0.59	0/1710
3	V	0.28	0/1720	0.63	0/2342
3	Y	0.27	0/1720	0.64	0/2342
4	A	0.23	0/5127	0.53	0/6966
4	G	0.24	0/5126	0.53	0/6962
5	B	0.23	0/7439	0.55	2/10073 (0.0%)
5	H	0.24	0/7439	0.55	2/10073 (0.0%)
6	J	0.21	0/4095	0.50	0/5542
6	L	0.22	0/4095	0.51	0/5542
7	N	0.27	0/691	0.62	0/923
7	Q	0.27	0/691	0.62	0/923
All	All	0.23	0/42157	0.54	4/57117 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	944	ASP	CA-C-N	5.23	131.52	121.54
5	H	944	ASP	C-N-CA	5.23	131.52	121.54
5	B	944	ASP	CA-C-N	5.14	131.36	121.54
5	B	944	ASP	C-N-CA	5.14	131.36	121.54

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	R	951	0	923	5	0
1	S	951	0	923	2	0
2	U	800	0	744	4	0
2	X	1228	0	1122	13	0
3	V	1666	0	1573	15	0
3	Y	1666	0	1572	17	0
4	A	5025	0	5084	20	0
4	G	5025	0	5084	21	0
5	B	7293	0	7217	36	0
5	H	7293	0	7217	38	0
6	J	4007	0	3994	15	0
6	L	4007	0	3994	20	0
7	N	683	0	697	7	0
7	Q	683	0	697	5	0
8	C	21	0	19	0	0
8	D	21	0	19	0	0
8	F	21	0	19	0	0
8	I	21	0	19	0	0
8	K	21	0	19	0	0
9	E	38	0	34	0	0
9	M	38	0	34	0	0
10	O	28	0	25	0	0
10	P	28	0	25	0	0
10	T	28	0	25	0	0
10	W	28	0	25	0	0
10	Z	28	0	25	0	0
10	a	28	0	25	0	0
10	b	28	0	25	0	0
10	c	28	0	25	0	0
11	U	22	0	20	0	0
11	V	77	0	70	0	0
11	X	55	0	50	1	0
11	Y	77	0	70	0	0
12	J	1	0	0	0	0
12	L	1	0	0	0	0
All	All	41916	0	41414	187	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 2.

All (187) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:80:ARG:NE	5:H:1010:GLU:OE2	2.13	0.80
4:A:80:ARG:NE	5:B:1010:GLU:OE2	2.20	0.72
5:H:843:GLU:OE2	5:H:859:ARG:NH1	2.19	0.71
2:X:58:LEU:HB3	3:Y:311:PRO:HA	1.80	0.63
4:G:291:ASN:ND2	4:G:296:ASP:OD2	2.32	0.62
5:H:1045:ALA:HB2	5:H:1052:PRO:HA	1.82	0.61
4:G:367:VAL:HA	4:G:404:THR:HA	1.83	0.60
3:Y:388:TRP:HB3	3:Y:401:ARG:HD2	1.85	0.58
5:B:1585:LEU:HD22	5:B:1587:SER:H	1.68	0.58
4:A:367:VAL:HA	4:A:404:THR:HA	1.85	0.58
6:L:241:SER:O	6:L:354:ARG:NH2	2.36	0.58
3:V:388:TRP:HB3	3:V:401:ARG:HD2	1.86	0.57
2:X:58:LEU:HB2	3:Y:274:GLY:HA2	1.87	0.56
5:H:840:VAL:HG22	5:H:894:VAL:HG12	1.88	0.56
4:G:10:ASN:HD22	4:G:623:THR:HG23	1.71	0.56
6:J:241:SER:O	6:J:354:ARG:NH2	2.39	0.56
1:S:105:VAL:HG11	3:V:279:MET:HB3	1.88	0.56
6:L:277:SER:O	6:L:685:ARG:NH1	2.40	0.55
5:B:1387:THR:HG22	5:B:1451:GLN:H	1.71	0.55
6:L:584:LEU:HD13	6:L:588:THR:HG21	1.89	0.55
5:H:1585:LEU:HD22	5:H:1587:SER:H	1.72	0.55
5:B:923:ARG:NH1	5:B:938:GLU:OE2	2.40	0.54
3:V:325:SER:HG	3:V:345:SER:H	1.56	0.54
2:X:159:ARG:NH2	11:X:208:MAN:O6	2.40	0.54
6:L:354:ARG:O	6:L:354:ARG:NH1	2.39	0.54
4:G:246:THR:HA	4:G:270:PRO:HA	1.89	0.53
5:H:742:ARG:HB3	5:H:775:ASP:HB3	1.90	0.53
5:B:809:ILE:N	5:B:901:ASP:OD2	2.35	0.53
5:B:873:SER:O	5:B:1420:ASN:ND2	2.41	0.53
1:R:105:VAL:HG11	3:Y:279:MET:HB3	1.91	0.52
5:B:1381:LEU:HB2	5:B:1424:ILE:HB	1.90	0.52
3:V:330:ARG:NH1	5:B:1512:ASP:OD2	2.43	0.52
6:J:584:LEU:HD13	6:J:588:THR:HG21	1.91	0.52
1:R:104:LEU:HD21	2:X:34:THR:HB	1.91	0.51
5:H:898:PHE:HB2	7:Q:50:LYS:HE2	1.92	0.51
6:L:320:GLU:HA	6:L:323:LYS:HB2	1.92	0.51
3:V:344:GLN:OE1	3:V:368:ARG:NH1	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:103:ARG:HH12	3:Y:464:PRO:HB2	1.75	0.51
5:B:1446:ASN:HB2	7:Q:4:LEU:HB2	1.93	0.51
1:S:75:ASN:ND2	3:V:281:GLN:OE1	2.43	0.51
5:B:1338:LYS:HA	5:B:1371:ARG:HB2	1.92	0.51
3:V:260:TRP:HB3	3:V:282:ARG:HD2	1.92	0.51
4:A:541:LEU:HD22	5:B:786:SER:HB3	1.93	0.51
6:L:425:GLN:HB2	7:N:34:GLY:HA3	1.93	0.50
5:H:1347:PRO:HA	5:H:1362:MET:HA	1.93	0.50
6:J:354:ARG:O	6:J:354:ARG:NH1	2.42	0.50
1:R:32:ILE:HD11	3:Y:268:PRO:HG2	1.93	0.50
5:B:1511:LEU:HD13	5:B:1630:PHE:HB2	1.94	0.49
3:Y:260:TRP:HB3	3:Y:282:ARG:HD2	1.93	0.49
6:J:320:GLU:HA	6:J:323:LYS:HB2	1.93	0.49
3:Y:344:GLN:OE1	3:Y:368:ARG:NH1	2.45	0.49
4:A:10:ASN:HD22	4:A:623:THR:HG23	1.75	0.49
5:B:1564:SER:HB2	5:B:1600:ILE:HD12	1.95	0.49
4:G:478:LEU:HD21	4:G:622:LEU:HD21	1.94	0.49
6:J:425:GLN:HB2	7:Q:34:GLY:HA3	1.95	0.49
2:U:103:ARG:HH12	3:V:464:PRO:HB2	1.77	0.49
5:H:965:VAL:HB	5:H:1267:HIS:HB3	1.94	0.49
5:H:947:ASP:OD1	5:H:947:ASP:N	2.46	0.49
5:B:732:ASP:OD1	7:N:62:LYS:NZ	2.46	0.49
5:H:1126:LEU:HD11	5:H:1147:ILE:HG23	1.95	0.49
5:B:1347:PRO:HA	5:B:1362:MET:HA	1.95	0.49
5:H:1178:GLY:O	5:H:1181:LYS:NZ	2.45	0.48
6:J:621:TYR:O	6:J:623:LYS:NZ	2.38	0.48
5:B:923:ARG:NH2	5:B:939:ASP:O	2.43	0.48
5:B:777:ILE:HG23	5:B:804:MET:HA	1.95	0.48
5:B:809:ILE:HG23	5:B:829:LEU:HG	1.95	0.48
2:U:58:LEU:HB3	3:V:311:PRO:HA	1.95	0.48
5:H:1511:LEU:HD13	5:H:1630:PHE:HB2	1.95	0.48
6:L:572:LEU:O	6:L:578:THR:OG1	2.29	0.48
5:B:843:GLU:OE2	5:B:859:ARG:NH1	2.36	0.48
2:X:47:LEU:HD21	3:Y:275:LEU:HB3	1.96	0.48
4:G:31:VAL:HG13	4:G:54:LEU:HB2	1.95	0.48
2:X:95:GLU:HB3	3:Y:456:LEU:HD12	1.96	0.48
4:G:81:ASN:ND2	5:H:1013:GLU:OE1	2.43	0.48
4:A:55:THR:HG22	4:A:57:ALA:H	1.79	0.47
5:B:1178:GLY:O	5:B:1181:LYS:NZ	2.46	0.47
5:H:1338:LYS:HA	5:H:1371:ARG:HB2	1.96	0.47
6:J:277:SER:O	6:J:685:ARG:NH1	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:L:478:ARG:NE	6:L:507:ASP:OD1	2.46	0.47
5:H:809:ILE:HG23	5:H:829:LEU:HG	1.96	0.47
5:H:1480:LEU:HD13	5:H:1493:GLU:HG3	1.96	0.47
2:X:47:LEU:O	3:Y:277:GLN:NE2	2.48	0.47
5:B:992:ASN:OD1	5:B:1033:GLN:NE2	2.47	0.47
5:B:1630:PHE:HA	5:B:1633:SER:HB3	1.96	0.47
5:H:1387:THR:HG22	5:H:1451:GLN:H	1.80	0.47
5:H:1477:ASP:OD1	5:H:1477:ASP:N	2.48	0.47
4:G:55:THR:HG22	4:G:57:ALA:H	1.80	0.47
5:H:1027:ILE:HG22	5:H:1071:ILE:HD13	1.97	0.46
4:A:635:ARG:NH2	4:A:638:LEU:O	2.48	0.46
3:Y:256:VAL:HB	3:Y:290:GLN:H	1.80	0.46
5:H:1396:LEU:HD23	5:H:1399:LEU:HD12	1.97	0.46
6:J:364:ASP:OD2	6:J:366:LEU:HB2	2.15	0.46
6:L:476:VAL:HG22	6:L:512:ILE:HG12	1.98	0.46
4:A:147:ASN:OD1	4:A:151:ILE:N	2.45	0.46
4:A:506:SER:HB2	4:A:530:TRP:HE1	1.80	0.46
5:H:837:GLU:HB3	5:H:868:PRO:HD3	1.97	0.46
2:X:66:LYS:HD2	2:X:66:LYS:HA	1.83	0.46
4:A:31:VAL:HG13	4:A:54:LEU:HB2	1.98	0.46
4:G:458:ASP:OD1	4:G:458:ASP:N	2.48	0.46
6:J:706:GLN:HG2	6:J:707:LYS:HG3	1.98	0.46
4:A:115:THR:OG1	4:A:584:ASN:O	2.33	0.46
4:G:19:THR:HB	4:G:478:LEU:HB2	1.98	0.46
6:J:478:ARG:NE	6:J:507:ASP:OD1	2.48	0.46
2:X:97:SER:HB3	2:X:124:LEU:HD11	1.99	0.45
6:L:621:TYR:O	6:L:623:LYS:NZ	2.37	0.45
3:Y:409:PRO:HG3	3:Y:437:PRO:HB3	1.97	0.45
5:H:1475:LYS:HD3	5:H:1480:LEU:HD23	1.97	0.45
3:Y:417:THR:HG22	3:Y:426:GLU:HG2	1.98	0.45
3:V:442:LEU:HD23	3:V:449:VAL:HG11	1.97	0.45
5:B:852:SER:HB3	5:B:878:ILE:HG22	1.99	0.45
6:J:253:SER:O	6:J:319:TYR:OH	2.29	0.45
4:G:572:VAL:HG12	5:H:753:VAL:HG22	1.99	0.45
6:L:320:GLU:HG2	6:L:323:LYS:HD2	1.99	0.45
5:B:742:ARG:HB3	5:B:775:ASP:HB3	1.97	0.45
6:J:603:ILE:HB	6:J:622:ILE:HB	1.99	0.45
5:H:923:ARG:NH1	5:H:938:GLU:OE2	2.50	0.45
5:H:1187:LYS:O	5:H:1191:THR:OG1	2.28	0.45
3:V:417:THR:HG22	3:V:426:GLU:HG2	1.99	0.44
2:X:160:ARG:HG2	2:X:179:GLN:HB3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:U:97:SER:HB3	2:U:124:LEU:HD11	1.99	0.44
5:H:1630:PHE:HA	5:H:1633:SER:HB3	1.99	0.44
4:A:20:MET:HE2	4:A:22:LEU:HD21	1.99	0.44
5:B:965:VAL:HB	5:B:1267:HIS:HB3	1.99	0.44
1:R:109:LYS:NZ	1:R:111:GLU:O	2.48	0.44
5:H:852:SER:HB3	5:H:878:ILE:HG22	2.00	0.44
5:B:730:ASP:OD1	7:N:56:LYS:NZ	2.41	0.44
6:L:364:ASP:OD2	6:L:366:LEU:HB2	2.18	0.44
6:J:320:GLU:HG2	6:J:323:LYS:HD2	2.00	0.43
3:V:326:PRO:HB2	3:V:328:ILE:HD12	2.01	0.43
3:V:409:PRO:HG3	3:V:437:PRO:HB3	1.99	0.43
5:H:1381:LEU:HB2	5:H:1424:ILE:HB	2.00	0.43
4:A:458:ASP:OD1	4:A:458:ASP:N	2.52	0.43
4:G:465:ILE:HD11	4:G:515:LEU:HD22	1.99	0.43
3:Y:359:ARG:HE	3:Y:359:ARG:HB2	1.71	0.43
5:B:1477:ASP:OD1	5:B:1477:ASP:N	2.45	0.43
6:L:706:GLN:HG2	6:L:707:LYS:HG3	2.01	0.43
6:L:481:LYS:NZ	6:L:507:ASP:OD2	2.51	0.43
7:Q:50:LYS:HG2	7:Q:66:ALA:HB2	2.00	0.43
5:B:898:PHE:HB2	7:N:50:LYS:HE2	2.00	0.43
4:A:147:ASN:OD1	4:A:150:GLY:N	2.52	0.42
4:A:7:ILE:HG12	4:A:624:PHE:HD1	1.85	0.42
5:B:1050:ARG:NH2	5:B:1101:PRO:O	2.51	0.42
3:Y:330:ARG:HE	3:Y:330:ARG:HB2	1.73	0.42
5:H:739:ILE:HB	5:H:891:LYS:HD3	2.01	0.42
5:H:958:ILE:HG23	5:H:1322:VAL:HG22	2.00	0.42
5:B:1261:GLN:O	5:B:1263:ASP:N	2.53	0.42
7:N:50:LYS:HG2	7:N:66:ALA:HB2	2.01	0.42
4:A:382:ASP:OD1	4:A:382:ASP:N	2.53	0.42
6:L:432:ASP:HA	7:N:27:ASN:HD21	1.85	0.42
7:Q:55:LEU:O	7:Q:58:LYS:NZ	2.42	0.42
4:A:334:HIS:HB3	4:A:336:THR:HG23	2.01	0.42
6:L:253:SER:O	6:L:319:TYR:OH	2.30	0.42
5:B:840:VAL:HG22	5:B:894:VAL:HG12	2.01	0.42
5:B:1396:LEU:HD23	5:B:1399:LEU:HD12	2.02	0.42
5:B:1641:ASN:O	6:L:255:SER:N	2.53	0.42
5:H:1494:GLU:HB3	5:H:1602:LYS:HB3	2.02	0.42
4:A:338:THR:OG1	4:A:351:MET:O	2.38	0.41
6:L:256:ILE:HD12	6:L:405:VAL:HG23	2.02	0.41
2:X:77:SER:HA	2:X:78:PRO:HD3	1.93	0.41
4:A:37:VAL:HB	4:A:47:LEU:HB3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:541:LEU:HD22	5:H:786:SER:HB3	2.01	0.41
1:R:92:THR:HG23	1:R:122:THR:HA	2.02	0.41
4:G:215:GLU:O	4:G:232:THR:N	2.47	0.41
2:U:51:VAL:HG11	3:V:275:LEU:HD21	2.02	0.41
4:G:334:HIS:HB3	4:G:336:THR:HG23	2.02	0.41
4:A:19:THR:HB	4:A:478:LEU:HB2	2.02	0.41
4:G:459:ARG:HE	4:G:459:ARG:HB2	1.69	0.41
4:G:508:ARG:NH1	4:G:602:ASP:OD2	2.34	0.41
5:H:1564:SER:HB2	5:H:1600:ILE:HD12	2.03	0.41
6:L:429:LYS:HG2	6:L:432:ASP:OD2	2.21	0.41
2:X:78:PRO:HA	2:X:106:GLY:HA3	2.03	0.41
4:G:175:GLU:O	5:H:915:ARG:NH2	2.53	0.41
6:J:626:ASP:N	6:J:626:ASP:OD1	2.54	0.41
6:L:438:ASP:OD2	6:L:459:HIS:HB2	2.21	0.41
5:B:1527:LEU:HA	5:B:1541:MET:HG2	2.03	0.41
4:G:635:ARG:NH2	4:G:638:LEU:O	2.54	0.41
5:H:981:LEU:HB3	5:H:998:PRO:HB2	2.02	0.41
3:V:310:VAL:HA	3:V:311:PRO:HD3	1.96	0.41
4:A:459:ARG:HE	4:A:459:ARG:HB2	1.71	0.41
5:B:917:ASN:HB3	5:B:1325:MET:HG3	2.02	0.41
5:B:990:GLU:OE2	5:B:1046:ALA:HB2	2.20	0.41
4:G:147:ASN:OD1	4:G:151:ILE:N	2.45	0.41
3:Y:294:PRO:HB2	3:Y:295:PHE:H	1.70	0.40
6:J:481:LYS:NZ	6:J:507:ASP:OD2	2.53	0.40
5:H:1261:GLN:O	5:H:1263:ASP:N	2.54	0.40
5:H:847:ASN:ND2	5:H:887:GLU:O	2.39	0.40
7:N:44:ILE:O	7:N:48:GLY:N	2.55	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	R	122/131 (93%)	122 (100%)	0	0	100	100
1	S	122/131 (93%)	122 (100%)	0	0	100	100
2	U	103/170 (61%)	94 (91%)	9 (9%)	0	100	100
2	X	161/170 (95%)	147 (91%)	13 (8%)	1 (1%)	21	59
3	V	213/221 (96%)	195 (92%)	12 (6%)	6 (3%)	4	24
3	Y	213/221 (96%)	193 (91%)	14 (7%)	6 (3%)	4	24
4	A	643/645 (100%)	623 (97%)	17 (3%)	3 (0%)	24	63
4	G	641/645 (99%)	621 (97%)	17 (3%)	3 (0%)	24	63
5	B	911/915 (100%)	859 (94%)	44 (5%)	8 (1%)	14	50
5	H	911/915 (100%)	858 (94%)	45 (5%)	8 (1%)	14	50
6	J	503/505 (100%)	478 (95%)	24 (5%)	1 (0%)	43	78
6	L	503/505 (100%)	479 (95%)	23 (5%)	1 (0%)	43	78
7	N	82/86 (95%)	81 (99%)	0	1 (1%)	10	43
7	Q	82/86 (95%)	81 (99%)	0	1 (1%)	10	43
All	All	5210/5346 (98%)	4953 (95%)	218 (4%)	39 (1%)	18	56

All (39) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	V	294	PRO
3	Y	294	PRO
5	B	1555	GLN
5	H	1349	PRO
6	J	326	SER
3	V	421	VAL
3	V	422	GLU
3	Y	421	VAL
3	Y	422	GLU
5	B	1262	LYS
5	B	1349	PRO
5	H	1262	LYS
5	H	1555	GLN
6	L	326	SER
7	Q	7	SER
3	V	288	VAL
3	Y	288	VAL
4	A	45	LEU
4	A	372	GLU

