



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 10, 2020 – 07:16 AM BST

PDB ID : 6RUV  
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 wwPDB X-ray Structure Validation Summary 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 : 2.13.1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13.1

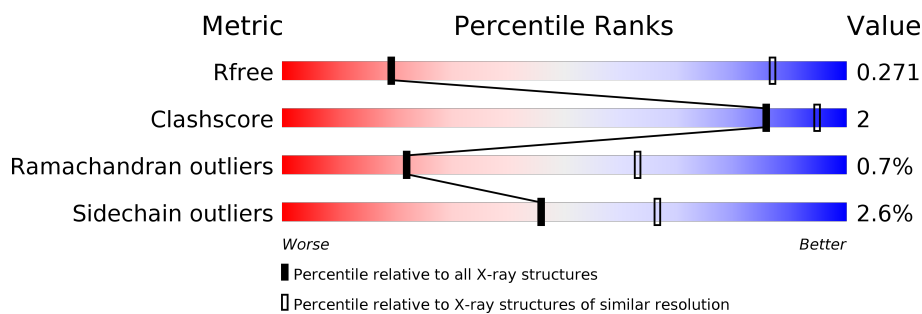
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 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.






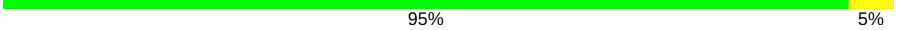



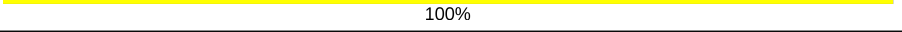
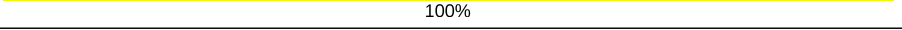
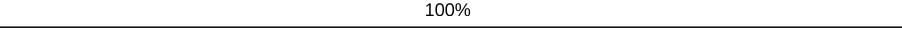
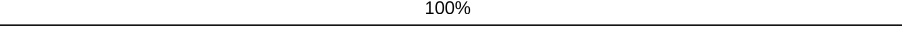
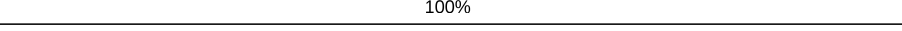

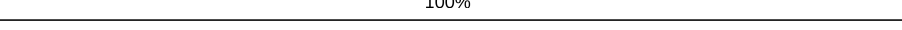


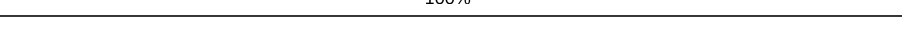

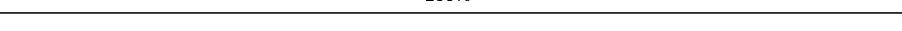
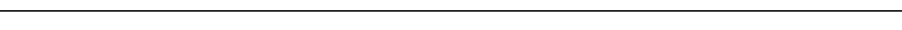
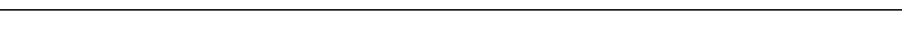
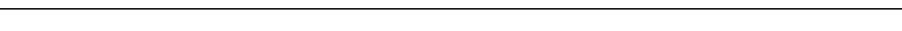
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1003 (8.40-3.88)
Clashscore	141614	1052 (8.40-3.90)
Ramachandran outliers	138981	1000 (8.40-3.88)
Sidechain outliers	138945	1000 (8.40-3.84)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	R	131	89% 5% • 5%
1	S	131	93% • 5%
2	U	170	55% 6% 38%
2	X	170	82% 12% • •
3	V	221	81% 14% • •
3	Y	221	79% 15% • •
4	A	645	94% 6% •

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Mol	Chain	Length	Quality of chain
4	G	645	 93% 7% .
5	B	915	 91% 9%
5	H	915	 90% 9%
6	J	505	 95% 5%
6	L	505	 93% 7%
7	N	86	 87% 10% .
7	Q	86	 91% 7% .
8	C	2	 100%
8	D	2	 100%
8	F	2	 100%
8	I	2	 100%
8	K	2	 100%
9	E	3	 33% 67%
9	M	3	 100%
10	O	2	 50% 50%
10	P	2	 50% 50%
10	T	2	 100%
10	W	2	 50% 50%
10	Z	2	 100%
10	a	2	 50% 50%
10	b	2	 100%
10	c	2	 50% 50%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	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 [i](#)

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

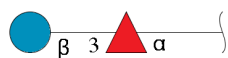
- Molecule 7 is a protein called Inhibitor.

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.



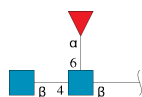
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
8	C	2	Total	C	O	0	0	0
			21	12	9			
8	D	2	Total	C	O	0	0	0
			21	12	9			
8	F	2	Total	C	O	0	0	0
			21	12	9			
8	I	2	Total	C	O	0	0	0
			21	12	9			

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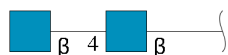
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
8	K	2	Total	C	O	0	0	0
			21	12	9			

- 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.



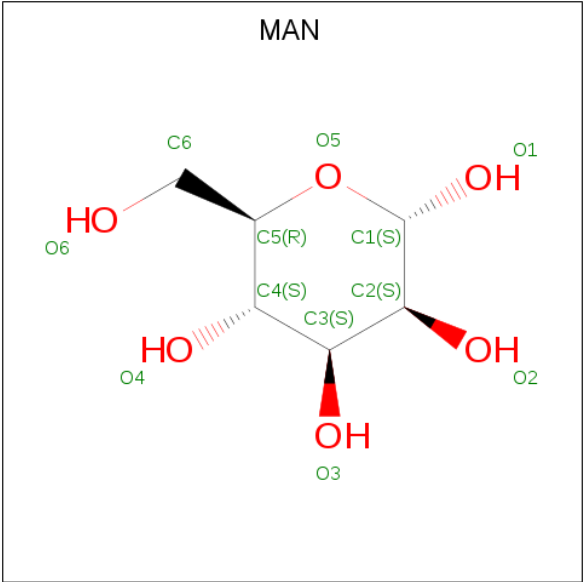
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	E	3	Total	C	N	O	0	0	0
			38	22	2	14			
9	M	3	Total	C	N	O	0	0	0
			38	22	2	14			

- 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 (three-letter code: MAN) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).



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 (three-letter code: 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. 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. 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

Chain R:  89% 5% • 5%



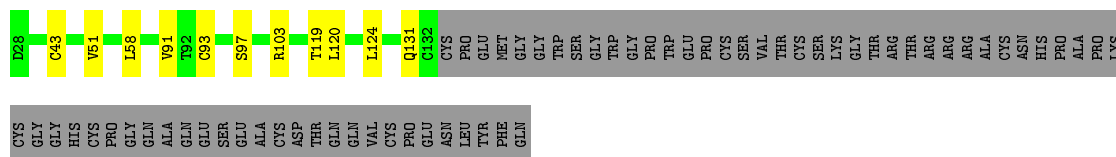
- Molecule 1: Nanobody hFPNb1

Chain S:  93% • 5%




- Molecule 2: Properdin

Chain U:  55% 6% 38%




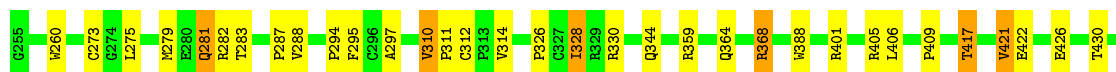
- Molecule 2: Properdin

Chain X:  82% 12% • •



- Molecule 3: Properdin

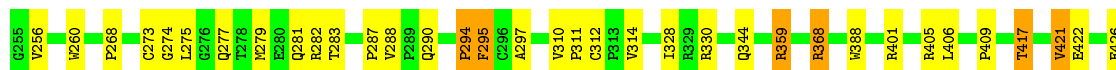
Chain V:  81% 14% • •





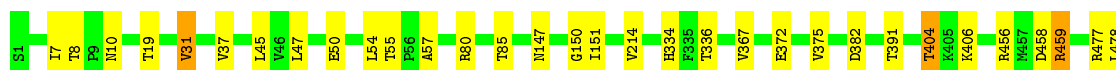
- Molecule 3: Properdin

Chain Y: 79% 15% . .



