



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 8, 2020 – 10:42 PM BST

PDB ID : 5FEC  
Title : Crystal structure of 3BNC60 Fab germline precursor in complex with 426c.TM4deltaV1-3 gp120  
Authors : Scharf, L.; Bjorkman, P.J.  
Deposited on : 2015-12-16  
Resolution : 3.17 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

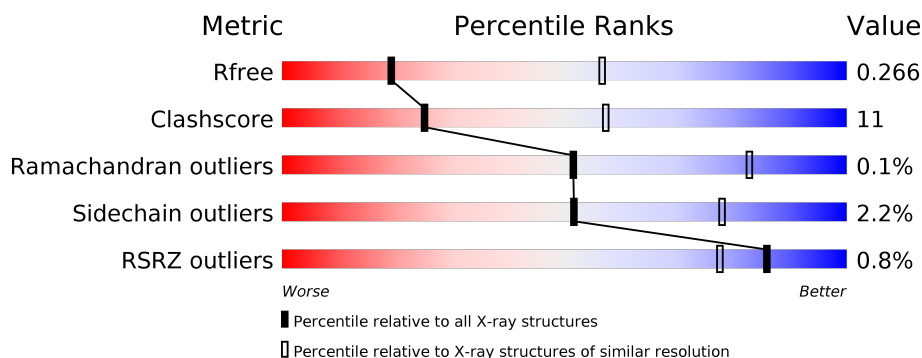
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.17 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	1467 (3.20-3.16)
Clashscore	141614	1599 (3.20-3.16)
Ramachandran outliers	138981	1574 (3.20-3.16)
Sidechain outliers	138945	1573 (3.20-3.16)
RSRZ outliers	127900	1423 (3.20-3.16)

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	230	<div> <div>71%</div> <div>21%</div> <div>7%</div> </div>
1	H	230	<div> <div>75%</div> <div>17%</div> <div>7%</div> </div>
2	B	210	<div> <div>70%</div> <div>29%</div> </div>
2	L	210	<div> <div>72%</div> <div>22%</div> </div>
3	C	353	<div> <div>77%</div> <div>18%</div> </div>
3	D	353	<div> <div>77%</div> <div>17%</div> <div>5%</div> </div>

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Mol	Chain	Length	Quality of chain
3	G	353	
3	I	353	
4	E	5	
5	F	4	
6	J	8	
7	K	2	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	BMA	F	3	-	-	-	X
5	MAN	F	4	-	-	-	X
6	MAN	J	8	-	-	-	X
8	NAG	C	604	-	-	-	X

## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 16613 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 germline 3BNC60 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	215	Total	C	N	O	S	0	0	0
			1614	1020	273	313	8			
1	A	214	Total	C	N	O	S	0	0	0
			1596	1008	268	312	8			

- Molecule 2 is a protein called germline 3BNC60 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	202	Total	C	N	O	S	0	0	0
			1486	932	242	307	5			
2	B	209	Total	C	N	O	S	0	0	0
			1549	969	254	321	5			

- Molecule 3 is a protein called 426c.TM4deltaV1-3 gp120.

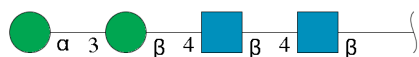
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	338	Total	C	N	O	S	0	0	0
			2536	1598	432	484	22			
3	D	337	Total	C	N	O	S	0	0	0
			2494	1574	428	470	22			
3	G	338	Total	C	N	O	S	0	0	0
			2508	1582	431	473	22			
3	I	329	Total	C	N	O	S	0	0	0
			2387	1502	409	455	21			

- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



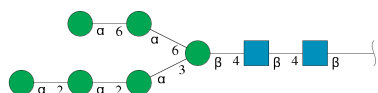
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	E	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



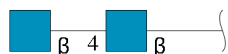
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	F	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 6 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)]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
6	J	8	Total	C	N	O	0	0	0
			94	52	2	40			

- Molecule 7 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
7	K	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 8 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
8	C	1	Total	C	N	O	0	0
			14	8	1	5		
8	C	1	Total	C	N	O	0	0
			14	8	1	5		
8	C	1	Total	C	N	O	0	0
			14	8	1	5		
8	C	1	Total	C	N	O	0	0
			14	8	1	5		
8	D	1	Total	C	N	O	0	0
			14	8	1	5		
8	D	1	Total	C	N	O	0	0
			14	8	1	5		
8	D	1	Total	C	N	O	0	0
			14	8	1	5		
8	D	1	Total	C	N	O	0	0
			14	8	1	5		
8	G	1	Total	C	N	O	0	0
			14	8	1	5		
8	G	1	Total	C	N	O	0	0
			14	8	1	5		
8	G	1	Total	C	N	O	0	0
			14	8	1	5		
8	G	1	Total	C	N	O	0	0
			14	8	1	5		
8	I	1	Total	C	N	O	0	0
			14	8	1	5		
8	I	1	Total	C	N	O	0	0
			14	8	1	5		

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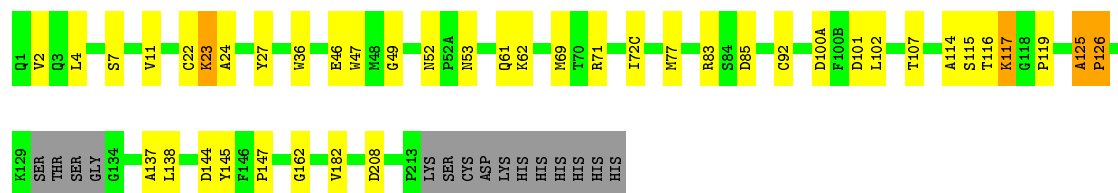
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
8	I	1	14	8	1	5	0	0

### 3 Residue-property plots

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.

