



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 7, 2021 – 12:12 AM EDT

PDB ID : 7KD6  
Title : Insulin Receptor L1-CR plus alphaCT fragment in co-complex with Fv 83-7 and single-chain insulin SCI-b  
Authors : Lawrence, M.C.; Menting, J.G.  
Deposited on : 2020-10-08  
Resolution : 2.60 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 : 2.23.2  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.23.2

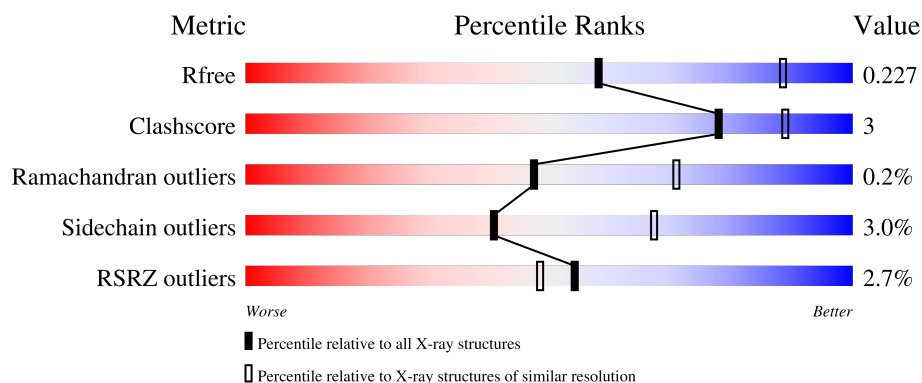
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	B	57	<div> <div>4%</div> <div> <div></div> <div>74%</div> <div>12%</div> <div>14%</div> </div> </div>
1	H	57	<div> <div>72%</div> <div>11%</div> <div>18%</div> </div>
1	N	57	<div> <div>5%</div> <div> <div></div> <div>74%</div> <div>9%</div> <div>18%</div> </div> </div>
1	T	57	<div> <div>5%</div> <div> <div></div> <div>72%</div> <div>11%</div> <div>18%</div> </div> </div>
2	C	126	<div> <div>90%</div> <div>7%</div> </div>

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Mol	Chain	Length	Quality of chain
2	I	126	% 83% 14% ..
2	O	126	87% 11% .
2	U	126	84% 10% 6%
3	D	121	84% 11% 5%
3	J	121	% 85% 10% 5%
3	P	121	2% 88% 7% 5%
3	V	121	2% 88% 7% 6%
4	E	317	2% 79% 10% 10%
4	K	317	4% 79% 10% 11%
4	Q	317	4% 83% 8% 9%
4	W	317	4% 75% 10% 15%
5	F	16	88% 6% 6%
5	L	16	81% 12% 6%
5	R	16	12% 88% 6% 6%
5	X	16	81% 6% 12%
6	1	4	25% 75%
6	M	4	50% 50%
6	S	4	25% 75%
6	Y	4	25% 75%
6	Z	4	50% 50%
7	A	3	67% 33%
8	2	2	50% 50%
8	3	2	50% 50%
8	4	2	100%
8	G	2	50% 50%

## 2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 19073 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 Single-chain Insulin SCI-b.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	49	Total	C	N	O	S	0	0	0
			391	244	70	71	6			
1	H	47	Total	C	N	O	S	0	0	0
			373	233	65	69	6			
1	N	47	Total	C	N	O	S	0	0	0
			373	233	65	69	6			
1	T	47	Total	C	N	O	S	0	0	0
			375	235	67	67	6			

- Molecule 2 is a protein called Fv 83-7 Heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	123	Total	C	N	O	S	0	0	0
			938	590	158	185	5			
2	I	123	Total	C	N	O	S	0	0	0
			938	590	158	185	5			
2	O	124	Total	C	N	O	S	0	0	0
			949	596	162	186	5			
2	U	119	Total	C	N	O	S	0	0	0
			910	571	154	180	5			

- Molecule 3 is a protein called Fv 83-7 Light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	115	Total	C	N	O	S	0	0	0
			891	564	147	176	4			
3	J	115	Total	C	N	O	S	0	0	0
			891	564	147	176	4			
3	P	115	Total	C	N	O	S	0	0	0
			890	564	147	175	4			
3	V	114	Total	C	N	O	S	0	0	0
			885	561	146	174	4			

- Molecule 4 is a protein called Insulin receptor subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	286	Total	C	N	O	S	0	1	0
			2297	1447	397	419	34			
4	K	282	Total	C	N	O	S	0	0	0
			2264	1424	392	416	32			
4	Q	290	Total	C	N	O	S	0	0	0
			2314	1455	400	425	34			
4	W	269	Total	C	N	O	S	0	0	0
			2155	1362	367	397	29			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	144	HIS	TYR	conflict	UNP P06213
E	311	SER	-	expression tag	UNP P06213
E	312	SER	-	expression tag	UNP P06213
E	313	SER	-	expression tag	UNP P06213
E	314	LEU	-	expression tag	UNP P06213
E	315	VAL	-	expression tag	UNP P06213
E	316	PRO	-	expression tag	UNP P06213
E	317	ARG	-	expression tag	UNP P06213
K	144	HIS	TYR	conflict	UNP P06213
K	311	SER	-	expression tag	UNP P06213
K	312	SER	-	expression tag	UNP P06213
K	313	SER	-	expression tag	UNP P06213
K	314	LEU	-	expression tag	UNP P06213
K	315	VAL	-	expression tag	UNP P06213
K	316	PRO	-	expression tag	UNP P06213
K	317	ARG	-	expression tag	UNP P06213
Q	144	HIS	TYR	conflict	UNP P06213
Q	311	SER	-	expression tag	UNP P06213
Q	312	SER	-	expression tag	UNP P06213
Q	313	SER	-	expression tag	UNP P06213
Q	314	LEU	-	expression tag	UNP P06213
Q	315	VAL	-	expression tag	UNP P06213
Q	316	PRO	-	expression tag	UNP P06213
Q	317	ARG	-	expression tag	UNP P06213
W	144	HIS	TYR	conflict	UNP P06213
W	311	SER	-	expression tag	UNP P06213
W	312	SER	-	expression tag	UNP P06213
W	313	SER	-	expression tag	UNP P06213
W	314	LEU	-	expression tag	UNP P06213
W	315	VAL	-	expression tag	UNP P06213

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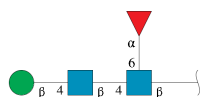
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Chain	Residue	Modelled	Actual	Comment	Reference
W	316	PRO	-	expression tag	UNP P06213
W	317	ARG	-	expression tag	UNP P06213

- Molecule 5 is a protein called Insulin receptor isoform A alphaCT peptide.

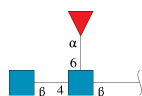
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	F	15	Total	C	N	O	0	0	0
			130	87	21	22			
5	L	15	Total	C	N	O	0	0	0
			130	87	21	22			
5	R	15	Total	C	N	O	0	0	0
			130	87	21	22			
5	X	14	Total	C	N	O	0	0	0
			123	82	20	21			

- Molecule 6 is an oligosaccharide called beta-D-mannopyranose-(1-4)-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
6	1	4	Total	C	N	O	0	0	0
			49	28	2	19			
6	M	4	Total	C	N	O	0	0	0
			49	28	2	19			
6	S	4	Total	C	N	O	0	0	0
			49	28	2	19			
6	Y	4	Total	C	N	O	0	0	0
			49	28	2	19			
6	Z	4	Total	C	N	O	0	0	0
			49	28	2	19			

- Molecule 7 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.



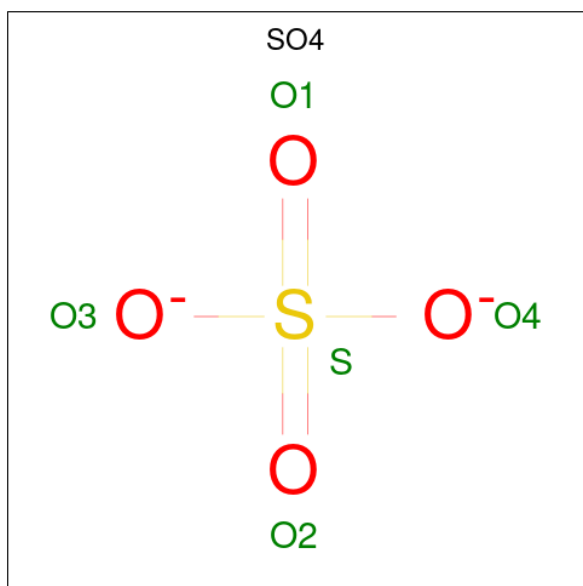
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	A	3	Total	C	N	O	0	0	0
			38	22	2	14			

- Molecule 8 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
8	G	2	Total	C	N	O	0	0	0
			28	16	2	10			
8	2	2	Total	C	N	O	0	0	0
			28	16	2	10			
8	3	2	Total	C	N	O	0	0	0
			28	16	2	10			
8	4	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 9 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



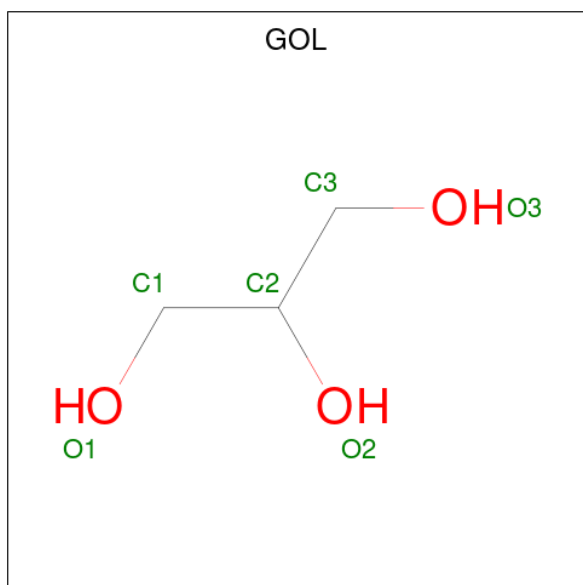
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	C	1	Total	O	S	0	0
			5	4	1		
9	I	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	O	1	Total	O	S	0	0
			5	4	1		
9	U	1	Total	O	S	0	0
			5	4	1		

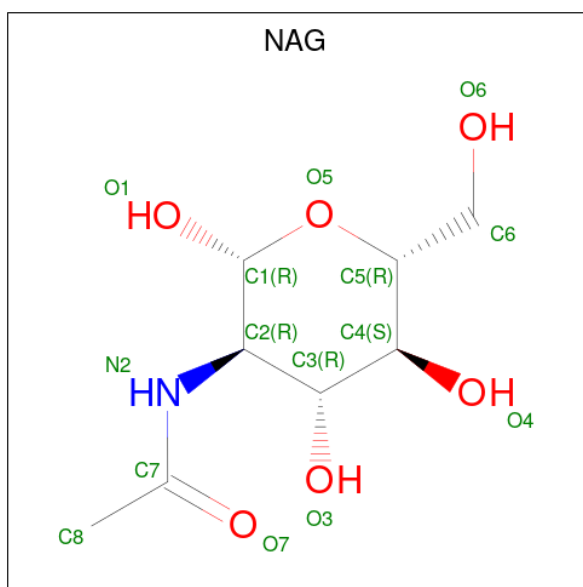
- Molecule 10 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 11 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	E	1	Total	C	N	O	0	0
			14	8	1	5		
11	K	1	Total	C	N	O	0	0
			14	8	1	5		
11	K	1	Total	C	N	O	0	0
			14	8	1	5		
11	K	1	Total	C	N	O	0	0
			14	8	1	5		
11	Q	1	Total	C	N	O	0	0
			14	8	1	5		
11	Q	1	Total	C	N	O	0	0
			14	8	1	5		
11	Q	1	Total	C	N	O	0	0
			14	8	1	5		
11	W	1	Total	C	N	O	0	0
			14	8	1	5		
11	W	1	Total	C	N	O	0	0
			14	8	1	5		
11	W	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	B	1	Total	O	0	0
			1	1		
12	C	26	Total	O	0	0
			26	26		

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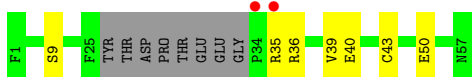
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	D	14	Total 14	O 14	0	0
12	E	17	Total 17	O 17	0	0
12	F	1	Total 1	O 1	0	0
12	H	1	Total 1	O 1	0	0
12	I	32	Total 32	O 32	0	0
12	J	11	Total 11	O 11	0	0
12	K	6	Total 6	O 6	0	0
12	O	23	Total 23	O 23	0	0
12	P	8	Total 8	O 8	0	0
12	Q	6	Total 6	O 6	0	0
12	T	1	Total 1	O 1	0	0
12	U	7	Total 7	O 7	0	0
12	V	2	Total 2	O 2	0	0
12	W	9	Total 9	O 9	0	0

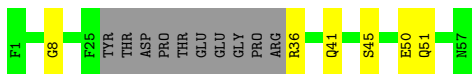
### 3 Residue-property plots [i](#)

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.