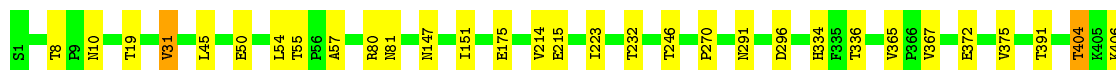
- Molecule 4: Complement C3

Chain A: 94% 6% . .



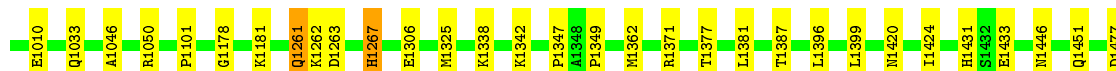
- Molecule 4: Complement C3

Chain G: 93% 7% . .




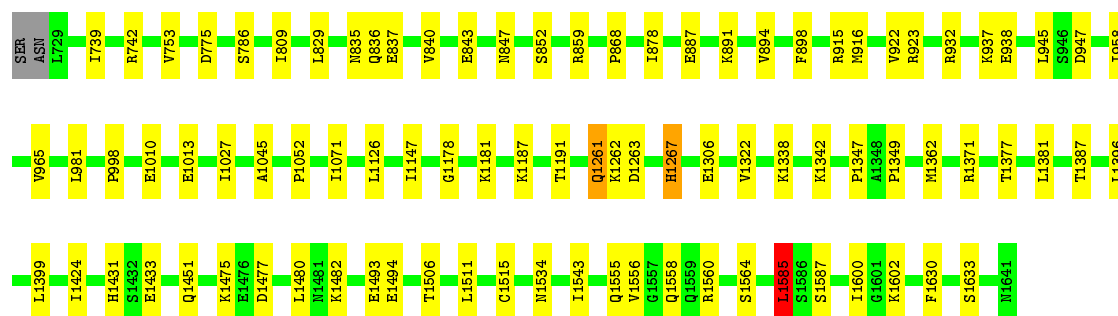
- Molecule 5: Complement C3

Chain B: 91% 9% . .



- Molecule 5: Complement C3

Chain H:  90% 9%



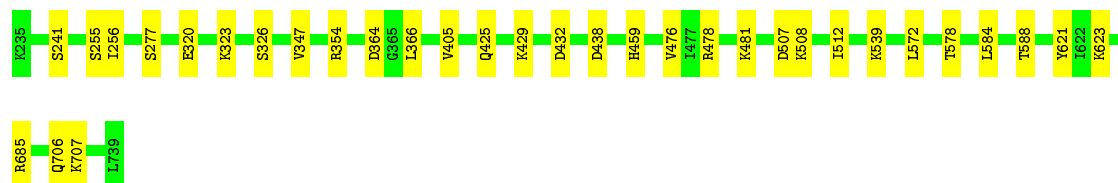
- Molecule 6: Complement factor B

Chain J:  95% 5%




- Molecule 6: Complement factor B

Chain L:  93% 7%



- Molecule 7: Inhibitor

Chain N:  87% 10%



- Molecule 7: Inhibitor

Chain Q:  91% 7%



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

Chain C:  100%

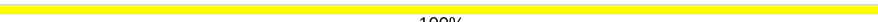


- Molecule 8: beta-D-glucopyranose-(1-3)-alpha-L-fucopyranose

Chain D:  100%

FUC1  
BGC2

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

Chain F:  100%

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:  50% 50%

NAG1  
NAG2

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

Chain P:  50% 50%



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

Chain T:  100%



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

Chain W:  50% 50%



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

Chain Z:  100%



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

Chain a:  50% 50%



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

Chain b:  100%



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

Chain c:  50% 50%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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) 99.8 (49.82-6.15)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.10 (at 6.15Å)	Xtriage
Refinement program	PHENIX (1.14 _3260: ???)	Depositor
R, $R_{free}$	0.242 , 0.271 0.242 , 0.271	Depositor DCC
$R_{free}$ test set	1990 reflections (5.18%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	436.1	Xtriage
Anisotropy	0.347	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.24 , 436.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.41$ , $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	0.030 for -h,l,k	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	41916	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<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: FUC, MG, BGC, NAG, MAN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	R	0.30	0/967	0.57	0/1305
1	S	0.30	0/967	0.55	0/1305
2	U	0.28	0/819	0.56	0/1109
2	X	0.30	0/1261	0.58	1/1710 (0.1%)
3	V	0.33	0/1720	0.58	0/2342
3	Y	0.33	0/1720	0.60	0/2342
4	A	0.30	0/5127	0.57	0/6966
4	G	0.30	0/5126	0.57	0/6962
5	B	0.29	0/7439	0.55	1/10073 (0.0%)
5	H	0.30	0/7439	0.55	1/10073 (0.0%)
6	J	0.28	0/4095	0.51	0/5542
6	L	0.28	0/4095	0.52	0/5542
7	N	0.30	0/691	0.53	0/923
7	Q	0.29	0/691	0.52	0/923
All	All	0.30	0/42157	0.55	3/57117 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1585	LEU	CA-CB-CG	7.02	131.45	115.30
5	H	1585	LEU	CA-CB-CG	6.33	129.86	115.30
2	X	47	LEU	CA-CB-CG	5.43	127.79	115.30

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	14	0
3	Y	1666	0	1572	17	0
4	A	5025	0	5084	17	0
4	G	5025	0	5084	21	0
5	B	7293	0	7217	35	0
5	H	7293	0	7217	38	0
6	J	4007	0	3994	14	0
6	L	4007	0	3994	19	0
7	N	683	0	697	6	0
7	Q	683	0	697	4	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	179	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.

