



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 8, 2020 – 06:47 PM BST

PDB ID : 4XHJ  
Title : gHgL of Varicella-zoster virus in complex with human neutralizing antibodies.  
Authors : Xing, Y.  
Deposited on : 2015-01-05  
Resolution : 3.16 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



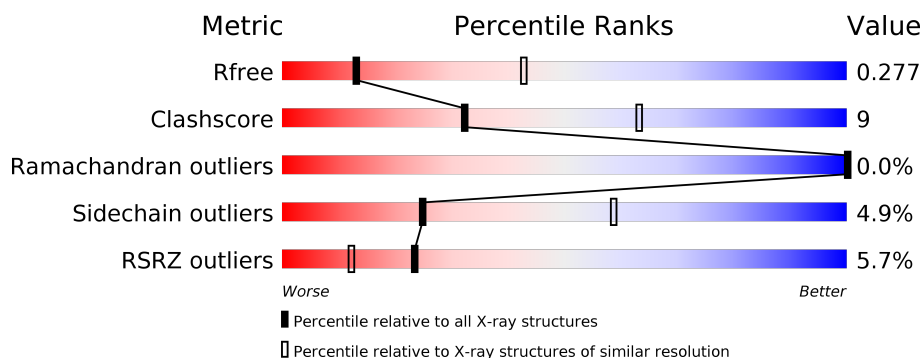
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.16 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	1665 (3.20-3.12)
Clashscore	141614	1804 (3.20-3.12)
Ramachandran outliers	138981	1770 (3.20-3.12)
Sidechain outliers	138945	1769 (3.20-3.12)
RSRZ outliers	127900	1616 (3.20-3.12)

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	833	<div> <div> <div></div> <div>63%</div> <div>22%</div> <div>•</div> <div>12%</div> </div> </div>
1	E	833	<div> <div>4%</div> <div> <div></div> <div>63%</div> <div>21%</div> <div>•</div> <div>15%</div> </div> </div>
2	B	138	<div> <div></div> <div> <div></div> <div>73%</div> <div>20%</div> <div>•</div> <div>•</div> </div> </div>
2	F	138	<div> <div>2%</div> <div> <div></div> <div>69%</div> <div>22%</div> <div>•</div> <div>6%</div> </div> </div>
3	C	215	<div> <div>13%</div> <div> <div></div> <div>79%</div> <div>17%</div> <div>•</div> </div> </div>
3	G	215	<div> <div>12%</div> <div> <div></div> <div>73%</div> <div>17%</div> <div>9%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
4	D	282	 7% 56% 16% 27%
4	H	282	 8% 57% 16% 27%
5	I	3	 33% 67%
6	J	5	 40% 40% 20%
6	M	5	 100%
7	K	2	 50% 50%
7	L	2	 50% 50%



## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 19505 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 Envelope glycoprotein H.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	729	Total	C	N	O	S	0	0	0
			5610	3602	936	1047	25			
1	E	705	Total	C	N	O	S	0	0	0
			5452	3508	906	1015	23			

There are 76 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	796	GLY	-	expression tag	UNP Q775J3
A	797	SER	-	expression tag	UNP Q775J3
A	798	GLU	-	expression tag	UNP Q775J3
A	799	ASN	-	expression tag	UNP Q775J3
A	800	LEU	-	expression tag	UNP Q775J3
A	801	TYR	-	expression tag	UNP Q775J3
A	802	PHE	-	expression tag	UNP Q775J3
A	803	GLN	-	expression tag	UNP Q775J3
A	804	GLY	-	expression tag	UNP Q775J3
A	805	SER	-	expression tag	UNP Q775J3
A	806	TRP	-	expression tag	UNP Q775J3
A	807	SER	-	expression tag	UNP Q775J3
A	808	HIS	-	expression tag	UNP Q775J3
A	809	PRO	-	expression tag	UNP Q775J3
A	810	GLN	-	expression tag	UNP Q775J3
A	811	PHE	-	expression tag	UNP Q775J3
A	812	GLU	-	expression tag	UNP Q775J3
A	813	LYS	-	expression tag	UNP Q775J3
A	814	GLY	-	expression tag	UNP Q775J3
A	815	GLY	-	expression tag	UNP Q775J3
A	816	GLY	-	expression tag	UNP Q775J3
A	817	SER	-	expression tag	UNP Q775J3
A	818	GLY	-	expression tag	UNP Q775J3
A	819	GLY	-	expression tag	UNP Q775J3
A	820	GLY	-	expression tag	UNP Q775J3

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Chain	Residue	Modelled	Actual	Comment	Reference
A	821	SER	-	expression tag	UNP Q775J3
A	822	GLY	-	expression tag	UNP Q775J3
A	823	GLY	-	expression tag	UNP Q775J3
A	824	GLY	-	expression tag	UNP Q775J3
A	825	SER	-	expression tag	UNP Q775J3
A	826	TRP	-	expression tag	UNP Q775J3
A	827	SER	-	expression tag	UNP Q775J3
A	828	HIS	-	expression tag	UNP Q775J3
A	829	PRO	-	expression tag	UNP Q775J3
A	830	GLN	-	expression tag	UNP Q775J3
A	831	PHE	-	expression tag	UNP Q775J3
A	832	GLU	-	expression tag	UNP Q775J3
A	833	LYS	-	expression tag	UNP Q775J3
E	796	GLY	-	expression tag	UNP Q775J3
E	797	SER	-	expression tag	UNP Q775J3
E	798	GLU	-	expression tag	UNP Q775J3
E	799	ASN	-	expression tag	UNP Q775J3
E	800	LEU	-	expression tag	UNP Q775J3
E	801	TYR	-	expression tag	UNP Q775J3
E	802	PHE	-	expression tag	UNP Q775J3
E	803	GLN	-	expression tag	UNP Q775J3
E	804	GLY	-	expression tag	UNP Q775J3
E	805	SER	-	expression tag	UNP Q775J3
E	806	TRP	-	expression tag	UNP Q775J3
E	807	SER	-	expression tag	UNP Q775J3
E	808	HIS	-	expression tag	UNP Q775J3
E	809	PRO	-	expression tag	UNP Q775J3
E	810	GLN	-	expression tag	UNP Q775J3
E	811	PHE	-	expression tag	UNP Q775J3
E	812	GLU	-	expression tag	UNP Q775J3
E	813	LYS	-	expression tag	UNP Q775J3
E	814	GLY	-	expression tag	UNP Q775J3
E	815	GLY	-	expression tag	UNP Q775J3
E	816	GLY	-	expression tag	UNP Q775J3
E	817	SER	-	expression tag	UNP Q775J3
E	818	GLY	-	expression tag	UNP Q775J3
E	819	GLY	-	expression tag	UNP Q775J3
E	820	GLY	-	expression tag	UNP Q775J3
E	821	SER	-	expression tag	UNP Q775J3
E	822	GLY	-	expression tag	UNP Q775J3
E	823	GLY	-	expression tag	UNP Q775J3
E	824	GLY	-	expression tag	UNP Q775J3

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Chain	Residue	Modelled	Actual	Comment	Reference
E	825	SER	-	expression tag	UNP Q775J3
E	826	TRP	-	expression tag	UNP Q775J3
E	827	SER	-	expression tag	UNP Q775J3
E	828	HIS	-	expression tag	UNP Q775J3
E	829	PRO	-	expression tag	UNP Q775J3
E	830	GLN	-	expression tag	UNP Q775J3
E	831	PHE	-	expression tag	UNP Q775J3
E	832	GLU	-	expression tag	UNP Q775J3
E	833	LYS	-	expression tag	UNP Q775J3

- Molecule 2 is a protein called Envelope glycoprotein L.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	132	Total	C	N	O	S	0	0	0
			1007	647	163	192	5			
2	F	130	Total	C	N	O	S	0	0	0
			997	641	161	190	5			

- Molecule 3 is a protein called Fab-RC light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	207	Total	C	N	O	S	0	0	0
			1569	984	265	315	5			
3	G	196	Total	C	N	O	S	0	0	0
			1481	936	247	293	5			

- Molecule 4 is a protein called Fab-RC heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	207	Total	C	N	O	S	0	0	0
			1569	992	265	299	13			
4	H	206	Total	C	N	O	S	0	0	0
			1561	988	264	296	13			

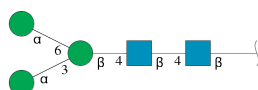
- Molecule 5 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.