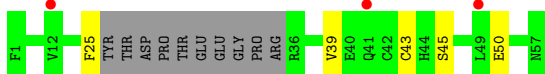
- Molecule 1: Single-chain Insulin SCI-b



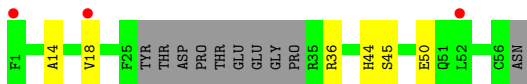
- Molecule 1: Single-chain Insulin SCI-b



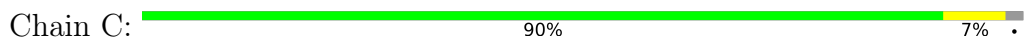
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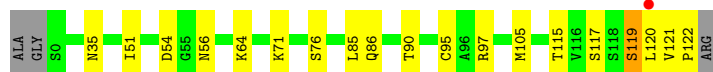
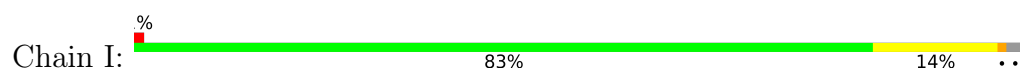
- Molecule 1: Single-chain Insulin SCI-b



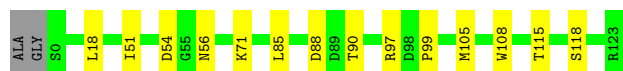
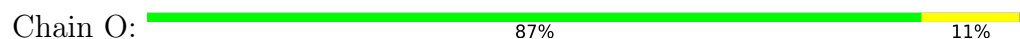
- Molecule 2: Fv 83-7 Heavy chain



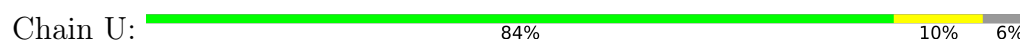
- Molecule 2: Fv 83-7 Heavy chain



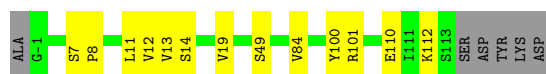
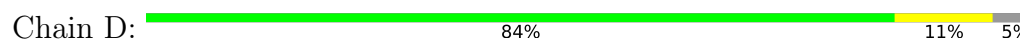
- Molecule 2: Fv 83-7 Heavy chain



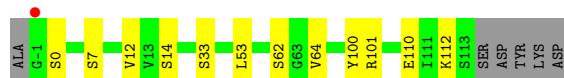
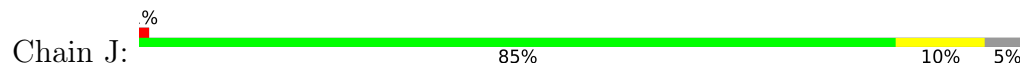
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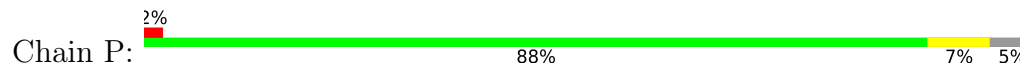
- Molecule 3: Fv 83-7 Light chain



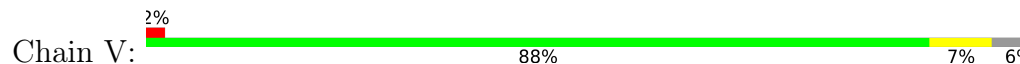
- Molecule 3: Fv 83-7 Light chain



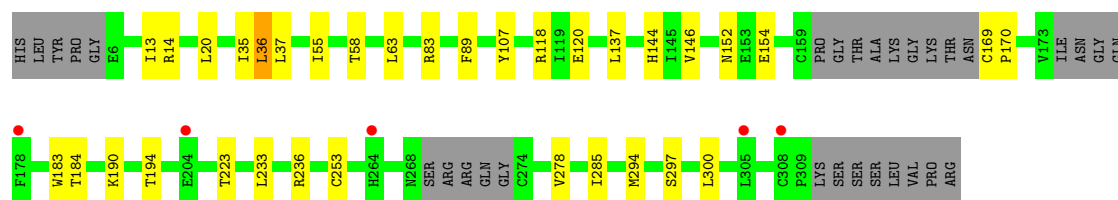
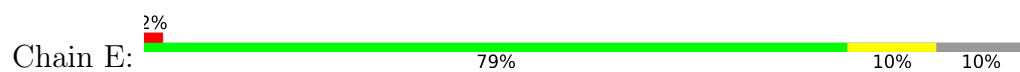
- Molecule 3: Fv 83-7 Light chain



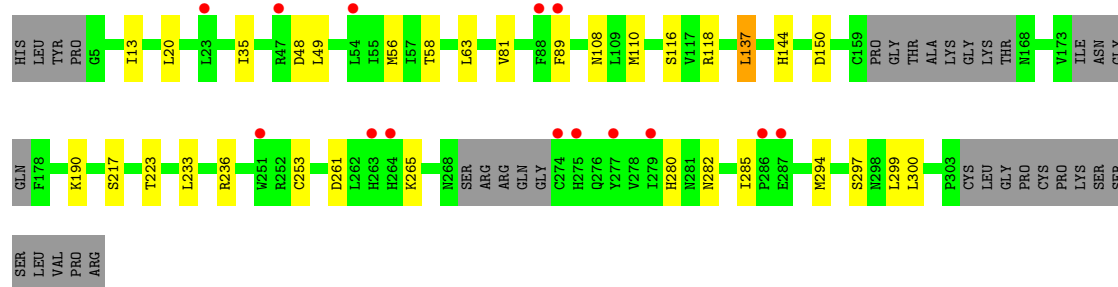
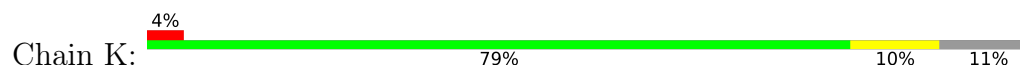
- Molecule 3: Fv 83-7 Light chain



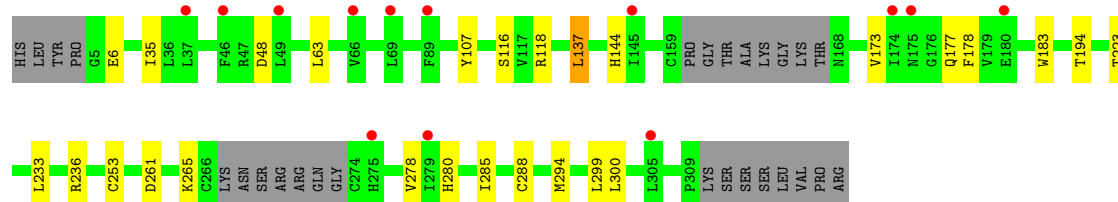
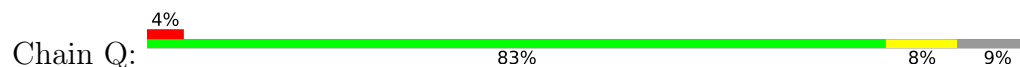
- Molecule 4: Insulin receptor subunit alpha



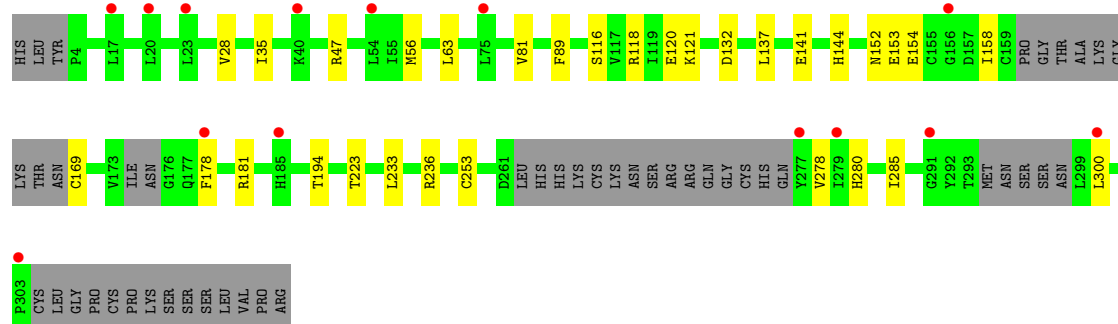
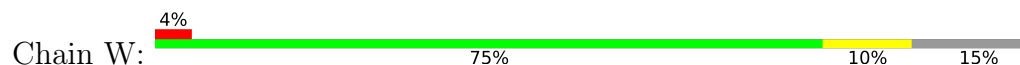
• Molecule 4: Insulin receptor subunit alpha




• Molecule 4: Insulin receptor subunit alpha



• Molecule 4: Insulin receptor subunit alpha




• Molecule 5: Insulin receptor isoform A alphaCT peptide

Chain F:  88% 6% 6%




- Molecule 5: Insulin receptor isoform A alphaCT peptide

Chain L:  81% 12% 6%




- Molecule 5: Insulin receptor isoform A alphaCT peptide

Chain R:  12% 88% 6% 6%



- Molecule 5: Insulin receptor isoform A alphaCT peptide

Chain X:  81% 6% 12%



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

Chain 1:  25% 75%

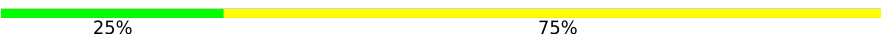


- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:  50% 50%



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

Chain S:  25% 75%



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

Chain Y:  25% 75%

  
MAG1  
MAG2  
BMA3  
FUC4

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

Chain Z:  50% 50%


  
MAG1  
MAG2  
BMA3  
FUC4

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

Chain A:  67% 33%

  
MAG1  
MAG2  
FUC3

- Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:  50% 50%

  
MAG1  
MAG2

- Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 2:  50% 50%

  
MAG1  
MAG2

- Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 3:  50% 50%

  
MAG1  
MAG2

- Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 4:  100%

MAG1  
MAG2



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	97.67Å 128.43Å 148.79Å 90.00° 90.18° 90.00°	Depositor
Resolution (Å)	45.65 – 2.60 45.65 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.2 (45.65-2.60) 98.2 (45.65-2.60)	Depositor EDS
$R_{merge}$	0.22	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.06 (at 2.61Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, $R_{free}$	0.189 , 0.221 0.210 , 0.227	Depositor DCC
$R_{free}$ test set	5626 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	56.1	Xtriage
Anisotropy	0.551	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 55.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.088 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	19073	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.45% 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: SO4, FUC, NAG, BMA, GOL

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	B	0.53	0/398	0.69	0/532
1	H	0.48	0/379	0.64	0/507
1	N	0.44	0/379	0.63	0/507
1	T	0.45	0/381	0.60	0/510
2	C	0.61	0/961	0.78	0/1307
2	I	0.65	0/961	0.80	0/1307
2	O	0.62	0/972	0.78	0/1321
2	U	0.55	0/932	0.75	0/1266
3	D	0.55	0/910	0.74	0/1228
3	J	0.55	0/910	0.74	0/1228
3	P	0.51	0/909	0.70	0/1227
3	V	0.48	0/904	0.68	0/1220
4	E	0.55	0/2355	0.75	0/3191
4	K	0.50	0/2316	0.72	0/3136
4	Q	0.48	0/2369	0.70	0/3212
4	W	0.49	0/2204	0.71	0/2985
5	F	0.55	0/135	0.68	0/185
5	L	0.54	0/135	0.71	0/185
5	R	0.48	0/135	0.62	0/185
5	X	0.50	0/127	0.60	0/173
All	All	0.53	0/18772	0.72	0/25412

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	B	391	0	366	2	0
1	H	373	0	345	2	0
1	N	373	0	345	2	0
1	T	375	0	352	1	0
2	C	938	0	916	4	0
2	I	938	0	916	10	0
2	O	949	0	929	8	0
2	U	910	0	884	7	0
3	D	891	0	877	7	0
3	J	891	0	877	5	0
3	P	890	0	877	3	0
3	V	885	0	872	3	0
4	E	2297	0	2191	16	0
4	K	2264	0	2157	18	0
4	Q	2314	0	2203	12	0
4	W	2155	0	2058	12	0
5	F	130	0	121	1	0
5	L	130	0	121	3	0
5	R	130	0	121	1	0
5	X	123	0	114	1	0
6	1	49	0	43	0	0
6	M	49	0	43	0	0
6	S	49	0	43	0	0
6	Y	49	0	43	0	0
6	Z	49	0	43	0	0
7	A	38	0	34	0	0
8	2	28	0	25	0	0
8	3	28	0	25	0	0
8	4	28	0	25	0	0
8	G	28	0	25	2	0
9	C	5	0	0	0	0
9	I	5	0	0	0	0
9	O	5	0	0	0	0
9	U	5	0	0	0	0
10	D	6	0	8	0	0
11	E	14	0	13	0	0
11	K	42	0	39	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	Q	42	0	39	0	0
11	W	42	0	39	0	0
12	B	1	0	0	0	0
12	C	26	0	0	0	0
12	D	14	0	0	0	0
12	E	17	0	0	0	0
12	F	1	0	0	0	0
12	H	1	0	0	0	0
12	I	32	0	0	0	0
12	J	11	0	0	0	0
12	K	6	0	0	0	0
12	O	23	0	0	0	0
12	P	8	0	0	0	0
12	Q	6	0	0	0	0
12	T	1	0	0	0	0
12	U	7	0	0	0	0
12	V	2	0	0	0	0
12	W	9	0	0	0	0
All	All	19073	0	18129	109	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 3.