The worst 5 of 179 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

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%)	25	66
3	V	213/221 (96%)	195 (92%)	12 (6%)	6 (3%)	5	30
3	Y	213/221 (96%)	193 (91%)	14 (7%)	6 (3%)	5	30
4	A	643/645 (100%)	623 (97%)	17 (3%)	3 (0%)	29	69
4	G	641/645 (99%)	621 (97%)	17 (3%)	3 (0%)	29	69
5	B	911/915 (100%)	859 (94%)	44 (5%)	8 (1%)	17	57
5	H	911/915 (100%)	858 (94%)	45 (5%)	8 (1%)	17	57
6	J	503/505 (100%)	478 (95%)	24 (5%)	1 (0%)	47	81
6	L	503/505 (100%)	479 (95%)	23 (5%)	1 (0%)	47	81

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
7	N	82/86 (95%)	81 (99%)	0	1 (1%)	13 50
7	Q	82/86 (95%)	81 (99%)	0	1 (1%)	13 50
All	All	5210/5346 (98%)	4953 (95%)	218 (4%)	39 (1%)	22 63

5 of 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

### 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%)	76 86
1	S	100/107 (94%)	100 (100%)	0	100 100
2	U	88/141 (62%)	82 (93%)	6 (7%)	16 41
2	X	134/141 (95%)	125 (93%)	9 (7%)	16 41
3	V	184/190 (97%)	167 (91%)	17 (9%)	9 29
3	Y	184/190 (97%)	168 (91%)	16 (9%)	10 31
4	A	567/567 (100%)	554 (98%)	13 (2%)	50 70
4	G	567/567 (100%)	553 (98%)	14 (2%)	47 68
5	B	808/810 (100%)	790 (98%)	18 (2%)	52 71
5	H	808/810 (100%)	790 (98%)	18 (2%)	52 71
6	J	444/444 (100%)	441 (99%)	3 (1%)	84 91
6	L	444/444 (100%)	441 (99%)	3 (1%)	84 91
7	N	76/77 (99%)	75 (99%)	1 (1%)	69 82
7	Q	76/77 (99%)	75 (99%)	1 (1%)	69 82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	4580/4672 (98%)	4460 (97%)	120 (3%)	46 66

5 of 120 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	391	THR
5	B	945	LEU
5	H	1560	ARG
4	A	404	THR
4	A	487	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	S	75	ASN
4	A	10	ASN
4	G	10	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

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	1.06	1 (7%)
8	BGC	C	2	8	11,11,12	1.76	2 (18%)	15,15,17	1.21	2 (13%)
8	FUC	D	1	8,3	10,10,11	1.28	1 (10%)	14,14,16	1.22	3 (21%)
8	BGC	D	2	8	11,11,12	1.77	3 (27%)	15,15,17	1.11	0
9	NAG	E	1	9,3	14,14,15	0.97	2 (14%)	17,19,21	1.25	2 (11%)
9	NAG	E	2	9	14,14,15	1.57	1 (7%)	17,19,21	2.42	3 (17%)
9	FUC	E	3	9	10,10,11	1.02	0	14,14,16	0.84	0
8	FUC	F	1	8,2	10,10,11	1.14	1 (10%)	14,14,16	0.91	1 (7%)
8	BGC	F	2	8	11,11,12	1.79	2 (18%)	15,15,17	1.24	2 (13%)
8	FUC	I	1	8,2	10,10,11	1.33	1 (10%)	14,14,16	1.29	2 (14%)
8	BGC	I	2	8	11,11,12	1.79	2 (18%)	15,15,17	1.23	1 (6%)
8	FUC	K	1	8,3	10,10,11	1.18	1 (10%)	14,14,16	1.18	2 (14%)
8	BGC	K	2	8	11,11,12	1.68	2 (18%)	15,15,17	0.94	1 (6%)
9	NAG	M	1	9,3	14,14,15	1.03	2 (14%)	17,19,21	1.48	2 (11%)
9	NAG	M	2	9	14,14,15	1.42	1 (7%)	17,19,21	2.44	3 (17%)
9	FUC	M	3	9	10,10,11	0.96	0	14,14,16	0.97	1 (7%)
10	NAG	O	1	10,4	14,14,15	0.58	0	17,19,21	0.64	0
10	NAG	O	2	10	14,14,15	0.72	1 (7%)	17,19,21	0.49	0
10	NAG	P	1	10,5	14,14,15	0.80	1 (7%)	17,19,21	0.83	1 (5%)
10	NAG	P	2	10	14,14,15	0.51	0	17,19,21	0.56	0
10	NAG	T	1	10,4	14,14,15	0.63	0	17,19,21	0.64	0
10	NAG	T	2	10	14,14,15	0.54	0	17,19,21	0.54	0
10	NAG	W	1	10,5	14,14,15	0.75	1 (7%)	17,19,21	0.73	0
10	NAG	W	2	10	14,14,15	0.59	0	17,19,21	0.58	0
10	NAG	Z	1	10,6	14,14,15	1.05	1 (7%)	17,19,21	1.95	5 (29%)
10	NAG	Z	2	10	14,14,15	1.61	2 (14%)	17,19,21	2.86	4 (23%)
10	NAG	a	1	10,6	14,14,15	1.54	2 (14%)	17,19,21	1.48	2 (11%)
10	NAG	a	2	10	14,14,15	0.45	0	17,19,21	0.61	0
10	NAG	b	1	10,6	14,14,15	1.05	1 (7%)	17,19,21	1.96	5 (29%)
10	NAG	b	2	10	14,14,15	1.64	2 (14%)	17,19,21	2.87	4 (23%)
10	NAG	c	1	10,6	14,14,15	1.47	2 (14%)	17,19,21	1.45	2 (11%)
10	NAG	c	2	10	14,14,15	0.46	0	17,19,21	0.62	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	-	3/6/23/26	0/1/1/1
9	NAG	E	2	9	-	5/6/23/26	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	3/6/23/26	0/1/1/1
9	NAG	M	2	9	-	5/6/23/26	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	-	1/6/23/26	0/1/1/1
10	NAG	P	2	10	-	2/6/23/26	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	-	3/6/23/26	0/1/1/1
10	NAG	a	1	10,6	-	4/6/23/26	0/1/1/1
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	-	3/6/23/26	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

The worst 5 of 34 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	b	2	NAG	O5-C1	5.31	1.52	1.43
10	Z	2	NAG	O5-C1	5.20	1.52	1.43
9	E	2	NAG	C1-C2	5.03	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	I	2	BGC	O5-C1	4.88	1.51	1.43
8	F	2	BGC	O5-C1	4.82	1.51	1.43

The worst 5 of 49 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	Z	2	NAG	C2-N2-C7	8.83	135.48	122.90
10	b	2	NAG	C2-N2-C7	8.81	135.45	122.90
9	M	2	NAG	C2-N2-C7	8.59	135.14	122.90
9	E	2	NAG	C2-N2-C7	8.53	135.05	122.90
10	b	2	NAG	C1-O5-C5	6.06	120.41	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

