



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 8, 2020 – 08:59 PM BST

PDB ID : 6VEP  
Title : Human insulin in complex with the human insulin microreceptor in turn in complex with Fv 83-7  
Authors : Lawrence, M.C.; Menting, J.G.T.  
Deposited on : 2020-01-02  
Resolution : 2.90 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.

---

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

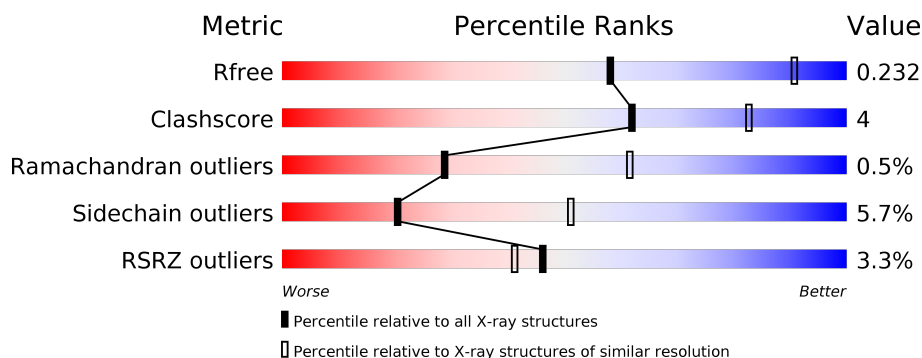
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	21	<div> <div style="width: 81%;"></div> <div style="width: 19%;"></div> </div> <div>81% 19%</div>
1	G	21	<div> <div style="width: 76%;"></div> <div style="width: 24%;"></div> </div> <div>76% 24%</div>
1	M	21	<div> <div style="width: 67%;"></div> <div style="width: 24%;"></div> <div style="width: 10%;"></div> </div> <div>67% 24% 10%</div>
1	S	21	<div> <div style="width: 67%;"></div> <div style="width: 24%;"></div> <div style="width: 10%;"></div> </div> <div>67% 24% 10%</div>
2	B	30	<div> <div style="width: 73%;"></div> <div style="width: 17%;"></div> <div style="width: 10%;"></div> </div> <div>73% 17% 10%</div>
2	H	30	<div> <div style="width: 73%;"></div> <div style="width: 10%;"></div> <div style="width: 17%;"></div> </div> <div>73% 10% 17%</div>




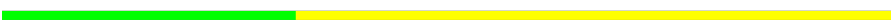

*Continued on next page...*

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	N	30	
2	T	30	
3	C	138	
3	I	138	
3	O	138	
3	U	138	
4	D	121	
4	J	121	
4	P	121	
4	V	121	
5	E	317	
5	K	317	
5	Q	317	
5	W	317	
6	F	16	
6	L	16	
6	R	16	
6	X	16	
7	Y	3	
7	c	3	
8	Z	4	
8	a	4	
8	f	4	
8	g	4	
8	j	4	

Continued on next page...

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
9	b	2	 100%
9	h	2	 100%
10	d	5	 40%60%
11	e	3	 33%67%
12	i	5	 40%60%

## 2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 19318 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 Insulin chain A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	21	Total	C	N	O	S	0	0	0
			163	99	25	35	4			
1	G	21	Total	C	N	O	S	0	0	0
			163	99	25	35	4			
1	M	21	Total	C	N	O	S	0	0	0
			163	99	25	35	4			
1	S	21	Total	C	N	O	S	0	0	0
			163	99	25	35	4			

- Molecule 2 is a protein called Insulin B chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	27	Total	C	N	O	S	0	0	0
			212	137	36	37	2			
2	H	25	Total	C	N	O	S	0	0	0
			200	129	34	35	2			
2	N	26	Total	C	N	O	S	0	0	0
			207	134	35	36	2			
2	T	26	Total	C	N	O	S	0	0	0
			207	134	35	36	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	121	Total	C	N	O	S	0	0	0
			925	582	156	182	5			
3	I	117	Total	C	N	O	S	0	0	0
			898	565	152	176	5			
3	O	122	Total	C	N	O	S	0	0	0
			932	587	157	183	5			
3	U	117	Total	C	N	O	S	0	0	0
			898	565	152	176	5			

- Molecule 4 is a protein called Fv 83-7 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	116	Total	C	N	O	S	0	0	0
			897	567	148	178	4			
4	J	113	Total	C	N	O	S	0	0	0
			881	559	145	173	4			
4	P	114	Total	C	N	O	S	0	0	0
			887	562	146	175	4			
4	V	114	Total	C	N	O	S	0	0	0
			881	558	145	174	4			

- Molecule 5 is a protein called Insulin receptor subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	293	Total	C	N	O	S	0	0	0
			2332	1467	403	428	34			
5	K	294	Total	C	N	O	S	0	0	0
			2339	1471	404	430	34			
5	Q	302	Total	C	N	O	S	0	0	0
			2400	1506	422	438	34			
5	W	296	Total	C	N	O	S	0	0	0
			2356	1481	408	433	34			

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

*Continued on next page...*

*Continued from previous page...*

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

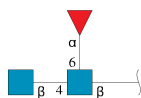
- Molecule 6 is a protein called Insulin receptor subunit beta.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	F	16	Total	C	N	O	0	0	0
			137	90	22	25			
6	L	16	Total	C	N	O	0	0	0
			137	90	22	25			
6	R	16	Total	C	N	O	0	0	0
			137	90	22	25			
6	X	16	Total	C	N	O	0	0	0
			137	90	22	25			

There are 8 discrepancies between the modelled and reference sequences:

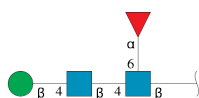
Chain	Residue	Modelled	Actual	Comment	Reference
F	718	PRO	LYS	conflict	UNP P06213
F	719	SER	THR	conflict	UNP P06213
L	718	PRO	LYS	conflict	UNP P06213
L	719	SER	THR	conflict	UNP P06213
R	718	PRO	LYS	conflict	UNP P06213
R	719	SER	THR	conflict	UNP P06213
X	718	PRO	LYS	conflict	UNP P06213
X	719	SER	THR	conflict	UNP P06213

- 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	Y	3	Total	C	N	O	0	0	0
			38	22	2	14			
7	c	3	Total	C	N	O	0	0	0
			38	22	2	14			

- Molecule 8 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
8	Z	4	Total	C	N	O	0	0	0
			49	28	2	19			
8	a	4	Total	C	N	O	0	0	0
			49	28	2	19			
8	f	4	Total	C	N	O	0	0	0
			49	28	2	19			
8	g	4	Total	C	N	O	0	0	0
			49	28	2	19			
8	j	4	Total	C	N	O	0	0	0
			49	28	2	19			

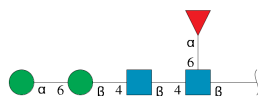
- Molecule 9 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	b	2	Total	C	N	O	0	0	0
			28	16	2	10			
9	h	2	Total	C	N	O	0	0	0
			28	16	2	10			



- Molecule 10 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-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.