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Mol	Chain	Res	Type
5	B	1534	ASN
4	G	45	LEU
4	G	372	GLU
5	H	1534	ASN
7	N	7	SER
3	V	297	ALA
3	Y	297	ALA
5	B	932	ARG
5	B	1261	GLN
5	H	932	ARG
5	H	1261	GLN
5	H	1377	THR
2	X	170	CYS
3	Y	287	PRO
5	B	1377	THR
5	B	1556	VAL
5	H	1556	VAL
3	V	287	PRO
4	A	50	GLU
4	G	50	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	R	100/107 (94%)	99 (99%)	1 (1%)	68	78
1	S	100/107 (94%)	100 (100%)	0	100	100
2	U	88/141 (62%)	81 (92%)	7 (8%)	11	31
2	X	134/141 (95%)	125 (93%)	9 (7%)	15	36
3	V	184/190 (97%)	170 (92%)	14 (8%)	12	33
3	Y	184/190 (97%)	169 (92%)	15 (8%)	10	31
4	A	567/567 (100%)	552 (97%)	15 (3%)	40	61
4	G	567/567 (100%)	553 (98%)	14 (2%)	42	62

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	B	808/810 (100%)	788 (98%)	20 (2%)	42	62
5	H	808/810 (100%)	787 (97%)	21 (3%)	40	61
6	J	444/444 (100%)	441 (99%)	3 (1%)	76	81
6	L	444/444 (100%)	439 (99%)	5 (1%)	65	76
7	N	76/77 (99%)	76 (100%)	0	100	100
7	Q	76/77 (99%)	76 (100%)	0	100	100
All	All	4580/4672 (98%)	4456 (97%)	124 (3%)	39	60

All (124) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	R	104	LEU
2	U	43	CYS
2	U	82	LEU
2	U	91	VAL
2	U	93	CYS
2	U	119	THR
2	U	120	LEU
2	U	131	GLN
3	V	281	GLN
3	V	283	THR
3	V	310	VAL
3	V	312	CYS
3	V	314	VAL
3	V	328	ILE
3	V	359	ARG
3	V	364	GLN
3	V	378	LEU
3	V	417	THR
3	V	421	VAL
3	V	430	THR
3	V	448	VAL
3	V	449	VAL
2	X	82	LEU
2	X	91	VAL
2	X	119	THR
2	X	120	LEU
2	X	133	CYS
2	X	135	GLU
2	X	169	LYS

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Mol	Chain	Res	Type
2	X	179	GLN
2	X	190	CYS
3	Y	273	CYS
3	Y	281	GLN
3	Y	283	THR
3	Y	310	VAL
3	Y	312	CYS
3	Y	314	VAL
3	Y	328	ILE
3	Y	359	ARG
3	Y	368	ARG
3	Y	378	LEU
3	Y	417	THR
3	Y	421	VAL
3	Y	430	THR
3	Y	448	VAL
3	Y	449	VAL
4	A	8	THR
4	A	31	VAL
4	A	85	THR
4	A	214	VAL
4	A	223	ILE
4	A	243	VAL
4	A	365	VAL
4	A	375	VAL
4	A	391	THR
4	A	404	THR
4	A	406	LYS
4	A	456	ARG
4	A	459	ARG
4	A	509	LEU
4	A	623	THR
5	B	809	ILE
5	B	835	ASN
5	B	836	GLN
5	B	916	MET
5	B	922	VAL
5	B	937	LYS
5	B	945	LEU
5	B	1267	HIS
5	B	1306	GLU
5	B	1342	LYS

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Mol	Chain	Res	Type
5	B	1433	GLU
5	B	1482	LYS
5	B	1498	ILE
5	B	1506	THR
5	B	1515	CYS
5	B	1543	ILE
5	B	1558	GLN
5	B	1560	ARG
5	B	1572	LEU
5	B	1585	LEU
4	G	8	THR
4	G	31	VAL
4	G	103	LEU
4	G	214	VAL
4	G	223	ILE
4	G	243	VAL
4	G	365	VAL
4	G	375	VAL
4	G	391	THR
4	G	404	THR
4	G	406	LYS
4	G	459	ARG
4	G	509	LEU
4	G	623	THR
5	H	809	ILE
5	H	835	ASN
5	H	836	GLN
5	H	916	MET
5	H	922	VAL
5	H	937	LYS
5	H	945	LEU
5	H	958	ILE
5	H	1267	HIS
5	H	1306	GLU
5	H	1342	LYS
5	H	1433	GLU
5	H	1482	LYS
5	H	1498	ILE
5	H	1506	THR
5	H	1515	CYS
5	H	1543	ILE
5	H	1558	GLN

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Mol	Chain	Res	Type
5	H	1560	ARG
5	H	1572	LEU
5	H	1585	LEU
6	J	347	VAL
6	J	383	LEU
6	J	508	LYS
6	L	236	ILE
6	L	255	SER
6	L	347	VAL
6	L	383	LEU
6	L	508	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (59) such sidechains are listed below:

Mol	Chain	Res	Type
1	R	2	GLN
1	S	75	ASN
3	V	307	ASN
3	V	364	GLN
2	X	98	GLN
2	X	131	GLN
3	Y	286	HIS
3	Y	331	ASN
4	A	10	ASN
4	A	132	HIS
4	A	181	GLN
4	A	225	ASN
5	B	752	ASN
5	B	770	ASN
5	B	831	ASN
5	B	1115	ASN
5	B	1160	ASN
5	B	1268	GLN
5	B	1277	GLN
5	B	1290	HIS
5	B	1333	GLN
5	B	1443	GLN
5	B	1499	GLN
5	B	1558	GLN
5	B	1620	ASN
4	G	10	ASN
4	G	132	HIS

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Mol	Chain	Res	Type
4	G	432	ASN
5	H	752	ASN
5	H	770	ASN
5	H	831	ASN
5	H	834	GLN
5	H	897	HIS
5	H	948	GLN
5	H	1160	ASN
5	H	1196	ASN
5	H	1268	GLN
5	H	1277	GLN
5	H	1290	HIS
5	H	1317	GLN
5	H	1333	GLN
5	H	1442	HIS
5	H	1443	GLN
5	H	1462	ASN
5	H	1555	GLN
5	H	1558	GLN
6	J	306	ASN
6	J	411	GLN
6	J	413	ASN
6	J	442	GLN
6	J	535	ASN
6	J	565	GLN
6	J	702	ASN
6	L	411	GLN
6	L	533	ASN
6	L	593	GLN
6	L	702	ASN
7	Q	11	GLN
7	Q	49	GLN

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 ⓘ

32 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	$\# Z > 2$
8	FUC	C	1	8,2	10,10,11	1.04	0	14,14,16	0.97	1 (7%)
8	BGC	C	2	8	11,11,12	1.70	2 (18%)	15,15,17	1.12	2 (13%)
8	FUC	D	1	8,3	10,10,11	1.25	1 (10%)	14,14,16	1.05	2 (14%)
8	BGC	D	2	8	11,11,12	1.72	3 (27%)	15,15,17	1.08	0
9	NAG	E	1	9,3	14,14,15	0.99	2 (14%)	17,19,21	1.31	3 (17%)
9	NAG	E	2	9	14,14,15	1.69	2 (14%)	17,19,21	2.56	3 (17%)
9	FUC	E	3	9	10,10,11	1.01	0	14,14,16	0.76	0
8	FUC	F	1	8,2	10,10,11	1.13	1 (10%)	14,14,16	0.82	0
8	BGC	F	2	8	11,11,12	1.73	2 (18%)	15,15,17	1.12	2 (13%)
8	FUC	I	1	8,2	10,10,11	1.31	1 (10%)	14,14,16	1.23	1 (7%)
8	BGC	I	2	8	11,11,12	1.73	2 (18%)	15,15,17	1.14	1 (6%)
8	FUC	K	1	8,3	10,10,11	1.15	1 (10%)	14,14,16	1.03	1 (7%)
8	BGC	K	2	8	11,11,12	1.62	2 (18%)	15,15,17	0.91	1 (6%)
9	NAG	M	1	9,3	14,14,15	1.05	2 (14%)	17,19,21	1.54	3 (17%)
9	NAG	M	2	9	14,14,15	1.52	1 (7%)	17,19,21	2.59	3 (17%)
9	FUC	M	3	9	10,10,11	0.94	0	14,14,16	0.87	1 (7%)
10	NAG	O	1	10,4	14,14,15	0.60	0	17,19,21	0.65	1 (5%)
10	NAG	O	2	10	14,14,15	0.75	1 (7%)	17,19,21	0.51	0
10	NAG	P	1	10,5	14,14,15	0.85	1 (7%)	17,19,21	0.86	1 (5%)
10	NAG	P	2	10	14,14,15	0.51	0	17,19,21	0.59	0
10	NAG	T	1	10,4	14,14,15	0.64	0	17,19,21	0.65	0
10	NAG	T	2	10	14,14,15	0.57	0	17,19,21	0.55	0
10	NAG	W	1	10,5	14,14,15	0.78	1 (7%)	17,19,21	0.75	0
10	NAG	W	2	10	14,14,15	0.59	0	17,19,21	0.61	0
10	NAG	Z	1	10,6	14,14,15	1.13	1 (7%)	17,19,21	2.01	5 (29%)
10	NAG	Z	2	10	14,14,15	1.58	2 (14%)	17,19,21	3.00	4 (23%)
10	NAG	a	1	10,6	14,14,15	1.57	2 (14%)	17,19,21	1.49	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	NAG	a	2	10	14,14,15	0.45	0	17,19,21	0.64	0
10	NAG	b	1	10,6	14,14,15	1.12	1 (7%)	17,19,21	2.01	5 (29%)
10	NAG	b	2	10	14,14,15	1.61	2 (14%)	17,19,21	3.01	4 (23%)
10	NAG	c	1	10,6	14,14,15	1.53	2 (14%)	17,19,21	1.47	2 (11%)
10	NAG	c	2	10	14,14,15	0.46	0	17,19,21	0.65	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	FUC	C	1	8,2	-	-	0/1/1/1
8	BGC	C	2	8	-	0/2/19/22	0/1/1/1
8	FUC	D	1	8,3	-	-	0/1/1/1
8	BGC	D	2	8	-	1/2/19/22	0/1/1/1
9	NAG	E	1	9,3	-	4/6/23/26	0/1/1/1
9	NAG	E	2	9	-	6/6/23/26	0/1/1/1
9	FUC	E	3	9	1/1/4/5	-	0/1/1/1
8	FUC	F	1	8,2	-	-	0/1/1/1
8	BGC	F	2	8	-	0/2/19/22	0/1/1/1
8	FUC	I	1	8,2	-	-	0/1/1/1
8	BGC	I	2	8	-	2/2/19/22	0/1/1/1
8	FUC	K	1	8,3	-	-	0/1/1/1
8	BGC	K	2	8	-	1/2/19/22	0/1/1/1
9	NAG	M	1	9,3	1/1/5/7	4/6/23/26	0/1/1/1
9	NAG	M	2	9	-	6/6/23/26	0/1/1/1
9	FUC	M	3	9	1/1/4/5	-	0/1/1/1
10	NAG	O	1	10,4	-	2/6/23/26	0/1/1/1
10	NAG	O	2	10	-	2/6/23/26	0/1/1/1
10	NAG	P	1	10,5	-	0/6/23/26	0/1/1/1
10	NAG	P	2	10	-	3/6/23/26	0/1/1/1
10	NAG	T	1	10,4	-	2/6/23/26	0/1/1/1
10	NAG	T	2	10	-	2/6/23/26	0/1/1/1
10	NAG	W	1	10,5	-	0/6/23/26	0/1/1/1
10	NAG	W	2	10	-	2/6/23/26	0/1/1/1
10	NAG	Z	1	10,6	1/1/5/7	3/6/23/26	0/1/1/1
10	NAG	Z	2	10	-	4/6/23/26	0/1/1/1
10	NAG	a	1	10,6	-	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	NAG	a	2	10	-	4/6/23/26	0/1/1/1
10	NAG	b	1	10,6	1/1/5/7	3/6/23/26	0/1/1/1
10	NAG	b	2	10	-	4/6/23/26	0/1/1/1
10	NAG	c	1	10,6	-	4/6/23/26	0/1/1/1
10	NAG	c	2	10	-	4/6/23/26	0/1/1/1

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	E	2	NAG	C1-C2	5.52	1.59	1.52
10	b	2	NAG	O5-C1	5.07	1.52	1.43
10	Z	2	NAG	O5-C1	4.96	1.52	1.43
9	M	2	NAG	C1-C2	4.89	1.59	1.52
8	I	2	BGC	O5-C1	4.65	1.51	1.43
8	F	2	BGC	O5-C1	4.60	1.51	1.43
8	C	2	BGC	O5-C1	4.58	1.51	1.43
8	D	2	BGC	O5-C1	4.43	1.51	1.43
10	c	1	NAG	C1-C2	4.29	1.58	1.52
8	K	2	BGC	O5-C1	4.25	1.50	1.43
10	a	1	NAG	C1-C2	4.06	1.57	1.52
10	Z	1	NAG	C1-C2	3.78	1.57	1.52
10	a	1	NAG	O5-C1	3.78	1.50	1.43
10	b	1	NAG	C1-C2	3.75	1.57	1.52
10	c	1	NAG	O5-C1	3.21	1.49	1.43
10	P	1	NAG	C1-C2	2.76	1.56	1.52
9	M	1	NAG	O5-C1	2.70	1.48	1.43
8	D	1	FUC	C2-C3	2.68	1.56	1.52
9	E	1	NAG	C1-C2	2.49	1.55	1.52
8	I	1	FUC	C2-C3	2.46	1.56	1.52
8	D	2	BGC	O5-C5	2.43	1.48	1.43
10	b	2	NAG	C1-C2	2.41	1.55	1.52
9	M	1	NAG	C1-C2	2.40	1.55	1.52
8	F	2	BGC	O5-C5	2.40	1.48	1.43
10	W	1	NAG	C1-C2	2.37	1.55	1.52
8	I	2	BGC	O5-C5	2.33	1.48	1.43
8	K	1	FUC	C2-C3	2.32	1.56	1.52
10	Z	2	NAG	C1-C2	2.31	1.55	1.52
10	O	2	NAG	C1-C2	2.24	1.55	1.52
9	E	1	NAG	O5-C1	2.19	1.47	1.43
8	K	2	BGC	O5-C5	2.17	1.47	1.43
8	F	1	FUC	C2-C3	2.17	1.55	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	C	2	BGC	O5-C5	2.12	1.47	1.43
8	D	2	BGC	C2-C3	-2.07	1.49	1.52
9	E	2	NAG	C3-C2	2.00	1.56	1.52

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	Z	2	NAG	C2-N2-C7	9.39	135.48	122.90
10	b	2	NAG	C2-N2-C7	9.37	135.45	122.90
9	M	2	NAG	C2-N2-C7	9.13	135.14	122.90
9	E	2	NAG	C2-N2-C7	9.07	135.05	122.90
10	b	2	NAG	C1-O5-C5	6.13	120.41	112.19
10	Z	2	NAG	C1-O5-C5	6.10	120.36	112.19
10	b	1	NAG	C2-N2-C7	4.32	128.69	122.90
10	Z	1	NAG	C2-N2-C7	4.23	128.56	122.90
9	M	1	NAG	C1-O5-C5	4.17	117.77	112.19
10	b	2	NAG	C1-C2-N2	4.00	116.73	110.43
10	Z	1	NAG	C1-C2-N2	3.95	116.65	110.43
10	Z	2	NAG	C1-C2-N2	3.94	116.64	110.43
10	b	1	NAG	C1-C2-N2	3.92	116.61	110.43
10	a	1	NAG	C1-O5-C5	3.90	117.42	112.19
9	M	2	NAG	C1-C2-N2	3.81	116.44	110.43
9	M	1	NAG	C2-N2-C7	3.76	127.94	122.90
9	E	1	NAG	C2-N2-C7	3.71	127.88	122.90
9	E	2	NAG	C1-C2-N2	3.71	116.27	110.43
10	c	1	NAG	C1-O5-C5	3.65	117.08	112.19
10	Z	1	NAG	C4-C3-C2	3.53	116.20	111.02
10	b	1	NAG	C4-C3-C2	3.50	116.15	111.02
10	b	1	NAG	C1-O5-C5	3.10	116.33	112.19
10	Z	1	NAG	C1-O5-C5	3.09	116.33	112.19
10	c	1	NAG	C4-C3-C2	3.08	115.54	111.02
10	a	1	NAG	C4-C3-C2	3.01	115.43	111.02
8	I	2	BGC	C2-C3-C4	2.92	116.00	110.86
8	I	1	FUC	O5-C5-C4	2.69	114.39	109.55
8	C	2	BGC	C2-C3-C4	2.66	115.54	110.86
10	P	1	NAG	C2-N2-C7	2.62	126.41	122.90
9	E	2	NAG	C8-C7-N2	2.57	120.38	116.12
10	b	2	NAG	C8-C7-N2	2.57	120.38	116.12
10	Z	2	NAG	C8-C7-N2	2.56	120.37	116.12
9	M	2	NAG	C8-C7-N2	2.54	120.34	116.12
9	E	1	NAG	C1-O5-C5	2.46	115.48	112.19
8	F	2	BGC	C1-C2-C3	2.43	113.18	109.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	C	1	FUC	C1-O5-C5	2.38	118.59	112.97
8	F	2	BGC	C2-C3-C4	2.25	114.81	110.86
8	D	1	FUC	C1-O5-C5	2.16	118.07	112.97
8	C	2	BGC	C1-C2-C3	2.15	112.77	109.64
9	M	3	FUC	C1-O5-C5	2.14	118.02	112.97
10	Z	1	NAG	C3-C4-C5	2.14	114.12	110.23
8	K	1	FUC	C1-O5-C5	2.11	117.94	112.97
8	K	2	BGC	C2-C3-C4	2.09	114.53	110.86
8	D	1	FUC	C1-C2-C3	2.09	112.68	109.64
10	b	1	NAG	C3-C4-C5	2.08	114.01	110.23
9	M	1	NAG	C1-C2-N2	2.06	113.68	110.43
9	E	1	NAG	C1-C2-N2	2.05	113.66	110.43
10	O	1	NAG	C1-O5-C5	2.02	114.89	112.19

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
9	E	3	FUC	C1
9	M	1	NAG	C1
9	M	3	FUC	C1
10	Z	1	NAG	C1
10	b	1	NAG	C1

All (67) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	a	1	NAG	O5-C5-C6-O6
10	c	1	NAG	O5-C5-C6-O6
9	E	2	NAG	C4-C5-C6-O6
9	M	2	NAG	C4-C5-C6-O6
10	a	1	NAG	C4-C5-C6-O6
10	c	2	NAG	O5-C5-C6-O6
10	c	1	NAG	C4-C5-C6-O6
10	a	2	NAG	O5-C5-C6-O6
10	O	1	NAG	O5-C5-C6-O6
10	T	1	NAG	O5-C5-C6-O6
9	E	1	NAG	C4-C5-C6-O6
10	a	2	NAG	C4-C5-C6-O6
9	M	1	NAG	C4-C5-C6-O6
10	O	1	NAG	C4-C5-C6-O6
10	c	2	NAG	C4-C5-C6-O6
10	b	1	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
9	E	2	NAG	O5-C5-C6-O6
9	M	2	NAG	O5-C5-C6-O6
10	T	1	NAG	C4-C5-C6-O6
10	Z	1	NAG	O5-C5-C6-O6
9	E	2	NAG	C8-C7-N2-C2
9	E	2	NAG	O7-C7-N2-C2
9	M	2	NAG	C8-C7-N2-C2
9	M	2	NAG	O7-C7-N2-C2
10	P	2	NAG	C8-C7-N2-C2
10	P	2	NAG	O7-C7-N2-C2
10	W	2	NAG	C8-C7-N2-C2
10	W	2	NAG	O7-C7-N2-C2
10	Z	2	NAG	C8-C7-N2-C2
10	Z	2	NAG	O7-C7-N2-C2
10	a	1	NAG	C8-C7-N2-C2
10	a	1	NAG	O7-C7-N2-C2
10	a	2	NAG	C8-C7-N2-C2
10	a	2	NAG	O7-C7-N2-C2
10	b	2	NAG	C8-C7-N2-C2
10	b	2	NAG	O7-C7-N2-C2
10	c	1	NAG	C8-C7-N2-C2
10	c	1	NAG	O7-C7-N2-C2
10	c	2	NAG	C8-C7-N2-C2
10	c	2	NAG	O7-C7-N2-C2
9	E	1	NAG	O5-C5-C6-O6
9	M	1	NAG	O5-C5-C6-O6
8	I	2	BGC	C4-C5-C6-O6
10	O	2	NAG	O5-C5-C6-O6
10	O	2	NAG	C4-C5-C6-O6
8	I	2	BGC	O5-C5-C6-O6
10	b	1	NAG	C4-C5-C6-O6
10	T	2	NAG	O5-C5-C6-O6
10	Z	1	NAG	C1-C2-N2-C7
10	b	1	NAG	C1-C2-N2-C7
10	T	2	NAG	C4-C5-C6-O6
10	Z	1	NAG	C4-C5-C6-O6
8	K	2	BGC	O5-C5-C6-O6
9	E	2	NAG	C3-C2-N2-C7
9	M	2	NAG	C3-C2-N2-C7
9	E	1	NAG	C1-C2-N2-C7
9	E	2	NAG	C1-C2-N2-C7
9	M	1	NAG	C1-C2-N2-C7