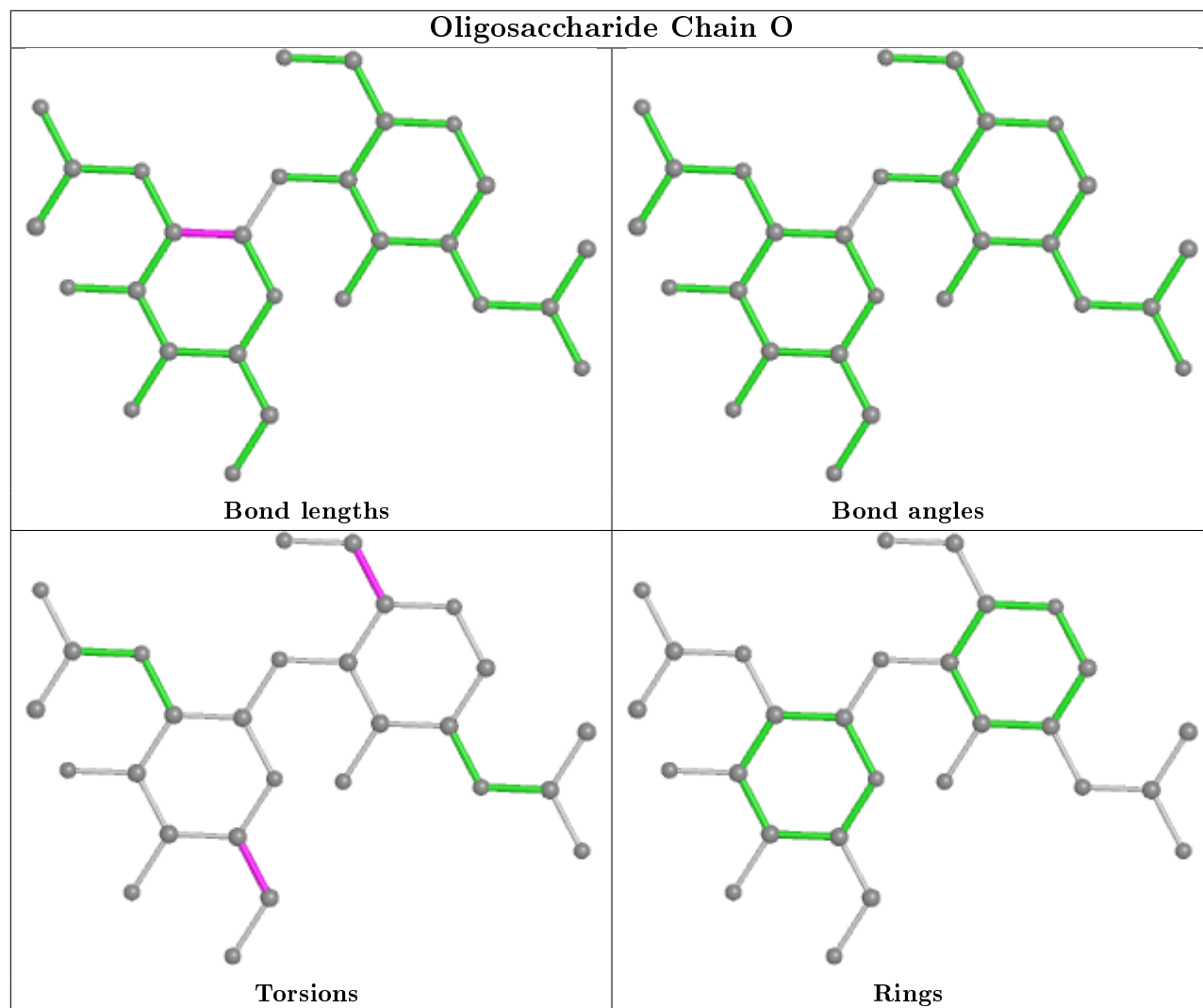
5 of 61 torsion outliers are listed below:

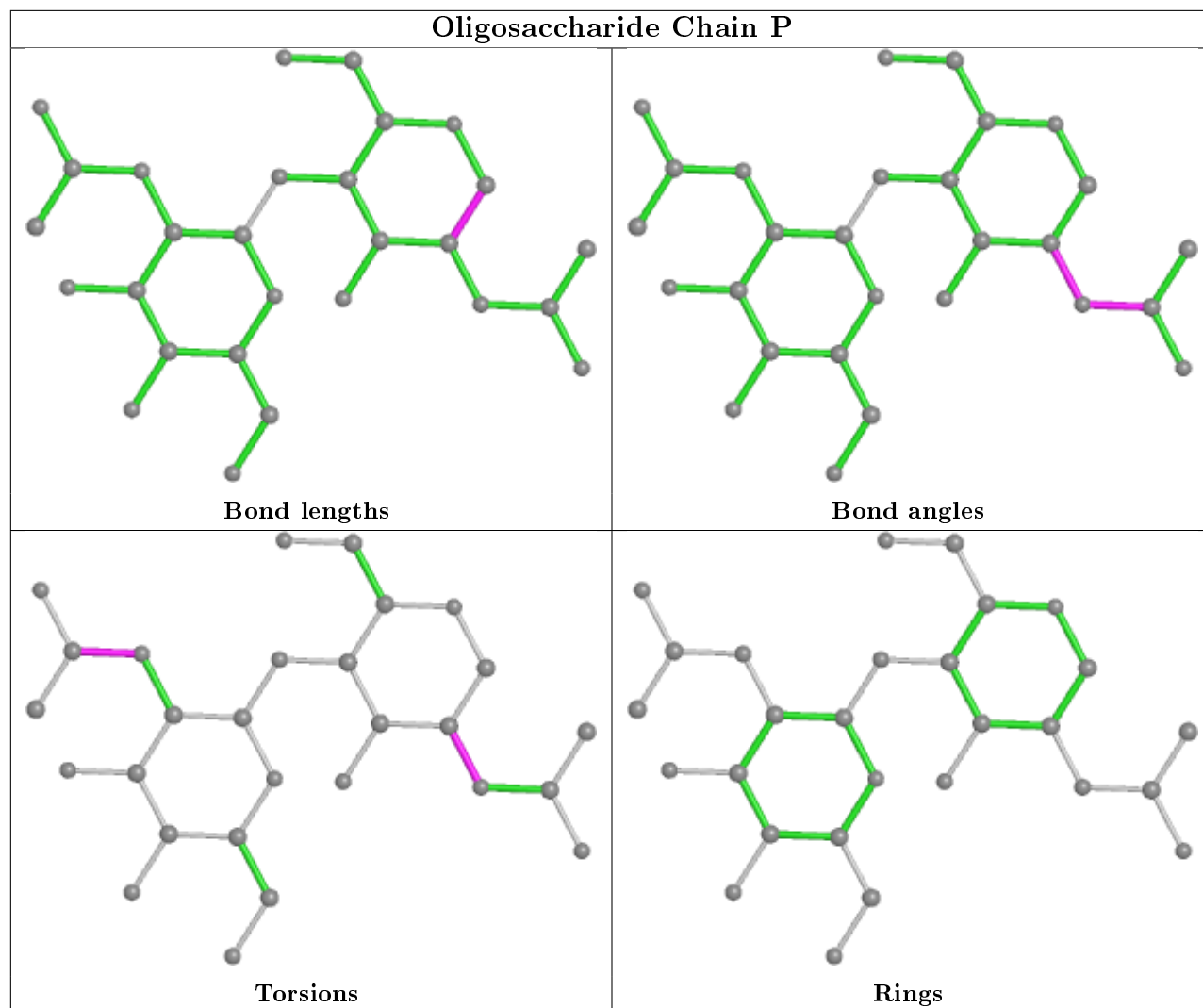
Mol	Chain	Res	Type	Atoms
10	a	1	NAG	O5-C5-C6-O6
10	c	1	NAG	O5-C5-C6-O6
9	E	2	NAG	C4-C5-C6-O6
9	M	2	NAG	C4-C5-C6-O6
10	a	1	NAG	C4-C5-C6-O6