All (109) 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:E:190:LYS:HD3	8:G:1:NAG:H81	1.56	0.87
4:K:89:PHE:HD2	5:L:705:PHE:HD1	1.28	0.80
2:C:90:THR:HG23	2:C:115:THR:HA	1.65	0.77
2:O:90:THR:HG23	2:O:115:THR:HA	1.67	0.75
2:I:90:THR:HG23	2:I:115:THR:HA	1.70	0.74
2:O:18:LEU:HB2	2:O:85:LEU:HD11	1.76	0.67
2:U:90:THR:HG23	2:U:115:THR:HA	1.77	0.67
4:Q:173:VAL:HG13	4:Q:177:GLN:H	1.60	0.67
4:E:223:THR:HG22	4:E:236:ARG:HG3	1.79	0.63
2:I:120:LEU:HB3	2:I:122:PRO:HD2	1.84	0.60
4:K:89:PHE:CD2	5:L:705:PHE:HD1	2.17	0.59
4:E:233:LEU:HD13	4:E:253:CYS:HB2	1.84	0.58
4:W:132:ASP:HB2	4:W:181:ARG:HD2	1.87	0.57
2:I:97:ARG:O	2:I:105:MET:HA	2.06	0.55
3:J:100:TYR:O	3:J:101:ARG:HD3	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:20:LEU:HD23	4:K:49:LEU:HD21	1.88	0.55
4:W:28:VAL:HG22	4:W:56:MET:HB3	1.88	0.55
4:W:118:ARG:HD2	4:W:144:HIS:HB3	1.89	0.54
4:K:118:ARG:HD2	4:K:144:HIS:HB3	1.90	0.54
4:Q:233:LEU:HD13	4:Q:253:CYS:HB2	1.90	0.53
2:I:51:ILE:HD13	2:I:71:LYS:HG2	1.90	0.53
2:C:11:LEU:HD13	2:C:120:LEU:HD22	1.91	0.53
4:E:118:ARG:HD2	4:E:144:HIS:HB3	1.91	0.52
3:D:8:PRO:HG2	3:D:11:LEU:HG	1.91	0.52
4:W:233:LEU:HD13	4:W:253:CYS:HB2	1.91	0.52
4:K:223:THR:HG22	4:K:236:ARG:HG3	1.91	0.52
3:D:100:TYR:O	3:D:101:ARG:HD3	2.09	0.52
4:W:223:THR:HG22	4:W:236:ARG:HG3	1.90	0.52
1:B:36:ARG:HD3	1:B:40:GLU:HG2	1.90	0.52
4:K:233:LEU:HD13	4:K:253:CYS:HB2	1.91	0.52
4:W:89:PHE:HB2	5:X:708:TYR:CE2	2.45	0.52
2:U:97:ARG:O	2:U:105:MET:HA	2.09	0.51
4:K:56:MET:HG3	4:K:81:VAL:HB	1.91	0.51
2:O:97:ARG:O	2:O:105:MET:HA	2.12	0.50
2:C:97:ARG:O	2:C:105:MET:HA	2.11	0.49
4:E:14:ARG:HB3	4:E:36:LEU:HD12	1.95	0.49
4:E:35:ILE:HB	4:E:63:LEU:HD23	1.94	0.49
4:K:190:LYS:HD3	11:K:403:NAG:H81	1.93	0.49
1:B:39:VAL:O	1:B:43:CYS:HB3	2.13	0.49
2:I:121:VAL:N	2:I:122:PRO:HD2	2.28	0.48
3:D:13:VAL:HG11	3:D:19:VAL:HG22	1.96	0.48
4:Q:278:VAL:HG12	4:Q:294:MET:HG3	1.96	0.48
4:E:278:VAL:HG12	4:E:294:MET:HG3	1.94	0.48
4:Q:35:ILE:HB	4:Q:63:LEU:HD23	1.96	0.48
4:E:278:VAL:HG23	4:E:285:ILE:HG13	1.96	0.47
4:Q:261:ASP:O	4:Q:265:LYS:HB2	2.14	0.47
4:K:261:ASP:O	4:K:265:LYS:HB2	2.14	0.47
3:V:12:VAL:HG22	3:V:110:GLU:HB2	1.97	0.47
4:Q:118:ARG:HD2	4:Q:144:HIS:HB3	1.97	0.47
4:K:280:HIS:HB3	4:K:285:ILE:HD11	1.97	0.47
2:U:18:LEU:CB	2:U:85:LEU:HD11	2.45	0.47
3:D:12:VAL:HG22	3:D:110:GLU:HB2	1.95	0.46
4:W:35:ILE:HB	4:W:63:LEU:HD23	1.98	0.46
4:W:120:GLU:HG2	4:W:121:LYS:HG3	1.97	0.46
4:K:294:MET:HE3	4:K:299:LEU:HA	1.98	0.46
3:P:17:GLU:O	3:P:84:VAL:HG23	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:294:MET:SD	4:Q:299:LEU:HA	2.56	0.46
4:K:217:SER:HA	11:K:403:NAG:H62	1.97	0.45
4:K:56:MET:CE	4:K:58:THR:HG22	2.46	0.45
4:K:13:ILE:HD13	4:K:20:LEU:HD12	1.97	0.45
3:J:12:VAL:HG22	3:J:110:GLU:HB2	1.98	0.45
4:K:35:ILE:HB	4:K:63:LEU:HD23	1.99	0.45
3:D:12:VAL:HG12	3:D:112:LYS:HG3	2.00	0.45
2:U:18:LEU:HB2	2:U:85:LEU:HD11	1.98	0.44
3:V:12:VAL:HG12	3:V:112:LYS:HG3	1.98	0.44
2:O:108:TRP:CE3	3:P:50:PRO:HD2	2.53	0.44
3:J:12:VAL:HG12	3:J:112:LYS:HG3	1.99	0.44
2:I:35:ASN:O	2:I:95:CYS:HA	2.17	0.44
1:H:41:GLN:HE21	1:H:51:GLN:HE21	1.65	0.44
3:D:8:PRO:CG	3:D:11:LEU:HG	2.47	0.44
4:W:280:HIS:HB3	4:W:285:ILE:HD11	2.00	0.44
2:C:18:LEU:HB2	2:C:85:LEU:HD11	1.99	0.44
4:E:89:PHE:CD2	5:F:705:PHE:HD1	2.36	0.44
2:I:120:LEU:C	2:I:122:PRO:HD2	2.39	0.43
4:W:56:MET:HG3	4:W:81:VAL:HB	2.00	0.43
4:Q:116:SER:HA	4:Q:137:LEU:HD21	2.01	0.43
4:W:116:SER:HA	4:W:137:LEU:HD21	2.01	0.43
4:E:190:LYS:CD	8:G:1:NAG:H81	2.40	0.42
2:I:51:ILE:CD1	2:I:71:LYS:HG2	2.49	0.42
2:O:99:PRO:C	4:Q:236:ARG:HH22	2.22	0.42
4:Q:107:TYR:HA	4:Q:183:TRP:CD1	2.55	0.42
4:E:36:LEU:HD13	4:E:37:LEU:HD12	2.00	0.42
4:E:58:THR:HA	4:E:83:ARG:HB2	2.02	0.42
3:P:12:VAL:HG12	3:P:112:LYS:HG3	2.01	0.42
1:N:39:VAL:O	1:N:43:CYS:HB3	2.20	0.42
4:Q:223:THR:HG22	4:Q:236:ARG:HG3	2.02	0.42
1:H:8:GLY:O	5:L:710:HIS:HE1	2.03	0.42
1:N:25:PHE:CD1	5:R:717:ARG:HG2	2.55	0.42
4:Q:280:HIS:HB3	4:Q:285:ILE:HD11	2.02	0.41
4:W:278:VAL:HG23	4:W:285:ILE:HG13	2.01	0.41
3:J:53:LEU:HA	3:J:64:VAL:HG21	2.03	0.41
2:O:51:ILE:HD13	2:O:71:LYS:HG2	2.02	0.41
2:I:117:SER:C	2:I:119:SER:HA	2.41	0.41
4:K:108:ASN:O	4:K:110:MET:HG2	2.21	0.41
1:T:14:ALA:O	1:T:18:VAL:HG23	2.20	0.41
4:E:107:TYR:HA	4:E:183:TRP:CD1	2.56	0.41
4:E:120:GLU:HA	4:E:146:VAL:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:54:ASP:OD1	2:O:56:ASN:HB2	2.21	0.41
3:V:11:LEU:HD12	3:V:13:VAL:HG13	2.02	0.41
2:U:35:ASN:O	2:U:95:CYS:HA	2.21	0.41
2:U:51:ILE:HD13	2:U:71:LYS:HG2	2.02	0.41
3:D:13:VAL:HG21	3:D:19:VAL:HG21	2.03	0.40
2:O:18:LEU:CB	2:O:85:LEU:HD11	2.47	0.40
4:E:14:ARG:HB3	4:E:36:LEU:CD1	2.52	0.40
2:I:54:ASP:OD1	2:I:56:ASN:HB2	2.21	0.40
4:K:116:SER:HA	4:K:137:LEU:HD21	2.04	0.40
4:E:13:ILE:HD13	4:E:20:LEU:HD12	2.04	0.40
2:U:67:LEU:HD22	2:U:80:LEU:HD11	2.02	0.40
3:J:33:SER:OG	4:K:282:ASN:HB2	2.22	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	B	45/57 (79%)	44 (98%)	1 (2%)	0	100	100
1	H	43/57 (75%)	42 (98%)	1 (2%)	0	100	100
1	N	43/57 (75%)	42 (98%)	1 (2%)	0	100	100
1	T	43/57 (75%)	41 (95%)	2 (5%)	0	100	100
2	C	121/126 (96%)	116 (96%)	5 (4%)	0	100	100
2	I	121/126 (96%)	111 (92%)	9 (7%)	1 (1%)	19	39
2	O	122/126 (97%)	115 (94%)	7 (6%)	0	100	100
2	U	117/126 (93%)	111 (95%)	6 (5%)	0	100	100
3	D	113/121 (93%)	106 (94%)	7 (6%)	0	100	100
3	J	113/121 (93%)	108 (96%)	5 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	P	113/121 (93%)	106 (94%)	7 (6%)	0	100	100
3	V	112/121 (93%)	106 (95%)	6 (5%)	0	100	100
4	E	279/317 (88%)	265 (95%)	13 (5%)	1 (0%)	34	57
4	K	274/317 (86%)	259 (94%)	14 (5%)	1 (0%)	34	57
4	Q	284/317 (90%)	269 (95%)	15 (5%)	0	100	100
4	W	259/317 (82%)	245 (95%)	13 (5%)	1 (0%)	34	57
5	F	13/16 (81%)	13 (100%)	0	0	100	100
5	L	13/16 (81%)	13 (100%)	0	0	100	100
5	R	13/16 (81%)	13 (100%)	0	0	100	100
5	X	12/16 (75%)	12 (100%)	0	0	100	100
All	All	2253/2548 (88%)	2137 (95%)	112 (5%)	4 (0%)	47	71

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	E	297	SER
2	I	64	LYS
4	K	297	SER
4	W	154	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	B	44/51 (86%)	41 (93%)	3 (7%)	16	32
1	H	42/51 (82%)	39 (93%)	3 (7%)	14	29
1	N	42/51 (82%)	40 (95%)	2 (5%)	25	49
1	T	42/51 (82%)	38 (90%)	4 (10%)	8	16
2	C	106/107 (99%)	105 (99%)	1 (1%)	78	91
2	I	106/107 (99%)	102 (96%)	4 (4%)	33	59

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	O	107/107 (100%)	105 (98%)	2 (2%)	57	79
2	U	102/107 (95%)	101 (99%)	1 (1%)	76	90
3	D	101/106 (95%)	97 (96%)	4 (4%)	31	57
3	J	101/106 (95%)	97 (96%)	4 (4%)	31	57
3	P	100/106 (94%)	97 (97%)	3 (3%)	41	67
3	V	100/106 (94%)	97 (97%)	3 (3%)	41	67
4	E	269/293 (92%)	259 (96%)	10 (4%)	34	60
4	K	264/293 (90%)	260 (98%)	4 (2%)	65	83
4	Q	270/293 (92%)	263 (97%)	7 (3%)	46	72
4	W	250/293 (85%)	241 (96%)	9 (4%)	35	61
5	F	15/16 (94%)	15 (100%)	0	100	100
5	L	15/16 (94%)	15 (100%)	0	100	100
5	R	15/16 (94%)	15 (100%)	0	100	100
5	X	14/16 (88%)	14 (100%)	0	100	100
All	All	2105/2292 (92%)	2041 (97%)	64 (3%)	41	67

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	9	SER
1	B	35	ARG
1	B	50	GLU
2	C	118	SER
3	D	7	SER
3	D	14	SER
3	D	49	SER
3	D	84	VAL
4	E	36	LEU
4	E	55	ILE
4	E	137	LEU
4	E	152	ASN
4	E	154	GLU
4	E	169	CYS
4	E	170	PRO
4	E	184	THR
4	E	194	THR
4	E	300	LEU

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Mol	Chain	Res	Type
1	H	36	ARG
1	H	45	SER
1	H	50	GLU
2	I	76	SER
2	I	85	LEU
2	I	86	GLN
2	I	119	SER
3	J	0	SER
3	J	7	SER
3	J	14	SER
3	J	62	SER
4	K	48	ASP
4	K	137	LEU
4	K	150	ASP
4	K	300	LEU
1	N	45	SER
1	N	50	GLU
2	O	88	ASP
2	O	118	SER
3	P	7	SER
3	P	14	SER
3	P	31	TYR
4	Q	6	GLU
4	Q	48	ASP
4	Q	137	LEU
4	Q	178	PHE
4	Q	194	THR
4	Q	288	CYS
4	Q	300	LEU
1	T	36	ARG
1	T	44	HIS
1	T	45	SER
1	T	50	GLU
2	U	11	LEU
3	V	7	SER
3	V	14	SER
3	V	62	SER
4	W	47	ARG
4	W	141	GLU
4	W	152	ASN
4	W	153	GLU
4	W	158	ILE

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Mol	Chain	Res	Type
4	W	169	CYS
4	W	178	PHE
4	W	194	THR
4	W	300	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
4	E	34	GLN
4	E	249	GLN
4	E	281	ASN
1	H	41	GLN
2	I	16	GLN
4	K	123	ASN
4	K	281	ASN
5	L	710	HIS
1	N	41	GLN
2	O	83	ASN
4	Q	34	GLN
4	Q	123	ASN
4	Q	175	ASN
4	Q	281	ASN
4	Q	282	ASN
1	T	41	GLN
4	W	32	HIS
4	W	34	GLN
4	W	123	ASN
4	W	152	ASN
4	W	230	ASN
5	X	710	HIS

### 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 ⓘ

31 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
6	NAG	1	1	6,4	14,14,15	0.38	0	17,19,21	0.96	0
6	NAG	1	2	6	14,14,15	0.45	0	17,19,21	1.48	5 (29%)
6	BMA	1	3	6	11,11,12	0.41	0	15,15,17	1.06	1 (6%)
6	FUC	1	4	6	10,10,11	0.45	0	14,14,16	0.97	1 (7%)
8	NAG	2	1	8,4	14,14,15	0.31	0	17,19,21	1.16	1 (5%)
8	NAG	2	2	8	14,14,15	0.31	0	17,19,21	0.52	0
8	NAG	3	1	8,4	14,14,15	0.37	0	17,19,21	1.21	3 (17%)
8	NAG	3	2	8	14,14,15	0.33	0	17,19,21	0.61	0
8	NAG	4	1	8,4	14,14,15	0.35	0	17,19,21	0.70	1 (5%)
8	NAG	4	2	8	14,14,15	0.34	0	17,19,21	0.96	2 (11%)
7	NAG	A	1	7,4	14,14,15	0.42	0	17,19,21	0.83	0
7	NAG	A	2	7	14,14,15	0.33	0	17,19,21	0.42	0
7	FUC	A	3	7	10,10,11	0.56	0	14,14,16	1.19	1 (7%)
8	NAG	G	1	8,4	14,14,15	0.31	0	17,19,21	1.76	4 (23%)
8	NAG	G	2	8	14,14,15	0.36	0	17,19,21	0.95	1 (5%)
6	NAG	M	1	6,4	14,14,15	0.37	0	17,19,21	0.83	1 (5%)
6	NAG	M	2	6	14,14,15	0.33	0	17,19,21	0.49	0
6	BMA	M	3	6	11,11,12	0.45	0	15,15,17	0.87	1 (6%)
6	FUC	M	4	6	10,10,11	0.39	0	14,14,16	0.64	0
6	NAG	S	1	6,4	14,14,15	0.29	0	17,19,21	0.75	0
6	NAG	S	2	6	14,14,15	0.35	0	17,19,21	0.75	1 (5%)
6	BMA	S	3	6	11,11,12	0.51	0	15,15,17	1.16	2 (13%)
6	FUC	S	4	6	10,10,11	0.50	0	14,14,16	0.94	1 (7%)
6	NAG	Y	1	6,4	14,14,15	0.31	0	17,19,21	0.54	0
6	NAG	Y	2	6	14,14,15	0.32	0	17,19,21	0.92	1 (5%)
6	BMA	Y	3	6	11,11,12	0.41	0	15,15,17	0.83	1 (6%)
6	FUC	Y	4	6	10,10,11	0.46	0	14,14,16	1.13	1 (7%)
6	NAG	Z	1	6,4	14,14,15	0.36	0	17,19,21	0.70	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	NAG	Z	2	6	14,14,15	0.36	0	17,19,21	0.90	1 (5%)
6	BMA	Z	3	6	11,11,12	0.54	0	15,15,17	0.87	1 (6%)
6	FUC	Z	4	6	10,10,11	0.48	0	14,14,16	0.63	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
6	NAG	1	1	6,4	-	2/6/23/26	0/1/1/1
6	NAG	1	2	6	-	0/6/23/26	0/1/1/1
6	BMA	1	3	6	-	0/2/19/22	0/1/1/1
6	FUC	1	4	6	-	-	0/1/1/1
8	NAG	2	1	8,4	-	0/6/23/26	0/1/1/1
8	NAG	2	2	8	-	1/6/23/26	0/1/1/1
8	NAG	3	1	8,4	-	1/6/23/26	0/1/1/1
8	NAG	3	2	8	-	0/6/23/26	0/1/1/1
8	NAG	4	1	8,4	-	0/6/23/26	0/1/1/1
8	NAG	4	2	8	-	2/6/23/26	0/1/1/1
7	NAG	A	1	7,4	-	1/6/23/26	0/1/1/1
7	NAG	A	2	7	-	0/6/23/26	0/1/1/1
7	FUC	A	3	7	-	-	0/1/1/1
8	NAG	G	1	8,4	-	3/6/23/26	0/1/1/1
8	NAG	G	2	8	-	0/6/23/26	0/1/1/1
6	NAG	M	1	6,4	-	0/6/23/26	0/1/1/1
6	NAG	M	2	6	-	0/6/23/26	0/1/1/1
6	BMA	M	3	6	-	0/2/19/22	0/1/1/1
6	FUC	M	4	6	-	-	0/1/1/1
6	NAG	S	1	6,4	-	0/6/23/26	0/1/1/1
6	NAG	S	2	6	-	0/6/23/26	0/1/1/1
6	BMA	S	3	6	-	0/2/19/22	0/1/1/1
6	FUC	S	4	6	-	-	0/1/1/1
6	NAG	Y	1	6,4	-	0/6/23/26	0/1/1/1
6	NAG	Y	2	6	-	1/6/23/26	0/1/1/1
6	BMA	Y	3	6	-	2/2/19/22	0/1/1/1
6	FUC	Y	4	6	-	-	0/1/1/1
6	NAG	Z	1	6,4	-	0/6/23/26	0/1/1/1
6	NAG	Z	2	6	-	1/6/23/26	0/1/1/1
6	BMA	Z	3	6	-	0/2/19/22	0/1/1/1
6	FUC	Z	4	6	-	-	0/1/1/1

There are no bond length outliers.