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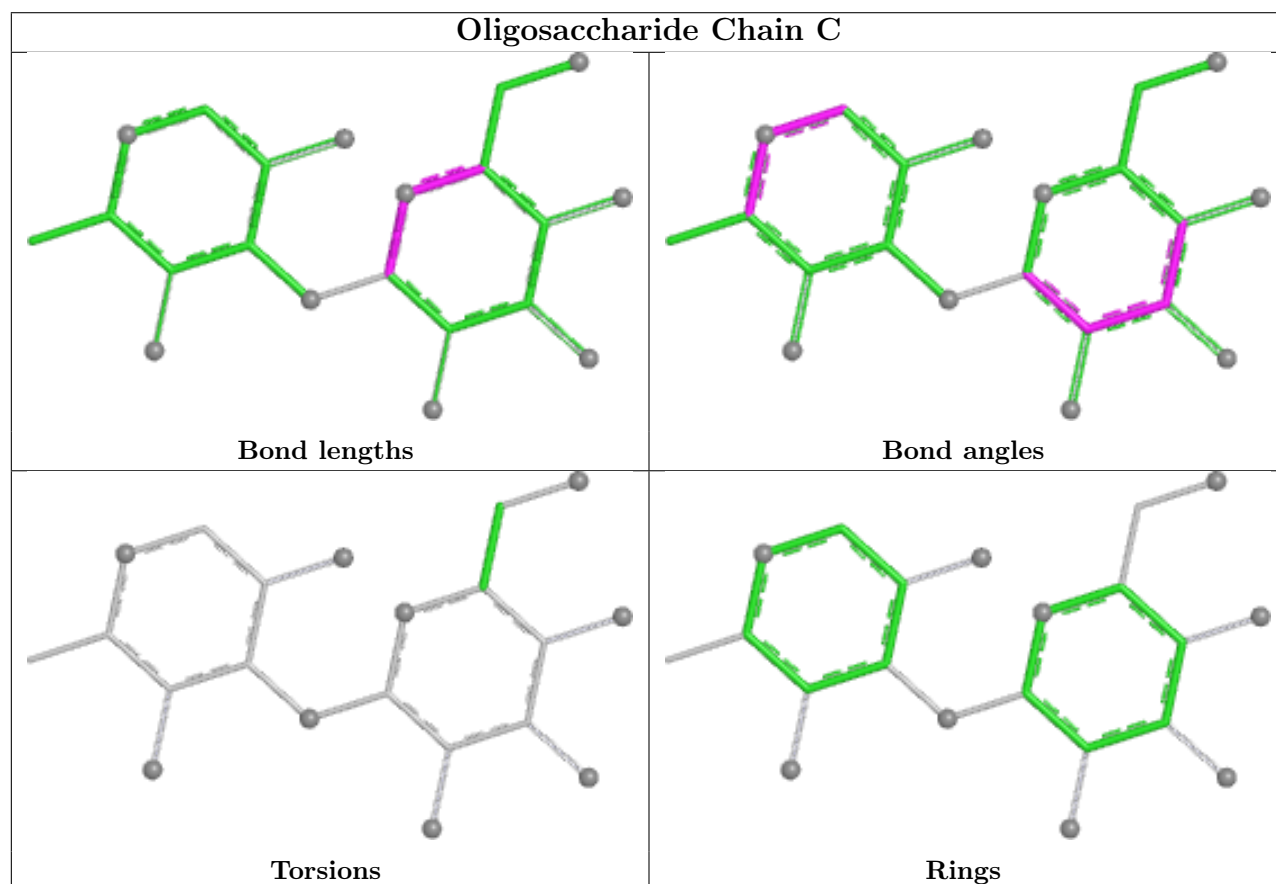
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Mol	Chain	Res	Type	Atoms
9	M	2	NAG	C1-C2-N2-C7
10	Z	2	NAG	C1-C2-N2-C7
10	b	2	NAG	C1-C2-N2-C7
8	D	2	BGC	O5-C5-C6-O6
9	E	1	NAG	C3-C2-N2-C7
9	M	1	NAG	C3-C2-N2-C7
10	Z	2	NAG	C3-C2-N2-C7
10	b	2	NAG	C3-C2-N2-C7
10	P	2	NAG	C4-C5-C6-O6

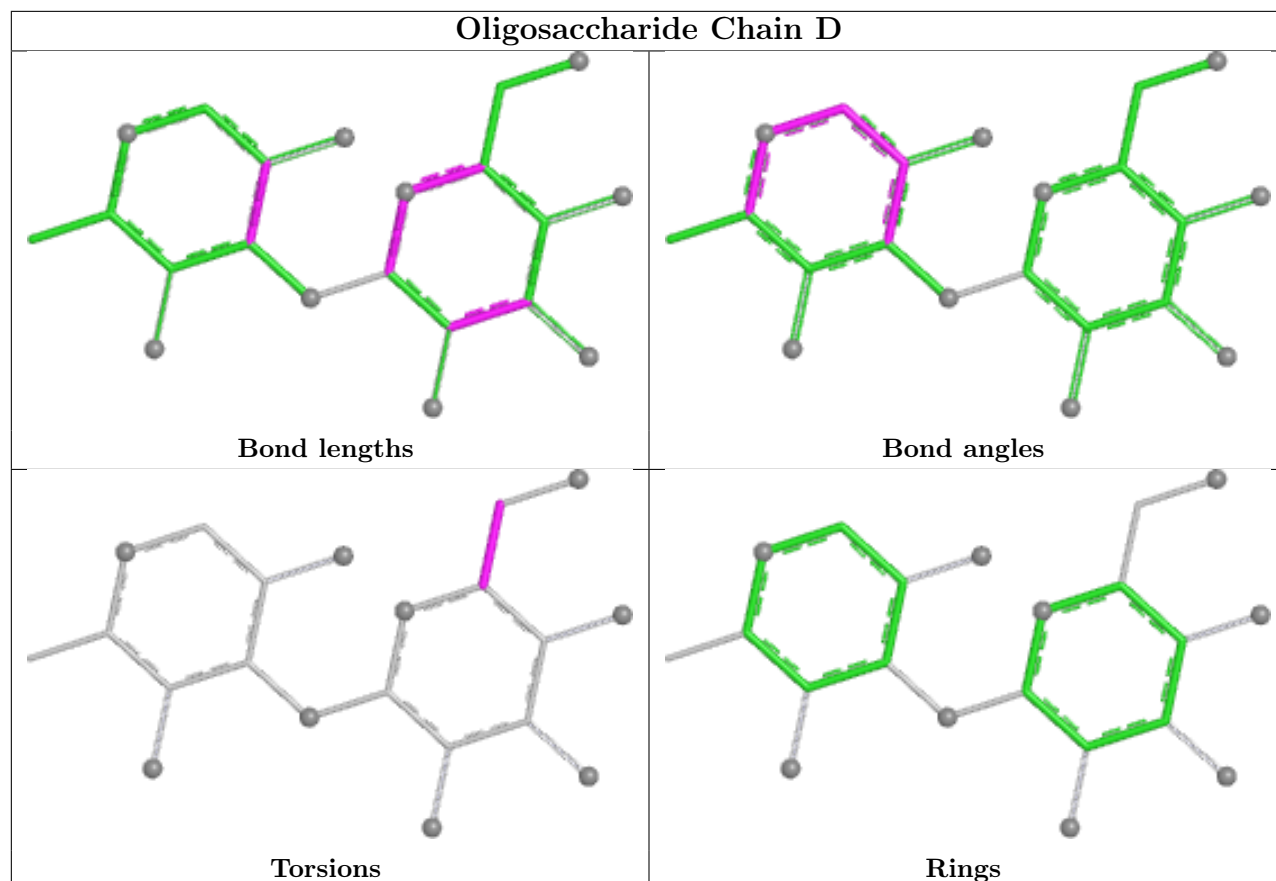
There are no ring outliers.

No monomer is involved in short contacts.

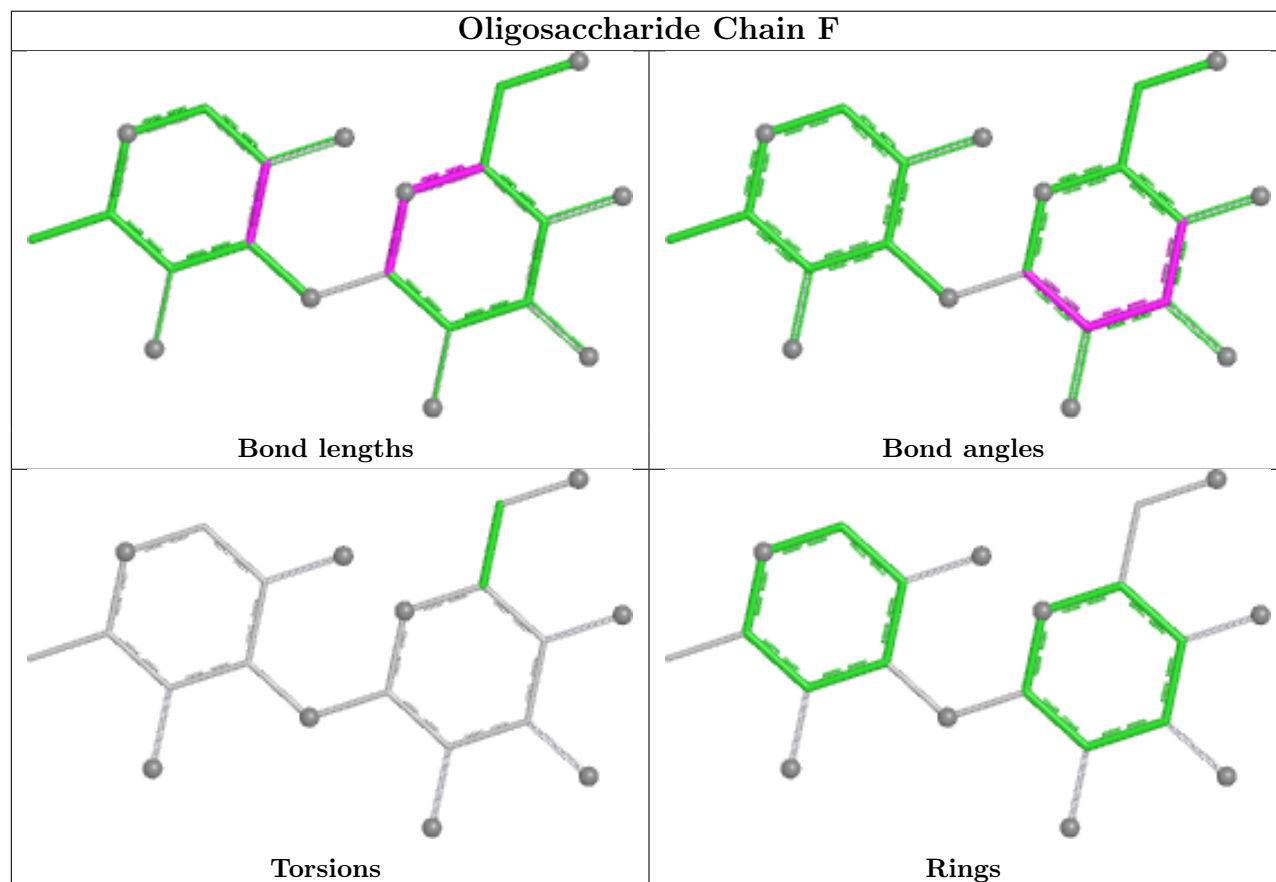
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