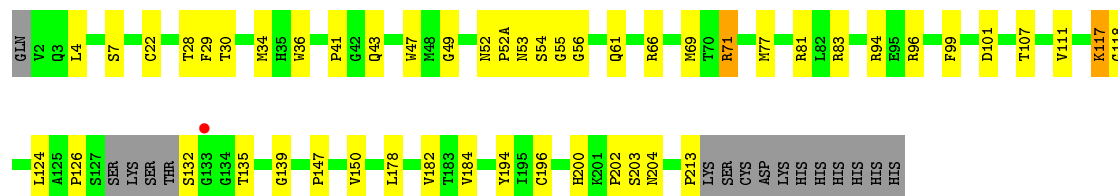
- Molecule 1: germline 3BNC60 heavy chain

Chain H: 



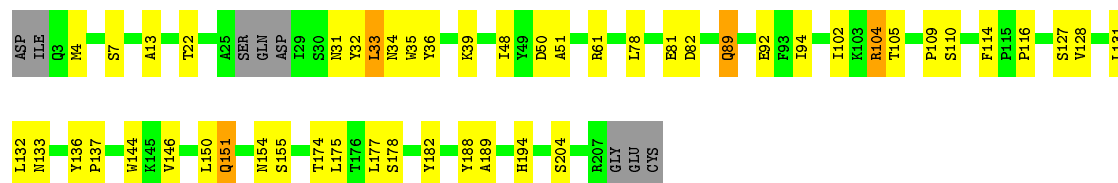
- Molecule 1: germline 3BNC60 heavy chain

Chain A: 



- Molecule 2: germline 3BNC60 light chain

Chain L: 

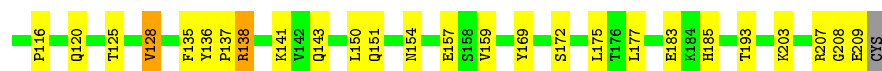


- Molecule 2: germline 3BNC60 light chain

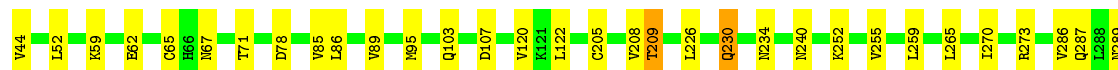
Chain B: 



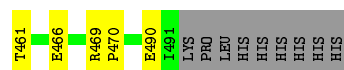
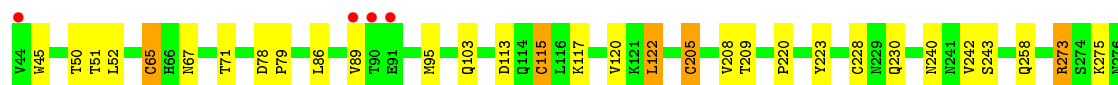
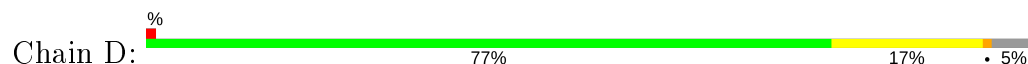