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	G	1	NAG	O5-C1-C2	-5.51	102.59	111.29
8	2	1	NAG	C1-O5-C5	3.96	117.56	112.19
6	S	3	BMA	C1-O5-C5	3.68	117.18	112.19
6	1	2	NAG	C1-O5-C5	3.33	116.70	112.19
6	Y	4	FUC	C1-C2-C3	3.20	113.60	109.67
7	A	3	FUC	C1-C2-C3	3.10	113.48	109.67
8	3	1	NAG	C1-O5-C5	3.03	116.29	112.19
8	G	1	NAG	C1-C2-N2	2.98	115.57	110.49
8	G	2	NAG	C1-O5-C5	2.92	116.14	112.19
8	3	1	NAG	O5-C1-C2	-2.90	106.71	111.29
6	Z	2	NAG	O5-C1-C2	-2.72	106.99	111.29
6	Y	3	BMA	C1-O5-C5	2.63	115.76	112.19
8	G	1	NAG	C2-N2-C7	2.57	126.57	122.90
6	S	4	FUC	C1-C2-C3	2.52	112.77	109.67
6	1	2	NAG	C1-C2-N2	2.45	114.67	110.49
6	1	2	NAG	O4-C4-C5	2.43	115.33	109.30
6	M	3	BMA	C1-O5-C5	2.43	115.48	112.19
6	Y	2	NAG	O5-C1-C2	-2.37	107.54	111.29
6	Z	3	BMA	C1-O5-C5	2.36	115.39	112.19
6	S	2	NAG	O5-C1-C2	-2.32	107.62	111.29
6	M	1	NAG	C1-O5-C5	-2.21	109.20	112.19
6	1	4	FUC	O2-C2-C1	2.21	113.67	109.15
6	1	2	NAG	O5-C1-C2	2.20	114.76	111.29
6	1	2	NAG	C4-C3-C2	-2.18	107.82	111.02
6	1	3	BMA	C1-O5-C5	-2.18	109.24	112.19
8	3	1	NAG	C1-C2-N2	2.14	114.15	110.49
8	4	1	NAG	C1-O5-C5	2.14	115.08	112.19
8	4	2	NAG	O5-C1-C2	-2.11	107.96	111.29
6	S	3	BMA	C1-C2-C3	2.07	112.21	109.67
8	G	1	NAG	C1-O5-C5	2.03	114.94	112.19
8	4	2	NAG	C1-C2-N2	2.00	113.91	110.49

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	Y	3	BMA	O5-C5-C6-O6
8	G	1	NAG	O5-C5-C6-O6
6	1	1	NAG	C4-C5-C6-O6
6	1	1	NAG	O5-C5-C6-O6

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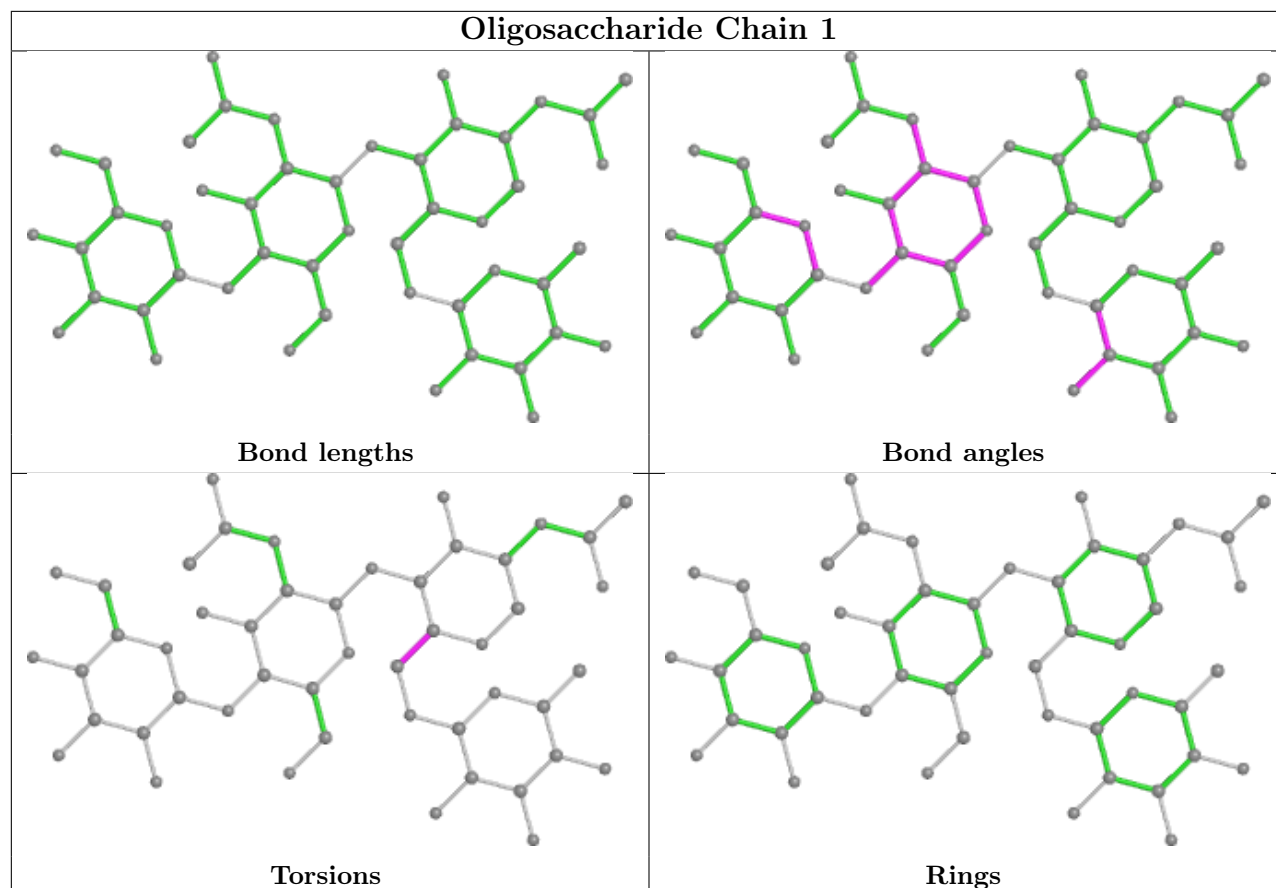
Mol	Chain	Res	Type	Atoms
8	2	2	NAG	O5-C5-C6-O6
6	Y	3	BMA	C4-C5-C6-O6
8	G	1	NAG	C4-C5-C6-O6
6	Y	2	NAG	O5-C5-C6-O6
8	G	1	NAG	C3-C2-N2-C7
8	4	2	NAG	C3-C2-N2-C7
8	4	2	NAG	C1-C2-N2-C7
8	3	1	NAG	C4-C5-C6-O6
6	Z	2	NAG	O5-C5-C6-O6
7	A	1	NAG	C4-C5-C6-O6

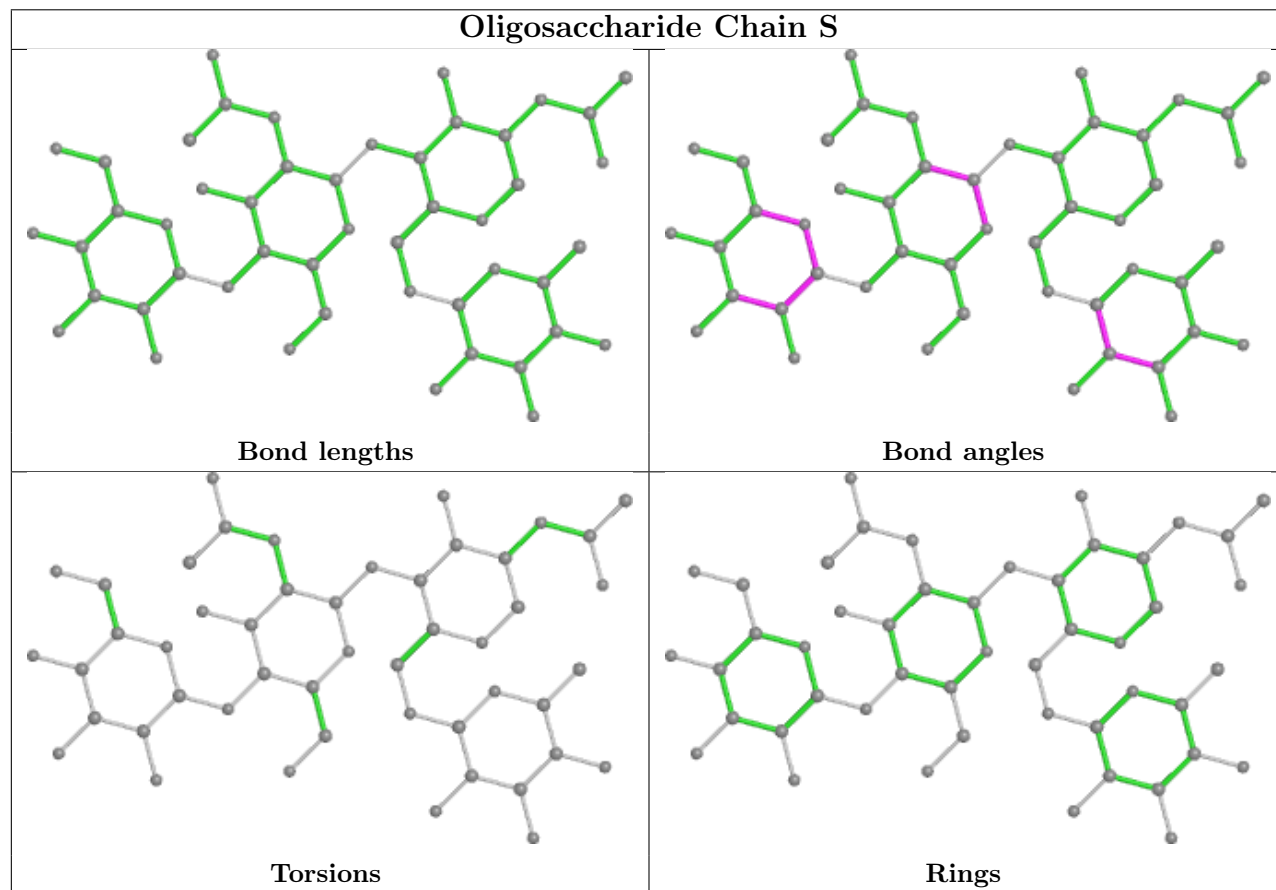
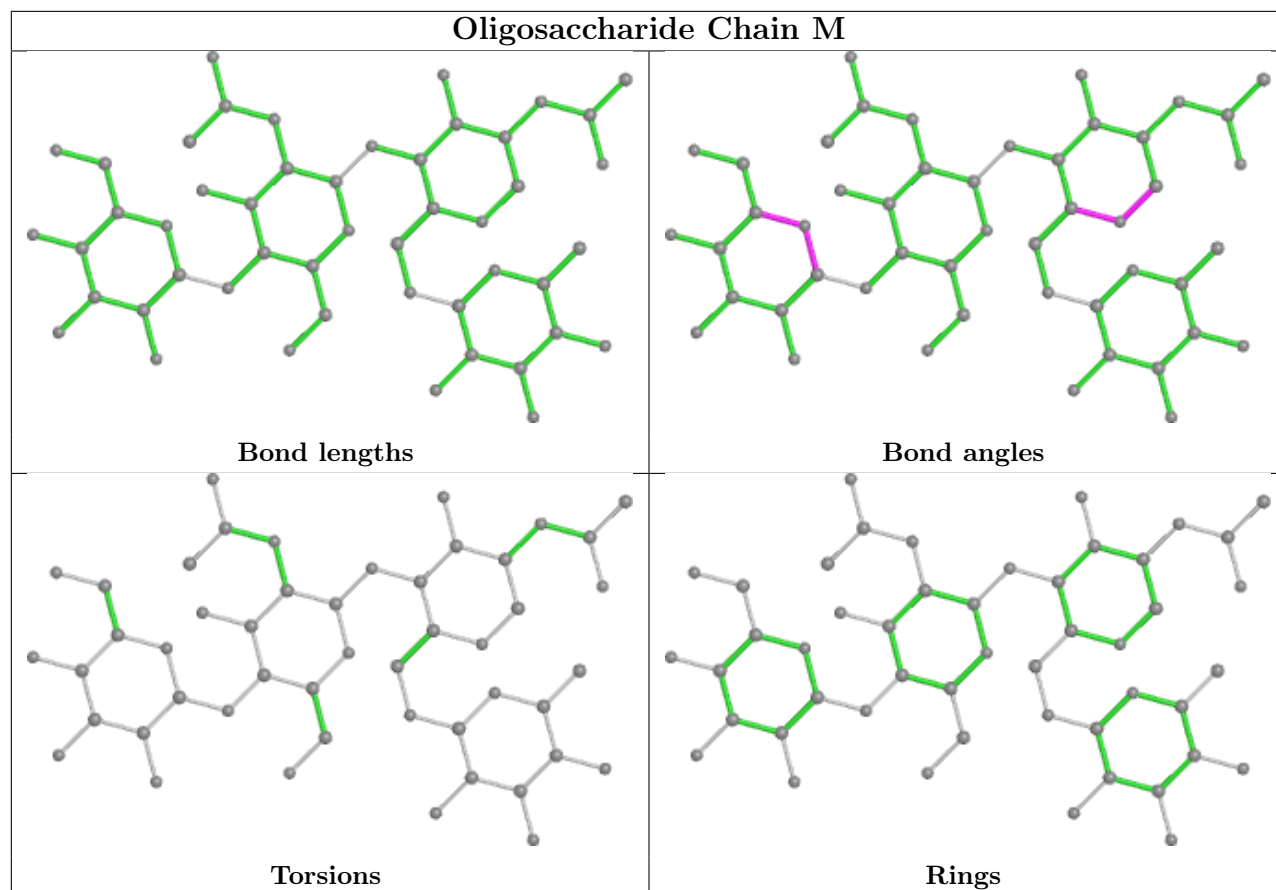
There are no ring outliers.