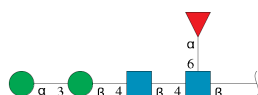
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	d	5	Total	C	N	O	0	0	0
			60	34	2	24			

- Molecule 11 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



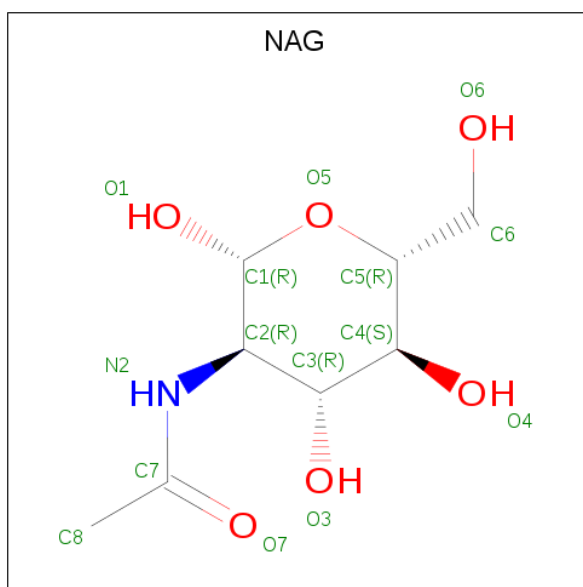
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	e	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 12 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-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
12	i	5	Total	C	N	O	0	0	0
			60	34	2	24			

- Molecule 13 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



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

- Molecule 14 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	C	4	Total	O	0	0
			4	4		
14	E	3	Total	O	0	0
			3	3		
14	I	1	Total	O	0	0
			1	1		
14	J	1	Total	O	0	0
			1	1		

*Continued on next page...*


*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	K	1	Total 1	O 1	0	0
14	O	2	Total 2	O 2	0	0
14	P	1	Total 1	O 1	0	0
14	Q	1	Total 1	O 1	0	0
14	R	1	Total 1	O 1	0	0
14	V	2	Total 2	O 2	0	0
14	W	1	Total 1	O 1	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: Insulin chain A

Chain A: 



- Molecule 1: Insulin chain A

Chain G: 



- Molecule 1: Insulin chain A

Chain M: 



- Molecule 1: Insulin chain A

Chain S: 



- Molecule 2: Insulin B chain

Chain B: 

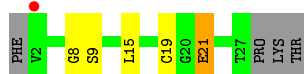


- Molecule 2: Insulin B chain

Chain H: 



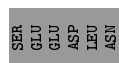
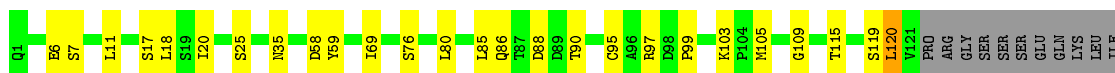
- Molecule 2: Insulin B chain



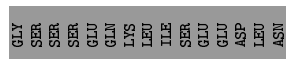
- Molecule 2: Insulin B chain



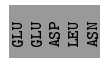
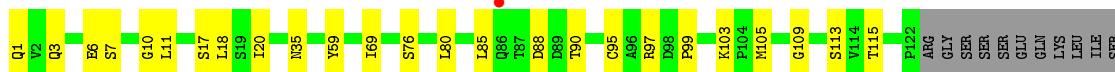
- Molecule 3: Fv 83-7 heavy chain



- Molecule 3: Fv 83-7 heavy chain

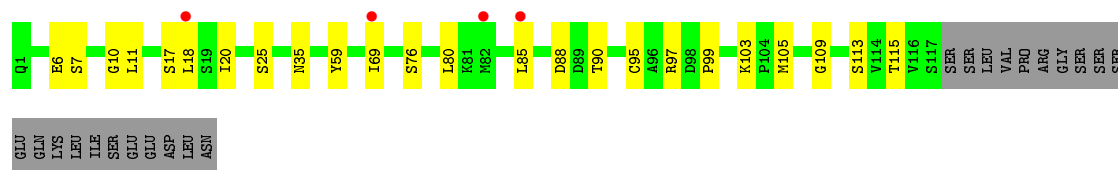


- Molecule 3: Fv 83-7 heavy chain

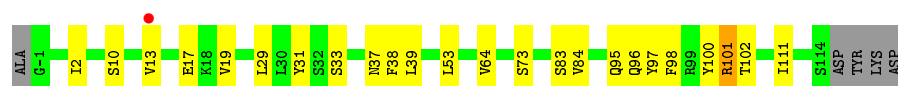
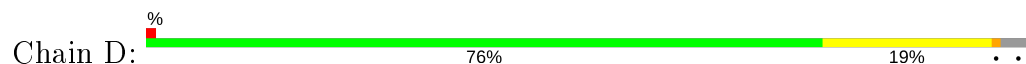


- Molecule 3: Fv 83-7 heavy chain

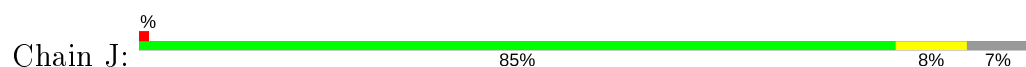




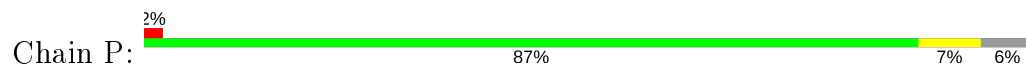
- Molecule 4: Fv 83-7 light chain



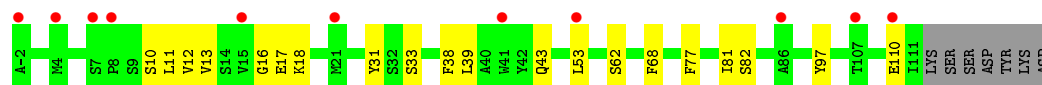
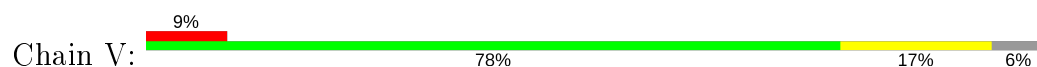
- Molecule 4: Fv 83-7 light chain



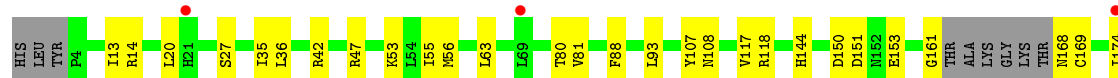
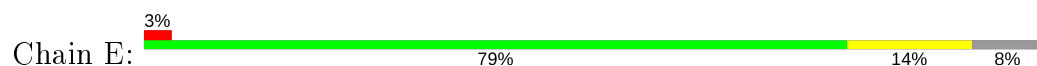
- Molecule 4: Fv 83-7 light chain