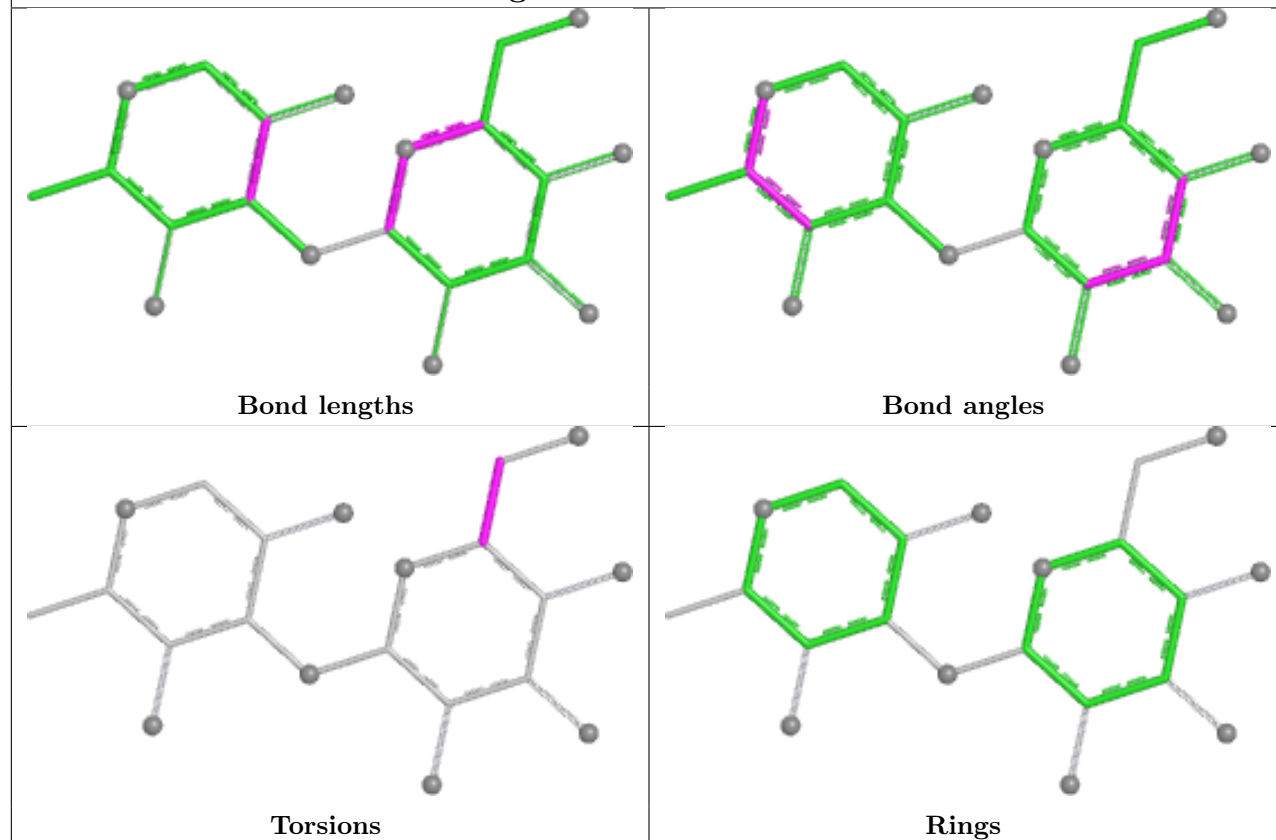
Oligosaccharide Chain D



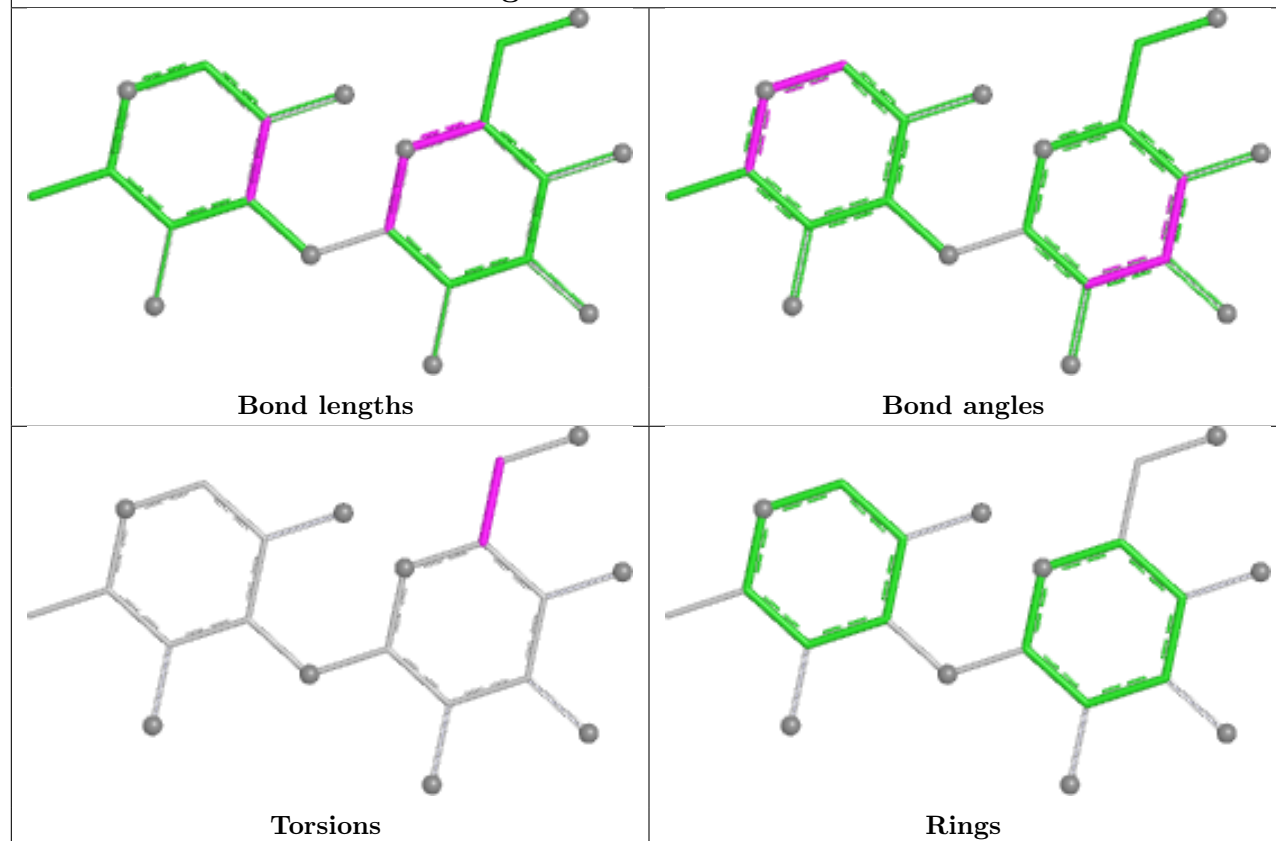
Oligosaccharide Chain F

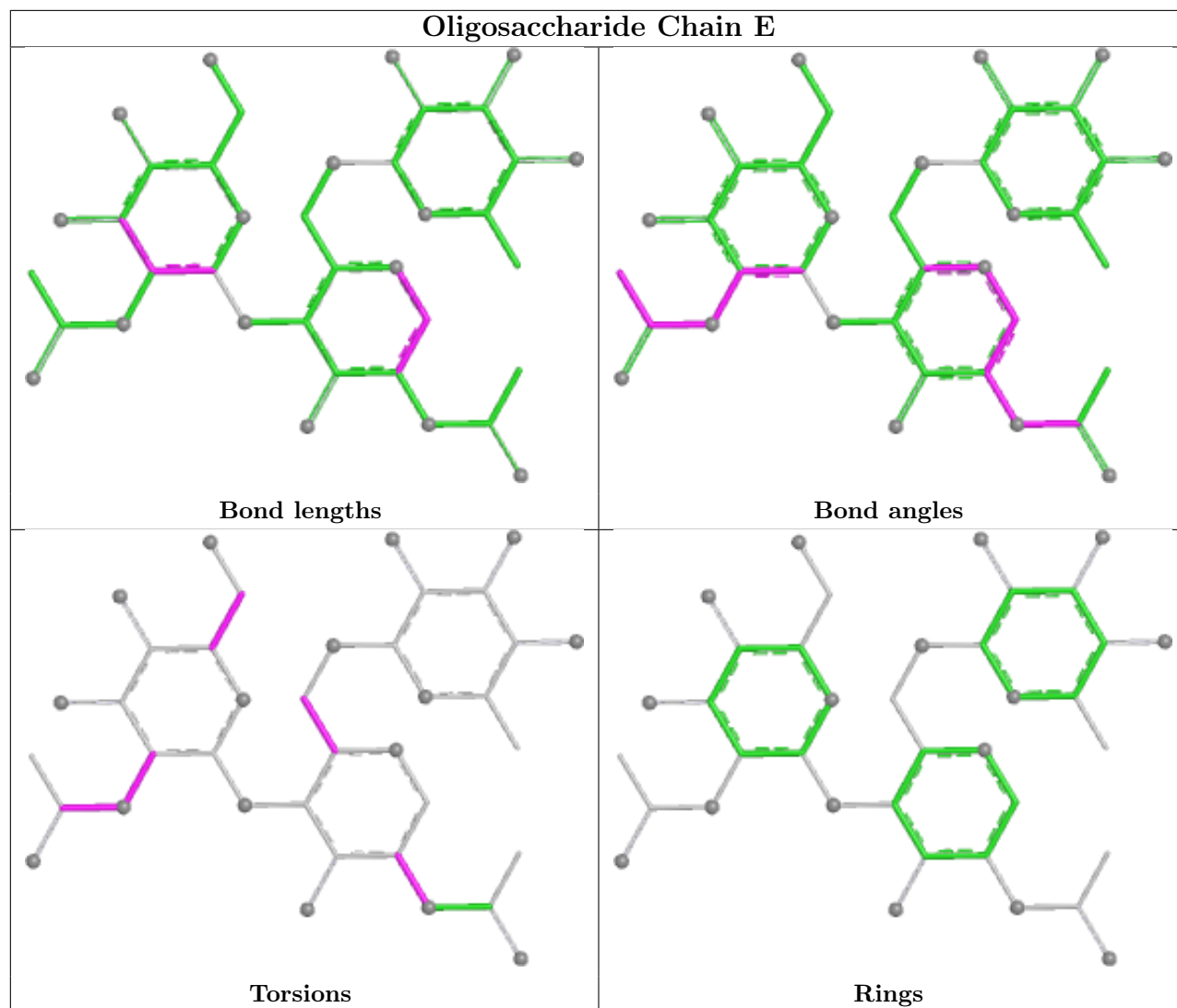


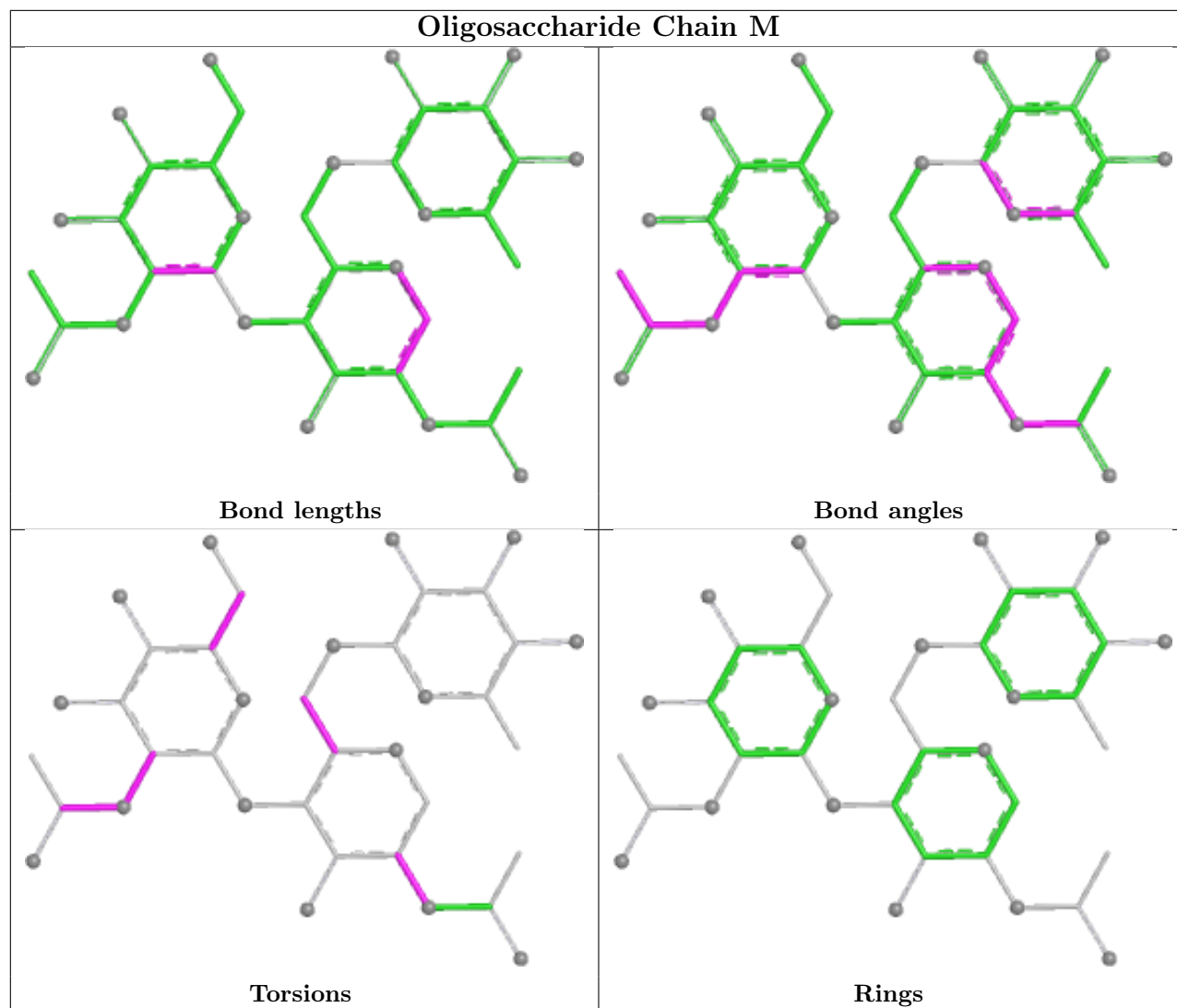
Oligosaccharide Chain I

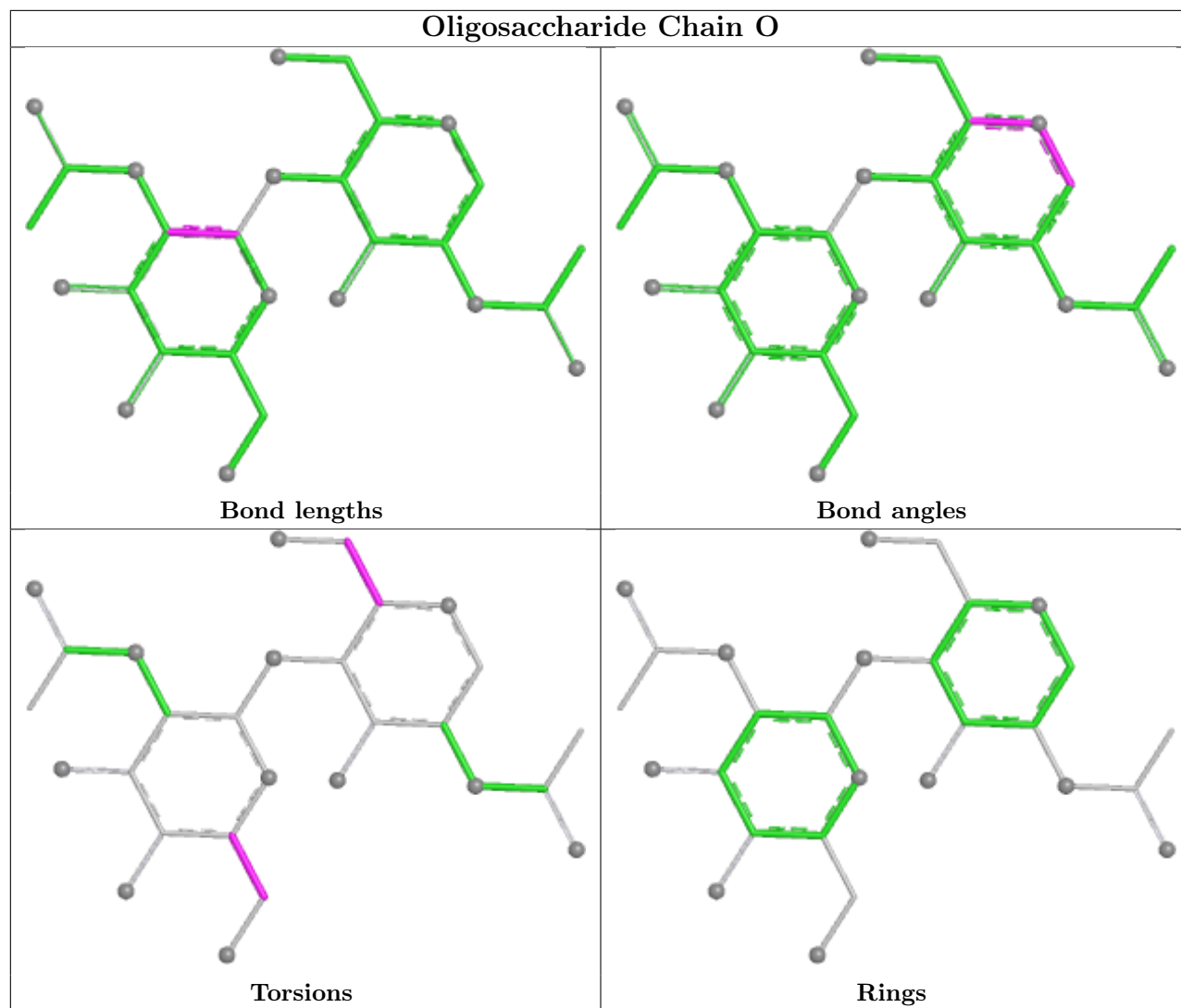


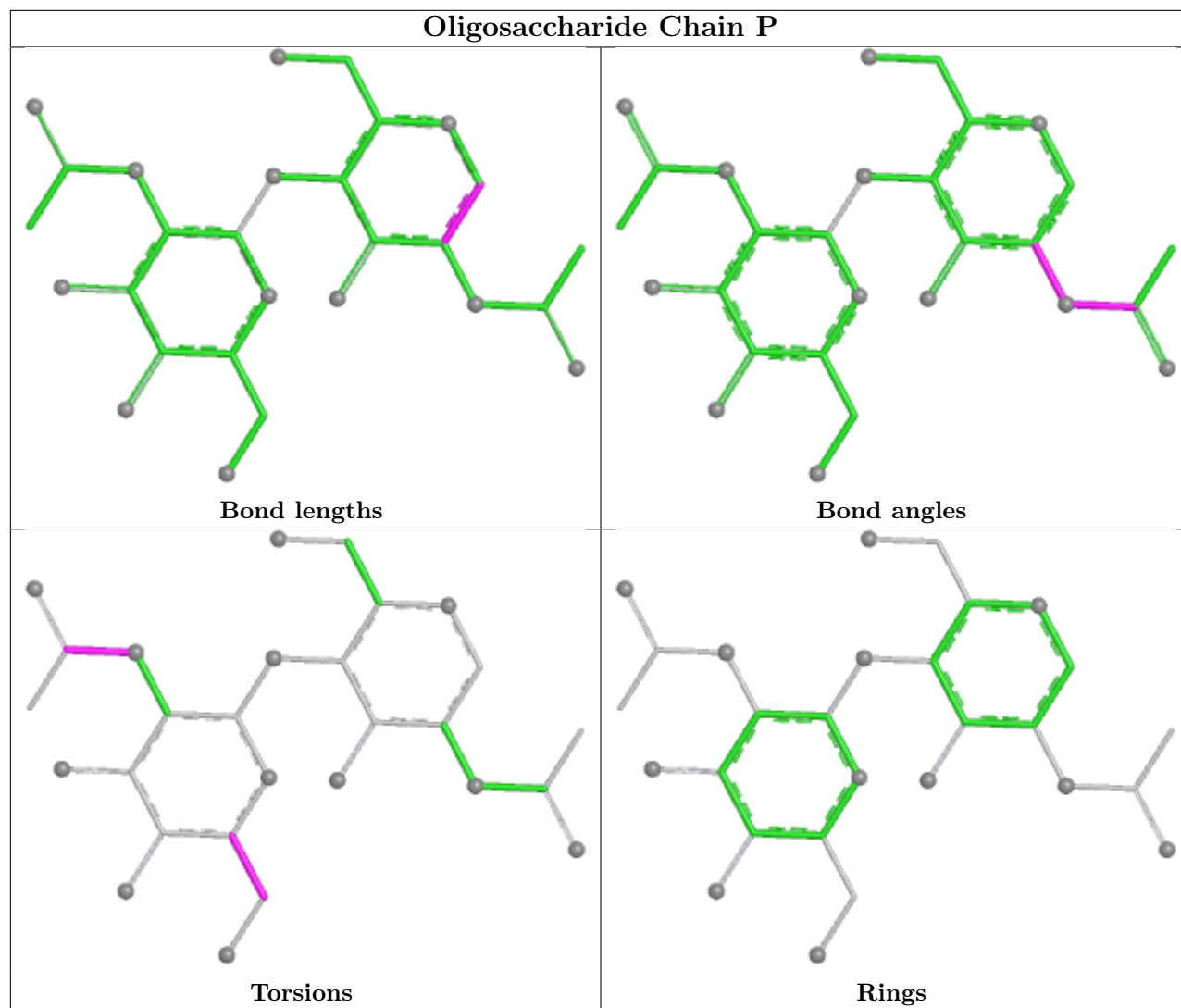
Oligosaccharide Chain K

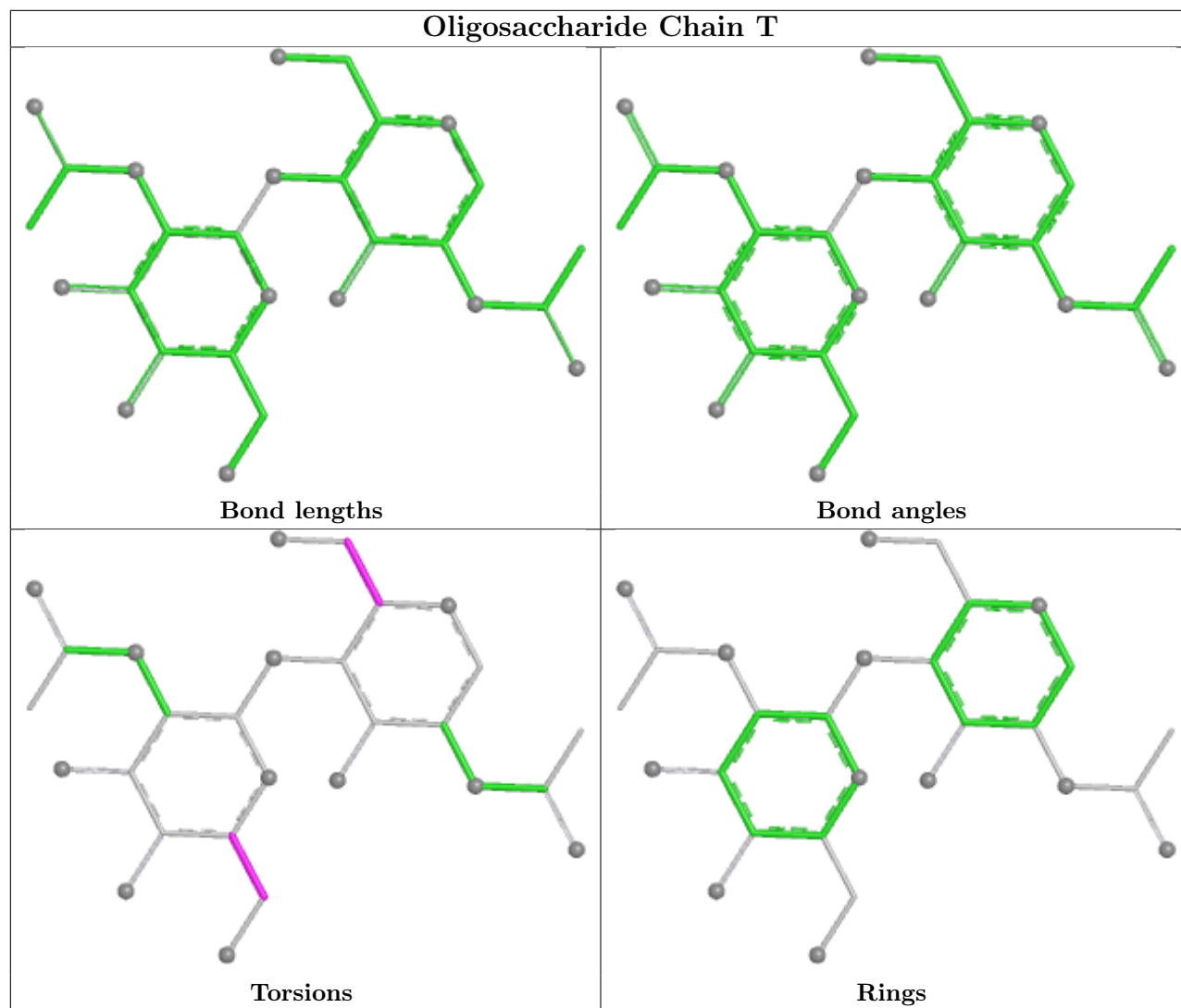


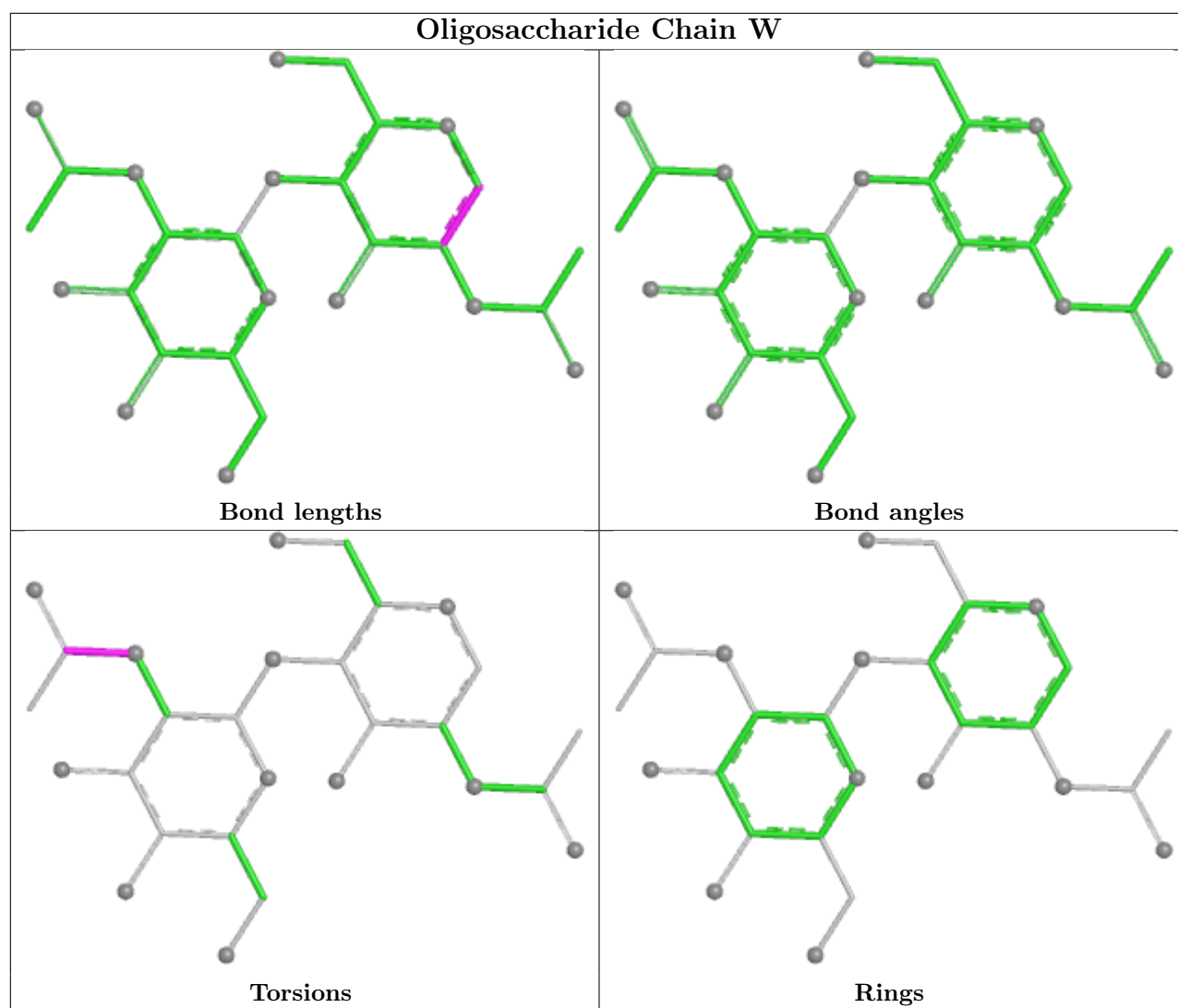


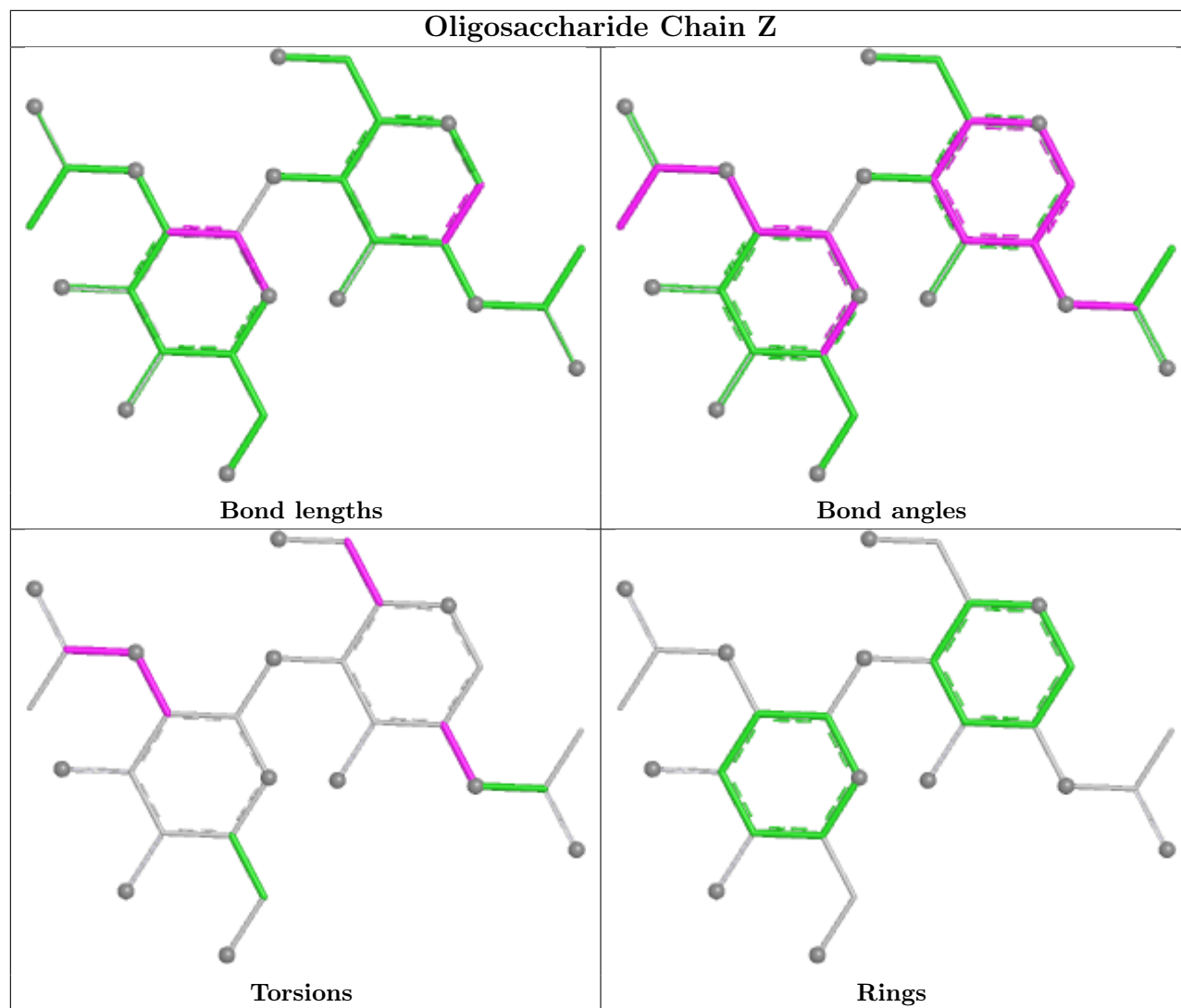


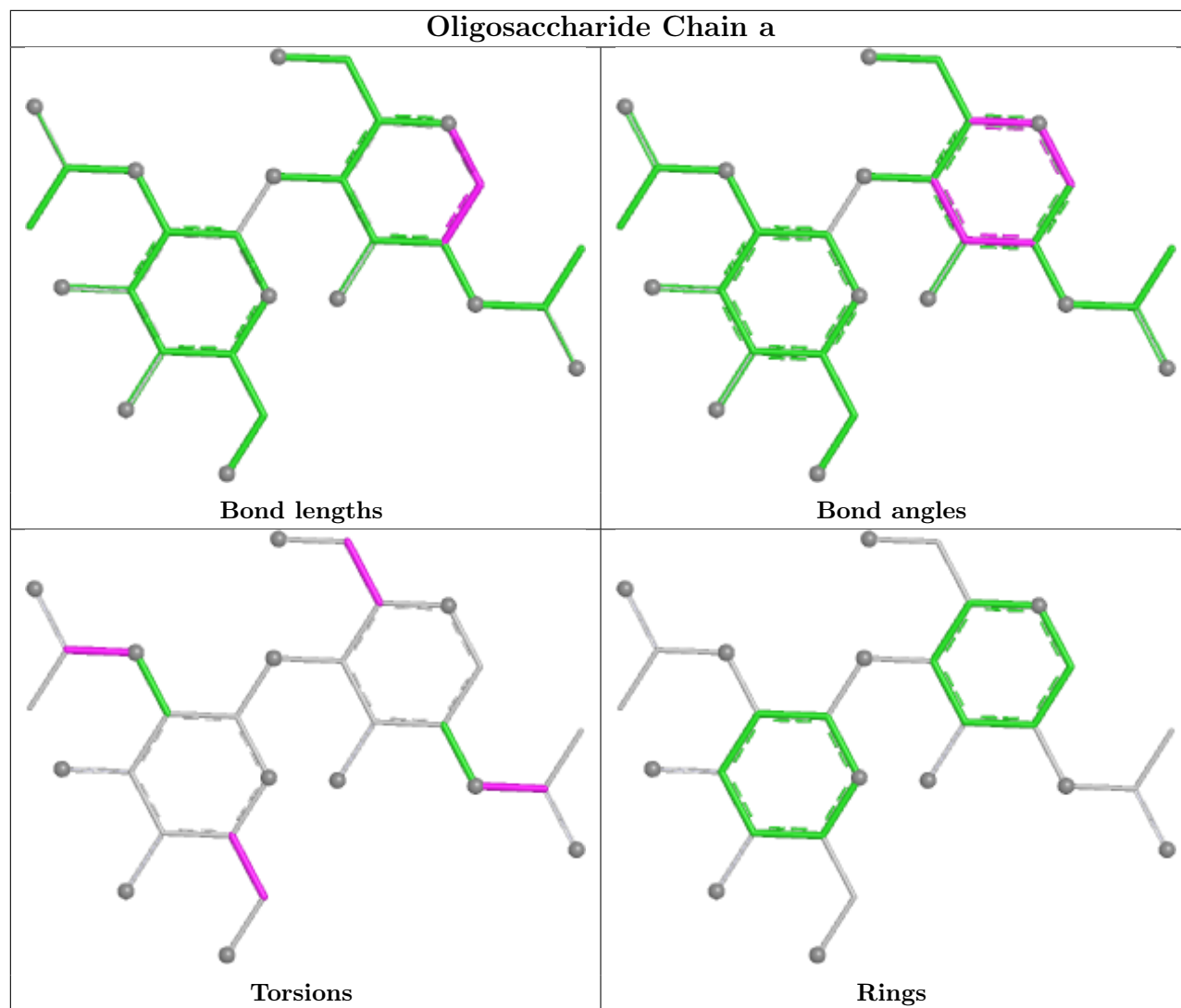


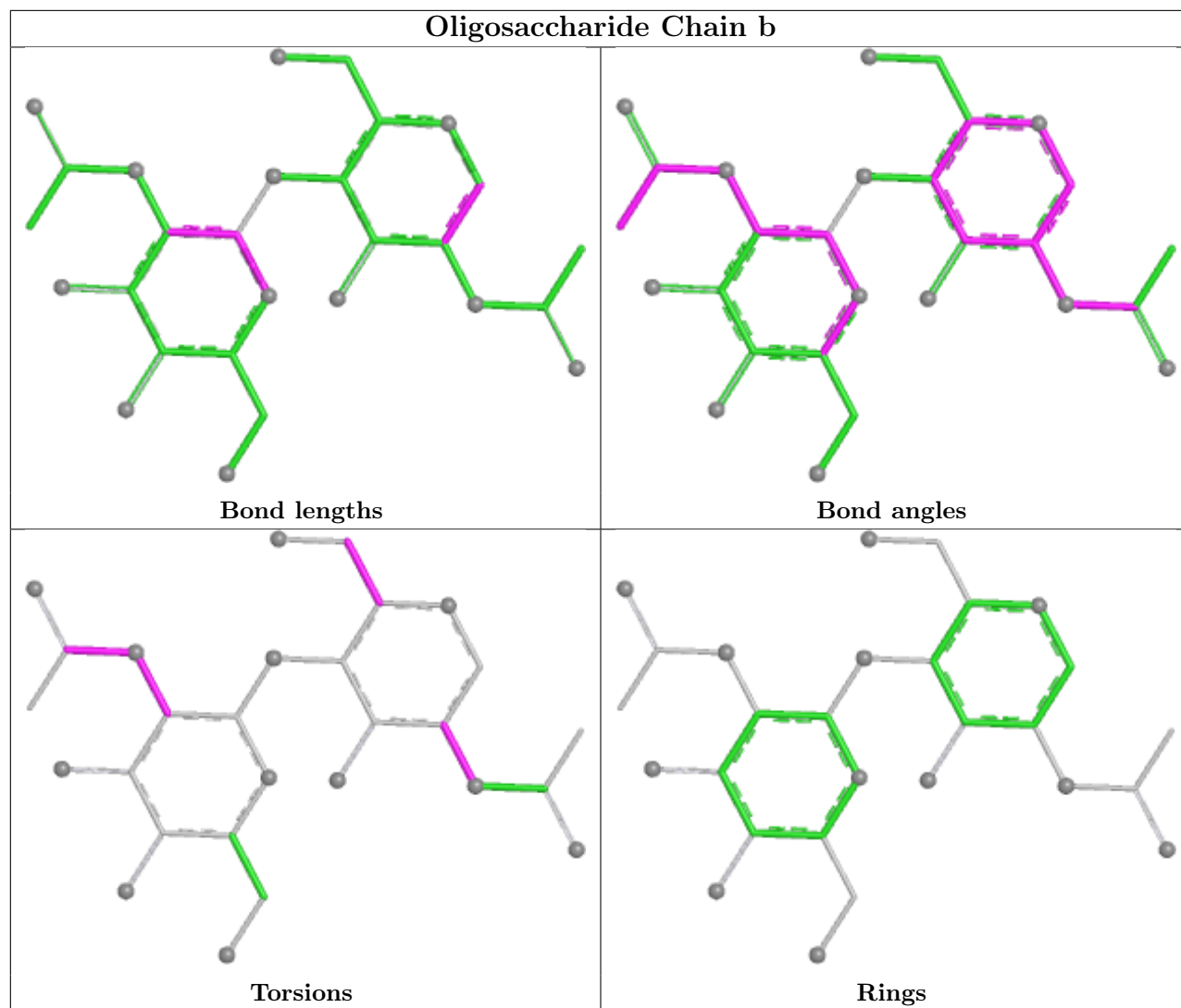


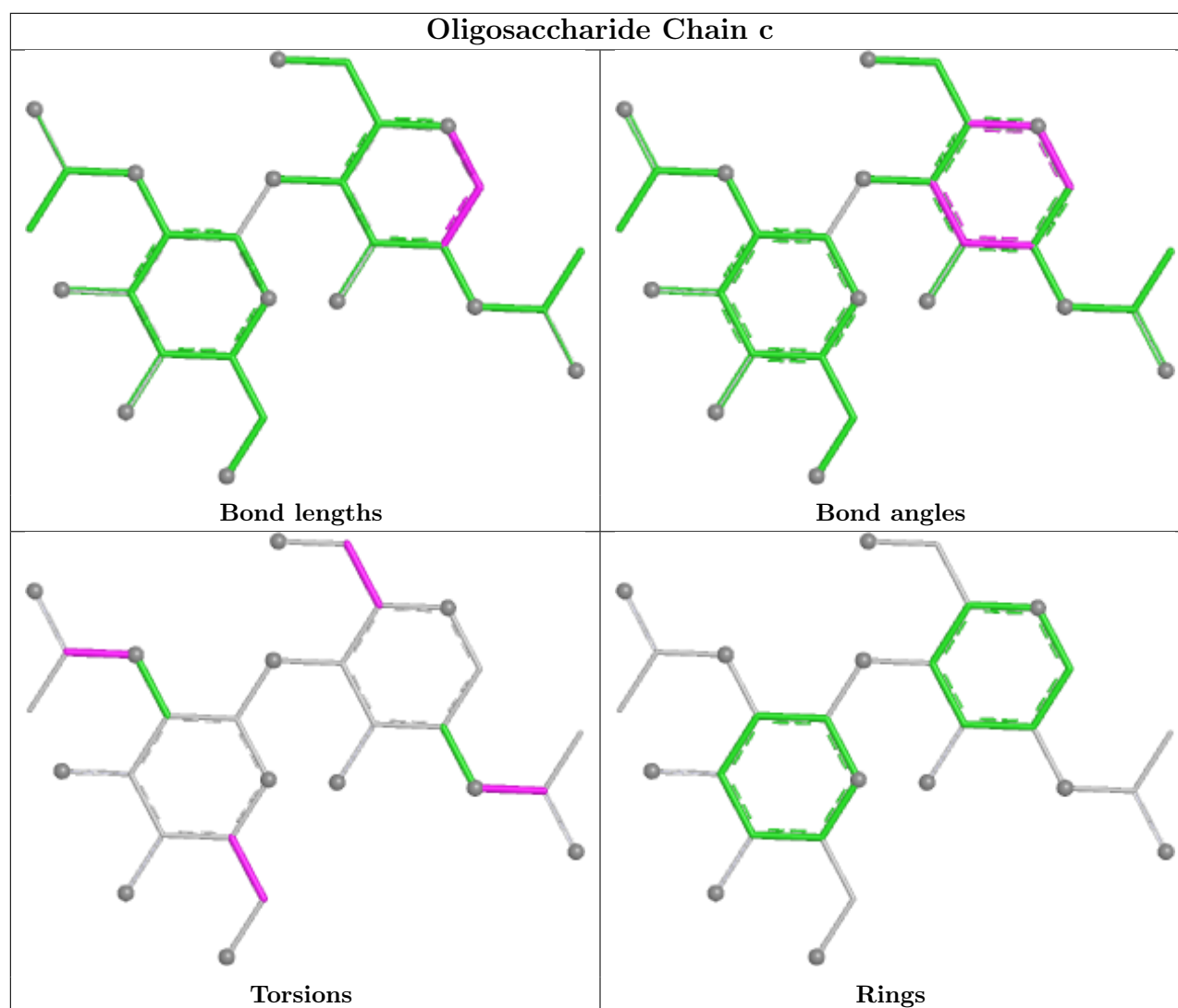












5.6 Ligand geometry [i](#)

Of 23 ligands modelled in this entry, 2 are monoatomic - leaving 21 for Mogul analysis.

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	$\# Z > 2$
11	MAN	Y	504	3	11,11,12	1.11	1 (9%)	15,15,17	1.74	2 (13%)
11	MAN	X	203	2	11,11,12	1.29	2 (18%)	15,15,17	1.64	2 (13%)
11	MAN	V	512	3	11,11,12	1.09	1 (9%)	15,15,17	1.85	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	MAN	Y	510	3	11,11,12	1.16	1 (9%)	15,15,17	1.73	2 (13%)
11	MAN	U	202	2	11,11,12	1.34	2 (18%)	15,15,17	1.70	2 (13%)
11	MAN	V	510	3	11,11,12	1.24	1 (9%)	15,15,17	1.82	2 (13%)
11	MAN	X	204	2	11,11,12	1.18	1 (9%)	15,15,17	1.72	2 (13%)
11	MAN	Y	509	3	11,11,12	1.20	1 (9%)	15,15,17	1.82	2 (13%)
11	MAN	X	207	2	11,11,12	1.45	2 (18%)	15,15,17	1.20	3 (20%)
11	MAN	X	209	2	11,11,12	1.39	1 (9%)	15,15,17	1.52	2 (13%)