1 monomer is involved in 2 short contacts:

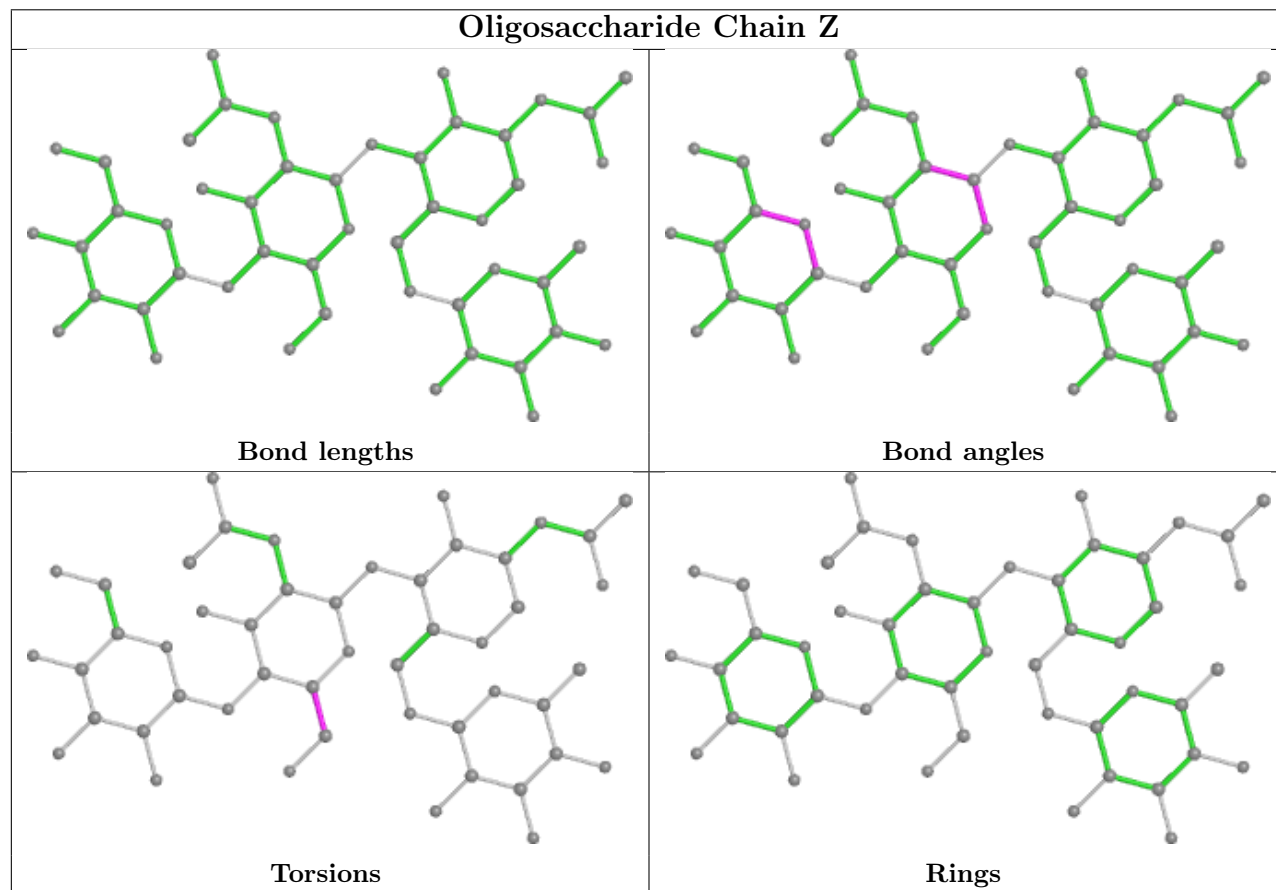
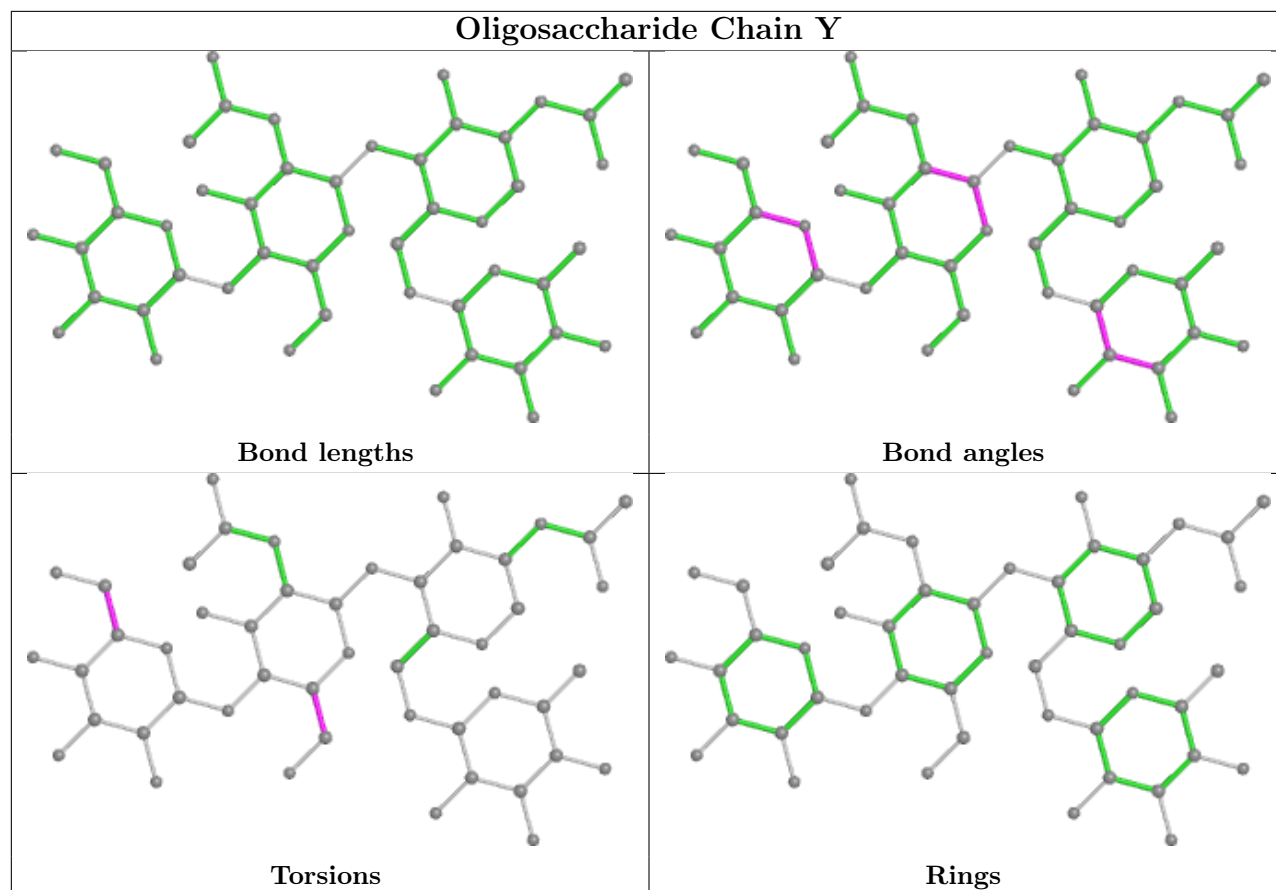
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	G	1	NAG	2	0

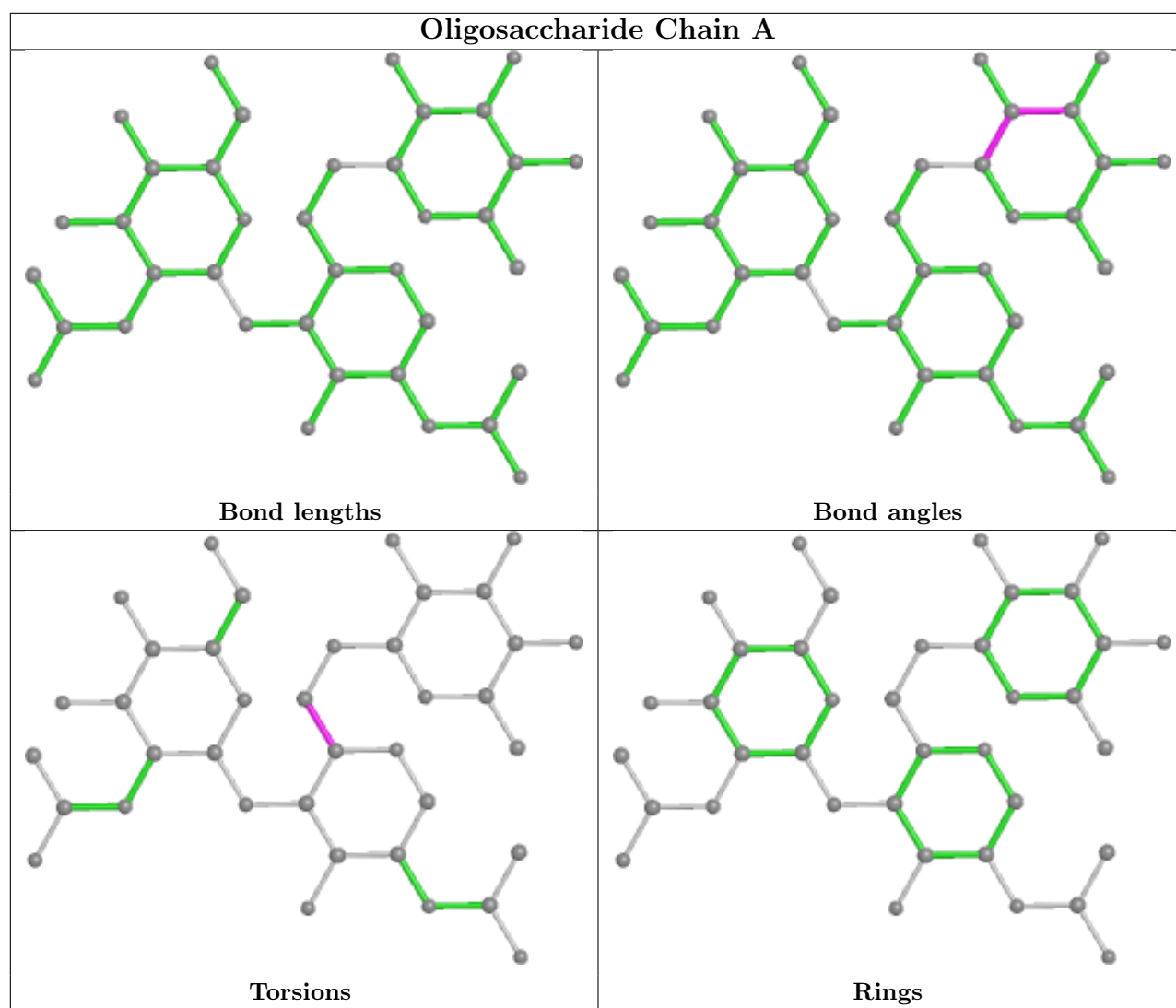
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