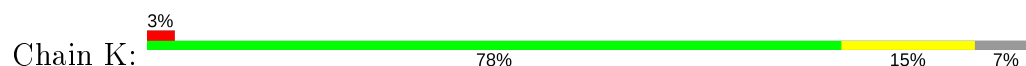
- Molecule 4: Fv 83-7 light chain

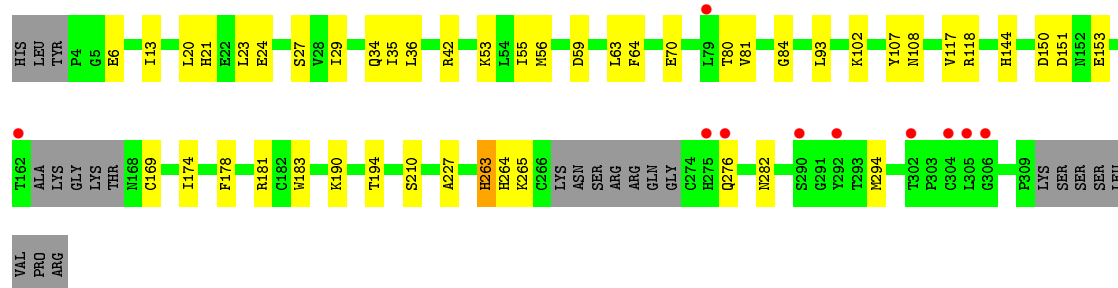


- Molecule 5: Insulin receptor subunit alpha

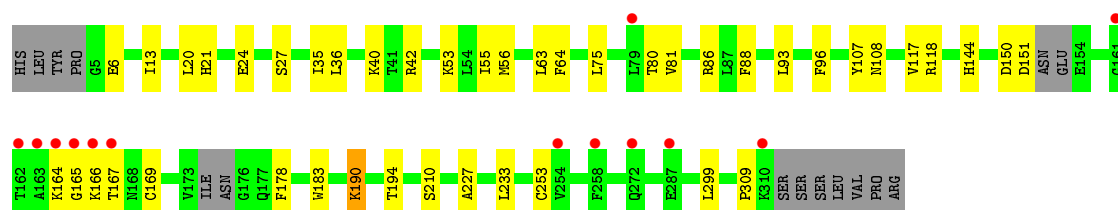
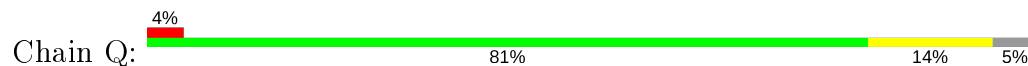


- Molecule 5: Insulin receptor subunit alpha

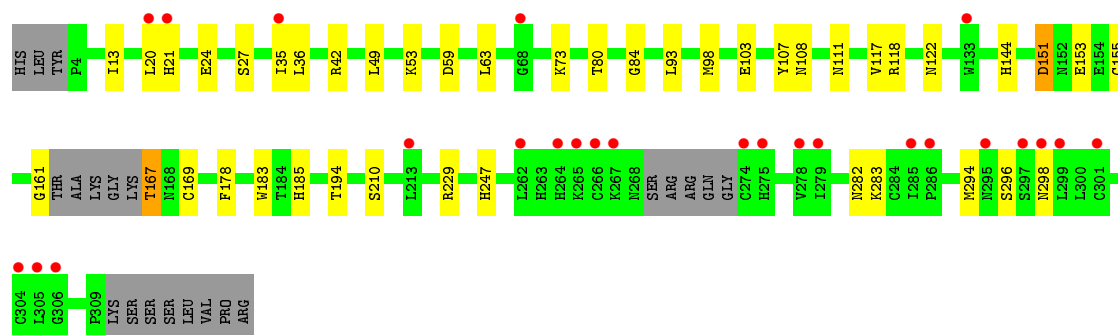
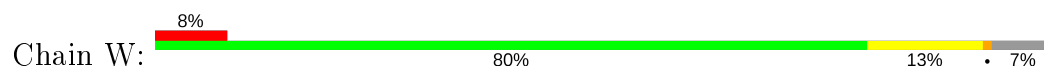




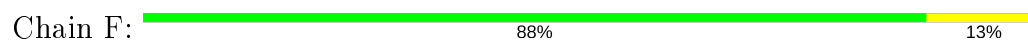
- Molecule 5: Insulin receptor subunit alpha



- Molecule 5: Insulin receptor subunit alpha




- Molecule 6: Insulin receptor subunit beta

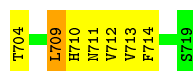


- Molecule 6: Insulin receptor subunit beta



- Molecule 6: Insulin receptor subunit beta

Chain R:  56% 38% 6%



- Molecule 6: Insulin receptor subunit beta

Chain X:  94% 6%



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

Chain Y:  33% 67%



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

Chain c:  67% 33%



- Molecule 8: 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%



- Molecule 8: 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 a:  75% 25%



- Molecule 8: 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 f:  25% 75%





- Molecule 8: 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 g:  75% 25%



- Molecule 8: 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 j:  50% 50%



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

Chain b:  100%



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

Chain h:  100%



- Molecule 10: alpha-D-mannopyranose-(1-6)-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 d:  40% 60%

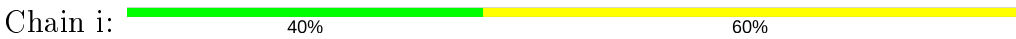


- Molecule 11: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain e:  33% 67%



- Molecule 12: alpha-D-mannopyranose-(1-3)-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



MAG1
MAG2
BCL3
MAL14
FUC5

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	100.03Å 130.12Å 148.18Å 90.00° 90.27° 90.00°	Depositor
Resolution (Å)	48.89 – 2.90 48.89 – 2.90	Depositor EDS
% Data completeness (in resolution range)	98.1 (48.89-2.90) 97.0 (48.89-2.90)	Depositor EDS
$R_{merge}$	0.26	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.06 (at 2.91Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, $R_{free}$	0.193 , 0.225 0.216 , 0.232	Depositor DCC
$R_{free}$ test set	4126 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	68.1	Xtriage
Anisotropy	0.622	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 65.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.127 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	19318	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	101.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.95% 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, BMA, NAG, MAN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	0.51	0/164	0.70	0/220
1	G	0.57	0/164	0.80	0/220
1	M	0.61	0/164	0.81	0/220
1	S	0.53	0/164	0.72	0/220
2	B	0.56	0/217	0.75	0/293
2	H	0.54	0/205	0.75	0/276
2	N	0.58	0/212	0.73	0/286
2	T	0.52	0/212	0.82	0/286
3	C	0.61	0/947	0.82	0/1287
3	I	0.55	0/920	0.75	0/1250
3	O	0.58	0/955	0.79	0/1299
3	U	0.52	0/920	0.74	0/1250
4	D	0.66	0/916	0.85	0/1236
4	J	0.50	0/900	0.71	0/1215
4	P	0.48	0/906	0.71	0/1223
4	V	0.43	0/900	0.66	0/1216
5	E	0.50	0/2389	0.72	0/3240
5	K	0.48	0/2396	0.72	0/3250
5	Q	0.49	0/2456	0.72	0/3324
5	W	0.49	0/2413	0.74	0/3272
6	F	0.55	0/142	0.72	0/193
6	L	0.59	0/142	0.81	0/193
6	R	0.70	0/142	0.84	0/193
6	X	0.62	0/142	0.70	0/193
All	All	0.52	0/19088	0.74	0/25855

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	163	0	149	0	0
1	G	163	0	149	2	0
1	M	163	0	149	3	0
1	S	163	0	149	3	0
2	B	212	0	198	3	0
2	H	200	0	184	1	0
2	N	207	0	193	4	0
2	T	207	0	193	2	0
3	C	925	0	904	11	0
3	I	898	0	874	10	0
3	O	932	0	911	10	0
3	U	898	0	874	9	0
4	D	897	0	882	17	0
4	J	881	0	869	4	0
4	P	887	0	874	3	0
4	V	881	0	864	12	0
5	E	2332	0	2221	19	0
5	K	2339	0	2228	19	0
5	Q	2400	0	2306	17	0
5	W	2356	0	2247	18	0
6	F	137	0	126	3	0
6	L	137	0	126	3	0
6	R	137	0	126	5	0
6	X	137	0	126	1	0
7	Y	38	0	34	2	0
7	c	38	0	34	0	0
8	Z	49	0	43	0	0
8	a	49	0	43	0	0
8	f	49	0	43	0	0
8	g	49	0	43	0	0
8	j	49	0	43	0	0
9	b	28	0	25	0	0
9	h	28	0	25	0	0
10	d	60	0	52	0	0
11	e	39	0	34	0	0
12	i	60	0	52	0	0
13	E	28	0	26	1	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	K	28	0	26	1	0
13	Q	42	0	39	2	0
13	W	14	0	13	1	0
14	C	4	0	0	0	0
14	E	3	0	0	0	0
14	I	1	0	0	0	0
14	J	1	0	0	0	0
14	K	1	0	0	0	0
14	O	2	0	0	0	0
14	P	1	0	0	0	0
14	Q	1	0	0	0	0
14	R	1	0	0	0	0
14	V	2	0	0	0	0
14	W	1	0	0	0	0
All	All	19318	0	18497	164	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 4.