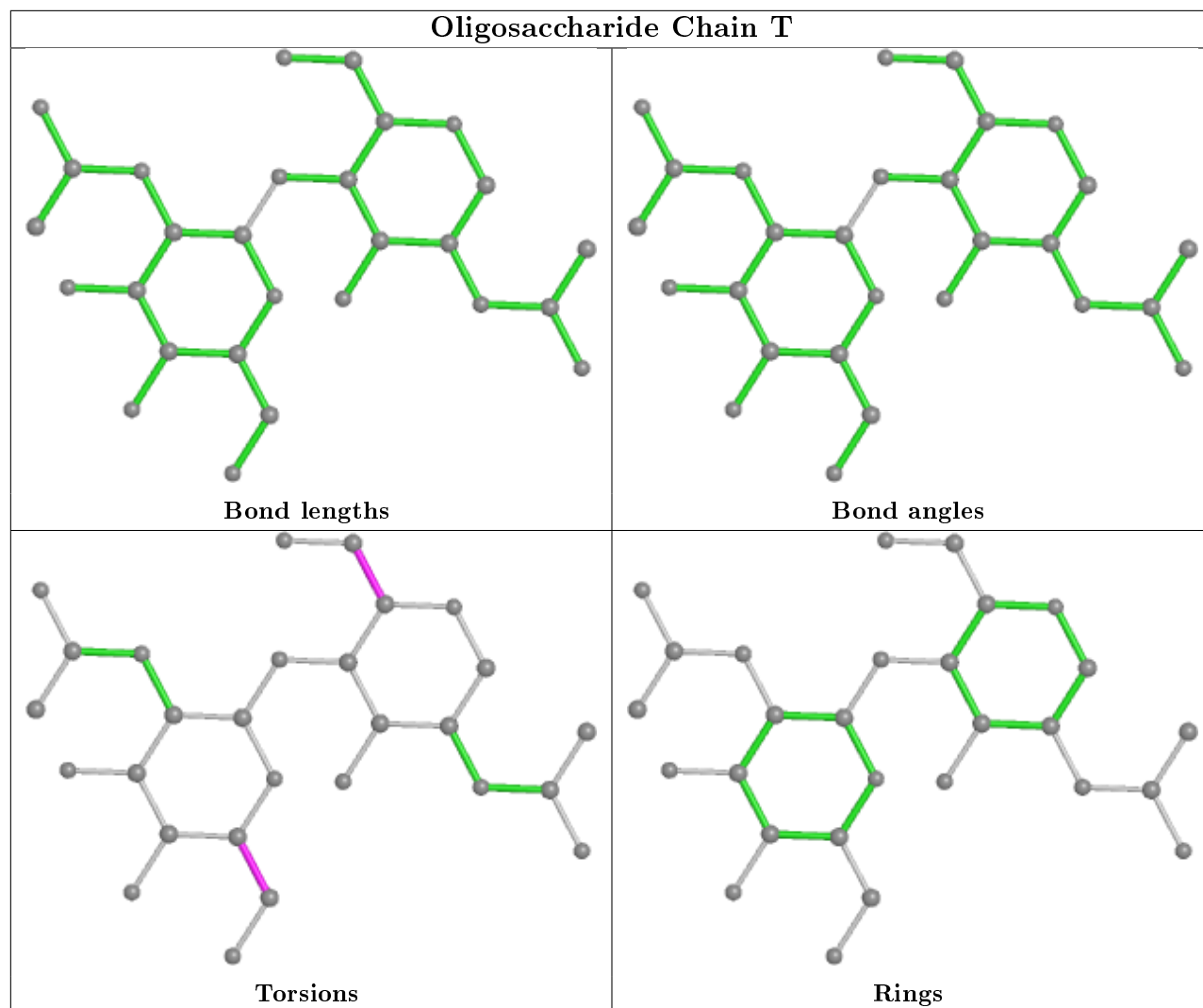
There are no ring outliers.

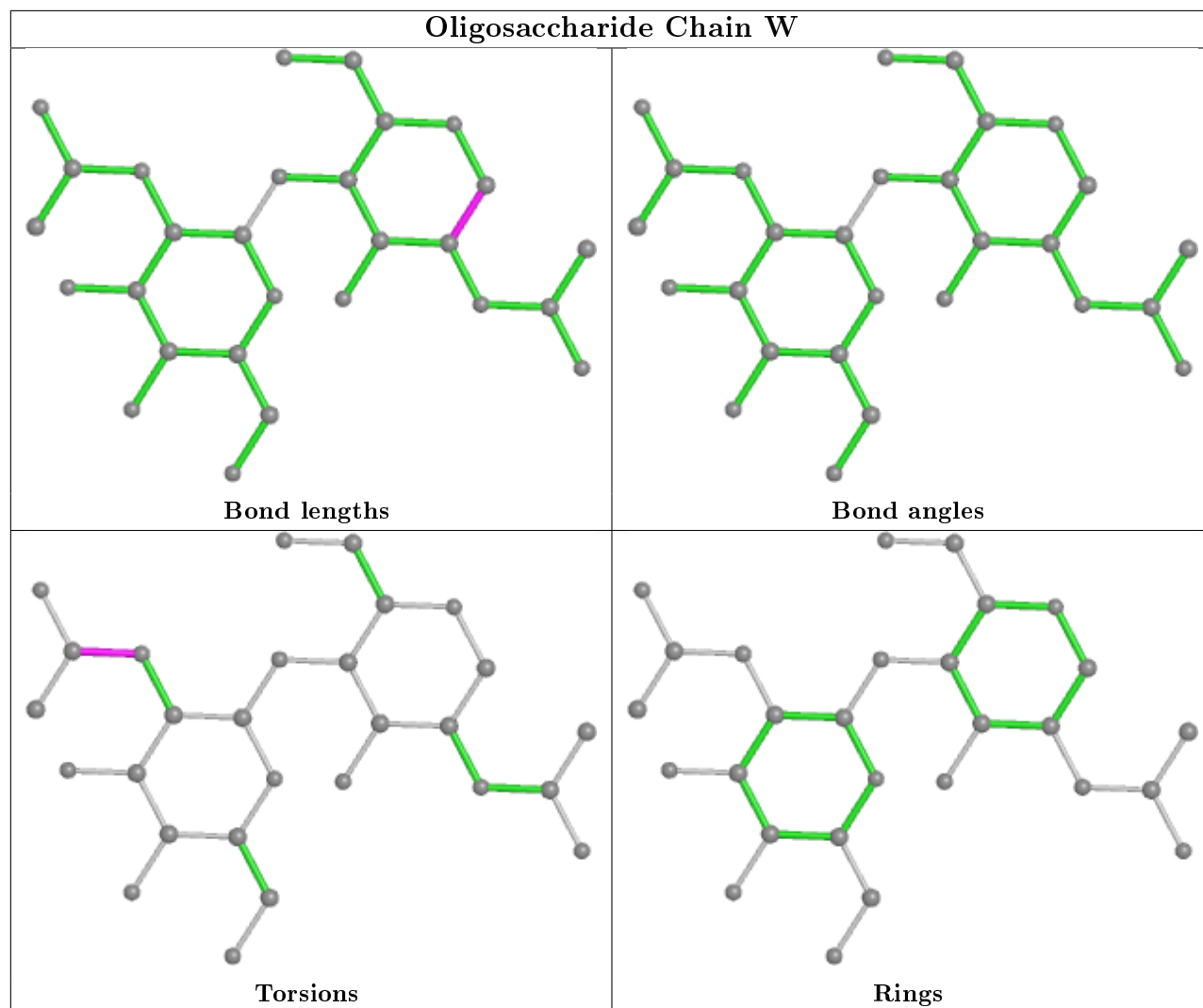
No monomer is involved in short contacts.