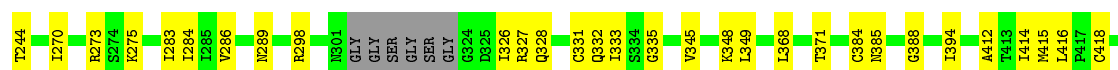
- Molecule 3: 426c.TM4deltaV1-3 gp120



- Molecule 3: 426c.TM4deltaV1-3 gp120

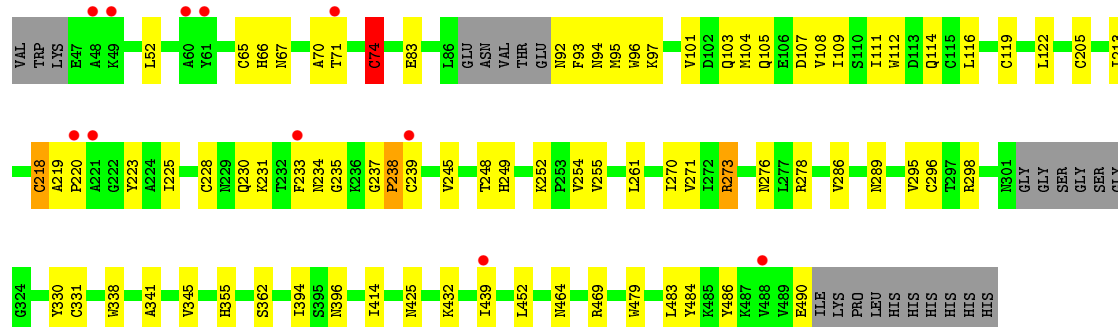


- Molecule 3: 426c.TM4deltaV1-3 gp120



- Molecule 3: 426c.TM4deltaV1-3 gp120





- Molecule 4: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E: 20% 80%



- Molecule 5: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F: 100%



- Molecule 6: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J: 75% 25%



- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K: 100%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	103.07Å 134.10Å 194.96Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.42 – 3.17 39.42 – 3.17	Depositor EDS
% Data completeness (in resolution range)	99.8 (39.42-3.17) 95.2 (39.42-3.17)	Depositor EDS
$R_{merge}$	0.56	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.10 (at 3.18Å)	Xtriage
Refinement program	PHENIX (1.10.1 _2155: ???)	Depositor
R, $R_{free}$	0.202 , 0.266 0.202 , 0.266	Depositor DCC
$R_{free}$ test set	1105 reflections (2.38%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	65.5	Xtriage
Anisotropy	0.059	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 33.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	16613	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.11% 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: 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	0.83	3/1638 (0.2%)	0.79	1/2239 (0.0%)
1	H	0.87	1/1656 (0.1%)	0.86	6/2261 (0.3%)
2	B	0.76	0/1583	0.76	2/2165 (0.1%)
2	L	0.77	0/1519	0.73	0/2079
3	C	0.77	2/2589 (0.1%)	0.82	8/3531 (0.2%)
3	D	0.82	2/2545 (0.1%)	0.76	3/3472 (0.1%)
3	G	0.83	3/2560 (0.1%)	0.77	1/3493 (0.0%)
3	I	0.69	1/2436 (0.0%)	0.79	4/3334 (0.1%)
All	All	0.79	12/16526 (0.1%)	0.79	25/22574 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	C	0	1

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	65	CYS	CB-SG	13.70	2.05	1.82
3	C	205	CYS	CB-SG	-10.75	1.64	1.82
1	A	182	VAL	CB-CG1	-8.53	1.34	1.52
1	H	22	CYS	CB-SG	-7.20	1.70	1.82
3	I	65	CYS	CB-SG	6.80	1.93	1.82

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	273	ARG	NE-CZ-NH2	10.25	125.42	120.30
3	C	65	CYS	CA-CB-SG	-8.96	97.88	114.00
3	D	65	CYS	CA-CB-SG	-7.82	99.93	114.00
3	I	273	ARG	NE-CZ-NH1	-7.78	116.41	120.30
3	G	115	CYS	CA-CB-SG	-7.62	100.29	114.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	396	ASN	Peptide

## 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	1596	0	1509	38	0
1	H	1614	0	1539	22	0
2	B	1549	0	1421	47	0
2	L	1486	0	1350	37	0
3	C	2536	0	2378	39	0
3	D	2494	0	2338	44	0
3	G	2508	0	2350	54	0
3	I	2387	0	2173	63	0
4	E	61	0	52	4	0
5	F	50	0	43	5	0
6	J	94	0	79	1	0
7	K	28	0	25	4	0
8	C	56	0	52	0	0
8	D	56	0	52	2	0
8	G	56	0	52	7	0
8	I	42	0	39	3	0
All	All	16613	0	15452	341	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 11.

The worst 5 of 341 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)
3:D:65:CYS:CB	3:D:65:CYS:SG	2.05	1.43
1:A:7:SER:O	1:A:107:THR:HG22	1.51	1.09
1:A:7:SER:O	1:A:107:THR:CG2	2.07	1.03
1:H:126:PRO:HB3	1:H:137:ALA:O	1.66	0.95
3:G:95:MET:HE1	3:G:273:ARG:HB3	1.51	0.92

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	210/230 (91%)	202 (96%)	8 (4%)	0	100	100
1	H	211/230 (92%)	204 (97%)	6 (3%)	1 (0%)	29	66
2	B	207/210 (99%)	199 (96%)	8 (4%)	0	100	100
2	L	198/210 (94%)	192 (97%)	6 (3%)	0	100	100
3	C	334/353 (95%)	325 (97%)	9 (3%)	0	100	100
3	D	333/353 (94%)	324 (97%)	9 (3%)	0	100	100
3	G	334/353 (95%)	325 (97%)	9 (3%)	0	100	100
3	I	323/353 (92%)	313 (97%)	9 (3%)	1 (0%)	41	73
All	All	2150/2292 (94%)	2084 (97%)	64 (3%)	2 (0%)	51	83

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	126	PRO
3	I	238	PRO

### 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	173/196 (88%)	169 (98%)	4 (2%)	50	77
1	H	175/196 (89%)	170 (97%)	5 (3%)	42	72
2	B	167/186 (90%)	162 (97%)	5 (3%)	41	72
2	L	159/186 (86%)	152 (96%)	7 (4%)	28	62
3	C	270/311 (87%)	265 (98%)	5 (2%)	57	80
3	D	261/311 (84%)	258 (99%)	3 (1%)	73	88
3	G	264/311 (85%)	261 (99%)	3 (1%)	73	88
3	I	244/311 (78%)	238 (98%)	6 (2%)	47	76
All	All	1713/2008 (85%)	1675 (98%)	38 (2%)	52	78

5 of 38 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	92	GLU
3	C	59	LYS
3	I	218	CYS
2	B	177	LEU
3	C	230	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 ⓘ