The worst 5 of 164 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)
5:W:98:MET:H	5:W:122:ASN:HD22	1.27	0.81
4:V:12:VAL:HG22	4:V:110:GLU:HB2	1.63	0.80
4:V:43:GLN:HB2	4:V:53:LEU:HD11	1.69	0.74
2:N:8:GLY:HA2	6:R:710:HIS:HE1	1.52	0.74
4:D:96:GLN:O	4:D:101:ARG:HA	1.88	0.72

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	A	19/21 (90%)	17 (90%)	2 (10%)	0	100	100
1	G	19/21 (90%)	18 (95%)	1 (5%)	0	100	100
1	M	19/21 (90%)	17 (90%)	1 (5%)	1 (5%)	2	6
1	S	19/21 (90%)	17 (90%)	2 (10%)	0	100	100
2	B	25/30 (83%)	23 (92%)	2 (8%)	0	100	100
2	H	23/30 (77%)	20 (87%)	3 (13%)	0	100	100
2	N	24/30 (80%)	22 (92%)	2 (8%)	0	100	100
2	T	24/30 (80%)	22 (92%)	1 (4%)	1 (4%)	3	10
3	C	119/138 (86%)	111 (93%)	8 (7%)	0	100	100
3	I	115/138 (83%)	108 (94%)	7 (6%)	0	100	100
3	O	120/138 (87%)	113 (94%)	7 (6%)	0	100	100
3	U	115/138 (83%)	108 (94%)	7 (6%)	0	100	100
4	D	114/121 (94%)	104 (91%)	10 (9%)	0	100	100
4	J	111/121 (92%)	106 (96%)	5 (4%)	0	100	100
4	P	112/121 (93%)	106 (95%)	6 (5%)	0	100	100
4	V	112/121 (93%)	107 (96%)	5 (4%)	0	100	100
5	E	287/317 (90%)	271 (94%)	15 (5%)	1 (0%)	41	71
5	K	288/317 (91%)	270 (94%)	15 (5%)	3 (1%)	15	45
5	Q	296/317 (93%)	280 (95%)	14 (5%)	2 (1%)	22	54
5	W	290/317 (92%)	271 (93%)	15 (5%)	4 (1%)	11	36
6	F	14/16 (88%)	14 (100%)	0	0	100	100
6	L	14/16 (88%)	14 (100%)	0	0	100	100
6	R	14/16 (88%)	14 (100%)	0	0	100	100
6	X	14/16 (88%)	14 (100%)	0	0	100	100
All	All	2307/2572 (90%)	2167 (94%)	128 (6%)	12 (0%)	29	61

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	M	9	SER
5	W	298	ASN
5	K	265	LYS
5	W	151	ASP
5	W	153	GLU

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	20/20 (100%)	16 (80%)	4 (20%)	1	4
1	G	20/20 (100%)	18 (90%)	2 (10%)	7	23
1	M	20/20 (100%)	16 (80%)	4 (20%)	1	4
1	S	20/20 (100%)	16 (80%)	4 (20%)	1	4
2	B	22/26 (85%)	20 (91%)	2 (9%)	9	28
2	H	21/26 (81%)	19 (90%)	2 (10%)	8	26
2	N	22/26 (85%)	18 (82%)	4 (18%)	1	5
2	T	22/26 (85%)	19 (86%)	3 (14%)	3	11
3	C	104/120 (87%)	96 (92%)	8 (8%)	13	35
3	I	100/120 (83%)	92 (92%)	8 (8%)	12	33
3	O	105/120 (88%)	98 (93%)	7 (7%)	16	43
3	U	100/120 (83%)	94 (94%)	6 (6%)	19	49
4	D	102/106 (96%)	100 (98%)	2 (2%)	55	82
4	J	100/106 (94%)	97 (97%)	3 (3%)	41	75
4	P	101/106 (95%)	98 (97%)	3 (3%)	41	75
4	V	99/106 (93%)	96 (97%)	3 (3%)	41	75
5	E	272/293 (93%)	262 (96%)	10 (4%)	34	68
5	K	273/293 (93%)	262 (96%)	11 (4%)	31	65
5	Q	278/293 (95%)	262 (94%)	16 (6%)	20	50
5	W	275/293 (94%)	263 (96%)	12 (4%)	28	61
6	F	16/16 (100%)	16 (100%)	0	100	100
6	L	16/16 (100%)	14 (88%)	2 (12%)	4	14
6	R	16/16 (100%)	11 (69%)	5 (31%)	0	1
6	X	16/16 (100%)	16 (100%)	0	100	100
All	All	2140/2324 (92%)	2019 (94%)	121 (6%)	20	51

5 of 121 residues with a non-rotameric sidechain are listed below:



Mol	Chain	Res	Type
1	M	2	ILE
3	O	76	SER
5	W	73	LYS
1	M	13	LEU
2	N	21	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
6	L	710	HIS
5	Q	34	GLN
5	W	34	GLN
5	K	263	HIS
5	W	122	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 ⓘ