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

- Molecule 6 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[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	5	Total	C	N	O	0	0	0
			61	34	2	25			
6	M	5	Total	C	N	O	0	0	0
			61	34	2	25			

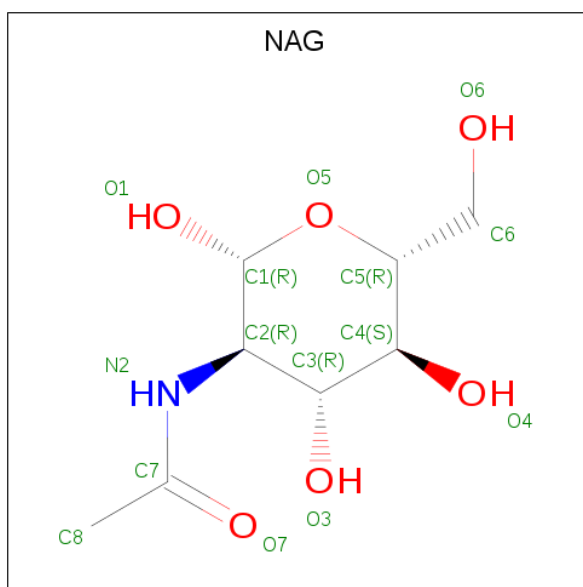
- Molecule 7 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	K	2	Total	C	N	O	0	0	0
			28	16	2	10			
7	L	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>).





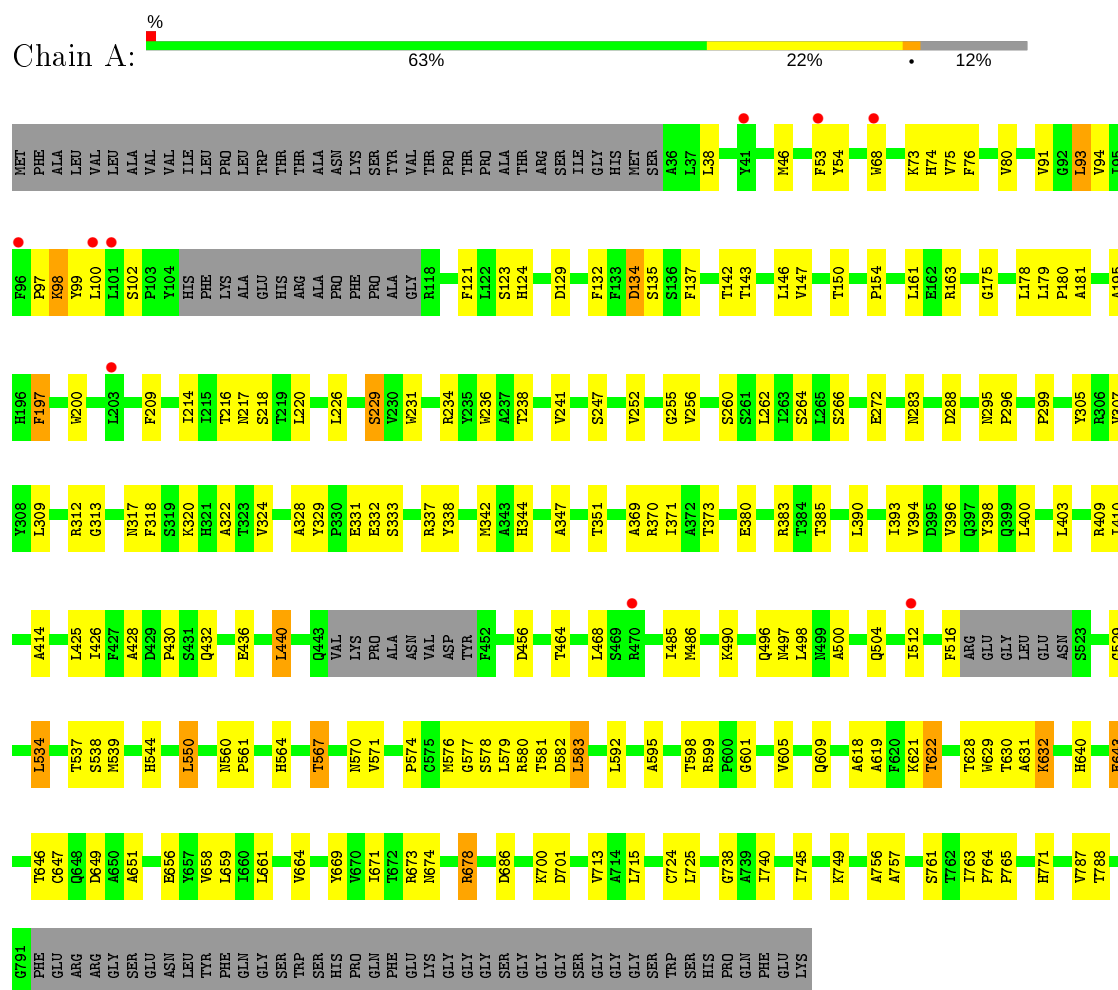
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	N	O	0	0
			14	8	1	5		
8	A	1	Total	C	N	O	0	0
			14	8	1	5		
8	E	1	Total	C	N	O	0	0
			14	8	1	5		



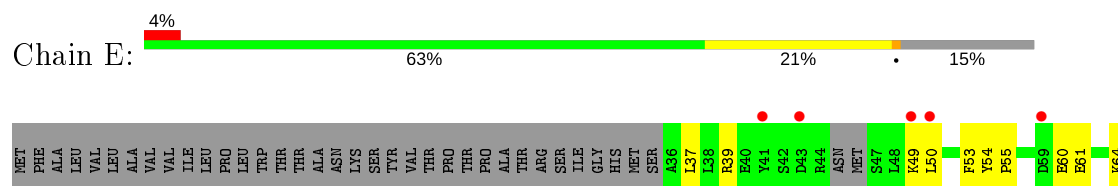
### 3 Residue-property plots

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.