19 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
4	NAG	E	1	3,4	14,14,15	1.21	1 (7%)	17,19,21	1.72	4 (23%)
4	NAG	E	2	4	14,14,15	1.26	1 (7%)	17,19,21	1.09	1 (5%)
4	BMA	E	3	4	11,11,12	1.52	3 (27%)	15,15,17	1.08	1 (6%)
4	MAN	E	4	4	11,11,12	1.66	2 (18%)	15,15,17	1.59	3 (20%)
4	MAN	E	5	4	11,11,12	1.84	4 (36%)	15,15,17	2.12	5 (33%)
5	NAG	F	1	3,5	14,14,15	0.62	0	17,19,21	1.97	2 (11%)
5	NAG	F	2	5	14,14,15	1.55	2 (14%)	17,19,21	1.80	3 (17%)
5	BMA	F	3	5	11,11,12	2.28	4 (36%)	15,15,17	2.09	7 (46%)
5	MAN	F	4	5	11,11,12	4.02	6 (54%)	15,15,17	1.98	5 (33%)
6	NAG	J	1	3,6	14,14,15	0.86	1 (7%)	17,19,21	1.20	3 (17%)
6	NAG	J	2	6	14,14,15	1.29	1 (7%)	17,19,21	1.37	3 (17%)
6	BMA	J	3	6	11,11,12	1.57	2 (18%)	15,15,17	1.85	6 (40%)
6	MAN	J	4	6	11,11,12	2.30	5 (45%)	15,15,17	1.34	1 (6%)
6	MAN	J	5	6	11,11,12	3.46	7 (63%)	15,15,17	3.16	9 (60%)
6	MAN	J	6	6	11,11,12	1.91	6 (54%)	15,15,17	1.55	3 (20%)
6	MAN	J	7	6	11,11,12	2.68	5 (45%)	15,15,17	1.79	6 (40%)
6	MAN	J	8	6	11,11,12	2.66	5 (45%)	15,15,17	1.70	4 (26%)
7	NAG	K	1	3,7	14,14,15	0.35	0	17,19,21	1.55	1 (5%)
7	NAG	K	2	7	14,14,15	1.19	1 (7%)	17,19,21	0.99	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
4	NAG	E	1	3,4	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	E	2	4	-	0/6/23/26	0/1/1/1
4	BMA	E	3	4	-	0/2/19/22	0/1/1/1
4	MAN	E	4	4	-	0/2/19/22	0/1/1/1
4	MAN	E	5	4	-	2/2/19/22	0/1/1/1
5	NAG	F	1	3,5	-	1/6/23/26	0/1/1/1
5	NAG	F	2	5	-	0/6/23/26	0/1/1/1
5	BMA	F	3	5	-	0/2/19/22	0/1/1/1
5	MAN	F	4	5	-	1/2/19/22	0/1/1/1
6	NAG	J	1	3,6	-	2/6/23/26	0/1/1/1
6	NAG	J	2	6	-	0/6/23/26	0/1/1/1
6	BMA	J	3	6	-	0/2/19/22	0/1/1/1
6	MAN	J	4	6	-	0/2/19/22	0/1/1/1
6	MAN	J	5	6	-	0/2/19/22	0/1/1/1
6	MAN	J	6	6	-	0/2/19/22	0/1/1/1
6	MAN	J	7	6	-	2/2/19/22	0/1/1/1
6	MAN	J	8	6	-	2/2/19/22	0/1/1/1
7	NAG	K	1	3,7	-	1/6/23/26	0/1/1/1
7	NAG	K	2	7	-	2/6/23/26	0/1/1/1

The worst 5 of 56 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	4	MAN	C2-C3	7.79	1.64	1.52
5	F	4	MAN	O5-C5	7.01	1.57	1.43
6	J	5	MAN	C4-C5	6.77	1.67	1.53
6	J	5	MAN	O3-C3	5.31	1.55	1.43
6	J	8	MAN	C2-C3	5.26	1.60	1.52

The worst 5 of 68 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	1	NAG	C1-O5-C5	6.80	121.40	112.19
6	J	5	MAN	C2-C3-C4	-5.91	100.67	110.89
4	E	5	MAN	O5-C1-C2	5.55	119.34	110.77
7	K	1	NAG	C1-O5-C5	5.49	119.63	112.19
5	F	4	MAN	O5-C5-C6	5.00	115.05	107.20

There are no chirality outliers.

5 of 15 torsion outliers are listed below:

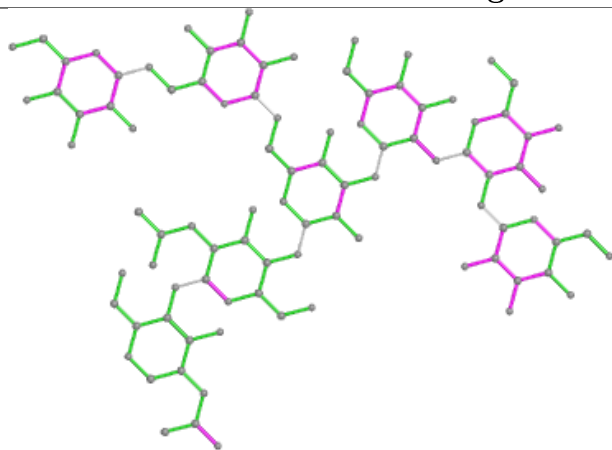
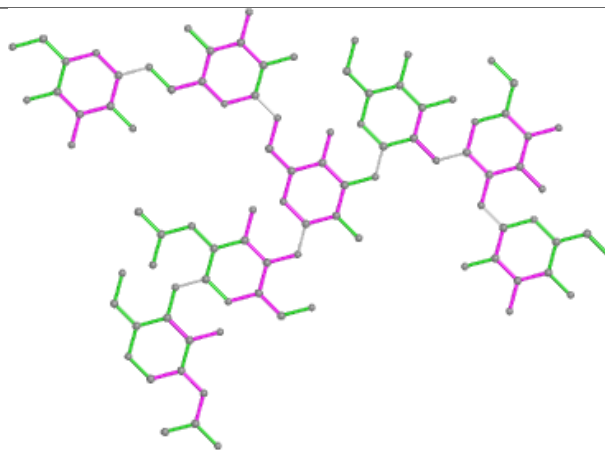
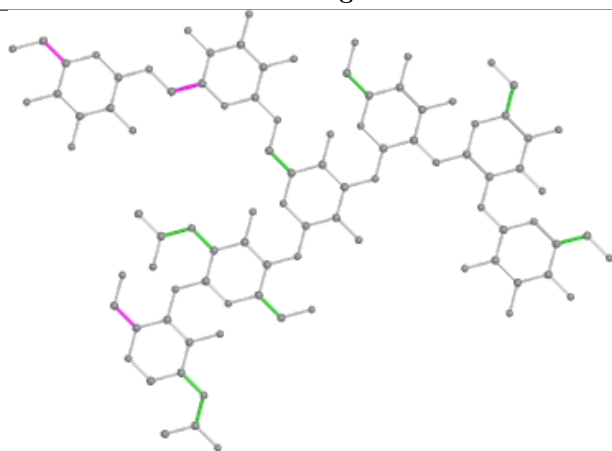
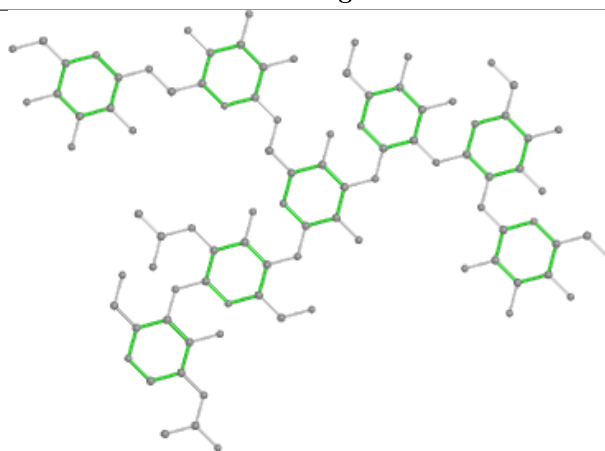
Mol	Chain	Res	Type	Atoms
6	J	1	NAG	O5-C5-C6-O6
6	J	1	NAG	C4-C5-C6-O6
6	J	8	MAN	C4-C5-C6-O6
6	J	8	MAN	O5-C5-C6-O6
7	K	2	NAG	O5-C5-C6-O6

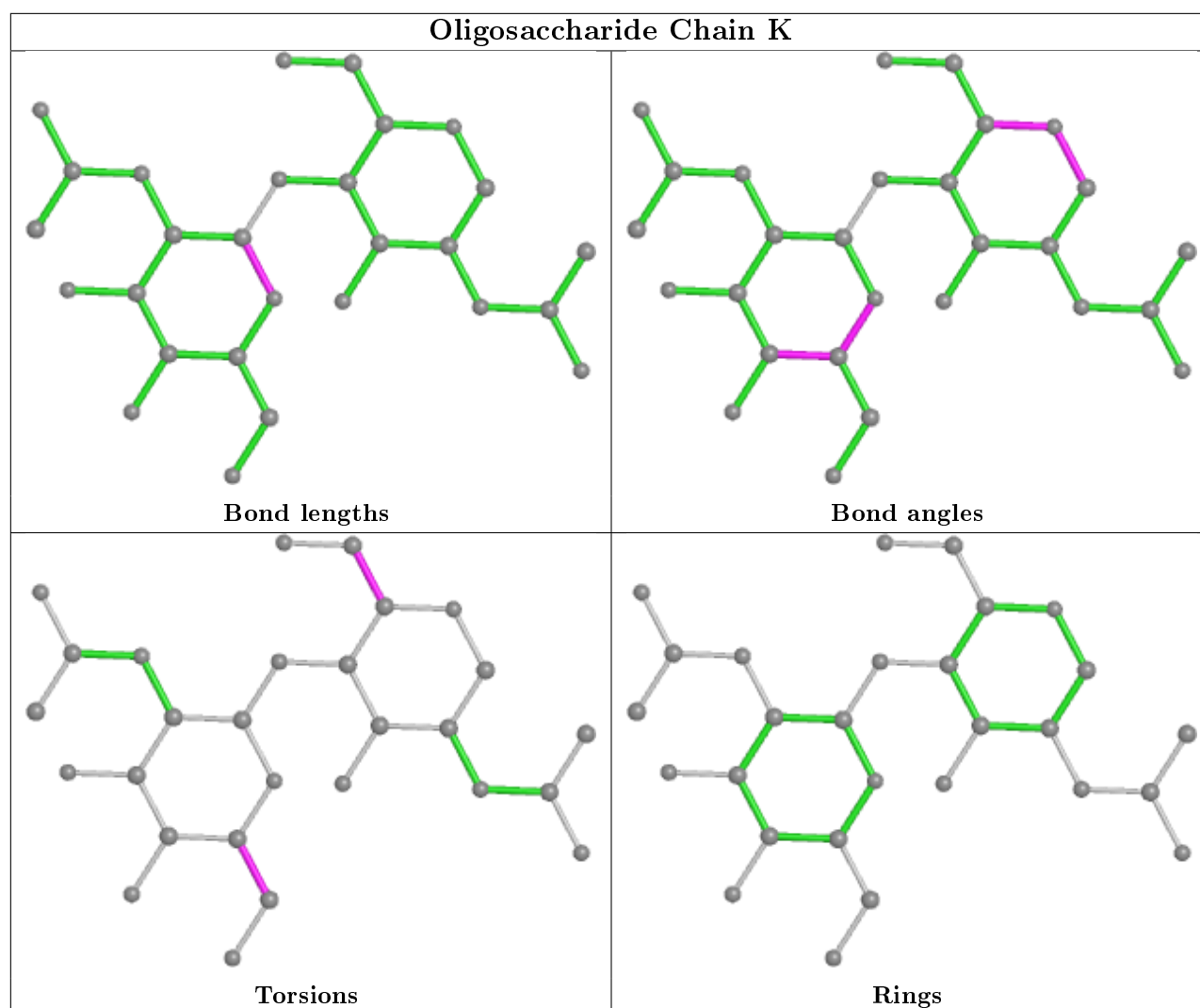
There are no ring outliers.