43 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
7	NAG	Y	1	5,7	14,14,15	0.38	0	17,19,21	1.26	2 (11%)
7	NAG	Y	2	7	14,14,15	0.42	0	17,19,21	0.97	1 (5%)
7	FUC	Y	3	7	10,10,11	0.50	0	14,14,16	0.83	1 (7%)
8	NAG	Z	1	8,5	14,14,15	0.34	0	17,19,21	1.01	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	NAG	Z	2	8	14,14,15	0.34	0	17,19,21	0.70	1 (5%)
8	BMA	Z	3	8	11,11,12	0.45	0	15,15,17	0.69	0
8	FUC	Z	4	8	10,10,11	0.51	0	14,14,16	0.80	0
8	NAG	a	1	8,5	14,14,15	0.33	0	17,19,21	0.64	0
8	NAG	a	2	8	14,14,15	0.27	0	17,19,21	1.04	2 (11%)
8	BMA	a	3	8	11,11,12	0.37	0	15,15,17	0.73	0
8	FUC	a	4	8	10,10,11	0.48	0	14,14,16	0.83	0
9	NAG	b	1	9,5	14,14,15	0.52	0	17,19,21	1.52	3 (17%)
9	NAG	b	2	9	14,14,15	0.32	0	17,19,21	0.90	1 (5%)
7	NAG	c	1	5,7	14,14,15	0.34	0	17,19,21	0.50	0
7	NAG	c	2	7	14,14,15	0.36	0	17,19,21	0.55	0
7	FUC	c	3	7	10,10,11	0.54	0	14,14,16	0.87	1 (7%)
10	NAG	d	1	10,5	14,14,15	0.41	0	17,19,21	0.70	0
10	NAG	d	2	10	14,14,15	0.30	0	17,19,21	0.90	1 (5%)
10	BMA	d	3	10	11,11,12	0.46	0	15,15,17	0.72	0
10	MAN	d	4	10	11,11,12	0.56	0	15,15,17	1.31	2 (13%)
10	FUC	d	5	10	10,10,11	0.45	0	14,14,16	0.91	1 (7%)
11	NAG	e	1	11,5	14,14,15	0.43	0	17,19,21	1.63	3 (17%)
11	NAG	e	2	11	14,14,15	0.41	0	17,19,21	1.39	4 (23%)
11	BMA	e	3	11	11,11,12	0.44	0	15,15,17	0.71	0
8	NAG	f	1	8,5	14,14,15	0.33	0	17,19,21	0.93	1 (5%)
8	NAG	f	2	8	14,14,15	0.32	0	17,19,21	1.02	2 (11%)
8	BMA	f	3	8	11,11,12	0.52	0	15,15,17	0.95	1 (6%)
8	FUC	f	4	8	10,10,11	0.40	0	14,14,16	0.73	0
8	NAG	g	1	8,5	14,14,15	0.32	0	17,19,21	0.65	0
8	NAG	g	2	8	14,14,15	0.36	0	17,19,21	0.64	1 (5%)
8	BMA	g	3	8	11,11,12	0.44	0	15,15,17	0.65	0
8	FUC	g	4	8	10,10,11	0.52	0	14,14,16	0.76	0
9	NAG	h	1	9,5	14,14,15	0.49	0	17,19,21	1.13	1 (5%)
9	NAG	h	2	9	14,14,15	0.37	0	17,19,21	1.06	3 (17%)
12	NAG	i	1	12,5	14,14,15	0.33	0	17,19,21	0.58	0
12	NAG	i	2	12	14,14,15	0.30	0	17,19,21	1.06	2 (11%)
12	BMA	i	3	12	11,11,12	0.44	0	15,15,17	0.73	0
12	MAN	i	4	12	11,11,12	0.51	0	15,15,17	0.77	1 (6%)
12	FUC	i	5	12	10,10,11	0.39	0	14,14,16	0.83	1 (7%)
8	NAG	j	1	8,5	14,14,15	0.41	0	17,19,21	0.70	0
8	NAG	j	2	8	14,14,15	0.33	0	17,19,21	1.07	1 (5%)
8	BMA	j	3	8	11,11,12	0.38	0	15,15,17	0.74	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	FUC	j	4	8	10,10,11	0.53	0	14,14,16	1.25	1 (7%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	Y	1	5,7	-	2/6/23/26	0/1/1/1
7	NAG	Y	2	7	-	1/6/23/26	0/1/1/1
7	FUC	Y	3	7	-	-	0/1/1/1
8	NAG	Z	1	8,5	-	0/6/23/26	0/1/1/1
8	NAG	Z	2	8	-	0/6/23/26	0/1/1/1
8	BMA	Z	3	8	-	0/2/19/22	0/1/1/1
8	FUC	Z	4	8	-	-	0/1/1/1
8	NAG	a	1	8,5	-	0/6/23/26	0/1/1/1
8	NAG	a	2	8	-	1/6/23/26	0/1/1/1
8	BMA	a	3	8	-	0/2/19/22	0/1/1/1
8	FUC	a	4	8	-	-	0/1/1/1
9	NAG	b	1	9,5	-	0/6/23/26	0/1/1/1
9	NAG	b	2	9	-	0/6/23/26	0/1/1/1
7	NAG	c	1	5,7	-	0/6/23/26	0/1/1/1
7	NAG	c	2	7	-	0/6/23/26	0/1/1/1
7	FUC	c	3	7	-	-	0/1/1/1
10	NAG	d	1	10,5	-	0/6/23/26	0/1/1/1
10	NAG	d	2	10	-	0/6/23/26	0/1/1/1
10	BMA	d	3	10	-	0/2/19/22	0/1/1/1
10	MAN	d	4	10	-	0/2/19/22	0/1/1/1
10	FUC	d	5	10	-	-	0/1/1/1
11	NAG	e	1	11,5	-	1/6/23/26	0/1/1/1
11	NAG	e	2	11	-	1/6/23/26	0/1/1/1
11	BMA	e	3	11	-	0/2/19/22	0/1/1/1
8	NAG	f	1	8,5	-	0/6/23/26	0/1/1/1
8	NAG	f	2	8	-	0/6/23/26	0/1/1/1
8	BMA	f	3	8	-	0/2/19/22	0/1/1/1
8	FUC	f	4	8	-	-	0/1/1/1
8	NAG	g	1	8,5	-	2/6/23/26	0/1/1/1
8	NAG	g	2	8	-	0/6/23/26	0/1/1/1
8	BMA	g	3	8	-	0/2/19/22	0/1/1/1
8	FUC	g	4	8	-	-	0/1/1/1
9	NAG	h	1	9,5	-	2/6/23/26	0/1/1/1
9	NAG	h	2	9	-	1/6/23/26	0/1/1/1

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	NAG	i	1	12,5	-	0/6/23/26	0/1/1/1
12	NAG	i	2	12	-	0/6/23/26	0/1/1/1
12	BMA	i	3	12	-	0/2/19/22	0/1/1/1
12	MAN	i	4	12	-	0/2/19/22	0/1/1/1
12	FUC	i	5	12	-	-	0/1/1/1
8	NAG	j	1	8,5	-	2/6/23/26	0/1/1/1
8	NAG	j	2	8	-	0/6/23/26	0/1/1/1
8	BMA	j	3	8	-	1/2/19/22	0/1/1/1
8	FUC	j	4	8	-	-	0/1/1/1

There are no bond length outliers.

The worst 5 of 39 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	e	1	NAG	C1-C2-N2	4.44	118.07	110.49
9	b	1	NAG	O5-C1-C2	-3.95	105.05	111.29
11	e	1	NAG	C2-N2-C7	3.88	128.43	122.90
10	d	4	MAN	C1-O5-C5	3.83	117.38	112.19
8	j	4	FUC	C1-C2-C3	3.53	114.00	109.67