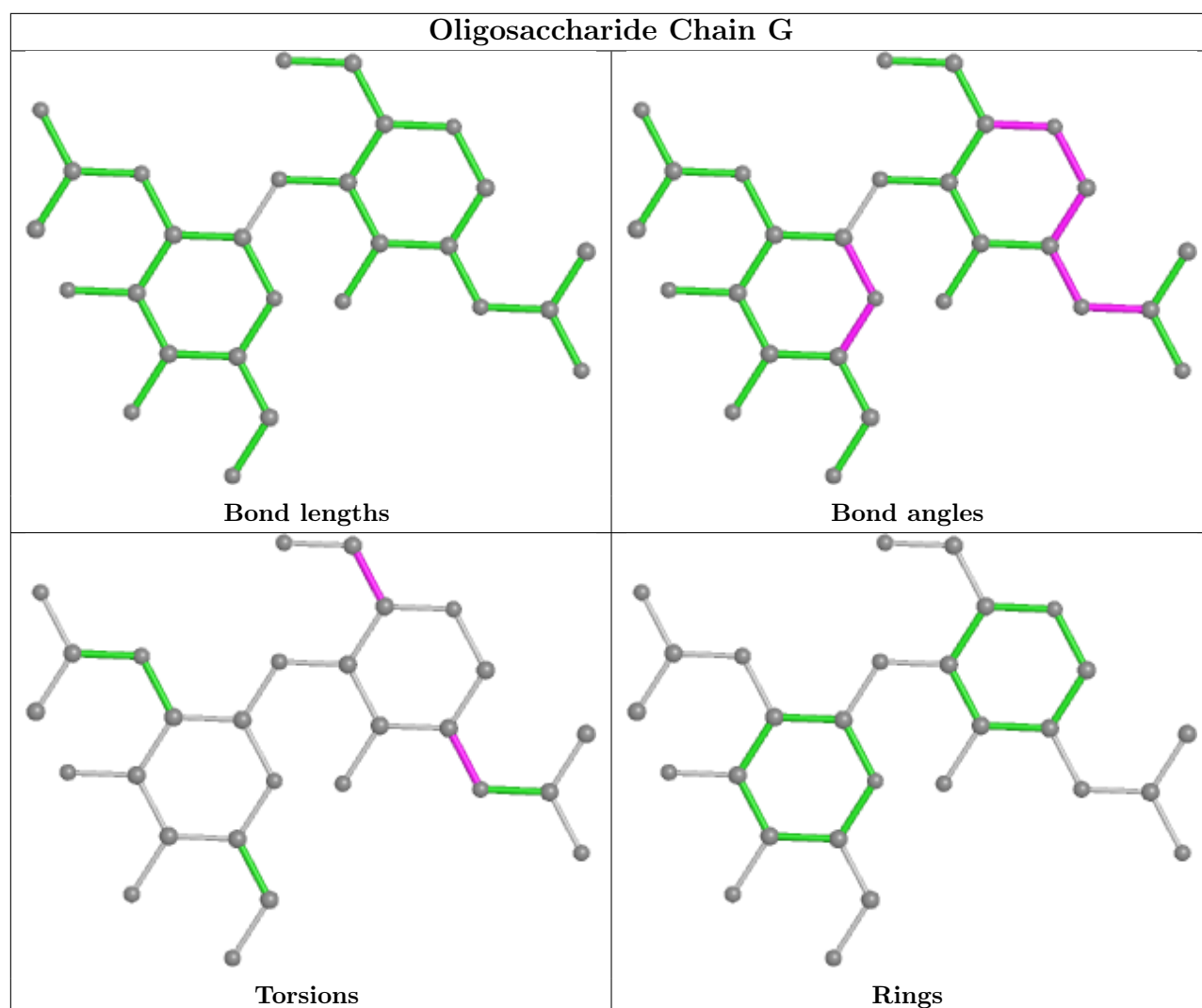


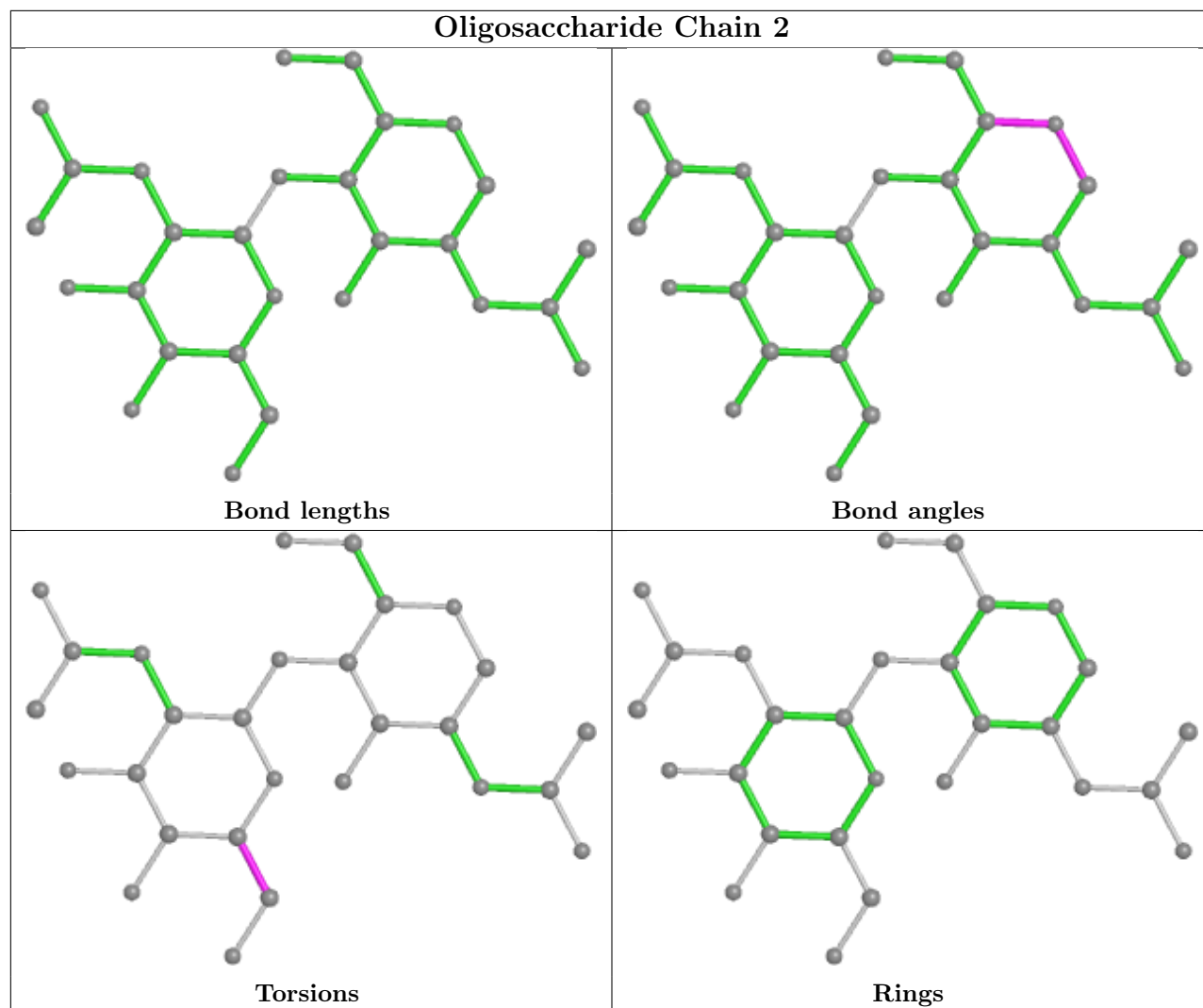


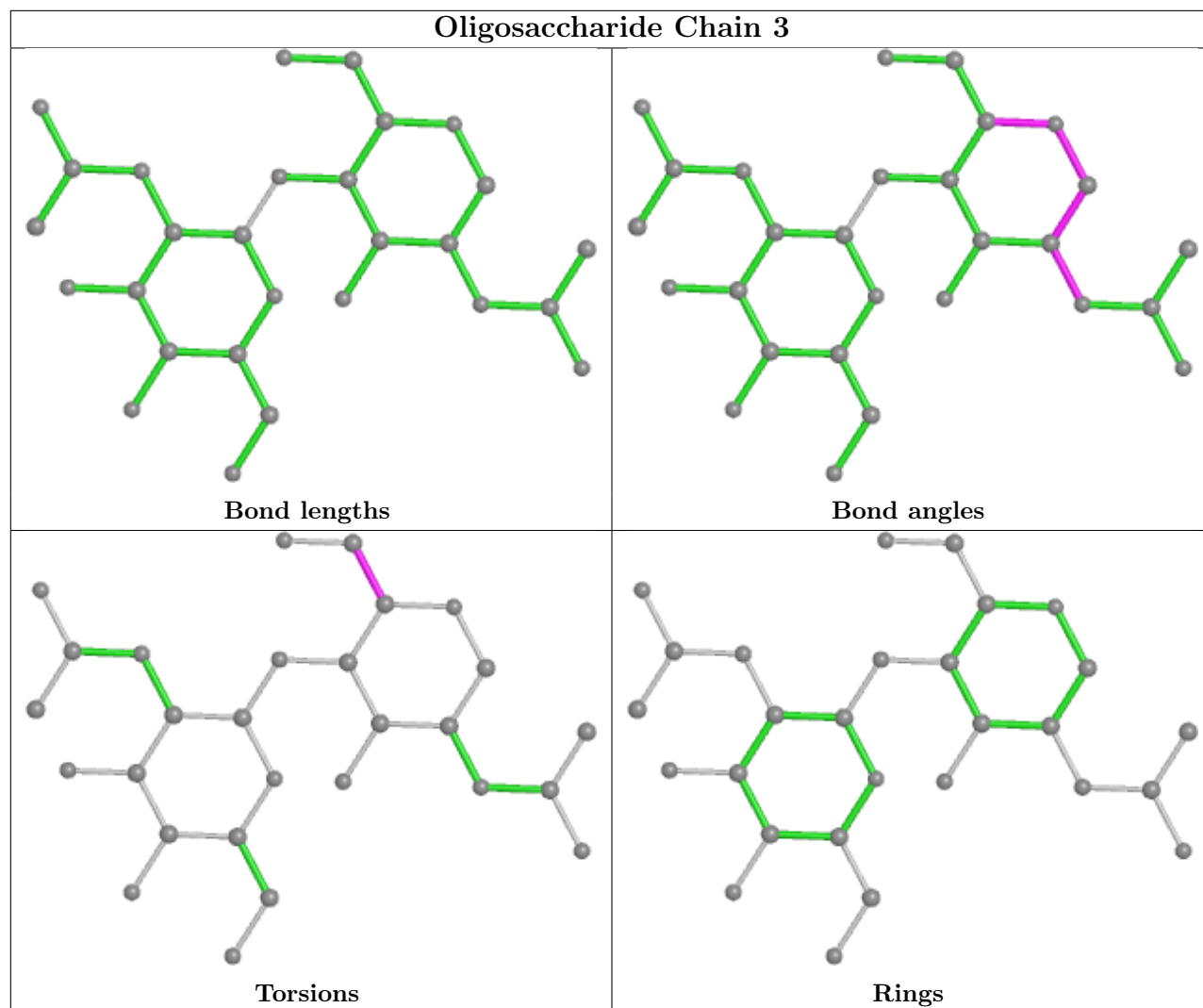


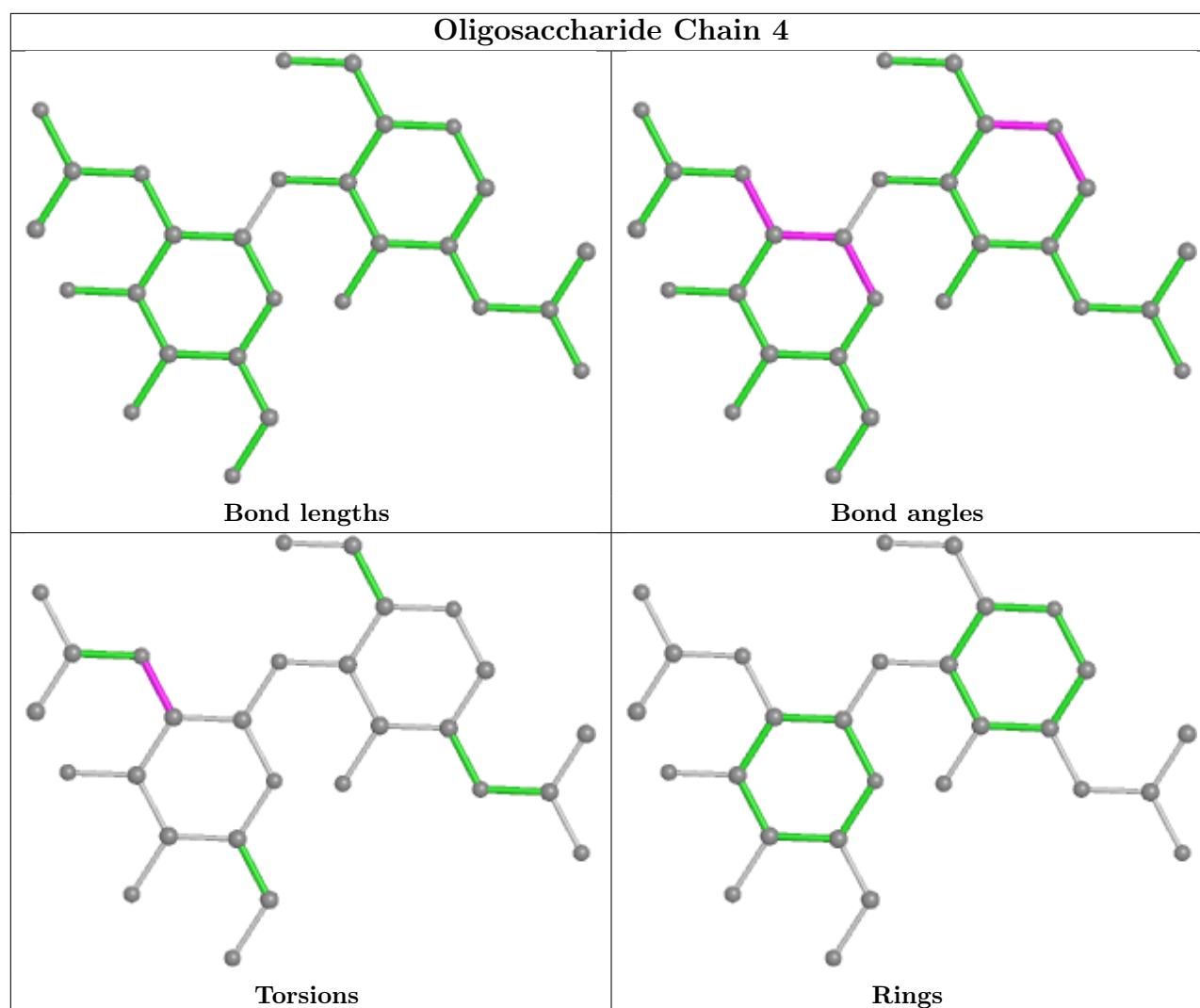












## 5.6 Ligand geometry [i](#)

15 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	$\# Z  > 2$
10	GOL	D	201	-	5,5,5	0.19	0	5,5,5	0.23	0
11	NAG	K	401	4	14,14,15	0.38	0	17,19,21	1.05	1 (5%)
9	SO4	C	201	-	4,4,4	0.13	0	6,6,6	0.39	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
11	NAG	Q	402	4	14,14,15	0.34	0	17,19,21	0.84	2 (11%)
11	NAG	W	403	4	14,14,15	0.31	0	17,19,21	1.02	2 (11%)
11	NAG	Q	403	4	14,14,15	0.40	0	17,19,21	0.76	1 (5%)
9	SO4	I	201	-	4,4,4	0.26	0	6,6,6	0.23	0
11	NAG	K	403	4	14,14,15	0.36	0	17,19,21	1.26	2 (11%)
9	SO4	U	201	-	4,4,4	0.20	0	6,6,6	0.15	0
11	NAG	Q	401	4	14,14,15	0.45	0	17,19,21	0.84	1 (5%)
11	NAG	W	402	4	14,14,15	0.33	0	17,19,21	1.02	1 (5%)
11	NAG	E	401	4	14,14,15	0.33	0	17,19,21	0.79	1 (5%)
11	NAG	K	402	4	14,14,15	0.36	0	17,19,21	1.49	2 (11%)
9	SO4	O	201	-	4,4,4	0.15	0	6,6,6	0.40	0
11	NAG	W	401	4	14,14,15	0.37	0	17,19,21	1.09	2 (11%)

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
10	GOL	D	201	-	-	3/4/4/4	-
11	NAG	K	401	4	-	0/6/23/26	0/1/1/1
11	NAG	Q	402	4	-	0/6/23/26	0/1/1/1
11	NAG	W	403	4	-	1/6/23/26	0/1/1/1
11	NAG	Q	403	4	-	2/6/23/26	0/1/1/1
11	NAG	K	403	4	-	4/6/23/26	0/1/1/1
11	NAG	Q	401	4	-	0/6/23/26	0/1/1/1
11	NAG	W	402	4	-	0/6/23/26	0/1/1/1
11	NAG	E	401	4	-	0/6/23/26	0/1/1/1
11	NAG	K	402	4	-	2/6/23/26	0/1/1/1
11	NAG	W	401	4	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	K	402	NAG	O5-C1-C2	-4.49	104.20	111.29
11	K	401	NAG	C1-O5-C5	4.08	117.72	112.19
11	K	403	NAG	C1-O5-C5	3.72	117.24	112.19
11	W	402	NAG	O5-C1-C2	-3.40	105.92	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	W	401	NAG	O5-C1-C2	-3.12	106.36	111.29
11	K	402	NAG	C1-O5-C5	2.94	116.17	112.19
11	W	403	NAG	O5-C1-C2	-2.74	106.96	111.29
11	W	403	NAG	C1-O5-C5	2.58	115.68	112.19
11	Q	401	NAG	C1-O5-C5	2.54	115.64	112.19
11	W	401	NAG	C1-C2-N2	2.54	114.82	110.49
11	Q	402	NAG	C1-O5-C5	2.49	115.56	112.19
11	E	401	NAG	C1-O5-C5	2.40	115.44	112.19
11	K	403	NAG	C1-C2-N2	2.25	114.33	110.49
11	Q	403	NAG	C3-C4-C5	2.05	113.90	110.24
11	Q	402	NAG	C1-C2-N2	2.00	113.91	110.49

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	Q	403	NAG	O5-C5-C6-O6
11	Q	403	NAG	C4-C5-C6-O6
10	D	201	GOL	O1-C1-C2-C3
10	D	201	GOL	O1-C1-C2-O2
11	K	402	NAG	C8-C7-N2-C2
11	K	402	NAG	O7-C7-N2-C2
11	K	403	NAG	C4-C5-C6-O6
11	K	403	NAG	C1-C2-N2-C7
11	K	403	NAG	O5-C5-C6-O6
11	W	403	NAG	O5-C5-C6-O6
11	K	403	NAG	C3-C2-N2-C7
10	D	201	GOL	C1-C2-C3-O3

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	K	403	NAG	2	0

## 5.7 Other polymers ⓘ

There are no such residues in this entry.