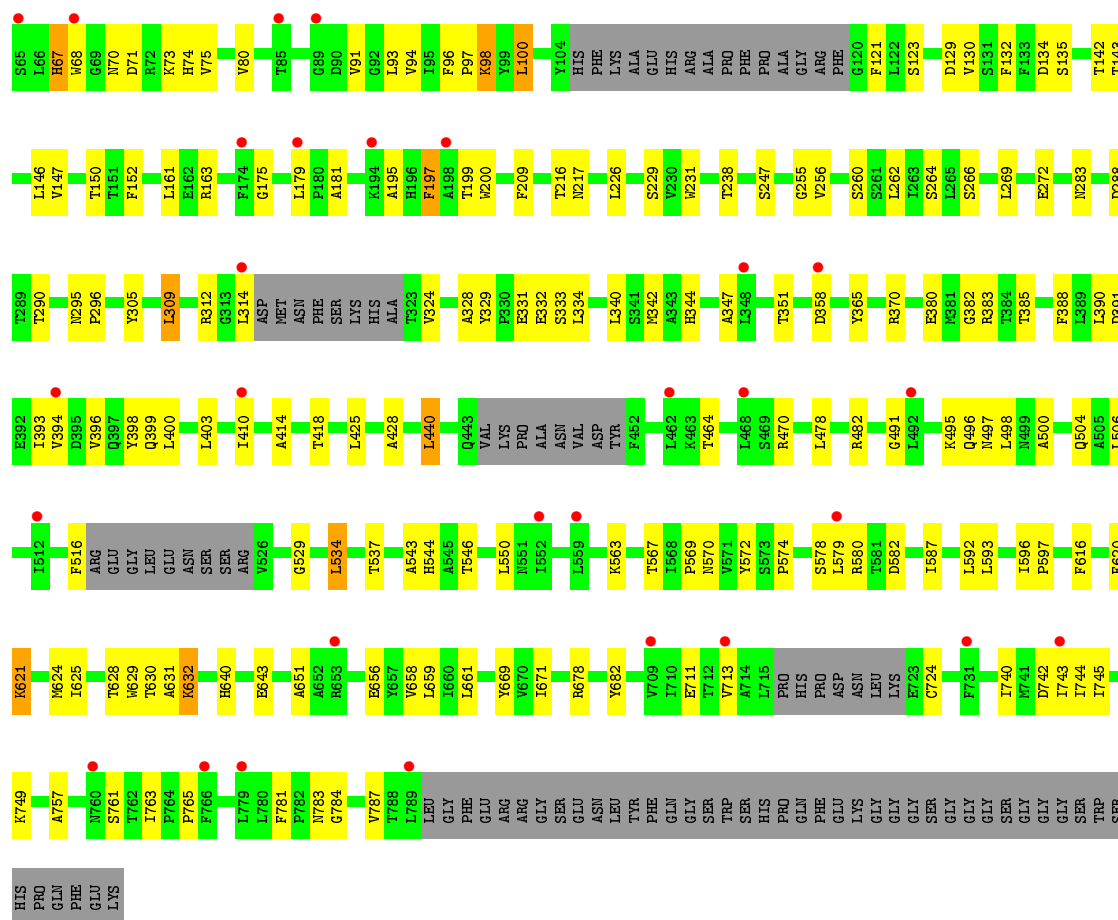
#### • Molecule 1: Envelope glycoprotein H



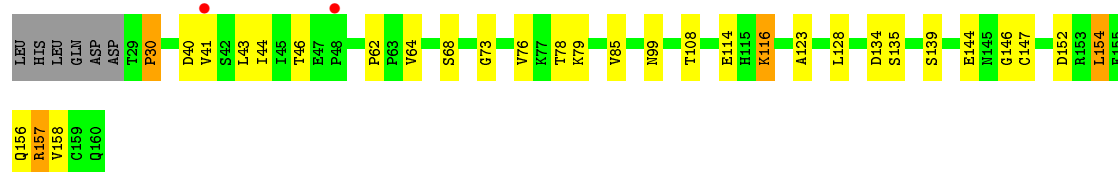
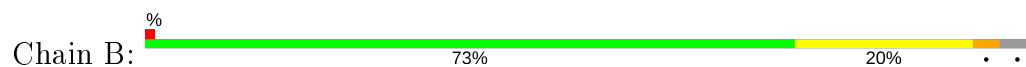
#### • Molecule 1: Envelope glycoprotein H