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

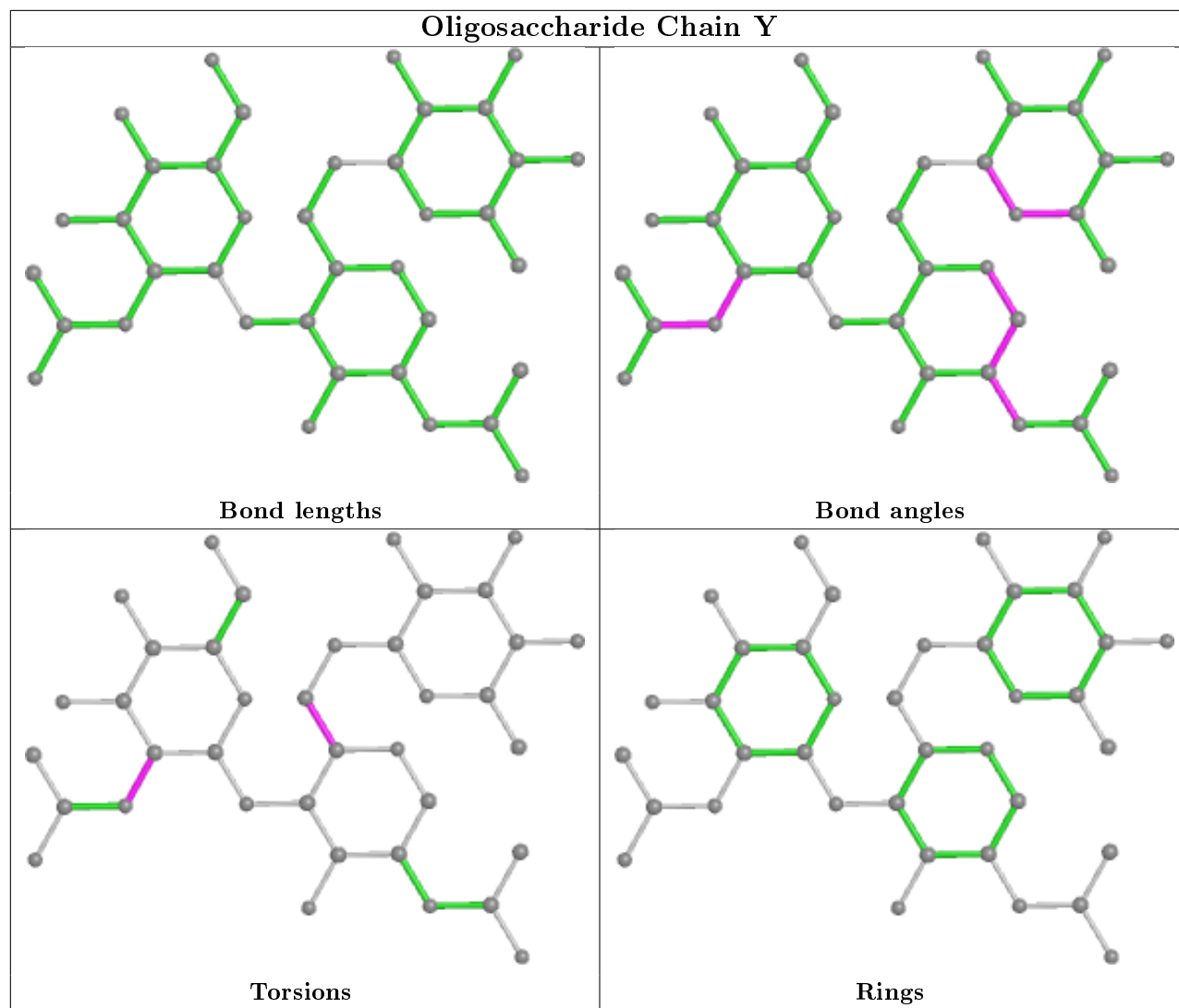
Mol	Chain	Res	Type	Atoms
7	Y	2	NAG	C3-C2-N2-C7
9	h	1	NAG	C1-C2-N2-C7
11	e	1	NAG	C1-C2-N2-C7
7	Y	1	NAG	O5-C5-C6-O6
8	j	1	NAG	O5-C5-C6-O6

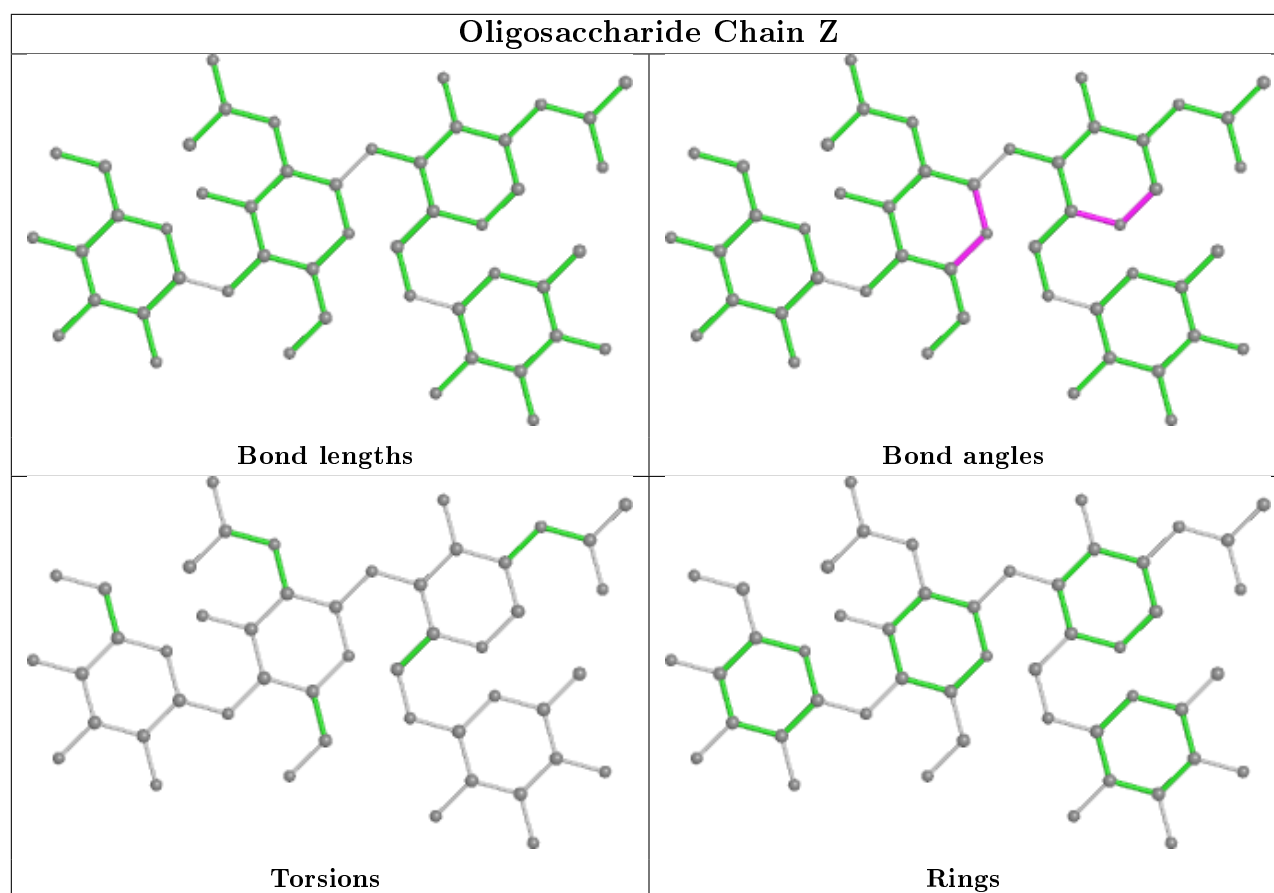
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	Y	3	FUC	2	0
7	Y	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](#)