12 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	F	4	MAN	3	0
4	E	4	MAN	1	0
7	K	2	NAG	2	0
6	J	1	NAG	1	0
7	K	1	NAG	4	0
4	E	1	NAG	2	0
6	J	2	NAG	1	0
4	E	2	NAG	2	0
5	F	3	BMA	1	0
5	F	2	NAG	2	0
5	F	1	NAG	1	0
4	E	3	BMA	1	0

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

**Oligosaccharide Chain J****Bond lengths****Bond angles****Torsions****Rings**



## 5.6 Ligand geometry ⓘ

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$
8	NAG	C	601	3	14,14,15	0.94	1 (7%)	17,19,21	0.80	0
8	NAG	G	601	3	14,14,15	1.00	1 (7%)	17,19,21	0.72	0
8	NAG	D	601	3	14,14,15	1.73	2 (14%)	17,19,21	0.74	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	NAG	C	604	3	14,14,15	0.56	0	17,19,21	0.80	0
8	NAG	I	603	3	14,14,15	1.09	2 (14%)	17,19,21	0.72	0
8	NAG	D	602	3	14,14,15	0.81	1 (7%)	17,19,21	0.76	0
8	NAG	C	603	3	14,14,15	0.63	0	17,19,21	0.83	0
8	NAG	D	603	3	14,14,15	1.11	1 (7%)	17,19,21	0.80	1 (5%)
8	NAG	G	603	3	14,14,15	0.91	1 (7%)	17,19,21	1.35	1 (5%)
8	NAG	G	604	3	14,14,15	0.20	0	17,19,21	1.13	1 (5%)
8	NAG	I	601	3	14,14,15	0.89	1 (7%)	17,19,21	1.38	4 (23%)
8	NAG	C	602	3	14,14,15	0.28	0	17,19,21	0.77	0
8	NAG	I	602	3	14,14,15	0.36	0	17,19,21	0.49	0
8	NAG	D	604	3	14,14,15	0.59	0	17,19,21	0.87	1 (5%)
8	NAG	G	602	3	14,14,15	1.35	1 (7%)	17,19,21	0.97	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
8	NAG	C	601	3	-	4/6/23/26	0/1/1/1
8	NAG	G	601	3	-	2/6/23/26	0/1/1/1
8	NAG	D	601	3	-	4/6/23/26	0/1/1/1
8	NAG	C	604	3	-	2/6/23/26	0/1/1/1
8	NAG	I	603	3	-	2/6/23/26	0/1/1/1
8	NAG	D	602	3	-	0/6/23/26	0/1/1/1
8	NAG	C	603	3	-	1/6/23/26	0/1/1/1
8	NAG	D	603	3	-	0/6/23/26	0/1/1/1
8	NAG	G	603	3	-	1/6/23/26	0/1/1/1
8	NAG	G	604	3	-	0/6/23/26	0/1/1/1
8	NAG	I	601	3	-	4/6/23/26	0/1/1/1
8	NAG	C	602	3	-	0/6/23/26	0/1/1/1
8	NAG	I	602	3	-	2/6/23/26	0/1/1/1
8	NAG	D	604	3	-	0/6/23/26	0/1/1/1
8	NAG	G	602	3	-	3/6/23/26	0/1/1/1

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	D	601	NAG	O5-C1	-5.07	1.35	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	G	602	NAG	O5-C1	-4.70	1.36	1.43
8	D	603	NAG	O5-C1	-3.88	1.37	1.43
8	D	601	NAG	C1-C2	-3.84	1.46	1.52
8	G	601	NAG	O5-C1	3.55	1.49	1.43

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	G	603	NAG	C1-O5-C5	4.46	118.24	112.19
8	G	604	NAG	C1-O5-C5	4.17	117.84	112.19
8	I	601	NAG	O3-C3-C2	2.54	114.73	109.47
8	I	601	NAG	O4-C4-C3	-2.36	104.90	110.35
8	D	604	NAG	O3-C3-C2	2.26	114.14	109.47

There are no chirality outliers.