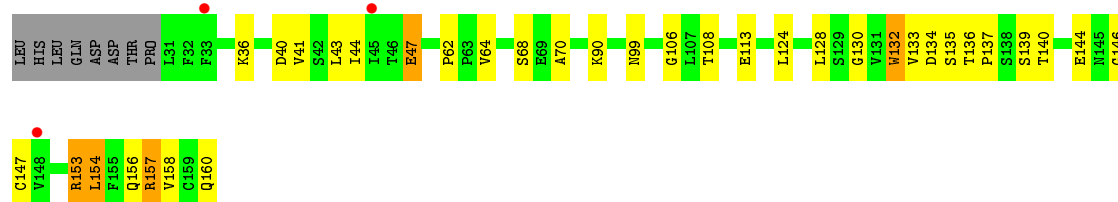




- Molecule 2: Envelope glycoprotein L

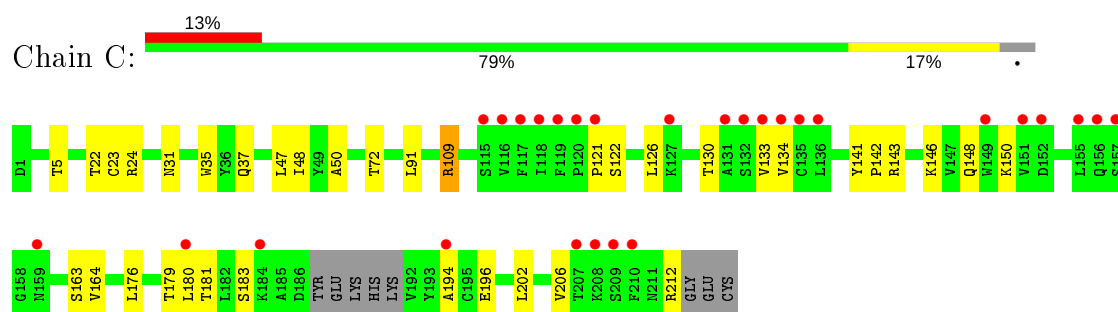


- Molecule 2: Envelope glycoprotein L

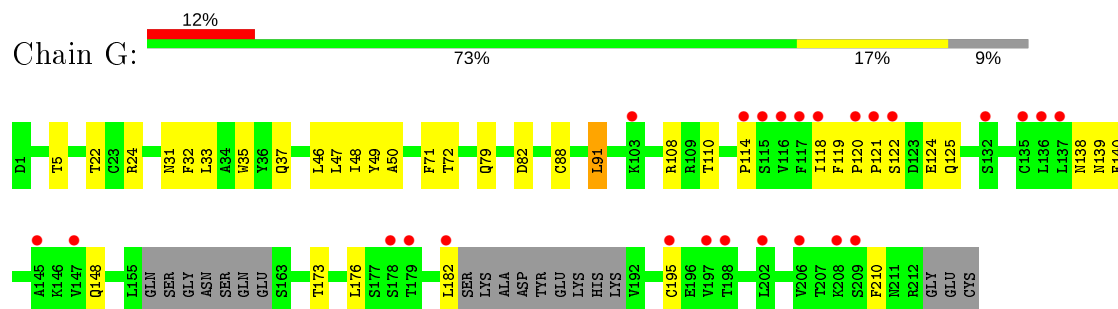


- Molecule 3: Fab-RC light chain

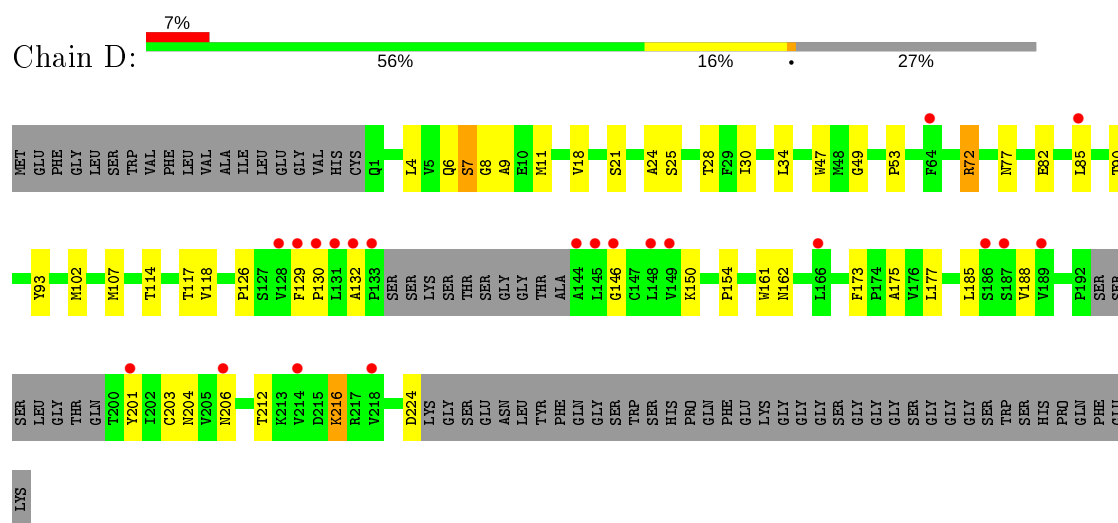




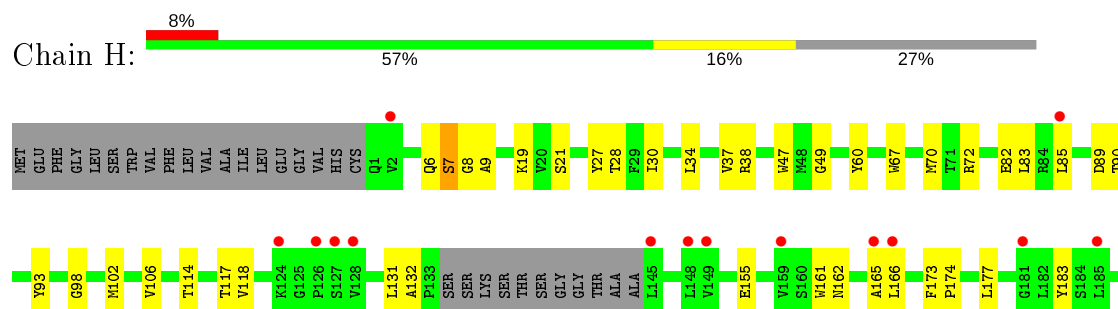
• Molecule 3: Fab-RC light chain



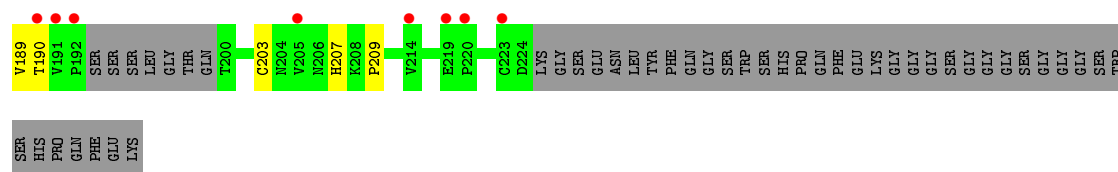
• Molecule 4: Fab-RC heavy chain



• Molecule 4: Fab-RC heavy chain







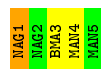
- Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I: 33% 67%



- Molecule 6: alpha-D-mannopyranose-(1-3)-[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: 40% 40% 20%



- Molecule 6: alpha-D-mannopyranose-(1-3)-[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 M: 100%



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

Chain K: 50% 50%



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

Chain L: 50% 50%





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	147.00Å 147.00Å 198.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.10 – 3.16 41.10 – 3.16	Depositor EDS
% Data completeness (in resolution range)	99.6 (41.10-3.16) 99.7 (41.10-3.16)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.57 (at 3.18Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1839)	Depositor
R, $R_{free}$	0.236 , 0.278 0.235 , 0.277	Depositor DCC
$R_{free}$ test set	3634 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	101.8	Xtriage
Anisotropy	0.601	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 44.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.047 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	19505	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 2.15% 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	0.25	0/5749	0.47	0/7854
1	E	0.23	0/5582	0.45	0/7619
2	B	0.26	0/1034	0.53	1/1416 (0.1%)
2	F	0.23	0/1024	0.51	0/1402
3	C	0.24	0/1600	0.46	0/2173
3	G	0.24	0/1511	0.46	0/2055
4	D	0.23	0/1608	0.47	0/2191
4	H	0.23	0/1600	0.46	0/2180
All	All	0.24	0/19708	0.47	1/26890 (0.0%)

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
4	D	0	1
4	H	0	1
All	All	0	2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
2	B	30	PRO	N-CA-CB	5.89	110.36	103.30

There are no chirality outliers.

All (2) planarity outliers are listed below:



Mol	Chain	Res	Type	Group
4	D	7	SER	Peptide
4	H	7	SER	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	5610	0	5452	119	0
1	E	5452	0	5349	109	0
2	B	1007	0	972	22	0
2	F	997	0	969	29	0
3	C	1569	0	1527	20	0
3	G	1481	0	1440	22	0
4	D	1569	0	1517	27	0
4	H	1561	0	1510	27	0
5	I	39	0	34	1	0
6	J	61	0	52	1	0
6	M	61	0	52	0	0
7	K	28	0	25	0	0
7	L	28	0	25	0	0
8	A	28	0	26	0	0
8	E	14	0	13	0	0
All	All	19505	0	18963	338	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 9.

The worst 5 of 338 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)
1:A:98:LYS:HD2	2:B:68:SER:HB3	1.57	0.86
1:E:175:GLY:HA3	1:E:333:SER:HA	1.63	0.79
1:E:73:LYS:O	1:E:98:LYS:NZ	2.17	0.78
3:G:5:THR:HB	3:G:24:ARG:HB2	1.69	0.75
1:E:61:GLU:HB3	1:E:64:LYS:HB2	1.68	0.74

There are no symmetry-related clashes.



## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	721/833 (87%)	687 (95%)	34 (5%)	0	100	100
1	E	691/833 (83%)	660 (96%)	31 (4%)	0	100	100
2	B	130/138 (94%)	119 (92%)	10 (8%)	1 (1%)	19	55
2	F	128/138 (93%)	115 (90%)	13 (10%)	0	100	100
3	C	203/215 (94%)	196 (97%)	7 (3%)	0	100	100
3	G	190/215 (88%)	182 (96%)	8 (4%)	0	100	100
4	D	201/282 (71%)	192 (96%)	9 (4%)	0	100	100
4	H	200/282 (71%)	192 (96%)	8 (4%)	0	100	100
All	All	2464/2936 (84%)	2343 (95%)	120 (5%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	30	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	604/717 (84%)	568 (94%)	36 (6%)	19	51
1	E	591/717 (82%)	564 (95%)	27 (5%)	27	60
2	B	111/121 (92%)	104 (94%)	7 (6%)	18	49
2	F	111/121 (92%)	105 (95%)	6 (5%)	22	55

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	176/187 (94%)	170 (97%)	6 (3%)	37	68
3	G	165/187 (88%)	159 (96%)	6 (4%)	35	67
4	D	173/233 (74%)	164 (95%)	9 (5%)	23	55
4	H	172/233 (74%)	167 (97%)	5 (3%)	42	72
All	All	2103/2516 (84%)	2001 (95%)	102 (5%)	25	59

5 of 102 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	91	LEU
4	D	216	LYS
3	G	91	LEU
3	C	109	ARG
4	D	72	ARG

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 ⓘ

17 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
5	NAG	I	1	1,5	14,14,15	0.60	0	17,19,21	0.88	1 (5%)
5	NAG	I	2	5	14,14,15	0.45	0	17,19,21	1.08	0
5	BMA	I	3	5	11,11,12	0.73	0	15,15,17	0.73	0
6	NAG	J	1	2,6	14,14,15	0.99	1 (7%)	17,19,21	1.13	2 (11%)
6	NAG	J	2	6	14,14,15	0.57	0	17,19,21	0.74	0
6	BMA	J	3	6	11,11,12	1.03	1 (9%)	15,15,17	1.34	2 (13%)
6	MAN	J	4	6	11,11,12	0.71	0	15,15,17	0.96	1 (6%)
6	MAN	J	5	6	11,11,12	0.66	0	15,15,17	0.60	0
7	NAG	K	1	1,7	14,14,15	0.67	0	17,19,21	1.01	0
7	NAG	K	2	7	14,14,15	0.60	0	17,19,21	0.92	1 (5%)
7	NAG	L	1	1,7	14,14,15	0.48	0	17,19,21	0.86	1 (5%)
7	NAG	L	2	7	14,14,15	0.62	0	17,19,21	0.74	0
6	NAG	M	1	2,6	14,14,15	0.54	0	17,19,21	0.96	1 (5%)
6	NAG	M	2	6	14,14,15	0.60	0	17,19,21	0.94	1 (5%)
6	BMA	M	3	6	11,11,12	1.21	1 (9%)	15,15,17	0.98	1 (6%)
6	MAN	M	4	6	11,11,12	0.61	0	15,15,17	1.02	2 (13%)
6	MAN	M	5	6	11,11,12	0.53	0	15,15,17	0.98	1 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	I	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	I	2	5	-	0/6/23/26	0/1/1/1
5	BMA	I	3	5	-	0/2/19/22	0/1/1/1
6	NAG	J	1	2,6	-	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	-	1/2/19/22	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
7	NAG	K	1	1,7	-	0/6/23/26	0/1/1/1
7	NAG	K	2	7	-	2/6/23/26	0/1/1/1
7	NAG	L	1	1,7	-	4/6/23/26	0/1/1/1
7	NAG	L	2	7	-	2/6/23/26	0/1/1/1
6	NAG	M	1	2,6	-	1/6/23/26	0/1/1/1
6	NAG	M	2	6	-	0/6/23/26	0/1/1/1
6	BMA	M	3	6	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	MAN	M	4	6	-	0/2/19/22	0/1/1/1
6	MAN	M	5	6	-	1/2/19/22	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	J	1	NAG	O5-C1	-3.36	1.38	1.43
6	J	3	BMA	O5-C1	-2.42	1.39	1.43
6	M	3	BMA	O5-C1	-2.05	1.40	1.43