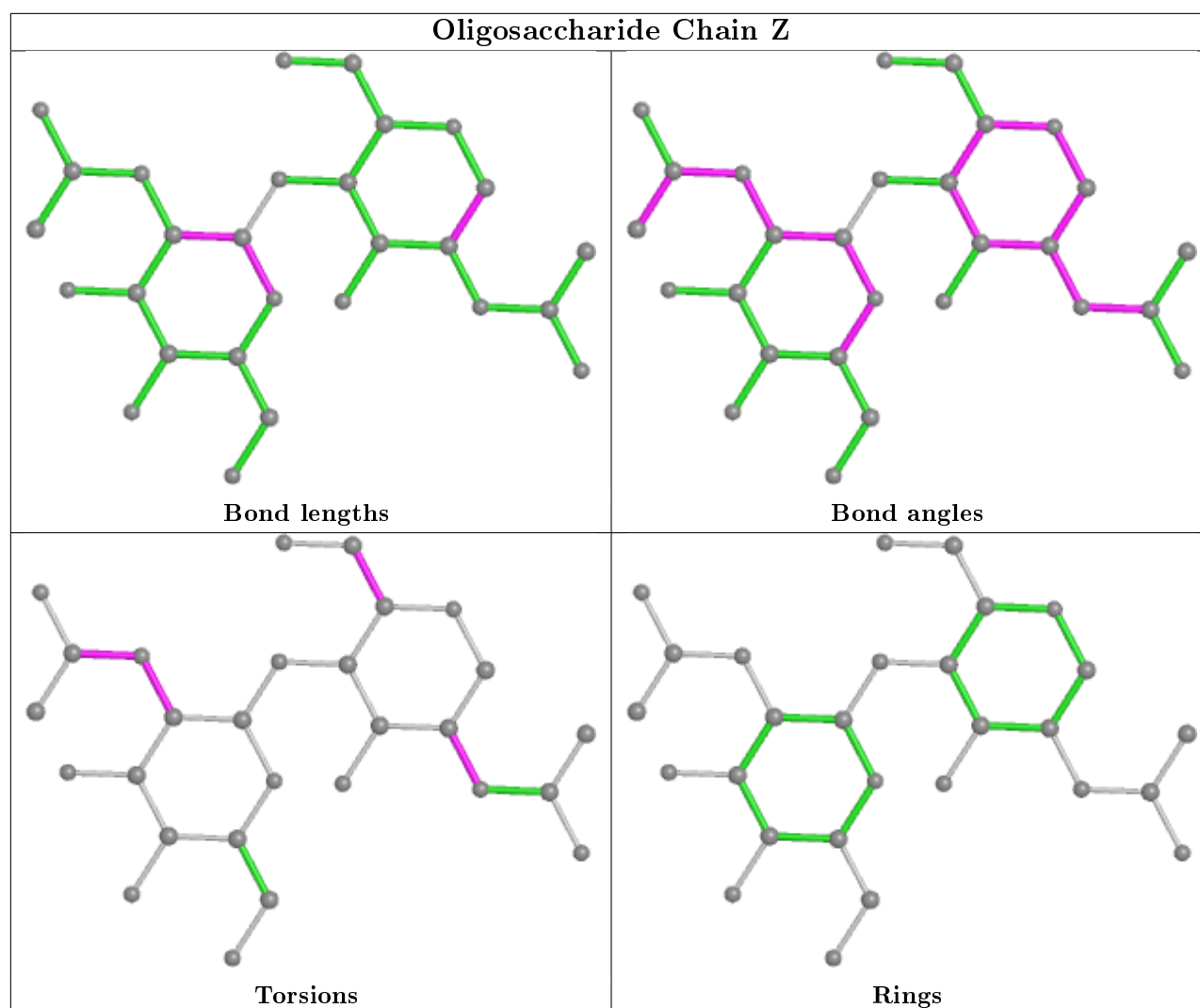
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











## 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	505	3	11,11,12	1.21	1 (9%)	15,15,17	1.90	2 (13%)
11	MAN	X	207	2	11,11,12	1.49	2 (18%)	15,15,17	1.27	3 (20%)
11	MAN	V	505	3	11,11,12	1.18	1 (9%)	15,15,17	2.32	3 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
11	MAN	V	510	3	11,11,12	1.24	1 (9%)	15,15,17	1.90	3 (20%)
11	MAN	Y	512	3	11,11,12	1.24	1 (9%)	15,15,17	1.89	2 (13%)
11	MAN	U	201	2	11,11,12	1.25	2 (18%)	15,15,17	2.01	4 (26%)
11	MAN	V	503	3	11,11,12	1.12	1 (9%)	15,15,17	1.75	2 (13%)
11	MAN	Y	511	3	11,11,12	1.30	2 (18%)	15,15,17	2.04	4 (26%)
11	MAN	V	511	3	11,11,12	1.24	1 (9%)	15,15,17	2.03	4 (26%)
11	MAN	Y	503	3	11,11,12	1.08	1 (9%)	15,15,17	1.85	4 (26%)
11	MAN	X	203	2	11,11,12	1.27	1 (9%)	15,15,17	1.70	2 (13%)
11	MAN	Y	510	3	11,11,12	1.16	1 (9%)	15,15,17	1.84	4 (26%)
11	MAN	V	509	3	11,11,12	1.17	1 (9%)	15,15,17	1.89	3 (20%)
11	MAN	Y	509	3	11,11,12	1.20	1 (9%)	15,15,17	1.93	4 (26%)
11	MAN	X	204	2	11,11,12	1.18	1 (9%)	15,15,17	1.77	2 (13%)
11	MAN	X	208	2	11,11,12	1.38	2 (18%)	15,15,17	1.42	3 (20%)
11	MAN	Y	504	3	11,11,12	1.11	1 (9%)	15,15,17	1.81	2 (13%)
11	MAN	X	209	2	11,11,12	1.38	2 (18%)	15,15,17	1.59	3 (20%)
11	MAN	U	202	2	11,11,12	1.34	2 (18%)	15,15,17	1.76	2 (13%)
11	MAN	V	512	3	11,11,12	1.10	1 (9%)	15,15,17	1.88	2 (13%)
11	MAN	V	504	3	11,11,12	1.29	1 (9%)	15,15,17	1.97	4 (26%)

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	505	3	-	0/2/19/22	0/1/1/1
11	MAN	X	207	2	-	0/2/19/22	0/1/1/1
11	MAN	V	505	3	-	0/2/19/22	0/1/1/1
11	MAN	V	510	3	-	0/2/19/22	0/1/1/1
11	MAN	Y	512	3	-	0/2/19/22	0/1/1/1
11	MAN	U	201	2	-	0/2/19/22	0/1/1/1
11	MAN	V	503	3	-	0/2/19/22	0/1/1/1
11	MAN	Y	511	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	503	3	-	0/2/19/22	0/1/1/1
11	MAN	X	203	2	-	0/2/19/22	0/1/1/1
11	MAN	Y	510	3	-	0/2/19/22	0/1/1/1
11	MAN	V	509	3	-	0/2/19/22	0/1/1/1

*Continued on next page...*

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	MAN	Y	509	3	-	0/2/19/22	0/1/1/1
11	MAN	X	204	2	-	0/2/19/22	0/1/1/1
11	MAN	X	208	2	-	0/2/19/22	0/1/1/1
11	MAN	Y	504	3	-	1/2/19/22	0/1/1/1
11	MAN	X	209	2	-	0/2/19/22	0/1/1/1
11	MAN	U	202	2	-	0/2/19/22	0/1/1/1
11	MAN	V	512	3	-	0/2/19/22	0/1/1/1
11	MAN	V	504	3	-	1/2/19/22	0/1/1/1