8 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	$\# Z  > 2$
13	NAG	Q	401	5	14,14,15	0.42	0	17,19,21	1.58	3 (17%)
13	NAG	W	416	5	14,14,15	0.46	0	17,19,21	1.49	2 (11%)
13	NAG	Q	405	5	14,14,15	0.40	0	17,19,21	1.09	2 (11%)
13	NAG	K	407	5	14,14,15	0.30	0	17,19,21	0.97	1 (5%)
13	NAG	K	406	5	14,14,15	0.39	0	17,19,21	1.12	2 (11%)
13	NAG	E	409	5	14,14,15	0.36	0	17,19,21	0.74	1 (5%)
13	NAG	E	408	5	14,14,15	0.34	0	17,19,21	0.99	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
13	NAG	Q	406	5	14,14,15	0.34	0	17,19,21	0.76	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	NAG	Q	401	5	-	0/6/23/26	0/1/1/1
13	NAG	W	416	5	-	2/6/23/26	0/1/1/1
13	NAG	Q	405	5	-	0/6/23/26	0/1/1/1
13	NAG	K	407	5	-	2/6/23/26	0/1/1/1
13	NAG	K	406	5	-	0/6/23/26	0/1/1/1
13	NAG	E	409	5	-	2/6/23/26	0/1/1/1
13	NAG	E	408	5	-	2/6/23/26	0/1/1/1
13	NAG	Q	406	5	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	W	416	NAG	O5-C1-C2	-4.97	103.44	111.29
13	Q	401	NAG	O5-C1-C2	-4.58	104.05	111.29
13	Q	401	NAG	C1-C2-N2	3.59	116.61	110.49
13	Q	405	NAG	O5-C1-C2	-3.47	105.81	111.29
13	K	407	NAG	C1-O5-C5	3.32	116.69	112.19

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	W	416	NAG	C8-C7-N2-C2
13	W	416	NAG	O7-C7-N2-C2
13	K	407	NAG	O5-C5-C6-O6
13	Q	406	NAG	O5-C5-C6-O6
13	K	407	NAG	C4-C5-C6-O6

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	W	416	NAG	1	0
13	K	407	NAG	1	0
13	E	409	NAG	1	0
13	Q	406	NAG	2	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	21/21 (100%)	0.14	0 100 100	80, 98, 118, 123	0
1	G	21/21 (100%)	0.26	0 100 100	80, 96, 120, 126	0
1	M	21/21 (100%)	-0.01	0 100 100	63, 89, 107, 116	0
1	S	21/21 (100%)	0.11	0 100 100	58, 99, 120, 132	0
2	B	27/30 (90%)	0.18	0 100 100	80, 95, 116, 131	0
2	H	25/30 (83%)	0.18	0 100 100	73, 95, 122, 133	0
2	N	26/30 (86%)	0.27	1 (3%) 40 36	62, 84, 119, 125	0
2	T	26/30 (86%)	0.14	0 100 100	78, 101, 133, 147	0
3	C	121/138 (87%)	0.11	0 100 100	50, 75, 104, 121	0
3	I	117/138 (84%)	0.23	0 100 100	54, 77, 115, 122	0
3	O	122/138 (88%)	0.18	1 (0%) 86 86	68, 85, 113, 145	0
3	U	117/138 (84%)	0.23	4 (3%) 45 40	68, 96, 144, 158	0
4	D	116/121 (95%)	0.24	1 (0%) 84 84	39, 100, 158, 172	0
4	J	113/121 (93%)	0.11	1 (0%) 84 84	57, 100, 137, 176	0
4	P	114/121 (94%)	0.15	2 (1%) 68 67	72, 100, 127, 162	0
4	V	114/121 (94%)	0.34	11 (9%) 8 6	87, 128, 161, 181	0
5	E	293/317 (92%)	0.24	8 (2%) 54 50	60, 98, 160, 190	0
5	K	294/317 (92%)	0.29	10 (3%) 45 40	57, 96, 181, 204	0
5	Q	302/317 (95%)	0.37	13 (4%) 35 31	60, 96, 168, 189	0
5	W	296/317 (93%)	0.53	25 (8%) 11 8	63, 99, 187, 211	0
6	F	16/16 (100%)	0.47	0 100 100	65, 74, 118, 140	0
6	L	16/16 (100%)	0.72	1 (6%) 20 16	70, 81, 138, 153	0
6	R	16/16 (100%)	0.25	0 100 100	62, 77, 132, 143	0
6	X	16/16 (100%)	0.18	0 100 100	71, 81, 130, 156	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
All	All	2371/2572 (92%)	0.28	78 (3%) 46 41	39, 95, 158, 211	0

The worst 5 of 78 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	Q	162	THR	10.6
5	Q	163	ALA	9.1
5	W	299	LEU	7.3
5	K	304	CYS	6.9
5	W	275	HIS	6.8

## 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
8	BMA	g	3	11/12	0.62	0.22	176,181,182,183	0
12	MAN	i	4	11/12	0.67	0.19	161,165,167,168	0
11	BMA	e	3	11/12	0.70	0.22	183,186,187,187	0
8	BMA	Z	3	11/12	0.76	0.17	187,189,191,191	0
8	BMA	a	3	11/12	0.76	0.19	145,149,155,157	0
10	MAN	d	4	11/12	0.76	0.16	170,174,175,176	0
8	NAG	g	2	14/15	0.80	0.33	173,175,179,182	0
8	BMA	f	3	11/12	0.81	0.14	147,150,154,154	0
12	BMA	i	3	11/12	0.81	0.12	158,160,163,166	0
8	FUC	j	4	10/11	0.81	0.25	157,161,161,162	0
8	FUC	Z	4	10/11	0.81	0.31	157,159,160,160	0
8	NAG	Z	1	14/15	0.82	0.11	150,157,162,165	0
9	NAG	b	2	14/15	0.82	0.19	146,152,154,154	0
9	NAG	h	2	14/15	0.83	0.30	150,152,155,156	0
7	NAG	c	2	14/15	0.84	0.18	162,175,178,178	0
11	NAG	e	1	14/15	0.85	0.17	148,156,163,168	0
10	BMA	d	3	11/12	0.85	0.12	158,161,170,173	0

*Continued on next page...*

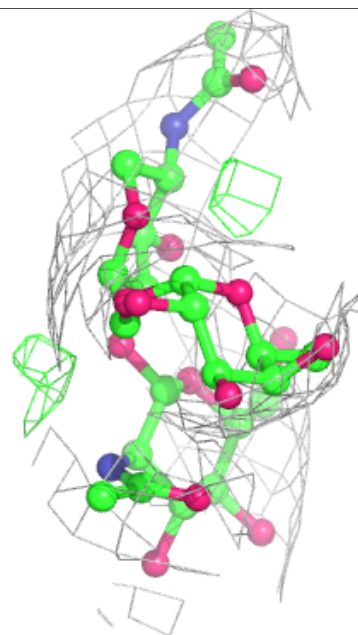
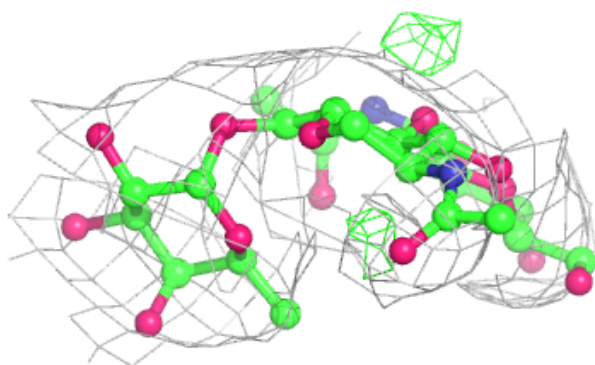
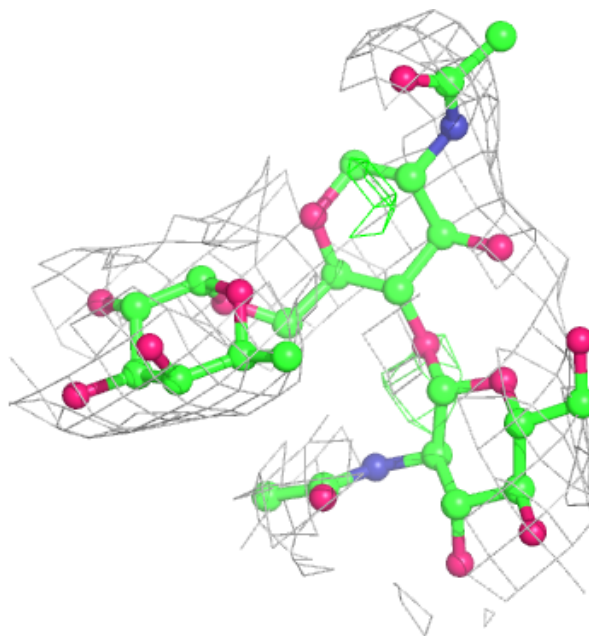
*Continued from previous page...*