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	M	5	MAN	C1-O5-C5	2.93	116.16	112.19
6	M	2	NAG	C4-C3-C2	2.86	115.21	111.02
6	J	3	BMA	C2-C3-C4	2.70	115.57	110.89
6	J	1	NAG	O5-C1-C2	-2.64	107.11	111.29
6	J	3	BMA	C1-C2-C3	2.43	112.66	109.67

There are no chirality outliers.

5 of 17 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	K	2	NAG	C8-C7-N2-C2
7	K	2	NAG	O7-C7-N2-C2
6	M	3	BMA	C4-C5-C6-O6
7	L	2	NAG	C8-C7-N2-C2
7	L	2	NAG	O7-C7-N2-C2

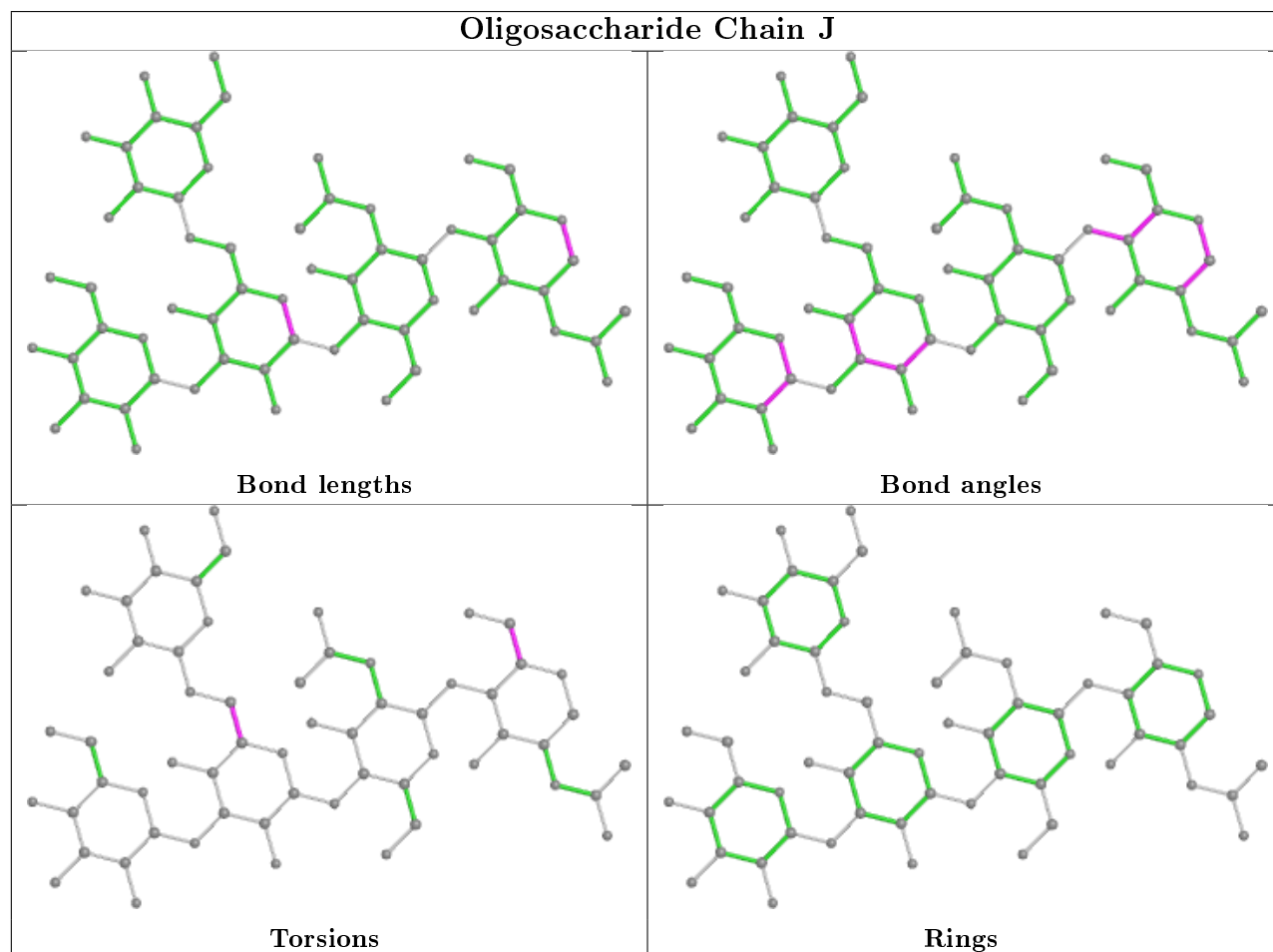
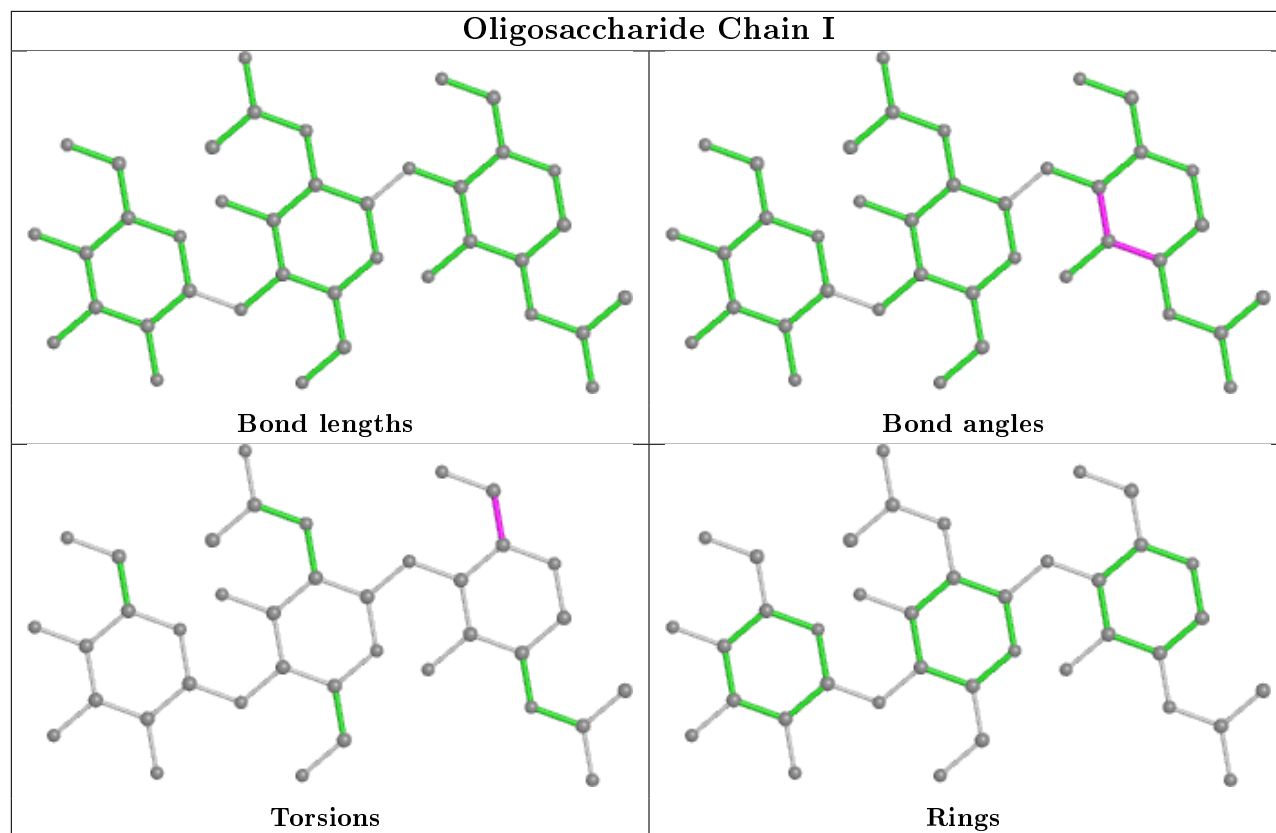
There are no ring outliers.