## 5.8 Polymer linkage issues ⓘ

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	B	49/57 (85%)	0.10	2 (4%) 37 30	69, 87, 114, 134	0
1	H	47/57 (82%)	0.12	0 100 100	75, 95, 119, 123	0
1	N	47/57 (82%)	0.36	3 (6%) 19 14	94, 115, 132, 146	0
1	T	47/57 (82%)	0.40	3 (6%) 19 14	97, 111, 140, 150	0
2	C	123/126 (97%)	-0.01	0 100 100	45, 57, 77, 97	0
2	I	123/126 (97%)	-0.02	1 (0%) 86 84	38, 57, 78, 109	0
2	O	124/126 (98%)	-0.07	0 100 100	42, 59, 81, 99	0
2	U	119/126 (94%)	-0.03	0 100 100	51, 73, 97, 111	0
3	D	115/121 (95%)	-0.20	0 100 100	48, 69, 94, 126	0
3	J	115/121 (95%)	-0.09	1 (0%) 84 82	45, 66, 93, 125	0
3	P	115/121 (95%)	0.09	2 (1%) 70 66	48, 83, 122, 146	0
3	V	114/121 (94%)	0.08	2 (1%) 68 64	52, 96, 118, 128	0
4	E	286/317 (90%)	0.10	5 (1%) 70 66	48, 71, 130, 148	0
4	K	282/317 (88%)	0.24	14 (4%) 28 23	55, 88, 153, 181	0
4	Q	290/317 (91%)	0.23	13 (4%) 33 26	57, 102, 148, 175	1 (0%)
4	W	269/317 (84%)	0.28	14 (5%) 27 21	72, 103, 163, 184	1 (0%)
5	F	15/16 (93%)	-0.04	0 100 100	64, 73, 97, 103	0
5	L	15/16 (93%)	0.18	0 100 100	75, 81, 110, 119	0
5	R	15/16 (93%)	0.62	2 (13%) 3 2	88, 97, 122, 124	0
5	X	14/16 (87%)	0.27	0 100 100	86, 96, 117, 139	0
All	All	2324/2548 (91%)	0.12	62 (2%) 54 48	38, 82, 137, 184	2 (0%)

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	W	156	GLY	5.3
4	W	277	TYR	5.2
4	W	20	LEU	5.0
1	T	1	PHE	4.8
1	T	52	LEU	4.7
4	W	303	PRO	4.4
1	B	34	PRO	4.3
4	Q	174	ILE	4.1
4	Q	275	HIS	3.9
4	Q	305	LEU	3.8
1	T	18	VAL	3.7
4	E	264	HIS	3.6
4	K	264	HIS	3.3
4	W	300	LEU	3.3
4	W	40	LYS	3.2
3	J	-1	GLY	3.2
4	E	305	LEU	3.1
4	K	286	PRO	3.1
2	I	120	LEU	3.0
4	Q	145	ILE	2.9
4	Q	279	ILE	2.8
4	W	23	LEU	2.8
4	Q	66	VAL	2.8
1	N	12	VAL	2.8
4	K	277	TYR	2.8
4	E	178	PHE	2.7
4	Q	175	ASN	2.7
4	K	47	ARG	2.7
4	W	17	LEU	2.7
4	E	308	CYS	2.7
4	K	275	HIS	2.7
5	R	705	PHE	2.5
1	N	49	LEU	2.5
4	K	287	GLU	2.5
4	K	251	TRP	2.5
4	K	279	ILE	2.4
4	Q	89	PHE	2.4
3	P	112	LYS	2.4
4	W	279	ILE	2.4
4	Q	46	PHE	2.4
4	K	263	HIS	2.4
4	K	23	LEU	2.4
4	Q	69	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
4	W	75	LEU	2.4
3	V	112	LYS	2.4
5	R	708	TYR	2.3
3	V	19	VAL	2.3
4	W	178	PHE	2.3
4	W	54	LEU	2.2
4	W	291	GLY	2.2
4	K	88	PHE	2.2
4	Q	49	LEU	2.2
4	Q	180	GLU	2.2
4	E	204	GLU	2.2
4	K	54	LEU	2.1
4	K	89	PHE	2.1
1	N	41	GLN	2.1
1	B	35	ARG	2.1
4	W	185	HIS	2.0
4	K	274	CYS	2.0
4	Q	37	LEU	2.0
3	P	12	VAL	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
6	BMA	Z	3	11/12	0.71	0.16	139,140,143,143	0
6	BMA	Y	3	11/12	0.78	0.21	148,151,154,156	0
8	NAG	4	1	14/15	0.79	0.17	157,159,161,162	0
6	BMA	1	3	11/12	0.81	0.12	135,139,142,143	0
6	NAG	Z	2	14/15	0.82	0.21	124,129,134,139	0
7	FUC	A	3	10/11	0.83	0.25	134,140,141,142	0
6	BMA	M	3	11/12	0.83	0.16	130,132,134,134	0
8	NAG	4	2	14/15	0.85	0.20	156,161,162,162	0
8	NAG	3	1	14/15	0.88	0.11	134,139,143,143	0

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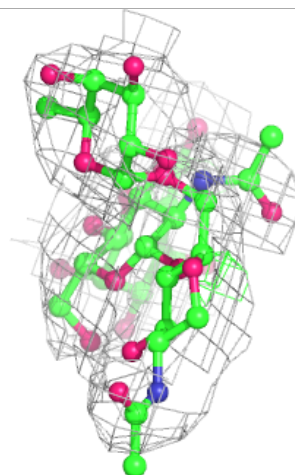
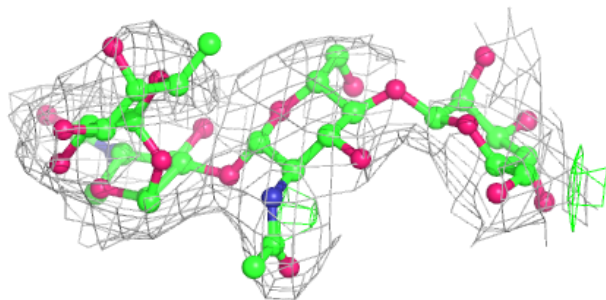
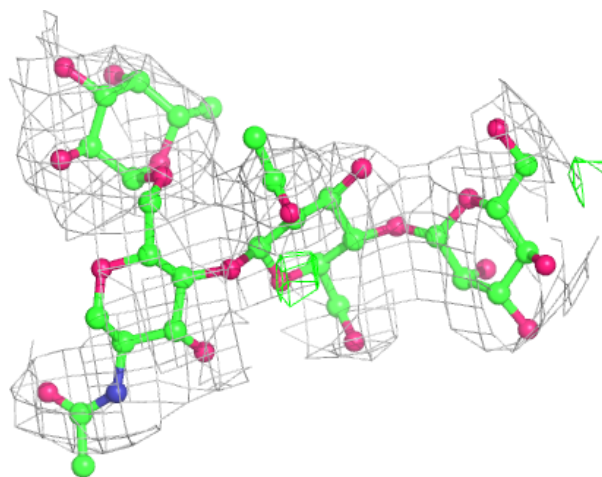
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	BMA	S	3	11/12	0.89	0.12	137,139,141,141	0
8	NAG	3	2	14/15	0.90	0.17	137,145,146,146	0
8	NAG	2	2	14/15	0.90	0.12	134,139,144,144	0
7	NAG	A	2	14/15	0.90	0.11	132,136,139,139	0
8	NAG	2	1	14/15	0.91	0.15	111,120,122,129	0
6	NAG	1	2	14/15	0.91	0.14	118,129,134,139	0
8	NAG	G	2	14/15	0.91	0.18	124,129,133,133	0
7	NAG	A	1	14/15	0.92	0.12	104,122,133,136	0
6	FUC	Z	4	10/11	0.93	0.18	128,132,135,137	0
6	FUC	1	4	10/11	0.93	0.15	123,127,129,131	0
6	NAG	M	2	14/15	0.93	0.13	98,105,115,123	0
6	NAG	1	1	14/15	0.93	0.13	104,110,117,121	0
8	NAG	G	1	14/15	0.93	0.14	102,107,114,120	0
6	NAG	S	2	14/15	0.93	0.12	102,113,123,131	0
6	NAG	Y	2	14/15	0.94	0.11	112,124,134,141	0
6	NAG	M	1	14/15	0.95	0.16	73,76,82,92	0
6	FUC	Y	4	10/11	0.95	0.14	88,90,96,98	0
6	NAG	Y	1	14/15	0.96	0.14	80,86,96,106	0
6	FUC	M	4	10/11	0.96	0.17	80,88,90,93	0
6	FUC	S	4	10/11	0.96	0.15	92,94,96,96	0
6	NAG	Z	1	14/15	0.97	0.16	112,115,120,124	0
6	NAG	S	1	14/15	0.98	0.14	80,86,93,99	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.

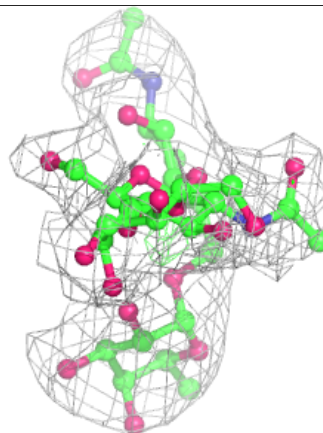
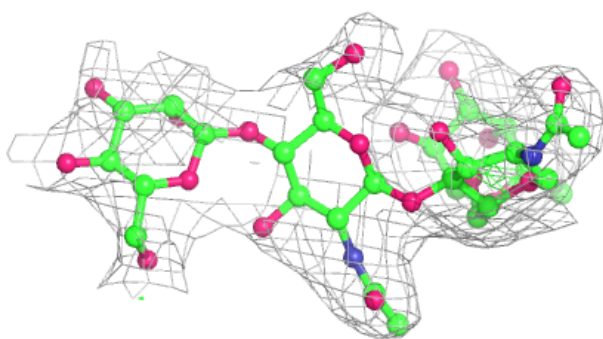
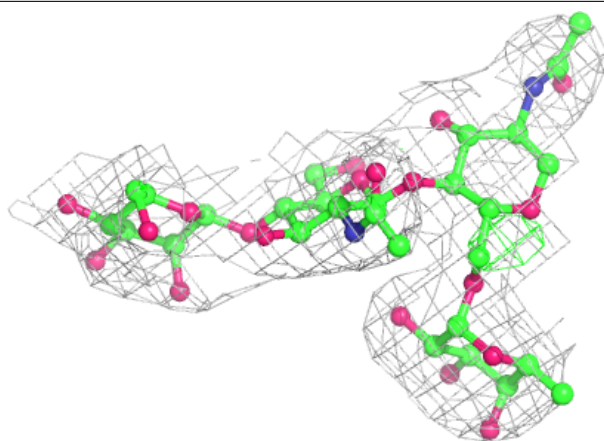
**Electron density around Chain 1:**

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

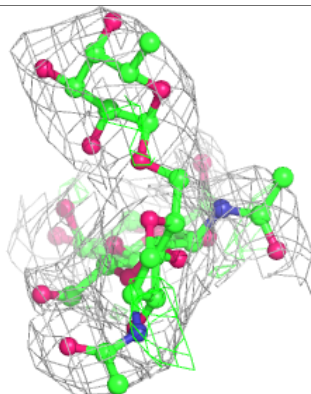
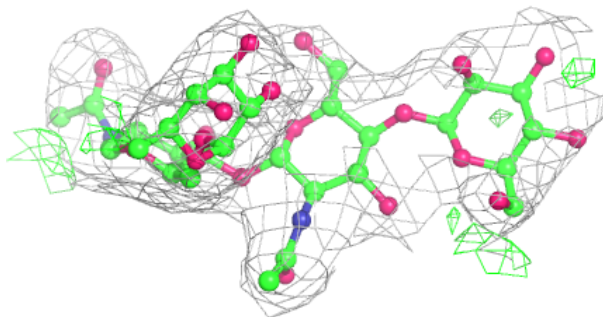
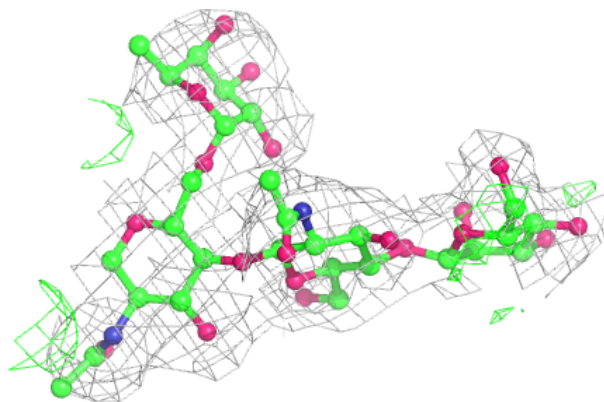


**Electron density around Chain M:**

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

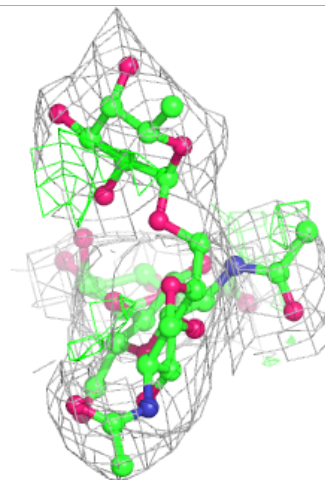
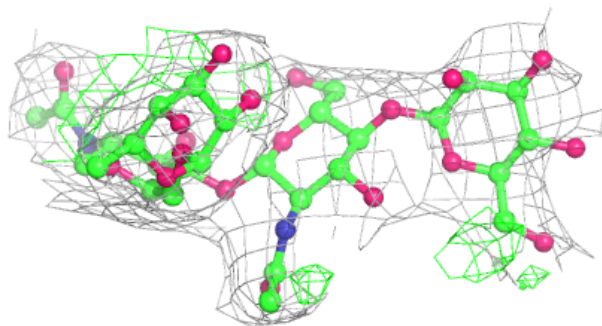
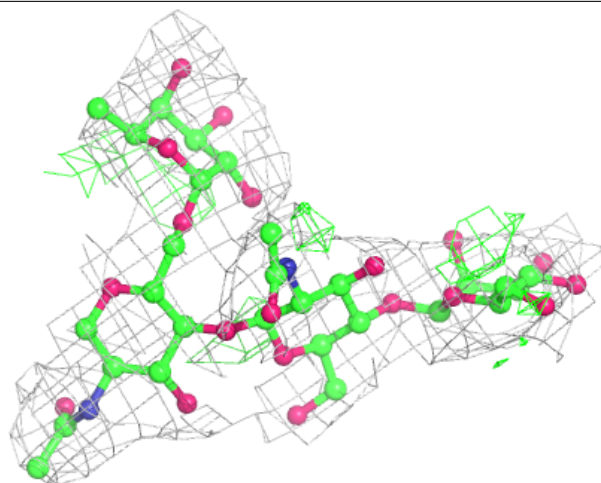
**Electron density around Chain S:**