5 of 25 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	C	601	NAG	C3-C2-N2-C7
8	I	601	NAG	C1-C2-N2-C7
8	G	602	NAG	C3-C2-N2-C7
8	C	601	NAG	O5-C5-C6-O6
8	I	601	NAG	O5-C5-C6-O6

There are no ring outliers.

5 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	G	601	NAG	3	0
8	D	601	NAG	2	0
8	G	603	NAG	4	0
8	I	601	NAG	2	0
8	I	602	NAG	1	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 [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	214/230 (93%)	-0.35	1 (0%) 91 86	30, 54, 79, 151	0
1	H	215/230 (93%)	-0.48	0 100 100	27, 50, 90, 134	0
2	B	209/210 (99%)	-0.41	0 100 100	35, 59, 95, 155	0
2	L	202/210 (96%)	-0.31	0 100 100	39, 68, 99, 122	0
3	C	338/353 (95%)	-0.30	0 100 100	31, 60, 99, 162	0
3	D	337/353 (95%)	-0.29	4 (1%) 79 67	34, 61, 100, 136	0
3	G	338/353 (95%)	-0.35	1 (0%) 94 92	32, 62, 105, 182	0
3	I	329/353 (93%)	-0.06	11 (3%) 46 30	43, 82, 133, 180	0
All	All	2182/2292 (95%)	-0.30	17 (0%) 86 77	27, 62, 109, 182	0

The worst 5 of 17 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	I	60	ALA	4.4
3	I	221	ALA	3.7
3	D	44	VAL	3.4
3	D	90	THR	3.3
3	I	239	CYS	3.2

### 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,



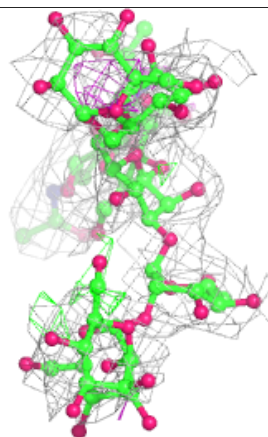
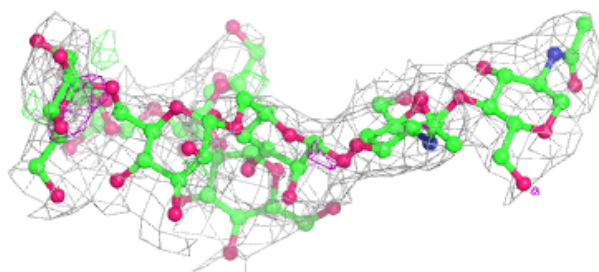
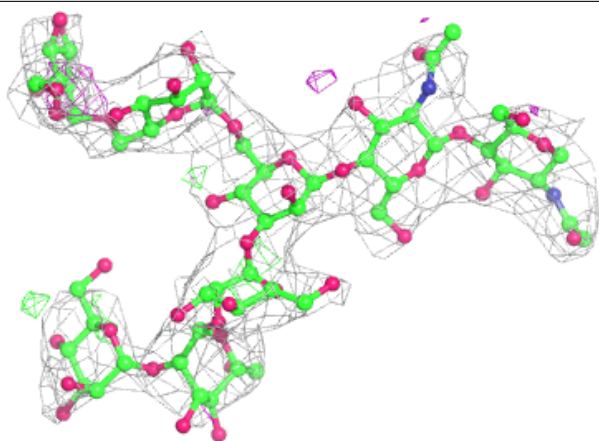
median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