2 monomers are involved in 2 short contacts:

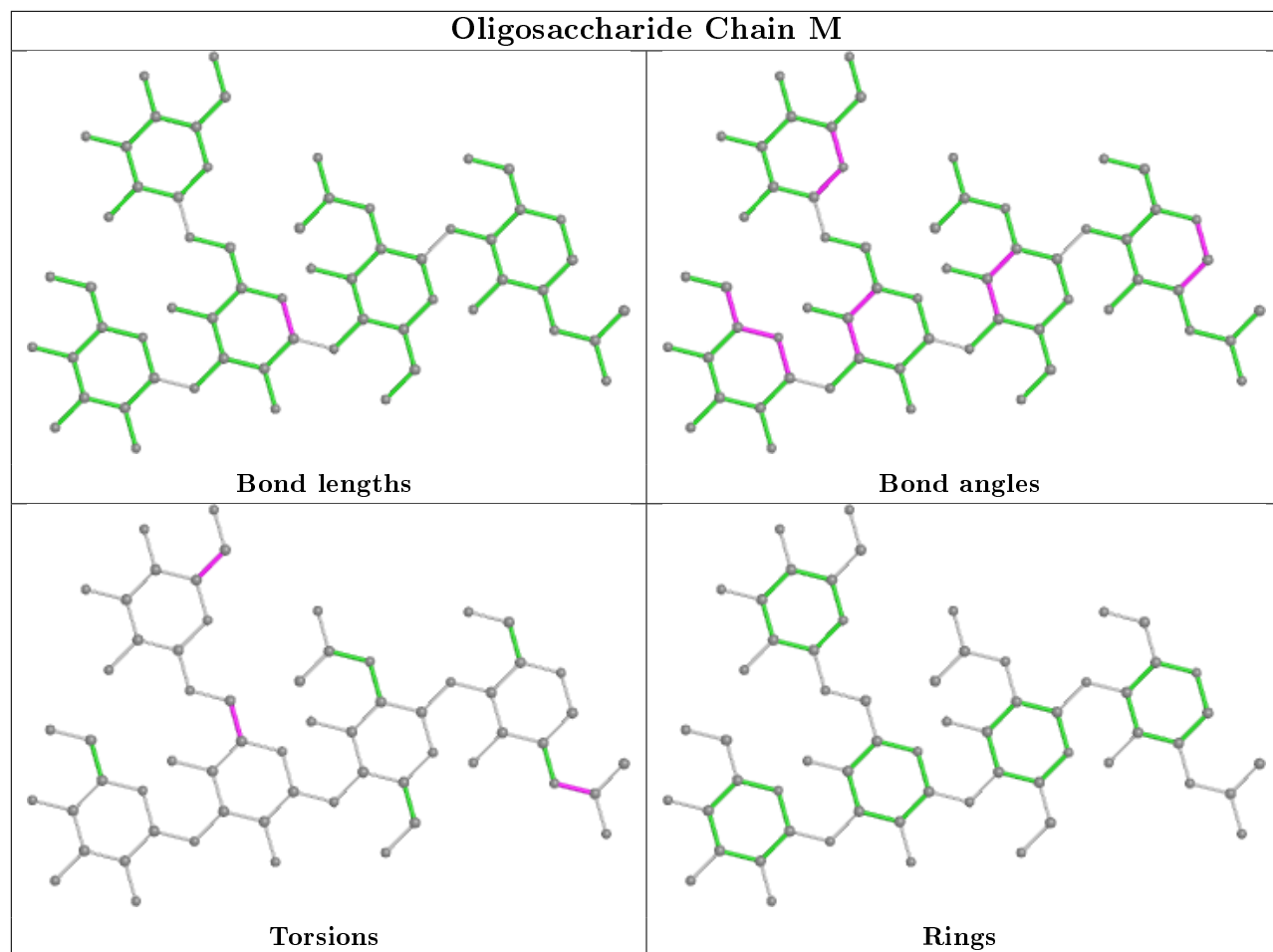
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	J	1	NAG	1	0
5	I	2	NAG	1	0