The worst 5 of 27 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	X	209	MAN	O5-C5	3.15	1.49	1.43
11	V	504	MAN	O5-C5	2.87	1.49	1.43
11	X	203	MAN	O5-C5	2.79	1.49	1.43
11	Y	505	MAN	O5-C5	2.74	1.49	1.43
11	X	207	MAN	O5-C1	-2.72	1.39	1.43

The worst 5 of 62 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	U	201	MAN	C1-O5-C5	5.80	120.05	112.19
11	Y	512	MAN	C1-O5-C5	5.60	119.78	112.19
11	V	512	MAN	C1-O5-C5	5.60	119.77	112.19
11	V	505	MAN	C1-O5-C5	5.57	119.74	112.19
11	V	504	MAN	C1-O5-C5	5.47	119.60	112.19

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 ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

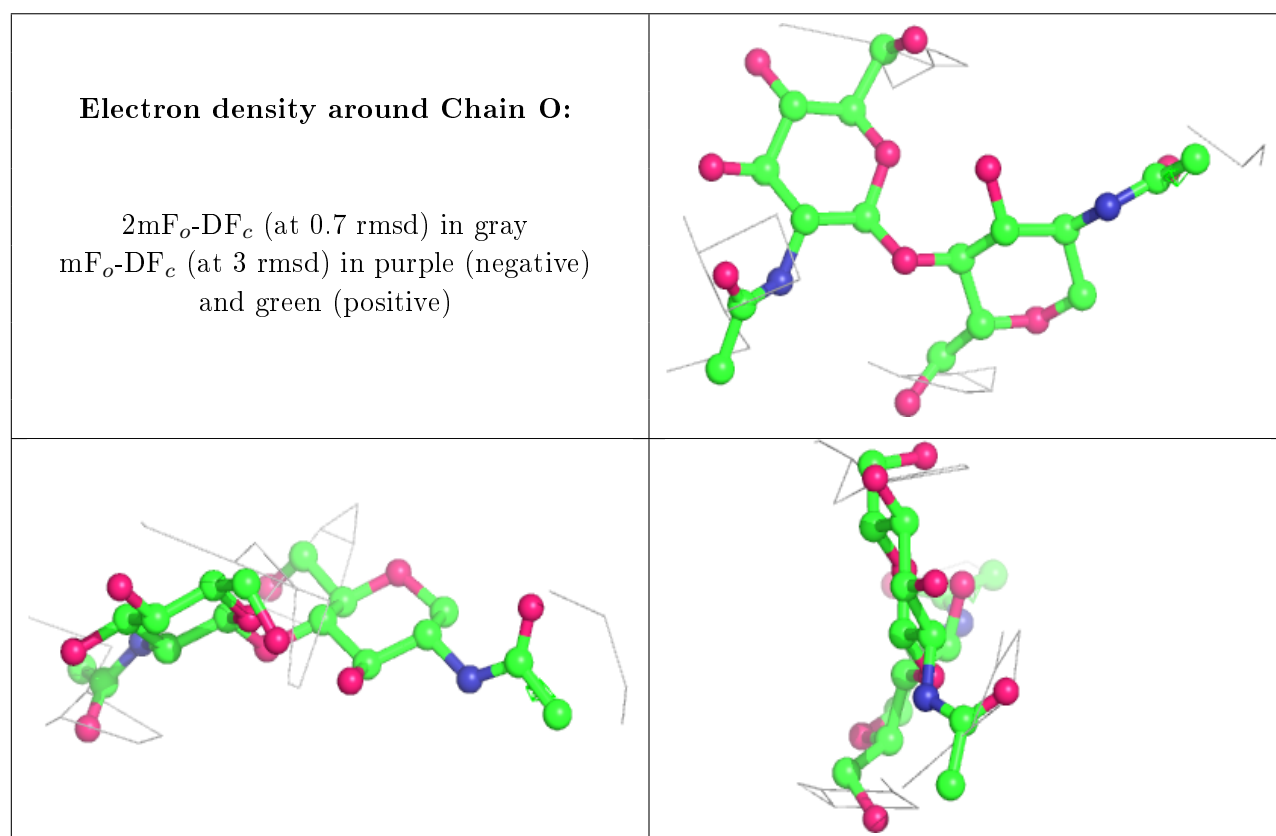
### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.3 Carbohydrates ⓘ

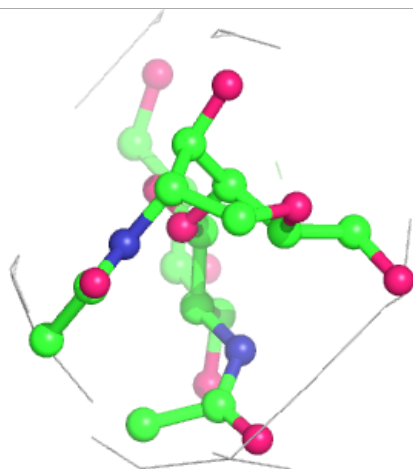
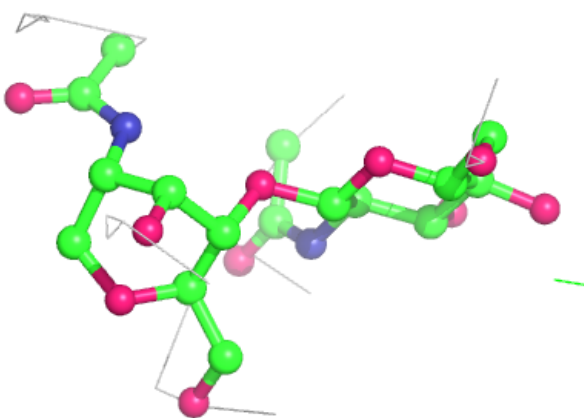
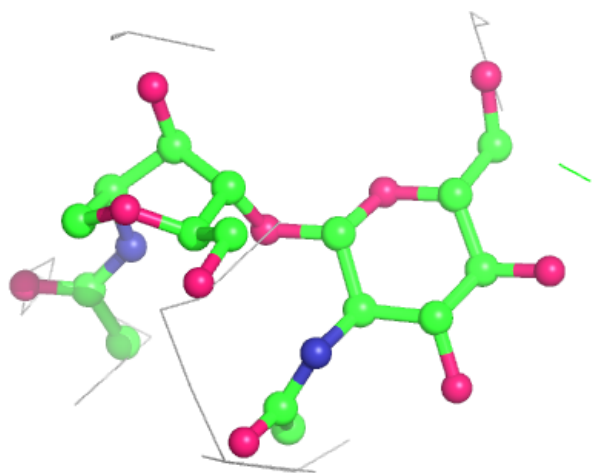
Unable to reproduce the depositors R factor - this section is therefore empty.

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.