11	MAN	V	505	3	11,11,12	1.17	1 (9%)	15,15,17	2.19	3 (20%)
11	MAN	Y	505	3	11,11,12	1.21	1 (9%)	15,15,17	1.86	2 (13%)
11	MAN	U	201	2	11,11,12	1.24	1 (9%)	15,15,17	1.96	3 (20%)
11	MAN	X	208	2	11,11,12	1.37	2 (18%)	15,15,17	1.35	2 (13%)
11	MAN	V	504	3	11,11,12	1.29	1 (9%)	15,15,17	1.87	3 (20%)
11	MAN	V	509	3	11,11,12	1.17	1 (9%)	15,15,17	1.80	2 (13%)
11	MAN	V	511	3	11,11,12	1.23	1 (9%)	15,15,17	1.94	2 (13%)
11	MAN	Y	511	3	11,11,12	1.28	2 (18%)	15,15,17	1.92	2 (13%)
11	MAN	Y	512	3	11,11,12	1.23	1 (9%)	15,15,17	1.85	2 (13%)
11	MAN	V	503	3	11,11,12	1.11	1 (9%)	15,15,17	1.67	2 (13%)
11	MAN	Y	503	3	11,11,12	1.07	1 (9%)	15,15,17	1.75	1 (6%)

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
11	MAN	Y	504	3	-	1/2/19/22	0/1/1/1
11	MAN	X	203	2	-	0/2/19/22	0/1/1/1
11	MAN	V	512	3	-	0/2/19/22	0/1/1/1
11	MAN	Y	510	3	-	0/2/19/22	0/1/1/1
11	MAN	U	202	2	-	0/2/19/22	0/1/1/1
11	MAN	V	510	3	-	0/2/19/22	0/1/1/1
11	MAN	X	204	2	-	0/2/19/22	0/1/1/1
11	MAN	Y	509	3	-	0/2/19/22	0/1/1/1
11	MAN	X	207	2	-	0/2/19/22	0/1/1/1
11	MAN	X	209	2	-	0/2/19/22	0/1/1/1
11	MAN	V	505	3	-	0/2/19/22	0/1/1/1
11	MAN	Y	505	3	-	0/2/19/22	0/1/1/1
11	MAN	U	201	2	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	MAN	X	208	2	-	0/2/19/22	0/1/1/1
11	MAN	V	504	3	-	1/2/19/22	0/1/1/1
11	MAN	V	509	3	-	0/2/19/22	0/1/1/1
11	MAN	V	511	3	-	0/2/19/22	0/1/1/1
11	MAN	Y	511	3	-	0/2/19/22	0/1/1/1
11	MAN	Y	512	3	-	0/2/19/22	0/1/1/1
11	MAN	V	503	3	-	0/2/19/22	0/1/1/1
11	MAN	Y	503	3	-	0/2/19/22	0/1/1/1