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

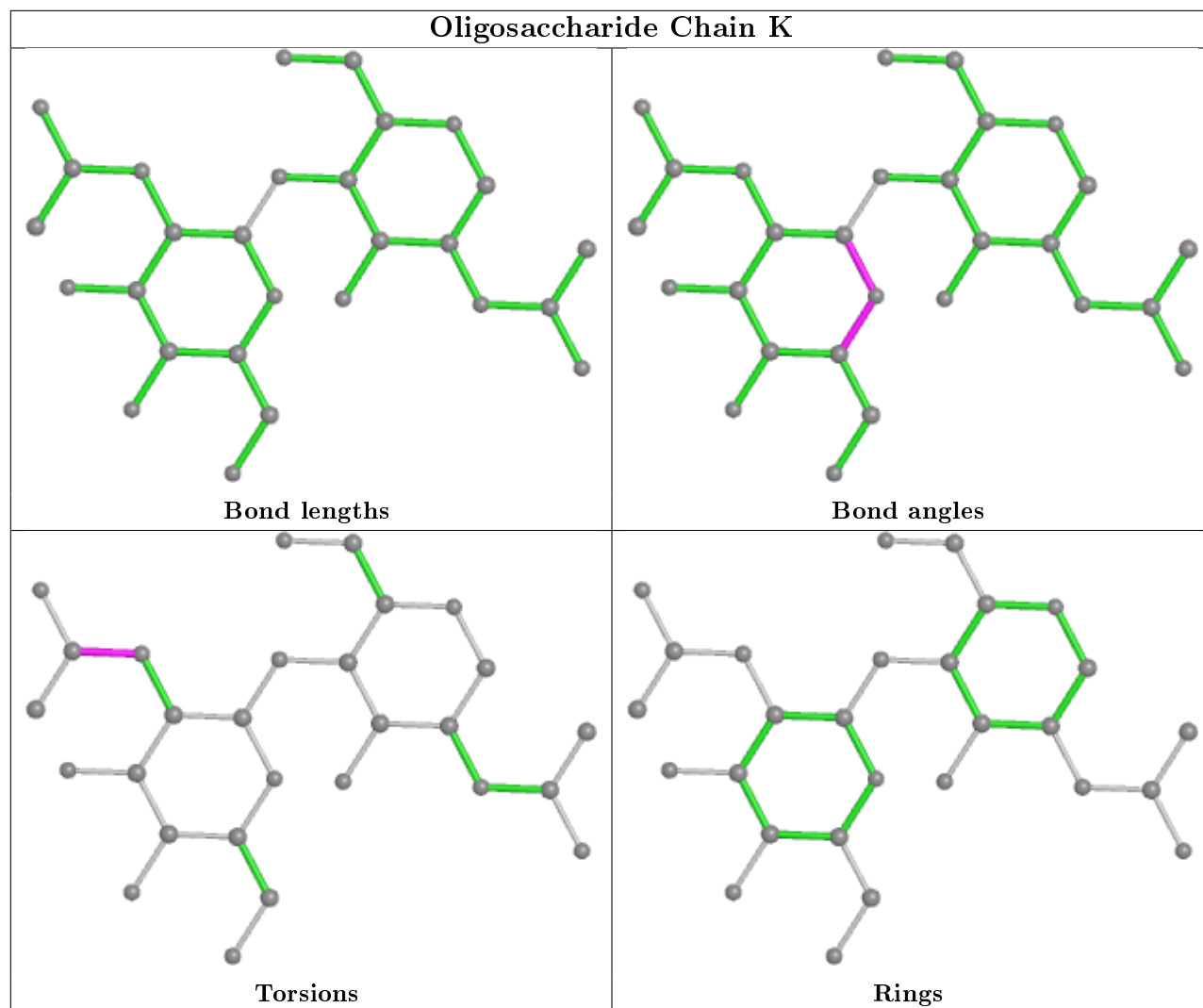




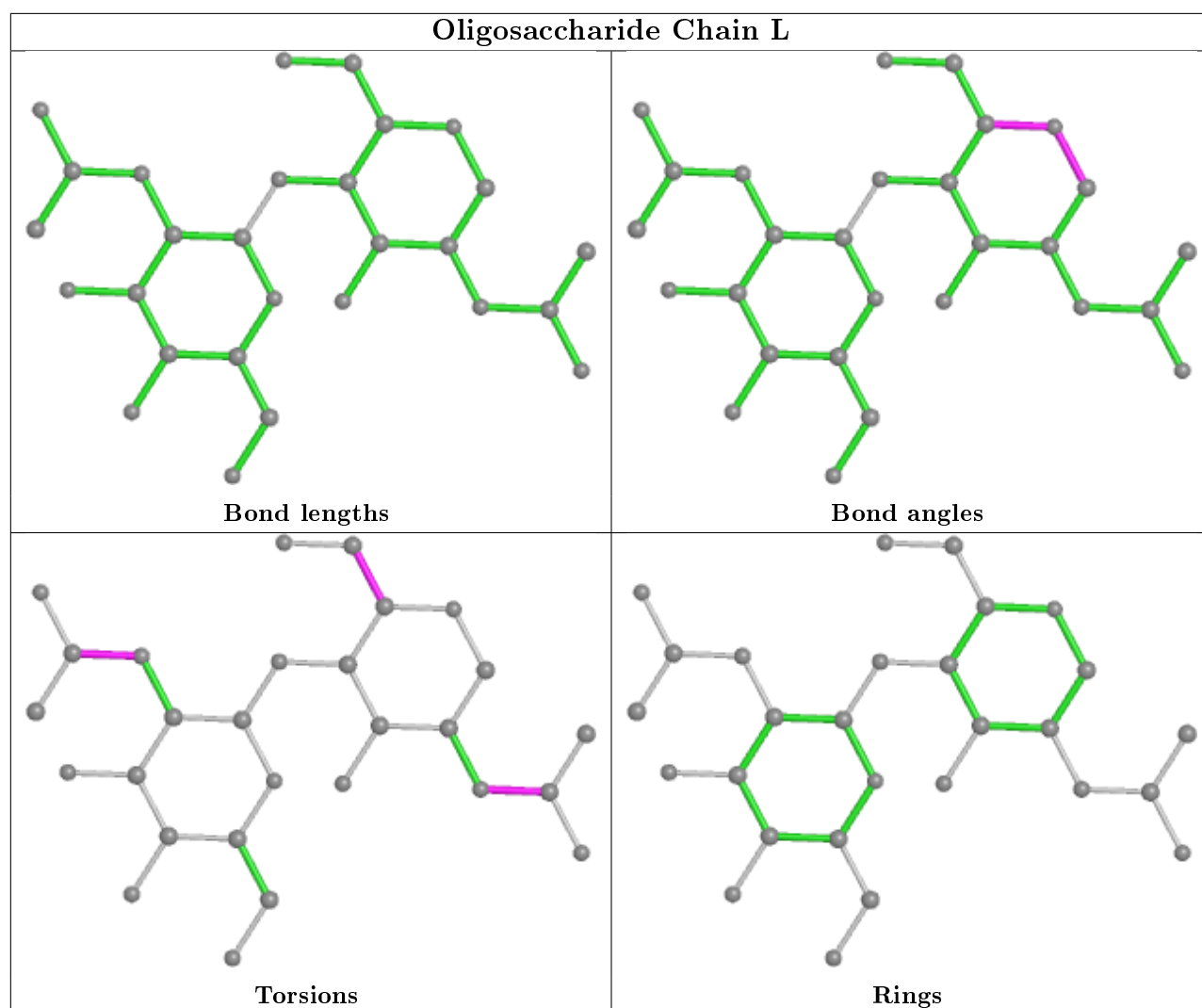












## 5.6 Ligand geometry [i](#)

3 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	A	901	1	14,14,15	0.48	0	17,19,21	0.86	1 (5%)
8	NAG	E	905	1	14,14,15	0.30	0	17,19,21	0.75	1 (5%)
8	NAG	A	902	1	14,14,15	0.49	0	17,19,21	1.05	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	A	901	1	-	0/6/23/26	0/1/1/1
8	NAG	E	905	1	-	0/6/23/26	0/1/1/1
8	NAG	A	902	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	902	NAG	C1-O5-C5	3.08	116.36	112.19
8	E	905	NAG	C1-O5-C5	2.46	115.53	112.19
8	A	901	NAG	O5-C5-C6	2.20	110.66	107.20

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	902	NAG	C8-C7-N2-C2
8	A	902	NAG	O7-C7-N2-C2

There are no ring outliers.

No monomer is involved in short contacts.

## 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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	729/833 (87%)	0.18	9 (1%) 79 68	25, 58, 145, 178	0
1	E	705/833 (84%)	0.31	34 (4%) 30 17	55, 112, 159, 213	0
2	B	132/138 (95%)	0.15	2 (1%) 73 61	53, 94, 138, 198	0
2	F	130/138 (94%)	0.04	3 (2%) 60 46	67, 93, 118, 140	0
3	C	207/215 (96%)	0.67	28 (13%) 3 2	52, 99, 201, 212	0
3	G	196/215 (91%)	0.59	25 (12%) 3 2	58, 94, 211, 221	0
4	D	207/282 (73%)	0.39	21 (10%) 7 3	52, 116, 184, 201	0
4	H	206/282 (73%)	0.52	22 (10%) 6 3	68, 126, 196, 205	0
All	All	2512/2936 (85%)	0.32	144 (5%) 23 12	25, 96, 182, 221	0

The worst 5 of 144 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	120	PRO	12.1
3	C	119	PHE	11.1
3	G	136	LEU	9.5
4	D	145	LEU	8.4
3	G	117	PHE	7.8