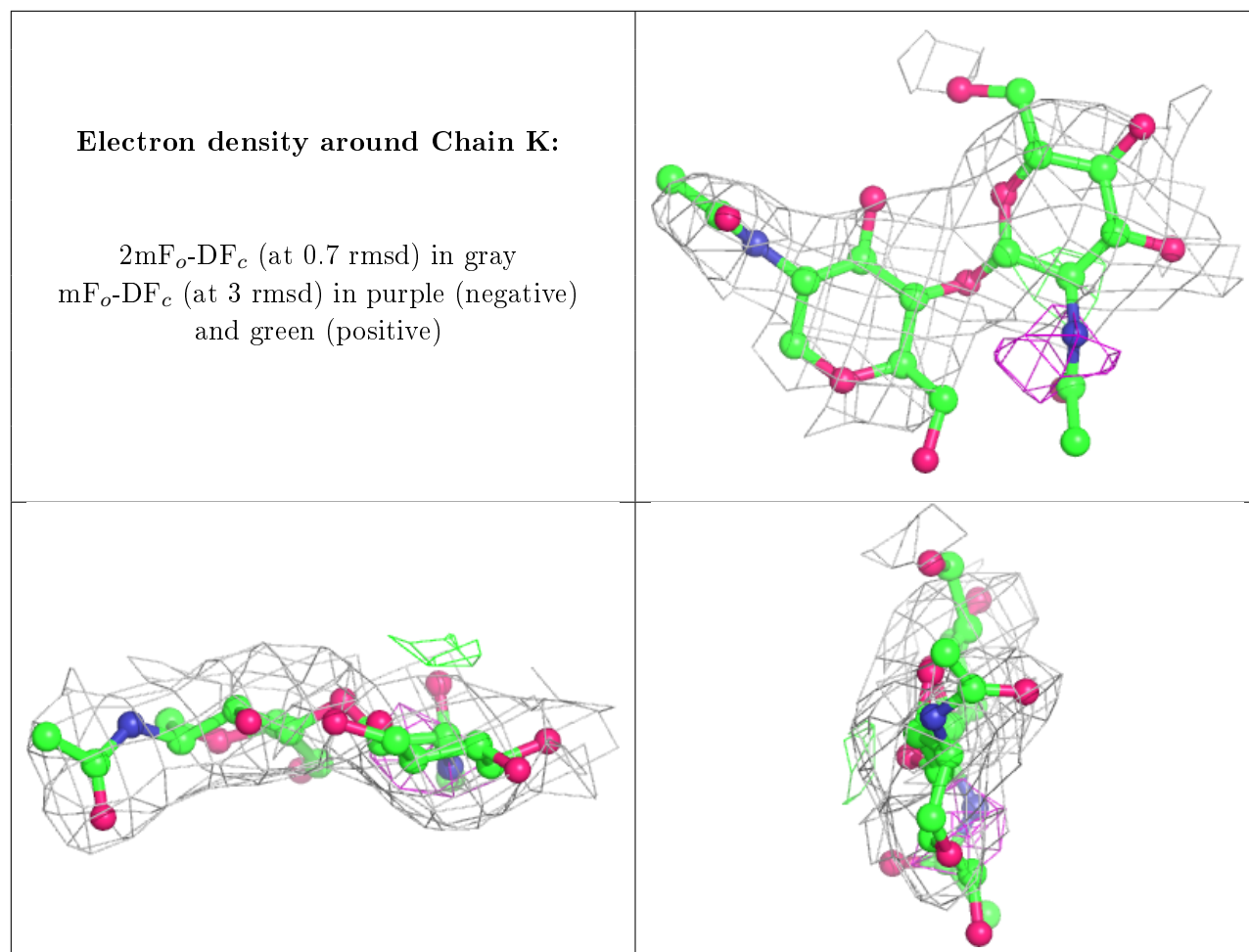
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
5	MAN	F	4	11/12	0.48	0.41	78,90,105,107	0
6	MAN	J	7	11/12	0.63	0.38	71,89,97,101	0
6	MAN	J	6	11/12	0.66	0.35	72,82,88,88	11
6	MAN	J	8	11/12	0.66	0.48	79,91,97,97	0
7	NAG	K	2	14/15	0.72	0.36	96,107,125,125	0
5	BMA	F	3	11/12	0.73	0.41	75,85,90,99	11
4	NAG	E	1	14/15	0.75	0.37	54,61,65,72	0
4	MAN	E	5	11/12	0.77	0.35	61,71,80,80	11
4	NAG	E	2	14/15	0.78	0.36	55,60,73,77	0
6	MAN	J	5	11/12	0.78	0.39	63,73,80,82	0
4	BMA	E	3	11/12	0.81	0.31	67,69,75,79	11
5	NAG	F	2	14/15	0.82	0.28	63,76,89,93	0
7	NAG	K	1	14/15	0.85	0.24	78,91,102,105	0
6	BMA	J	3	11/12	0.86	0.24	63,74,83,87	0
4	MAN	E	4	11/12	0.86	0.30	66,71,78,79	11
6	NAG	J	2	14/15	0.88	0.25	56,64,70,75	0
6	MAN	J	4	11/12	0.89	0.25	68,72,81,81	0
6	NAG	J	1	14/15	0.91	0.18	48,56,68,76	0
5	NAG	F	1	14/15	0.93	0.19	51,55,66,67	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 J:**

$2mF_o-DF_c$  (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
8	NAG	G	604	14/15	0.73	0.37	157,169,176,177	0
8	NAG	D	603	14/15	0.77	0.35	96,106,115,115	0
8	NAG	C	604	14/15	0.79	0.47	130,137,146,151	0
8	NAG	D	604	14/15	0.82	0.31	62,92,102,102	14
8	NAG	I	603	14/15	0.85	0.21	95,107,124,126	0
8	NAG	C	602	14/15	0.86	0.29	69,89,101,109	0
8	NAG	I	602	14/15	0.86	0.46	59,73,83,91	14
8	NAG	D	602	14/15	0.87	0.24	89,95,101,102	0
8	NAG	G	601	14/15	0.88	0.43	83,97,126,135	0
8	NAG	G	603	14/15	0.88	0.33	70,75,84,92	14
8	NAG	I	601	14/15	0.88	0.23	34,68,77,95	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
8	NAG	C	601	14/15	0.90	0.27	55,68,87,141	14
8	NAG	D	601	14/15	0.91	0.24	69,93,102,108	0
8	NAG	C	603	14/15	0.93	0.26	65,72,79,83	0
8	NAG	G	602	14/15	0.93	0.24	60,66,82,96	14

## 6.5 Other polymers [i](#)

There are no such residues in this entry.