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	X	209	MAN	O5-C5	3.29	1.49	1.43
11	V	504	MAN	O5-C5	2.99	1.49	1.43
11	X	203	MAN	O5-C5	2.90	1.49	1.43
11	Y	505	MAN	O5-C5	2.86	1.49	1.43
11	Y	509	MAN	O5-C5	2.78	1.48	1.43
11	U	202	MAN	O5-C5	2.77	1.48	1.43
11	V	510	MAN	O5-C5	2.74	1.48	1.43
11	Y	510	MAN	O5-C5	2.70	1.48	1.43
11	X	208	MAN	O5-C5	2.67	1.48	1.43
11	V	509	MAN	O5-C5	2.65	1.48	1.43
11	X	207	MAN	O5-C1	-2.57	1.39	1.43
11	X	204	MAN	O5-C5	2.55	1.48	1.43
11	Y	512	MAN	O5-C5	2.55	1.48	1.43
11	U	201	MAN	O5-C5	2.53	1.48	1.43
11	V	511	MAN	O5-C5	2.53	1.48	1.43
11	Y	511	MAN	O5-C5	2.47	1.48	1.43
11	X	207	MAN	C2-C3	2.45	1.56	1.52
11	Y	504	MAN	O5-C5	2.44	1.48	1.43
11	V	505	MAN	O5-C5	2.36	1.48	1.43
11	X	208	MAN	O5-C1	-2.29	1.39	1.43
11	Y	503	MAN	O5-C5	2.27	1.47	1.43
11	V	503	MAN	O5-C5	2.12	1.47	1.43
11	V	512	MAN	O5-C5	2.09	1.47	1.43
11	U	202	MAN	O2-C2	-2.04	1.39	1.43
11	Y	511	MAN	O4-C4	-2.03	1.37	1.43
11	X	203	MAN	O2-C2	-2.00	1.39	1.43

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	U	201	MAN	C1-O5-C5	5.86	120.05	112.19
11	Y	512	MAN	C1-O5-C5	5.67	119.78	112.19
11	V	512	MAN	C1-O5-C5	5.66	119.77	112.19
11	V	505	MAN	C1-O5-C5	5.64	119.74	112.19
11	V	504	MAN	C1-O5-C5	5.53	119.60	112.19
11	V	511	MAN	C1-O5-C5	5.49	119.55	112.19
11	Y	509	MAN	C1-O5-C5	5.45	119.49	112.19
11	Y	505	MAN	C1-O5-C5	5.41	119.44	112.19
11	Y	504	MAN	C1-O5-C5	5.37	119.38	112.19
11	Y	511	MAN	C1-O5-C5	5.30	119.30	112.19
11	Y	503	MAN	C1-O5-C5	5.30	119.28	112.19
11	V	510	MAN	C1-O5-C5	5.26	119.24	112.19
11	V	509	MAN	C1-O5-C5	5.23	119.20	112.19
11	X	204	MAN	C1-O5-C5	4.94	118.81	112.19
11	Y	510	MAN	C1-O5-C5	4.92	118.78	112.19
11	V	503	MAN	C1-O5-C5	4.91	118.77	112.19
11	X	209	MAN	C1-O5-C5	4.84	118.67	112.19
11	X	203	MAN	C1-O5-C5	4.75	118.55	112.19
11	U	202	MAN	C1-O5-C5	4.58	118.33	112.19
11	V	505	MAN	O2-C2-C3	-4.42	101.00	110.15
11	X	208	MAN	C1-O5-C5	3.75	117.22	112.19
11	Y	505	MAN	O2-C2-C3	-3.28	103.36	110.15
11	U	201	MAN	O2-C2-C3	-3.25	103.42	110.15
11	X	204	MAN	O2-C2-C3	-3.19	103.54	110.15
11	V	511	MAN	O2-C2-C3	-3.10	103.73	110.15
11	Y	511	MAN	O2-C2-C3	-2.96	104.01	110.15
11	V	510	MAN	O2-C2-C3	-2.90	104.15	110.15
11	U	202	MAN	O2-C2-C3	-2.85	104.26	110.15
11	X	203	MAN	O2-C2-C3	-2.81	104.34	110.15
11	Y	512	MAN	O2-C2-C3	-2.81	104.34	110.15
11	X	207	MAN	C1-O5-C5	2.67	115.77	112.19
11	Y	510	MAN	O2-C2-C3	-2.61	104.74	110.15
11	V	509	MAN	O2-C2-C3	-2.55	104.86	110.15
11	V	512	MAN	O2-C2-C3	-2.55	104.87	110.15
11	Y	509	MAN	O2-C2-C3	-2.28	105.42	110.15
11	V	504	MAN	O2-C2-C3	-2.26	105.47	110.15
11	X	208	MAN	O2-C2-C3	-2.26	105.47	110.15
11	X	207	MAN	C2-C3-C4	2.18	114.69	110.86
11	X	207	MAN	O2-C2-C3	-2.16	105.67	110.15
11	V	505	MAN	O5-C1-C2	2.16	115.95	110.79
11	V	504	MAN	C1-C2-C3	2.15	112.78	109.64
11	U	201	MAN	O4-C4-C3	-2.08	105.48	110.38
11	Y	504	MAN	O2-C2-C3	-2.08	105.85	110.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	X	209	MAN	O2-C2-C3	-2.06	105.87	110.15
11	V	503	MAN	O2-C2-C3	-2.02	105.97	110.15

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	V	504	MAN	C4-C5-C6-O6
11	Y	504	MAN	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	X	208	MAN	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
4	G	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	G	68:ILE	C	69:PRO	N	3.37

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	R	124/131 (94%)	0.28	3 (2%) 59 51	548, 627, 733, 762	0
1	S	124/131 (94%)	0.62	10 (8%) 18 24	702, 778, 805, 820	0
2	U	105/170 (61%)	0.74	13 (12%) 8 16	675, 735, 871, 891	0
2	X	163/170 (95%)	0.40	11 (6%) 24 29	506, 590, 642, 667	0
3	V	215/221 (97%)	0.66	27 (12%) 8 15	527, 675, 764, 811	0
3	Y	215/221 (97%)	0.84	28 (13%) 7 15	456, 572, 681, 714	0
4	A	645/645 (100%)	0.46	65 (10%) 12 19	340, 405, 469, 583	0
4	G	645/645 (100%)	0.39	45 (6%) 22 28	341, 414, 475, 611	0
5	B	913/915 (99%)	0.29	55 (6%) 27 32	335, 473, 577, 652	0
5	H	913/915 (99%)	0.53	88 (9%) 13 20	350, 490, 561, 613	0
6	J	505/505 (100%)	0.61	53 (10%) 11 19	437, 540, 646, 678	0
6	L	505/505 (100%)	0.74	73 (14%) 6 14	370, 452, 523, 589	0
7	N	84/86 (97%)	0.35	5 (5%) 27 32	393, 448, 515, 576	0
7	Q	84/86 (97%)	0.18	6 (7%) 22 28	380, 452, 514, 583	0
All	All	5240/5346 (98%)	0.50	482 (9%) 14 21	335, 476, 717, 891	0

All (482) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
6	L	697	VAL	15.4
6	J	510	HIS	12.5
6	L	696	VAL	12.2
6	J	511	SER	11.6
6	J	478	ARG	9.3
6	J	697	VAL	9.3
6	L	639	PRO	8.6
6	J	512	ILE	8.4

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Mol	Chain	Res	Type	RSRZ
4	A	341	TYR	8.4
6	J	477	ILE	8.1
6	L	565	GLN	7.7
5	H	1045	ALA	7.6
5	B	915	ARG	7.5
6	L	698	ASP	7.5
6	L	695	GLY	7.5
4	G	638	LEU	7.5
6	L	713	ALA	7.4
6	J	546	GLU	7.3
6	L	397	TYR	7.1
6	J	507	ASP	7.1
4	A	348	PHE	7.0
4	A	179	MET	7.0
5	H	1443	GLN	7.0
6	L	668	ASN	6.8
6	J	479	PRO	6.7
6	J	561	LEU	6.7
6	L	451	SER	6.6
4	A	422	LEU	6.5
6	J	506	ASP	6.4
6	L	661	VAL	6.3
6	J	508	LYS	6.2
5	H	1046	ALA	6.2
5	H	1148	THR	6.2
5	H	1044	PHE	6.1
6	L	288	THR	6.0
4	A	176	LEU	5.8
4	A	340	LYS	5.6
4	A	456	ARG	5.6
2	U	71	LEU	5.5
3	Y	350	CYS	5.4
5	H	1047	PHE	5.4
4	G	4	TYR	5.4
4	A	458	ASP	5.3
5	H	1535	ASP	5.3
5	B	914	ILE	5.3
6	L	441	TYR	5.2
4	A	433	TYR	5.2
6	L	699	VAL	5.2
5	H	1360	ASN	5.1
4	A	350	LEU	5.1

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Mol	Chain	Res	Type	RSRZ
6	L	287	VAL	5.1
6	L	449	SER	5.1
1	R	57	GLU	5.1
4	A	177	VAL	5.1
6	J	504	THR	5.0
6	L	677	PRO	5.0
4	A	387	LEU	5.0
5	H	1152	ASP	4.9
4	A	389	ILE	4.9
4	A	344	PRO	4.9
5	H	1439	PHE	4.9
4	G	636	ALA	4.8
5	H	1616	GLN	4.7
5	B	1535	ASP	4.7
4	G	639	GLN	4.7
5	H	1082	VAL	4.7
5	H	1444	TYR	4.7
5	B	1434	ASP	4.7
4	A	112	THR	4.7
6	J	662	SER	4.6
5	H	988	CYS	4.5
6	L	461	LYS	4.5
5	B	1482	LYS	4.5
5	B	953	GLU	4.5
2	X	163	CYS	4.4
5	B	954	SER	4.4
4	A	178	ASN	4.4
4	A	352	VAL	4.4
6	J	698	ASP	4.4
4	A	457	MET	4.4
5	H	968	MET	4.4
6	J	639	PRO	4.4
6	J	281	LYS	4.3
2	X	95	GLU	4.3
4	G	112	THR	4.3
5	H	1607	GLU	4.3
4	A	335	PHE	4.2
5	B	783	LEU	4.2
5	H	1483	LEU	4.2
4	G	78	LYS	4.2
5	B	1011	GLN	4.2
5	B	1291	TRP	4.1

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Mol	Chain	Res	Type	RSRZ
4	G	179	MET	4.1
5	B	1305	ASN	4.1
6	L	384	LEU	4.1
3	V	431	PHE	4.1
5	H	1634	MET	4.1
2	U	101	TYR	4.0
5	H	1319	THR	4.0
4	G	177	VAL	4.0
3	Y	387	THR	4.0
7	N	81	LEU	4.0
2	X	178	ALA	4.0
6	J	475	SER	4.0
2	X	162	ALA	4.0
5	B	1292	GLU	4.0
6	J	476	VAL	4.0
5	B	1553	GLU	4.0
6	L	375	THR	4.0
6	L	671	ARG	4.0
4	G	79	GLY	3.9
6	L	711	ALA	3.9
4	A	78	LYS	3.9
6	L	319	TYR	3.9
5	B	1156	ALA	3.9
5	H	1048	VAL	3.9
6	L	356	ARG	3.8
5	H	1388	GLY	3.8
5	H	915	ARG	3.8
7	Q	40	TYR	3.8
3	Y	455	CYS	3.8
4	G	180	GLY	3.8
2	U	103	ARG	3.8
3	Y	437	PRO	3.7
6	L	648	SER	3.7
4	G	353	PHE	3.7
4	G	110	ILE	3.7
5	H	1442	HIS	3.7
2	U	129	ASP	3.7
4	G	352	VAL	3.7
4	G	556	GLY	3.6
5	H	1534	ASN	3.6
6	J	481	LYS	3.6
4	A	343	LYS	3.6

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Mol	Chain	Res	Type	RSRZ
5	H	1155	GLU	3.6
5	H	1638	GLY	3.6
4	A	421	ALA	3.6
4	A	388	SER	3.5
7	N	29	ASN	3.5
6	L	238	LEU	3.5
5	B	1083	LYS	3.5
6	J	509	GLU	3.5
4	A	342	PHE	3.5
5	B	1009	THR	3.5
5	B	1481	ASN	3.5
5	H	1054	THR	3.5
5	B	1483	LEU	3.5
2	U	89	CYS	3.5
6	J	699	VAL	3.5
3	V	341	PRO	3.5
4	G	81	ASN	3.4
5	B	1327	HIS	3.4
6	L	379	GLU	3.4
4	G	198	THR	3.4
6	J	269	VAL	3.4
3	Y	408	THR	3.4
4	G	514	THR	3.4
1	R	103	ILE	3.4
6	J	696	VAL	3.3
5	H	1009	THR	3.3
4	G	178	ASN	3.3
4	A	331	TYR	3.3
7	N	77	ILE	3.3
4	A	339	PRO	3.3
5	B	1340	ASP	3.3
5	H	1363	ILE	3.3
3	Y	439	CYS	3.3
6	L	457	TRP	3.3
5	B	1002	ALA	3.2
4	A	423	PRO	3.2
4	A	424	TYR	3.2
4	G	349	ASP	3.2
6	L	576	GLU	3.2
4	A	589	LEU	3.2
5	B	865	THR	3.2
3	Y	341	PRO	3.2

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Mol	Chain	Res	Type	RSRZ
4	G	523	GLU	3.2
5	H	1637	PHE	3.2
6	J	385	TYR	3.1
6	L	237	VAL	3.1
3	Y	386	SER	3.1
5	H	1261	GLN	3.1
5	H	1052	PRO	3.1
5	H	1157	ASN	3.1
6	J	573	PRO	3.1
6	L	254	GLY	3.1
3	Y	257	ALA	3.1
2	X	124	LEU	3.1
3	Y	447	LEU	3.1
4	A	76	SER	3.1
4	G	102	SER	3.1
4	G	589	LEU	3.1
6	L	323	LYS	3.1
4	A	111	GLN	3.1
5	B	1166	THR	3.1
5	B	1321	SER	3.1
5	H	1490	ARG	3.1
3	Y	468	GLU	3.1
6	L	653	PRO	3.0
1	S	67	GLY	3.0
4	A	109	PHE	3.0
5	B	1359	LYS	3.0
5	H	838	LEU	3.0
5	H	1441	VAL	3.0
6	L	452	LEU	3.0
5	H	1445	PHE	3.0
3	V	303	THR	3.0
3	V	464	PRO	3.0
6	L	278	TYR	3.0
6	L	676	GLY	3.0
4	G	587	ASN	3.0
4	G	25	HIS	2.9
5	H	810	ASP	2.9
4	A	431	ASN	2.9
5	B	1592	GLU	2.9
4	A	349	ASP	2.9
4	A	461	HIS	2.9
5	H	987	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
4	A	542	VAL	2.9
5	H	1484	CYS	2.9
6	L	450	LEU	2.9
6	L	568	ARG	2.8
4	A	180	GLY	2.8
6	L	548	TYR	2.8
6	J	513	LYS	2.8
3	V	465	GLU	2.8
3	Y	384	GLU	2.8
5	H	948	GLN	2.8
6	L	252	GLY	2.8
5	H	1235	ASN	2.8
3	V	282	ARG	2.8
6	L	446	GLU	2.8
4	G	103	LEU	2.8
3	V	286	HIS	2.8
4	G	215	GLU	2.8
6	L	258	ALA	2.8
5	H	1017	LEU	2.8
6	L	459	HIS	2.8
3	V	451	GLU	2.8
4	G	111	GLN	2.8
5	B	1616	GLN	2.8
1	S	91	ASP	2.8
3	V	292	GLY	2.8
3	Y	389	GLY	2.8
2	U	88	PRO	2.8
3	V	301	THR	2.7
5	H	1387	THR	2.7
5	H	1446	ASN	2.7
6	L	709	VAL	2.7
3	Y	406	LEU	2.7
2	U	65	GLN	2.7
5	B	1319	THR	2.7
6	L	739	LEU	2.7
5	B	1023	ALA	2.7
5	B	1120	ALA	2.7
5	B	1326	TYR	2.7
5	H	1481	ASN	2.7
1	S	87	LEU	2.7
6	J	602	ASP	2.7
4	A	175	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
5	H	1362	MET	2.7
5	H	1621	GLN	2.7
4	G	251	PHE	2.7
3	V	285	ASN	2.6
4	A	455	LEU	2.6
5	H	1364	LEU	2.6
5	H	1043	ALA	2.6
5	H	1539	TYR	2.6
4	A	419	MET	2.6
5	H	1608	HIS	2.6
3	Y	351	ARG	2.6
4	G	319	ALA	2.6
5	H	772	PHE	2.6
5	H	1103	ILE	2.6
5	B	1121	LEU	2.6
4	A	26	ASP	2.6
2	U	31	LEU	2.6
3	Y	279	MET	2.6
6	J	480	SER	2.6
5	H	1389	PHE	2.6
3	V	279	MET	2.6
5	H	777	ILE	2.5
5	H	1563	ILE	2.5
5	H	1599	ILE	2.5
3	V	342	GLY	2.5
1	S	8	SER	2.5
4	G	634	GLN	2.5
4	A	338	THR	2.5
6	J	555	ILE	2.5
3	V	291	HIS	2.5
6	J	552	VAL	2.5
4	A	222	TYR	2.5
6	L	563	TYR	2.5
6	L	394	ARG	2.5
5	H	1321	SER	2.5
5	B	1493	GLU	2.5
4	G	297	LEU	2.5
6	L	606	LEU	2.5
5	B	1484	CYS	2.5
5	B	1432	SER	2.5
7	Q	39	TYR	2.5
4	A	367	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
5	B	1003	VAL	2.5
2	U	70	GLY	2.5
4	G	176	LEU	2.4
6	J	485	SER	2.4
4	A	168	PRO	2.4
6	L	690	GLY	2.4
5	H	1132	ALA	2.4
7	Q	81	LEU	2.4
5	H	1037	PHE	2.4
6	J	725	PRO	2.4
6	L	382	ASP	2.4
5	H	1440	LYS	2.4
4	A	400	ILE	2.4
2	X	101	TYR	2.4
3	V	278	THR	2.4
5	H	924	THR	2.4
6	L	250	LEU	2.4
3	V	283	THR	2.4
5	H	865	THR	2.4
6	L	466	HIS	2.4
4	G	558	GLN	2.4
6	L	573	PRO	2.4
5	H	1035	LEU	2.4
1	S	23	CYS	2.4
6	L	694	TRP	2.4
2	X	164	ASN	2.4
5	H	969	THR	2.4
4	G	101	VAL	2.4
4	A	305	SER	2.3
5	B	1371	ARG	2.3
5	H	922	VAL	2.3
5	B	1456	LYS	2.3
1	S	97	CYS	2.3
4	A	432	ASN	2.3
3	V	255	GLY	2.3
4	G	335	PHE	2.3
5	H	1086	ILE	2.3
2	U	92	THR	2.3
5	B	1480	LEU	2.3
2	X	168	PRO	2.3
3	Y	304	HIS	2.3
3	Y	409	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
6	J	638	ALA	2.3
6	L	567	ILE	2.3
5	B	1561	THR	2.3
6	L	516	VAL	2.3
3	V	447	LEU	2.3
3	V	340	ILE	2.3
4	A	110	ILE	2.3
4	A	402	VAL	2.3
4	A	224	TYR	2.3
3	V	457	HIS	2.3
5	H	1201	PRO	2.3
4	A	369	VAL	2.3
5	H	1482	LYS	2.3
6	L	678	LEU	2.3
3	Y	459	PRO	2.3
2	X	126	ALA	2.3
6	L	429	LYS	2.3
4	G	515	LEU	2.3
6	L	353	ASN	2.3
6	J	525	ILE	2.3
1	S	17	GLY	2.3
3	Y	342	GLY	2.3
5	H	989	GLY	2.3
5	H	1145	GLY	2.3
6	J	482	GLY	2.3
3	Y	266	VAL	2.3
2	X	97	SER	2.2
5	H	1564	SER	2.2
5	H	1390	ALA	2.2
6	L	249	VAL	2.2
6	L	646	ASP	2.2
6	J	493	GLU	2.2
5	H	914	ILE	2.2
5	B	952	THR	2.2
6	J	363	THR	2.2
6	L	628	LYS	2.2
4	G	305	SER	2.2
6	L	691	VAL	2.2
6	J	362	MET	2.2
4	A	25	HIS	2.2
5	H	990	GLU	2.2
4	A	391	THR	2.2