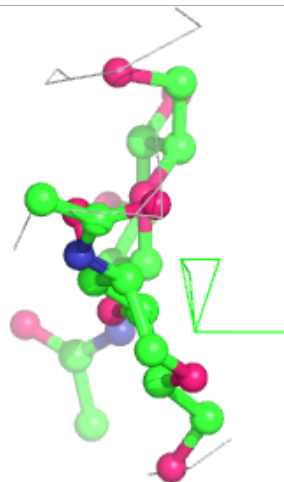
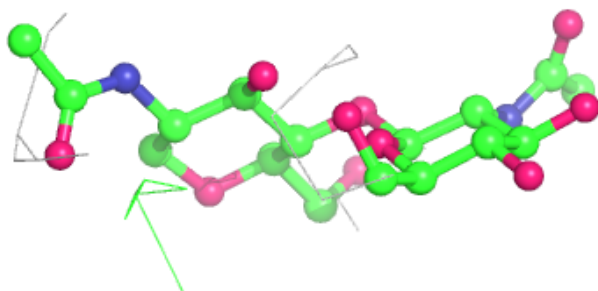
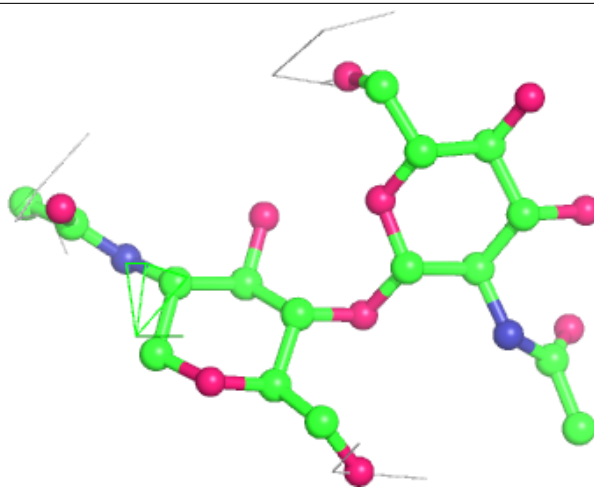
**Electron density around Chain P:**

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



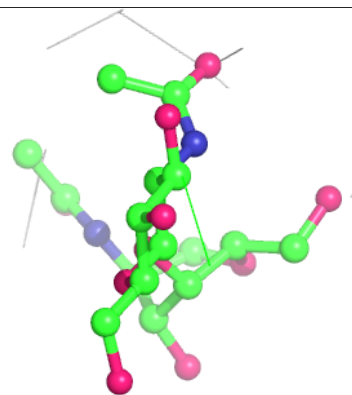
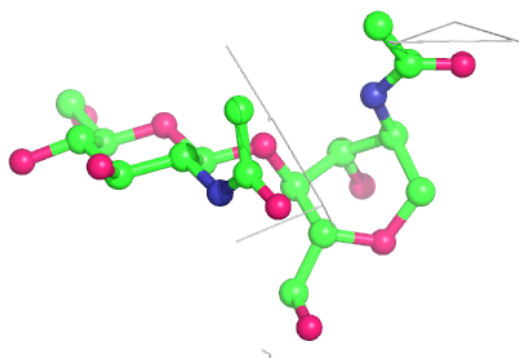
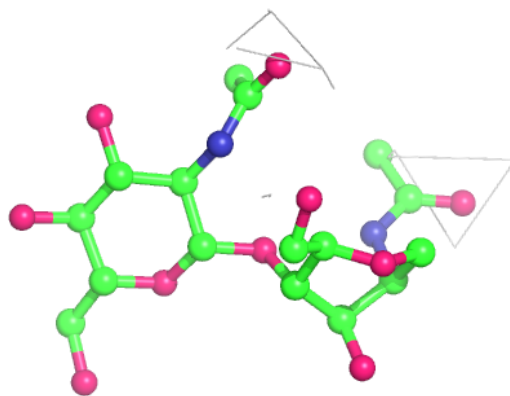
**Electron density around Chain T:**

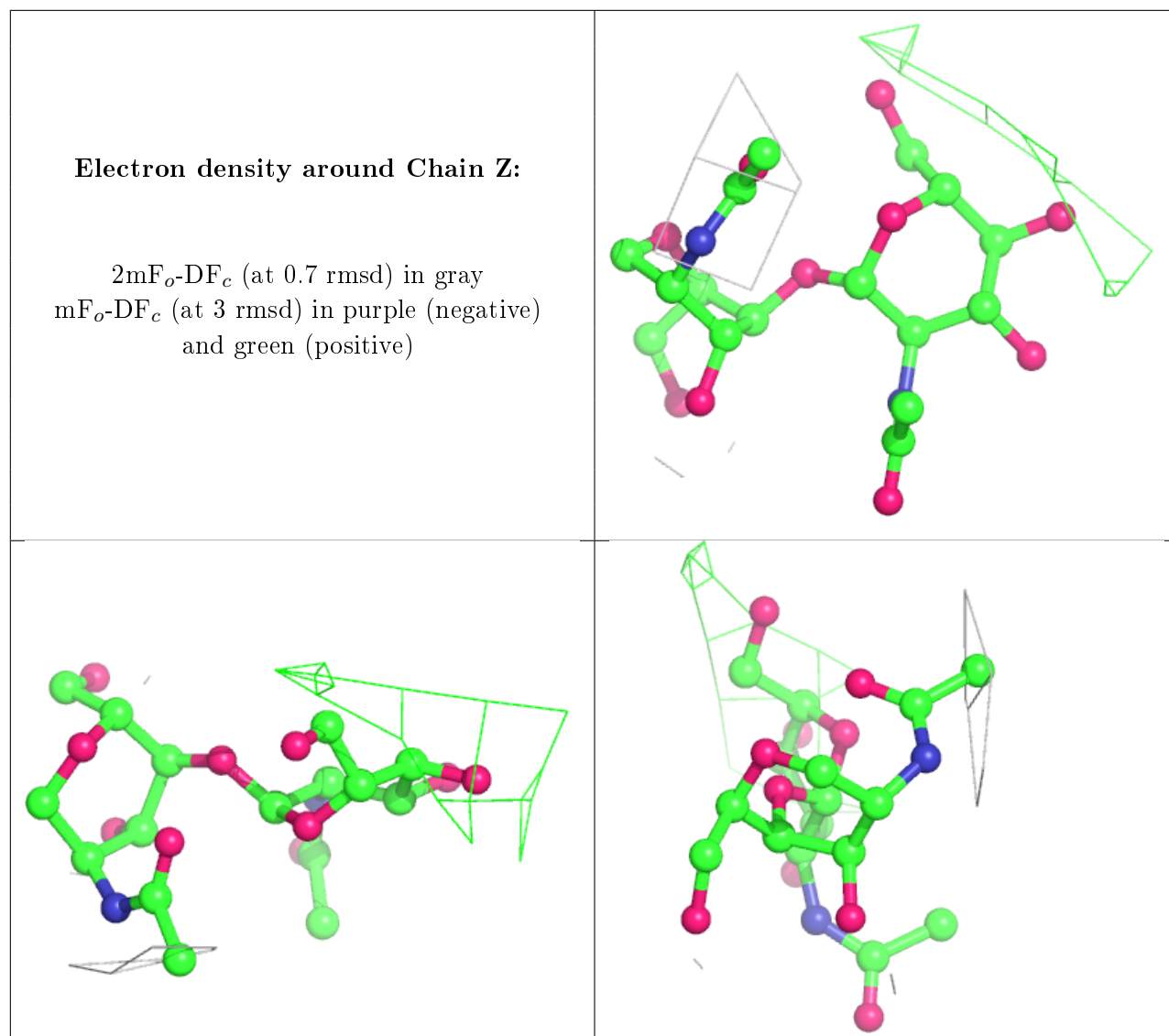
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**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)





## 6.4 Ligands ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

## 6.5 Other polymers ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.