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



**Electron density around Chain Y:**

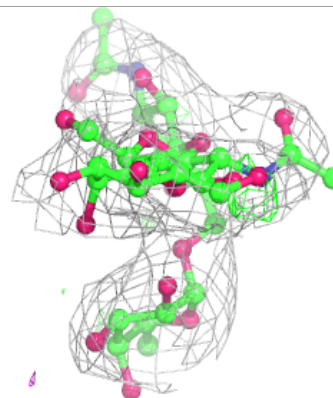
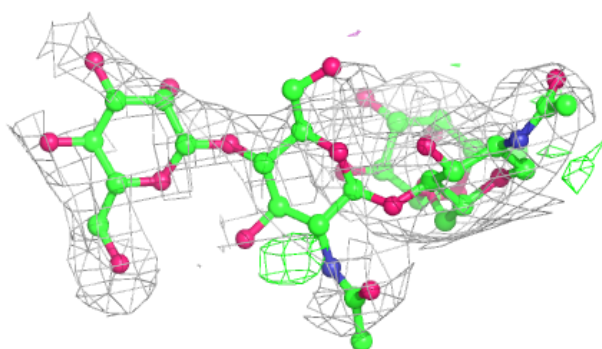
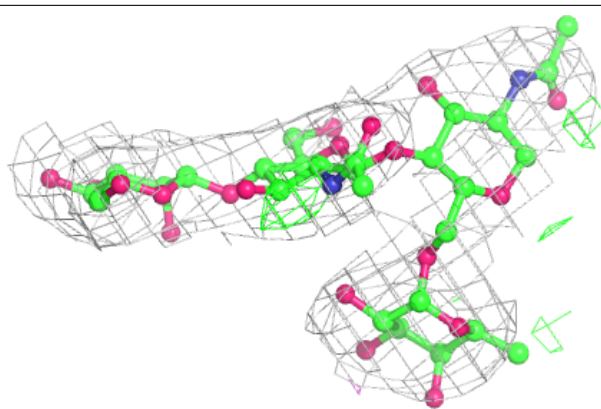
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





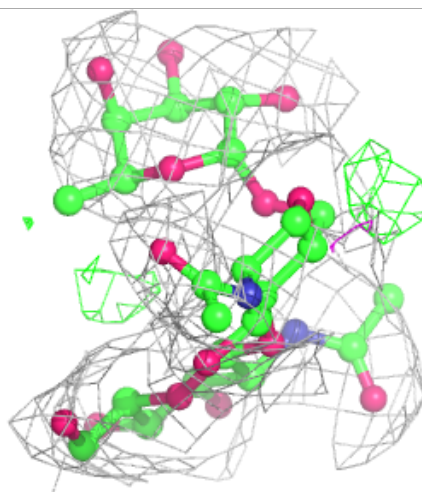
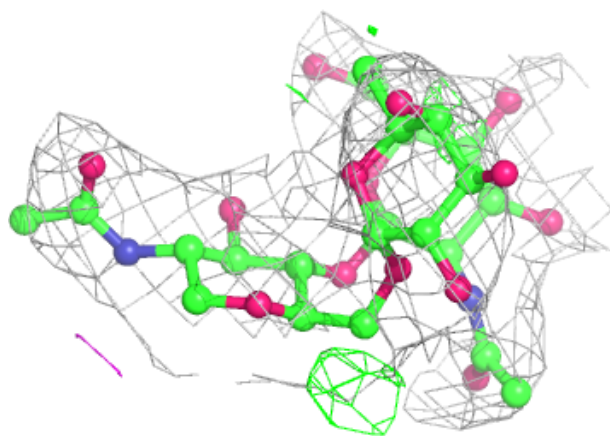
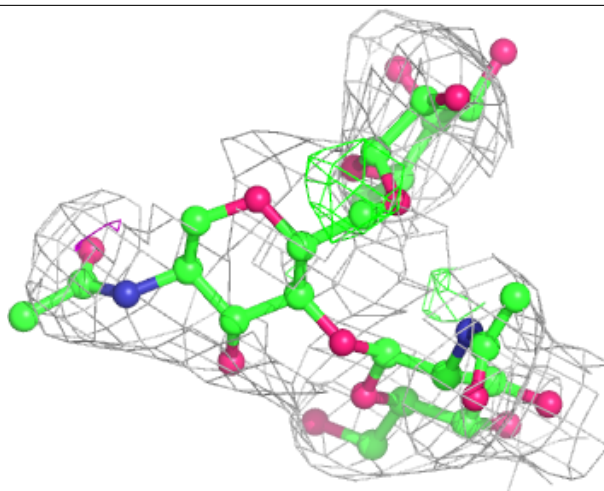
**Electron density around Chain Z:**

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



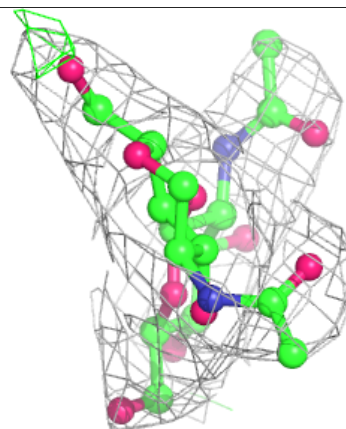
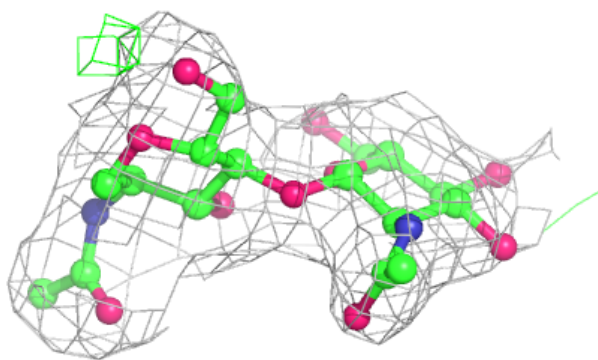
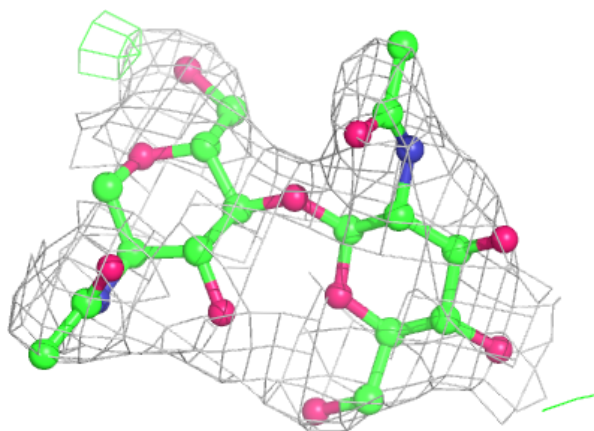
**Electron density around Chain A:**

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



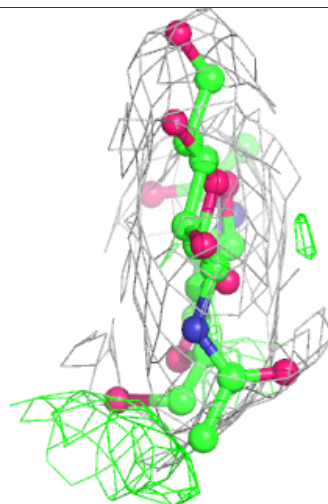
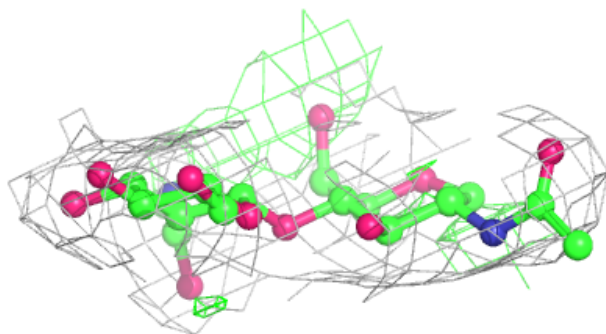
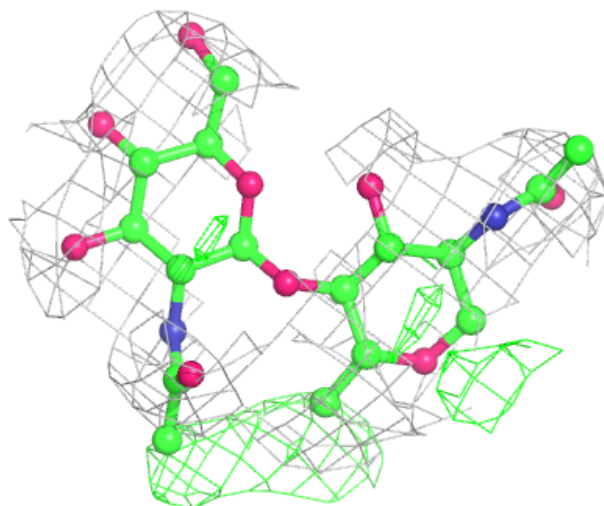
**Electron density around Chain G:**

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



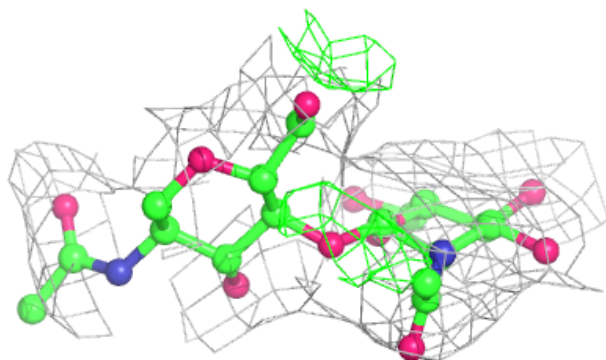
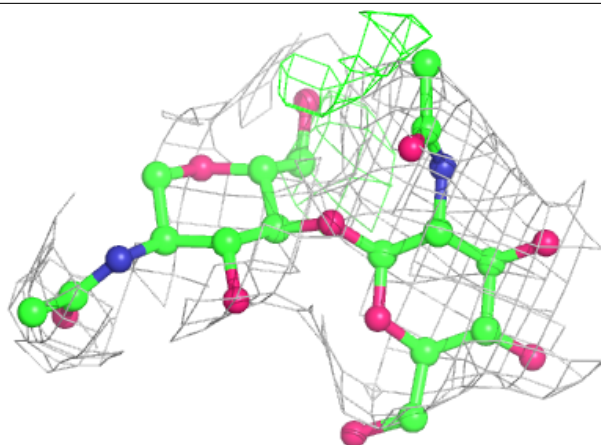
**Electron density around Chain 2:**

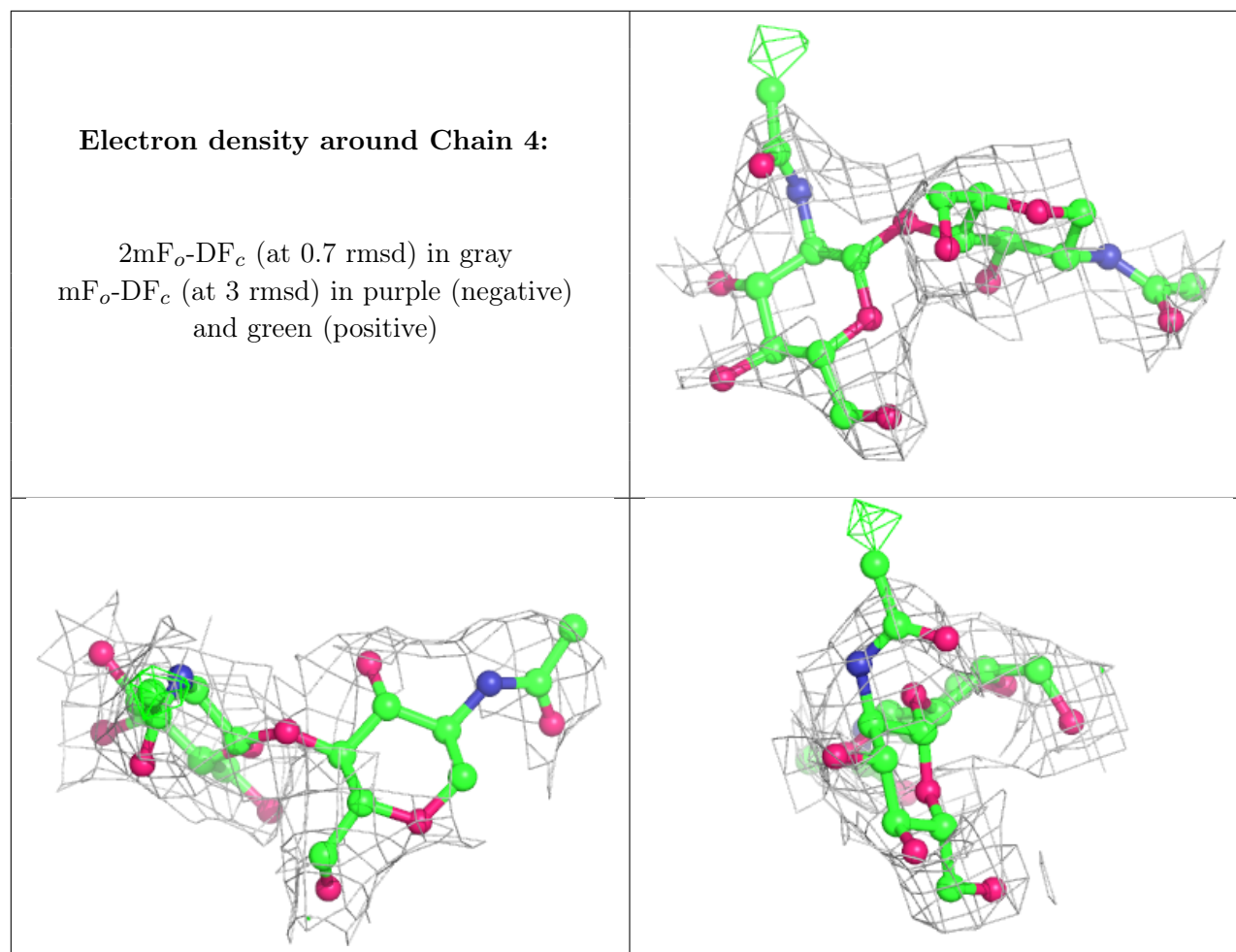
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around Chain 3:**

$2mF_o-DF_c$  (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(Å <sup>2</sup> )	Q<0.9
11	NAG	Q	401	14/15	0.74	0.17	134,141,143,144	0
11	NAG	W	401	14/15	0.75	0.16	130,136,139,139	0
11	NAG	K	401	14/15	0.84	0.12	112,121,123,124	0
11	NAG	Q	403	14/15	0.88	0.23	127,131,134,135	0
9	SO4	U	201	5/5	0.88	0.83	186,186,186,186	0
11	NAG	K	403	14/15	0.89	0.20	95,111,116,117	0
11	NAG	W	403	14/15	0.91	0.24	118,122,128,130	0
11	NAG	K	402	14/15	0.92	0.19	70,77,81,82	0
10	GOL	D	201	6/6	0.93	0.22	66,70,74,74	0
9	SO4	C	201	5/5	0.94	0.39	135,135,135,137	0
11	NAG	W	402	14/15	0.95	0.16	77,84,86,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
9	SO4	O	201	5/5	0.95	0.45	117,118,119,121	0
9	SO4	I	201	5/5	0.96	0.55	136,137,137,137	0
11	NAG	Q	402	14/15	0.96	0.15	70,75,80,82	0
11	NAG	E	401	14/15	0.97	0.14	60,67,71,73	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.