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Mol	Chain	Res	Type	RSRZ
6	J	650	VAL	2.2
5	B	1254	PHE	2.2
5	B	970	GLU	2.2
6	L	593	GLN	2.2
7	Q	77	ILE	2.2
2	U	64	TYR	2.2
4	G	433	TYR	2.2
4	A	346	MET	2.2
3	Y	407	CYS	2.2
5	H	1065	SER	2.2
4	A	398	LEU	2.2
5	B	1559	GLN	2.2
5	H	1581	LEU	2.2
6	J	563	TYR	2.2
5	H	1057	THR	2.2
4	A	425	SER	2.2
6	J	431	LYS	2.2
4	G	148	PRO	2.2
5	B	1599	ILE	2.2
2	X	71	LEU	2.2
5	B	1087	LEU	2.2
5	H	1239	TYR	2.2
3	V	263	TRP	2.2
6	J	369	MET	2.2
6	J	532	PRO	2.1
6	L	605	ALA	2.1
5	H	1422	LEU	2.1
6	J	274	LYS	2.1
7	Q	41	LYS	2.1
3	Y	303	THR	2.1
5	H	776	SER	2.1
5	H	1179	ARG	2.1
5	B	1593	LYS	2.1
7	N	41	LYS	2.1
7	Q	44	ILE	2.1
1	S	22	SER	2.1
5	B	780	TRP	2.1
5	H	1438	ALA	2.1
6	L	561	LEU	2.1
3	Y	398	ASN	2.1
4	A	420	GLN	2.1
5	B	1555	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
5	H	1432	SER	2.1
6	L	688	GLN	2.1
4	G	100	LEU	2.1
4	A	202	VAL	2.1
6	L	283	ARG	2.1
3	V	424	GLN	2.1
3	Y	383	SER	2.1
4	G	337	LYS	2.1
5	B	959	LEU	2.1
6	L	448	GLN	2.1
6	L	665	ALA	2.1
4	A	397	PRO	2.1
1	R	97	CYS	2.1
3	Y	353	ARG	2.1
5	B	1119	MET	2.1
5	B	1290	HIS	2.1
2	U	46	LEU	2.1
4	A	610	GLY	2.1
4	G	416	THR	2.1
6	J	270	ASN	2.1
5	H	1559	GLN	2.1
6	J	503	PHE	2.1
6	L	647	ILE	2.1
3	Y	415	PRO	2.1
4	A	410	SER	2.1
6	J	531	HIS	2.1
1	S	92	THR	2.1
4	A	19	THR	2.1
4	G	104	GLN	2.1
3	V	468	GLU	2.1
5	H	753	VAL	2.1
6	J	324	LEU	2.0
4	A	62	GLY	2.0
6	J	291	THR	2.0
2	U	94	SER	2.0
4	G	314	SER	2.0
6	J	684	SER	2.0
4	G	20	MET	2.0
6	J	695	GLY	2.0
6	L	710	PRO	2.0
3	V	337	CYS	2.0
4	A	514	THR	2.0

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Mol	Chain	Res	Type	RSRZ
5	B	1323	VAL	2.0
5	H	1352	GLU	2.0
6	J	355	THR	2.0
3	V	302	ARG	2.0
5	B	1005	TYR	2.0
3	V	281	GLN	2.0
1	S	122	THR	2.0
3	Y	349	THR	2.0
6	L	341	MET	2.0
7	N	30	GLU	2.0
3	V	350	CYS	2.0
5	B	1551	SER	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.

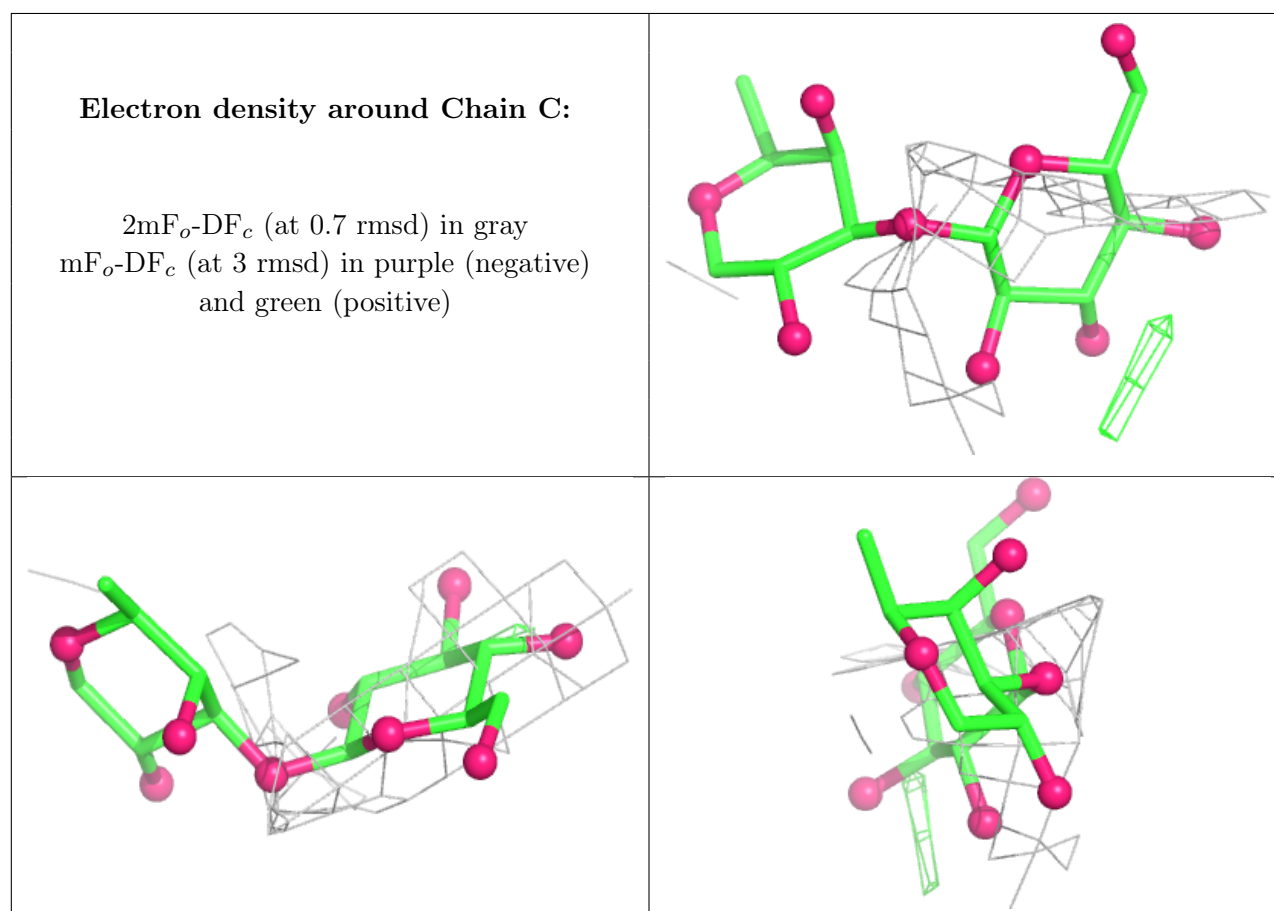
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
8	FUC	C	1	10/11	-	-	832,849,863,871	0
8	BGC	C	2	11/12	-	-	842,857,865,867	0
8	FUC	D	1	10/11	-	-	720,740,750,763	0
8	BGC	D	2	11/12	-	-	715,719,726,728	0
8	FUC	F	1	10/11	-	-	637,648,658,666	0
8	BGC	F	2	11/12	-	-	625,632,643,649	0
8	FUC	I	1	10/11	-	-	508,526,532,542	0
8	BGC	I	2	11/12	-	-	532,536,548,552	0
8	FUC	K	1	10/11	-	-	608,613,617,619	0
8	BGC	K	2	11/12	-	-	623,626,629,630	0
9	NAG	E	1	14/15	-	-	688,693,698,698	0
9	NAG	E	2	14/15	-	-	689,693,699,699	0
9	FUC	E	3	10/11	-	-	699,701,702,703	0
9	NAG	M	1	14/15	-	-	629,631,633,635	0
9	NAG	M	2	14/15	-	-	692,701,711,711	0
9	FUC	M	3	10/11	-	-	652,657,662,664	0

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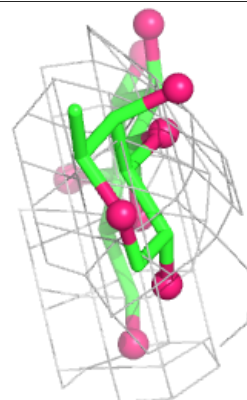
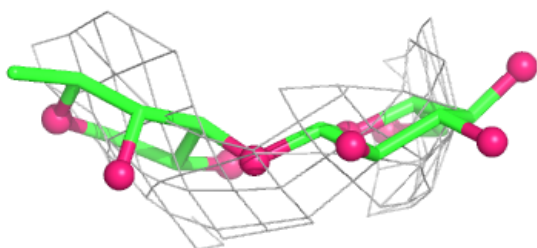
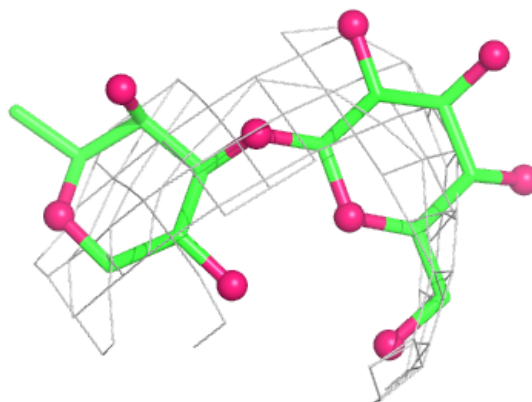
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
10	NAG	O	1	14/15	-	-	404,407,409,409	0
10	NAG	O	2	14/15	-	-	470,471,472,472	0
10	NAG	P	1	14/15	-	-	503,514,532,537	0
10	NAG	P	2	14/15	-	-	546,559,572,576	0
10	NAG	T	1	14/15	-	-	437,439,440,440	0
10	NAG	T	2	14/15	-	-	486,487,488,488	0
10	NAG	W	1	14/15	0.24	0.18	499,504,510,515	0
10	NAG	Z	2	14/15	0.48	0.13	566,572,581,584	0
10	NAG	W	2	14/15	0.72	0.09	513,516,519,520	0
10	NAG	Z	1	14/15	0.78	0.14	547,552,559,562	0
10	NAG	a	1	14/15	-	-	592,599,611,611	0
10	NAG	a	2	14/15	-	-	623,629,634,634	0
10	NAG	b	1	14/15	-	-	535,543,553,558	0
10	NAG	b	2	14/15	-	-	554,561,564,568	0
10	NAG	c	1	14/15	-	-	547,554,563,565	0
10	NAG	c	2	14/15	-	-	553,561,567,570	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.

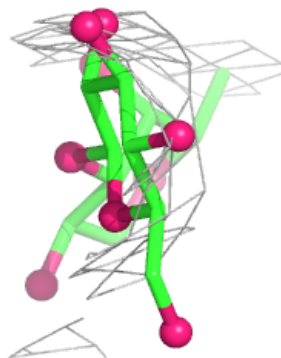
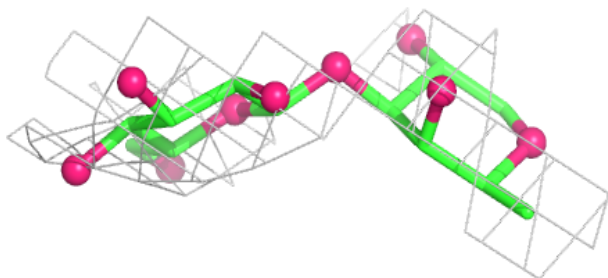
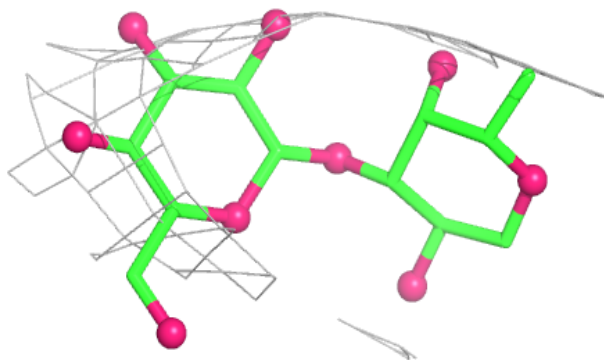


Electron density around Chain D:

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

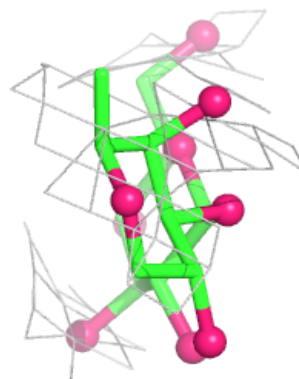
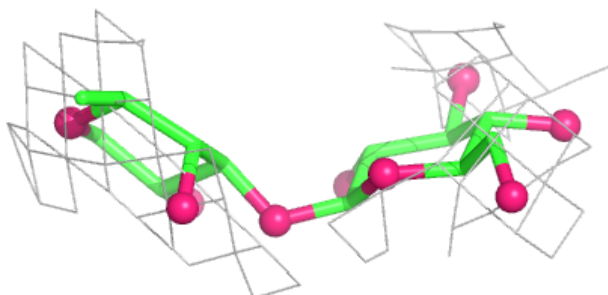
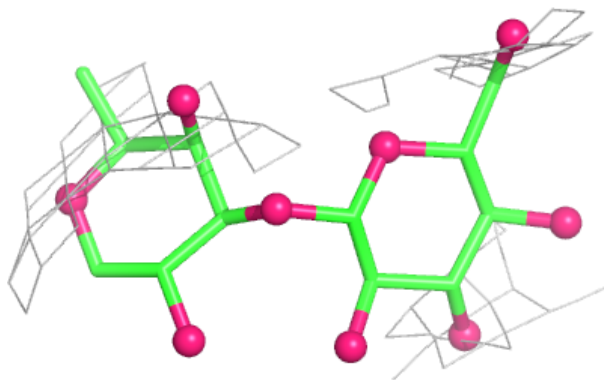
**Electron density around Chain F:**

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

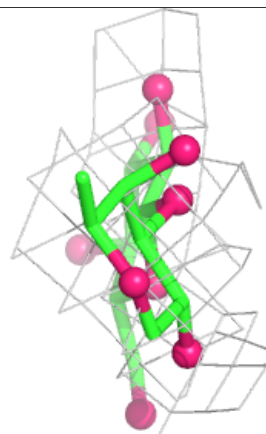
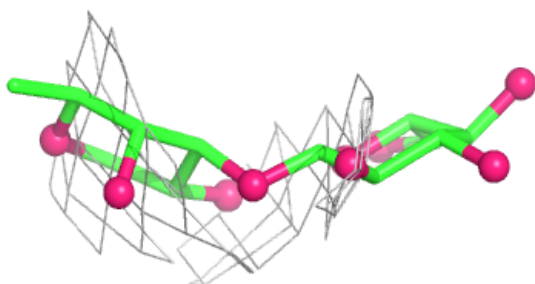
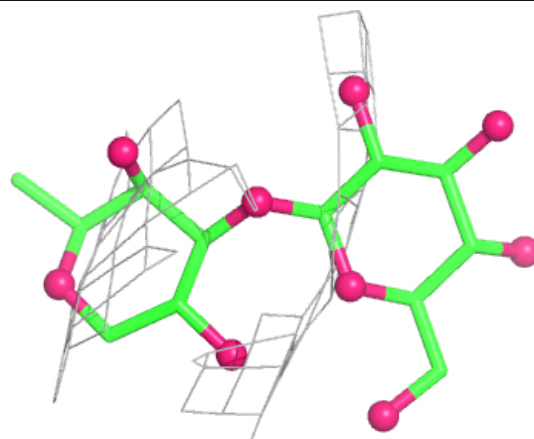


Electron density around Chain I:

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

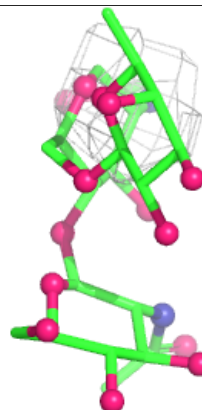
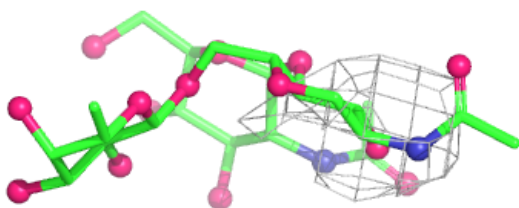
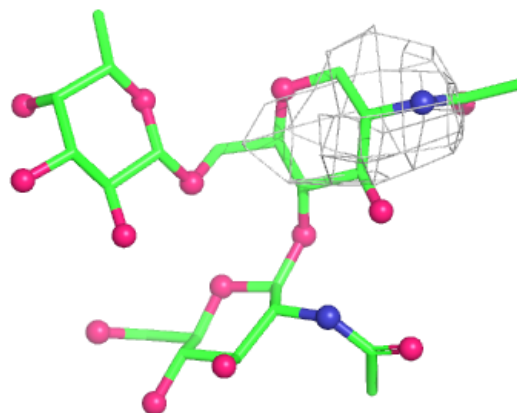
**Electron density around Chain K:**

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



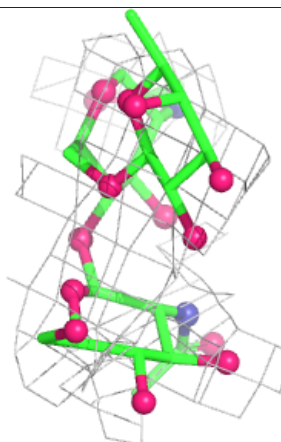
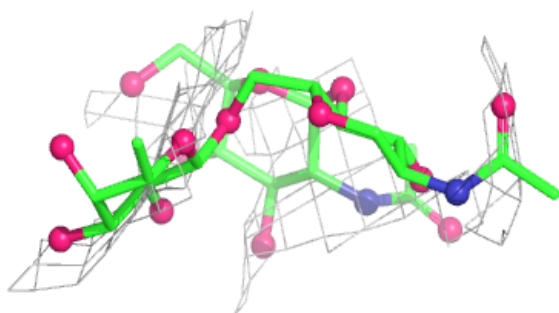
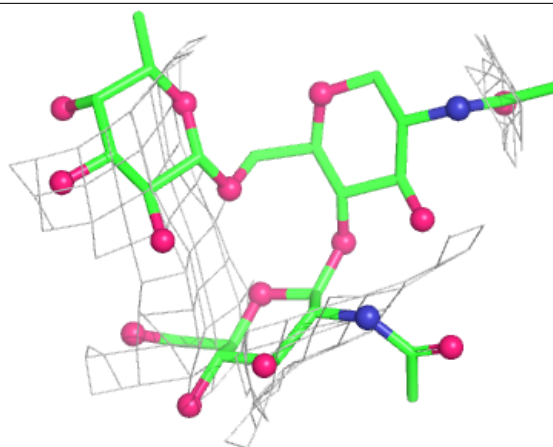
Electron density around Chain E:

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

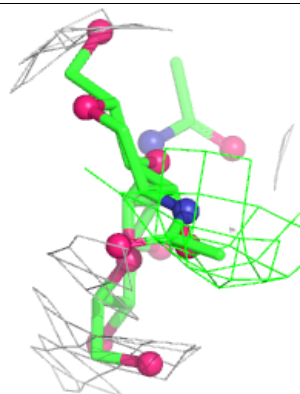
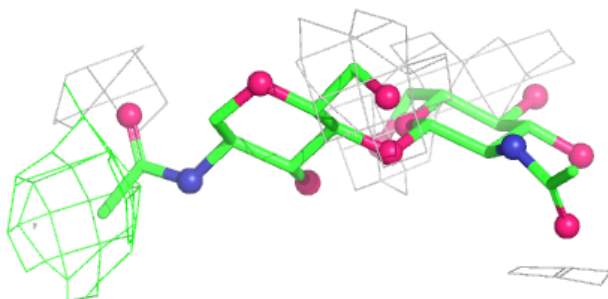
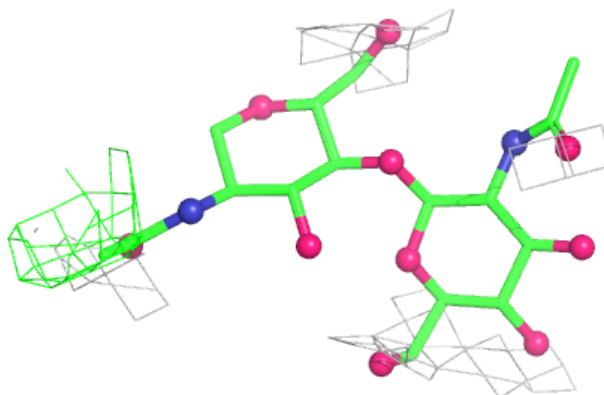


Electron density around Chain M:

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

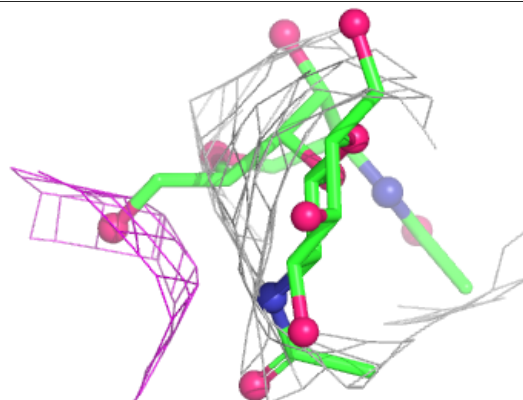
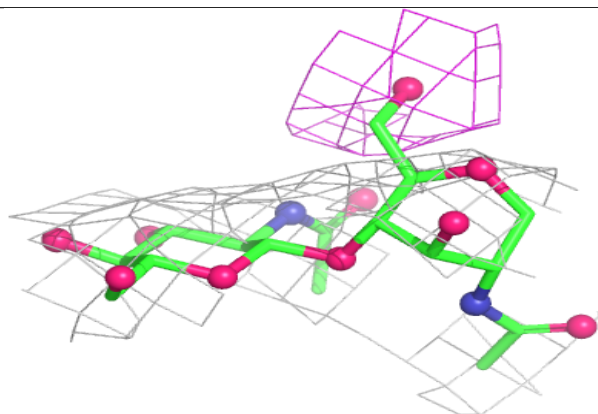
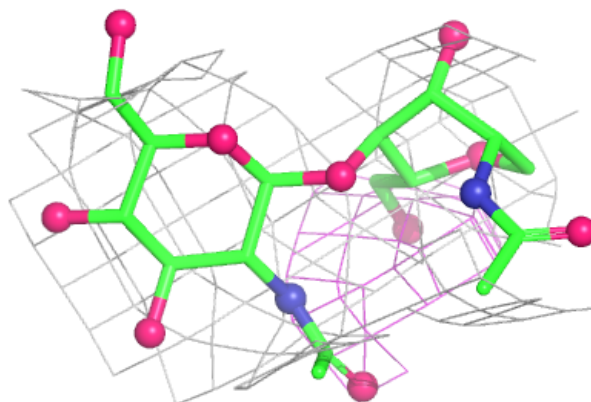
**Electron density around Chain O:**

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



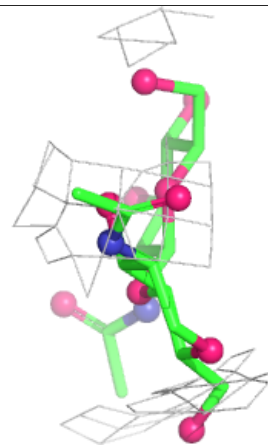
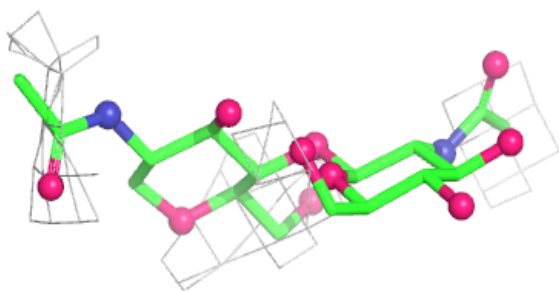
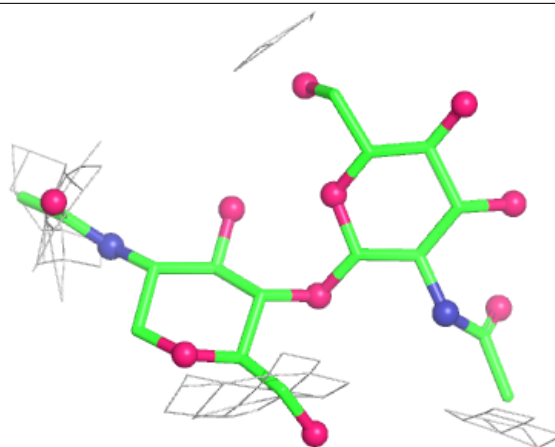
Electron density around Chain P:

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



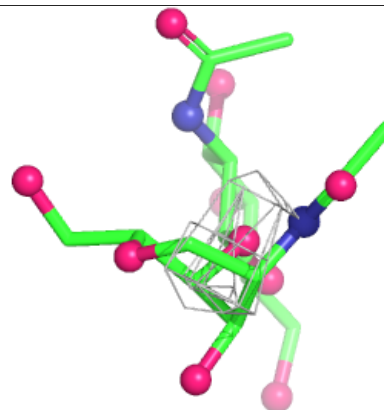
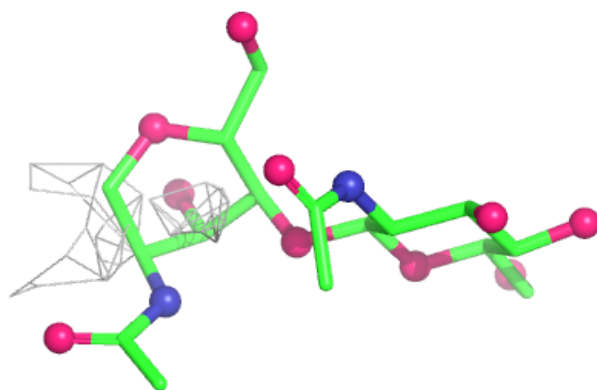
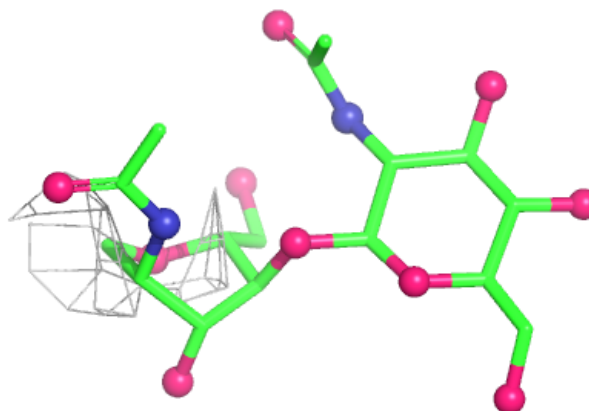
Electron density around Chain T:

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



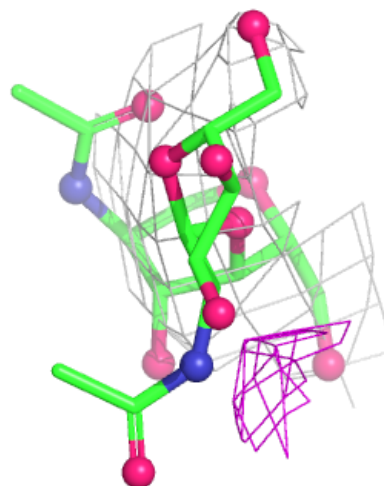
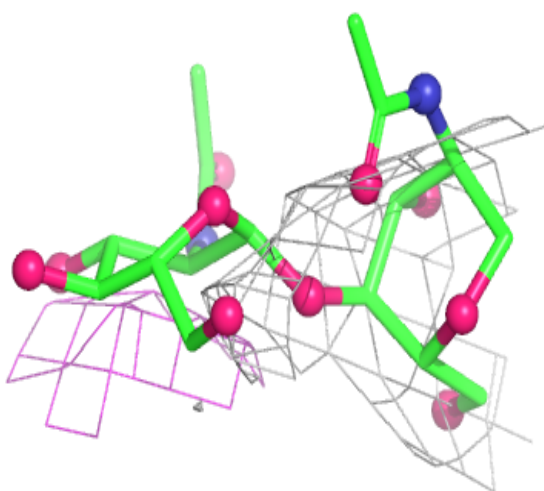
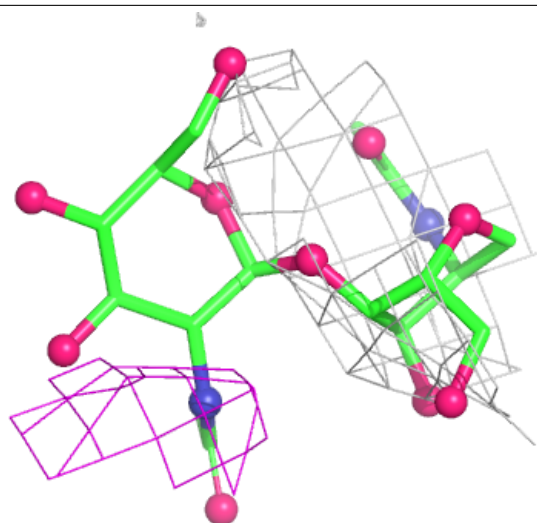
Electron density around Chain W:

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



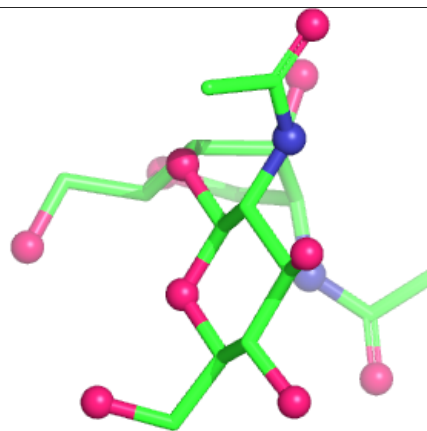
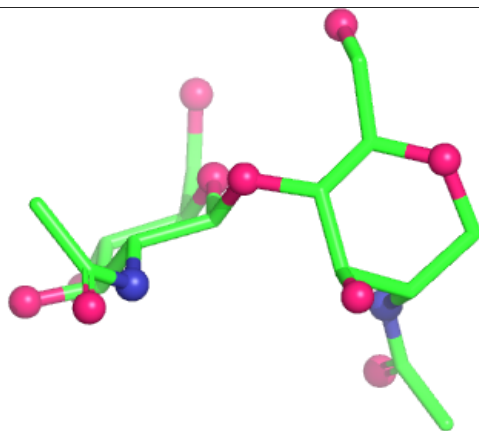
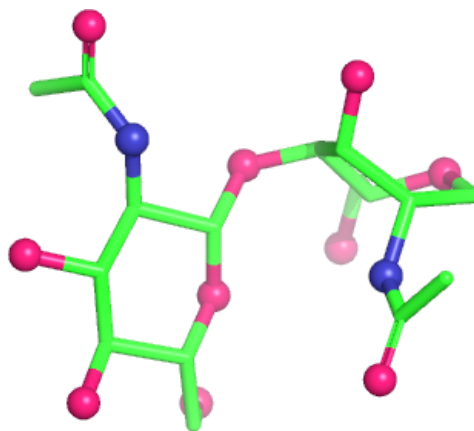
Electron density around Chain Z:

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



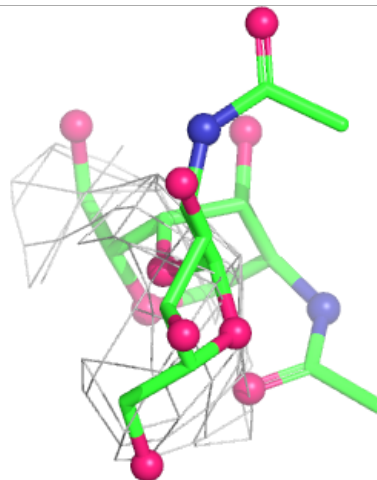
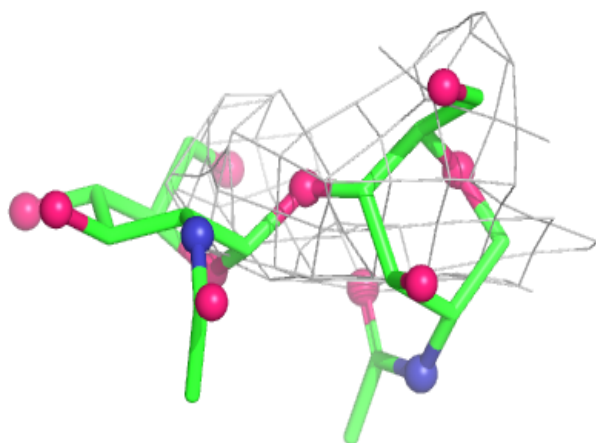
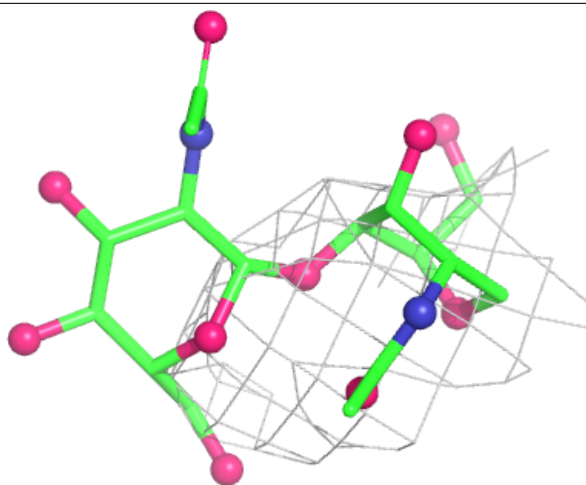
Electron density around Chain a:

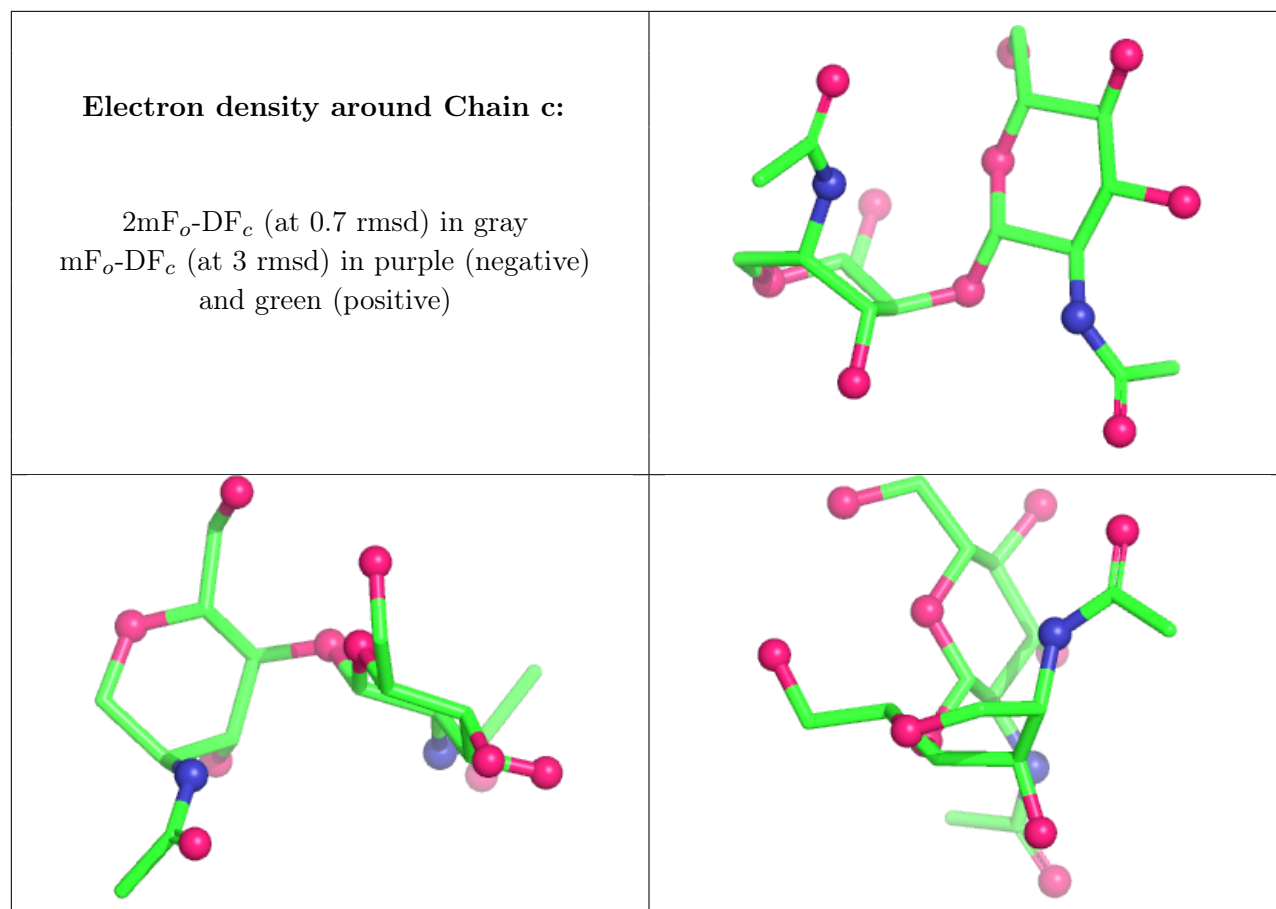
$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain b:

$2mF_o-DF_c$ (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, 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
11	MAN	V	512	11/12	-0.09	0.13	736,746,759,761	0
11	MAN	U	201	11/12	-0.01	0.13	775,792,812,818	0
11	MAN	U	202	11/12	0.33	0.11	810,827,843,849	0
11	MAN	V	503	11/12	0.49	0.07	559,580,593,602	0
11	MAN	Y	503	11/12	0.52	0.06	474,479,496,496	0
11	MAN	Y	512	11/12	0.52	0.08	689,699,706,706	0
11	MAN	Y	509	11/12	0.55	0.21	532,537,542,545	0
11	MAN	V	509	11/12	0.57	0.09	709,715,719,720	0
11	MAN	X	203	11/12	0.58	0.10	564,571,581,585	0
11	MAN	X	204	11/12	0.63	0.10	593,606,613,613	0
11	MAN	Y	510	11/12	0.67	0.15	574,580,586,592	0
11	MAN	X	209	11/12	0.67	0.10	635,644,656,657	0
11	MAN	X	208	11/12	0.70	0.17	601,612,624,624	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
11	MAN	X	207	11/12	0.73	0.11	570,583,596,598	0
11	MAN	Y	505	11/12	0.76	0.11	594,599,602,605	0
11	MAN	V	504	11/12	0.76	0.10	605,621,627,630	0
11	MAN	Y	511	11/12	0.77	0.11	678,686,689,695	0
11	MAN	V	505	11/12	0.84	0.13	638,646,651,656	0
11	MAN	V	510	11/12	0.84	0.05	690,694,698,702	0
11	MAN	Y	504	11/12	0.87	0.04	478,489,496,496	0
11	MAN	V	511	11/12	0.89	0.11	723,737,745,747	0
12	MG	L	801	1/1	0.96	0.04	464,464,464,464	0
12	MG	J	801	1/1	0.99	0.06	427,427,427,427	0

6.5 Other polymers

There are no such residues in this entry.