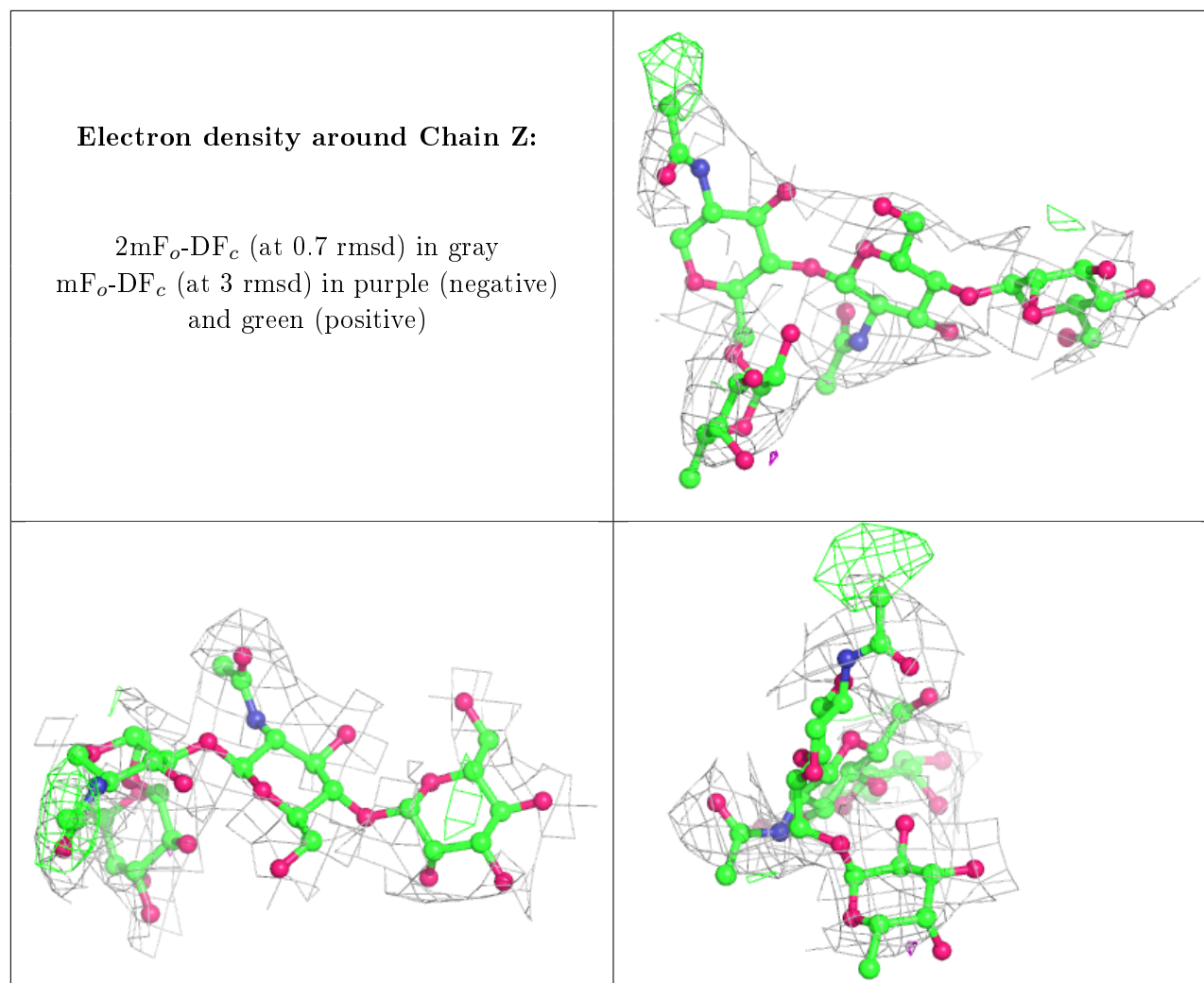
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
8	NAG	j	2	14/15	0.85	0.15	152,160,165,168	0
7	NAG	Y	2	14/15	0.85	0.15	158,160,162,163	0
9	NAG	b	1	14/15	0.86	0.14	113,137,140,144	0
8	NAG	j	1	14/15	0.87	0.14	148,150,157,160	0
8	FUC	g	4	10/11	0.87	0.17	169,170,171,172	0
8	BMA	j	3	11/12	0.88	0.13	167,169,170,170	0
8	NAG	g	1	14/15	0.88	0.16	146,158,168,169	0
11	NAG	e	2	14/15	0.88	0.17	166,170,176,182	0
8	NAG	f	2	14/15	0.89	0.16	109,127,134,142	0
8	NAG	Z	2	14/15	0.90	0.12	156,174,179,183	0
7	NAG	Y	1	14/15	0.90	0.12	140,145,154,154	0
9	NAG	h	1	14/15	0.91	0.18	121,129,135,143	0
7	NAG	c	1	14/15	0.91	0.13	155,163,173,177	0
12	NAG	i	1	14/15	0.91	0.16	115,117,121,124	0
12	NAG	i	2	14/15	0.92	0.13	131,136,144,152	0
7	FUC	Y	3	10/11	0.92	0.14	160,162,163,164	0
7	FUC	c	3	10/11	0.92	0.30	178,180,180,180	0
10	NAG	d	2	14/15	0.92	0.17	119,126,135,148	0
8	NAG	a	2	14/15	0.94	0.14	116,121,129,138	0
8	NAG	a	1	14/15	0.94	0.19	92,97,105,112	0
12	FUC	i	5	10/11	0.94	0.35	116,123,126,127	0
8	NAG	f	1	14/15	0.94	0.19	104,113,120,121	0
8	FUC	f	4	10/11	0.94	0.17	103,104,107,108	0
8	FUC	a	4	10/11	0.95	0.17	110,116,119,122	0
10	FUC	d	5	10/11	0.95	0.15	100,102,104,104	0
10	NAG	d	1	14/15	0.96	0.16	84,96,103,111	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 Y:**

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





## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
13	NAG	E	409	14/15	0.80	0.27	134,137,141,141	0
13	NAG	Q	401	14/15	0.82	0.18	114,120,122,122	0
13	NAG	K	407	14/15	0.87	0.21	113,120,124,125	0
13	NAG	W	416	14/15	0.88	0.20	74,80,91,95	0
13	NAG	Q	406	14/15	0.91	0.24	109,116,122,126	0
13	NAG	K	406	14/15	0.92	0.21	70,85,98,102	0
13	NAG	E	408	14/15	0.93	0.20	74,78,89,92	0
13	NAG	Q	405	14/15	0.94	0.16	80,90,92,92	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.