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

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

### 6.3 Carbohydrates ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,



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

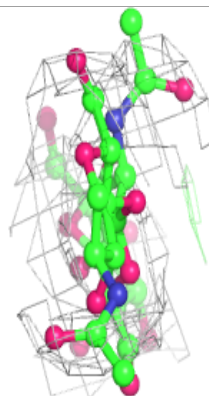
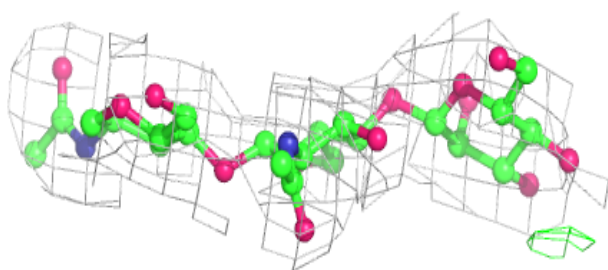
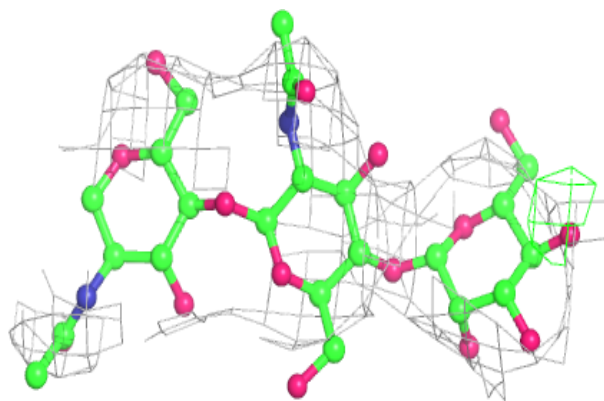
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
6	MAN	J	5	11/12	0.71	0.24	138,153,163,169	0
7	NAG	L	1	14/15	0.76	0.22	139,150,156,157	0
6	BMA	J	3	11/12	0.80	0.14	131,144,153,158	0
5	BMA	I	3	11/12	0.81	0.20	136,150,161,163	0
7	NAG	K	1	14/15	0.82	0.22	125,141,149,152	0
7	NAG	L	2	14/15	0.85	0.23	132,150,160,160	0
5	NAG	I	2	14/15	0.85	0.29	104,130,144,148	0
7	NAG	K	2	14/15	0.85	0.23	133,145,153,157	0
6	NAG	J	1	14/15	0.88	0.26	181,206,217,218	0
6	BMA	M	3	11/12	0.88	0.12	118,127,138,151	0
6	MAN	J	4	11/12	0.88	0.15	140,150,161,166	0
6	MAN	M	5	11/12	0.89	0.17	101,131,141,149	0
6	NAG	M	2	14/15	0.90	0.24	86,112,133,133	0
6	NAG	M	1	14/15	0.93	0.13	95,104,111,111	0
6	MAN	M	4	11/12	0.93	0.09	120,138,144,146	0
6	NAG	J	2	14/15	0.94	0.15	119,134,149,160	0
5	NAG	I	1	14/15	0.97	0.16	78,95,114,115	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.

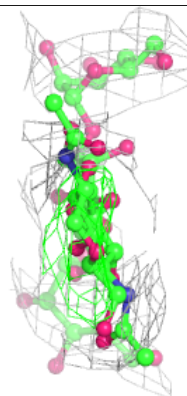
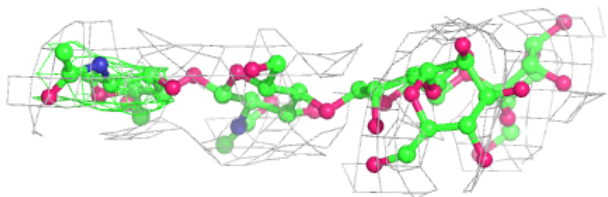
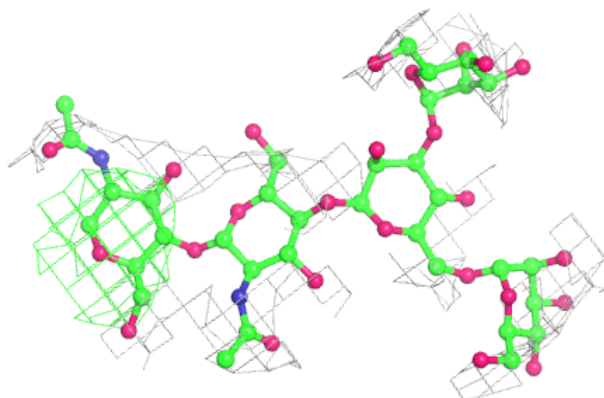


**Electron density around Chain I:**

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

**Electron density around Chain J:**

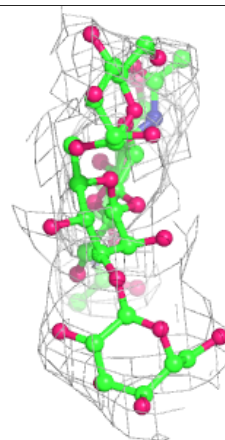
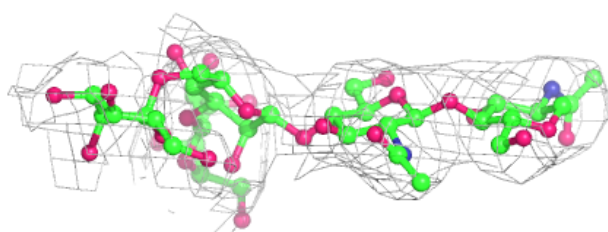
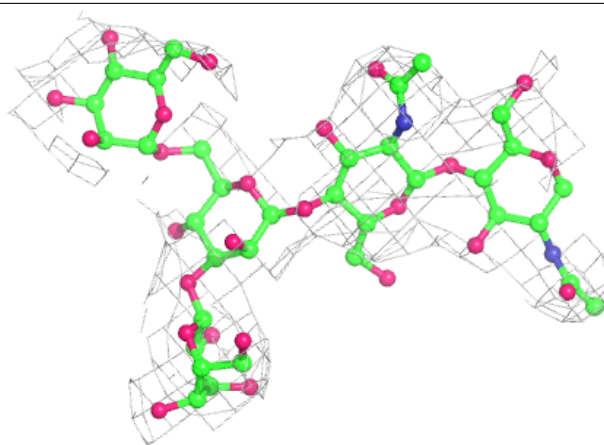
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



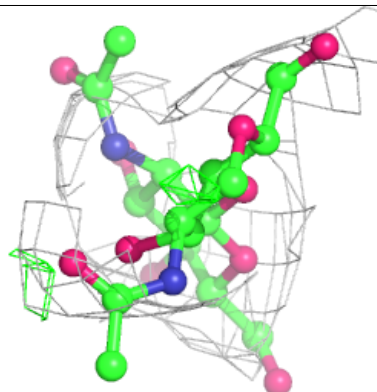
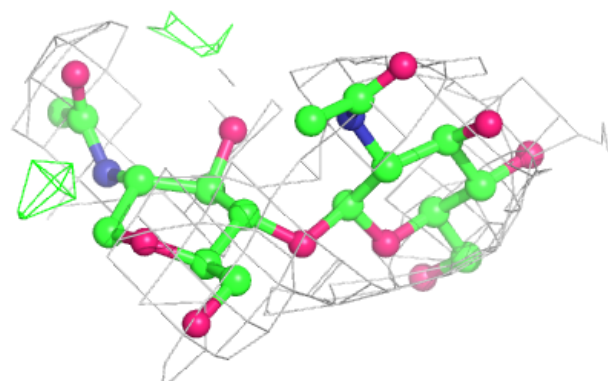
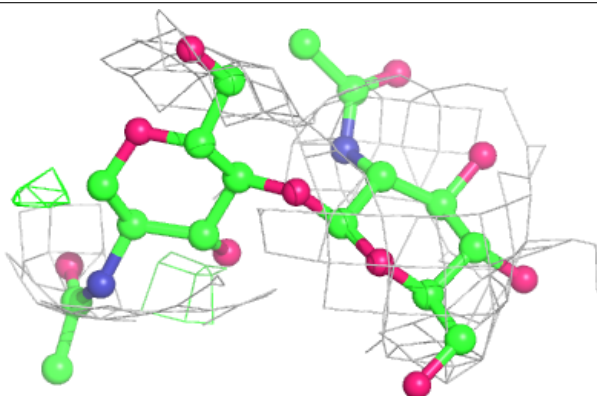


**Electron density around Chain M:**

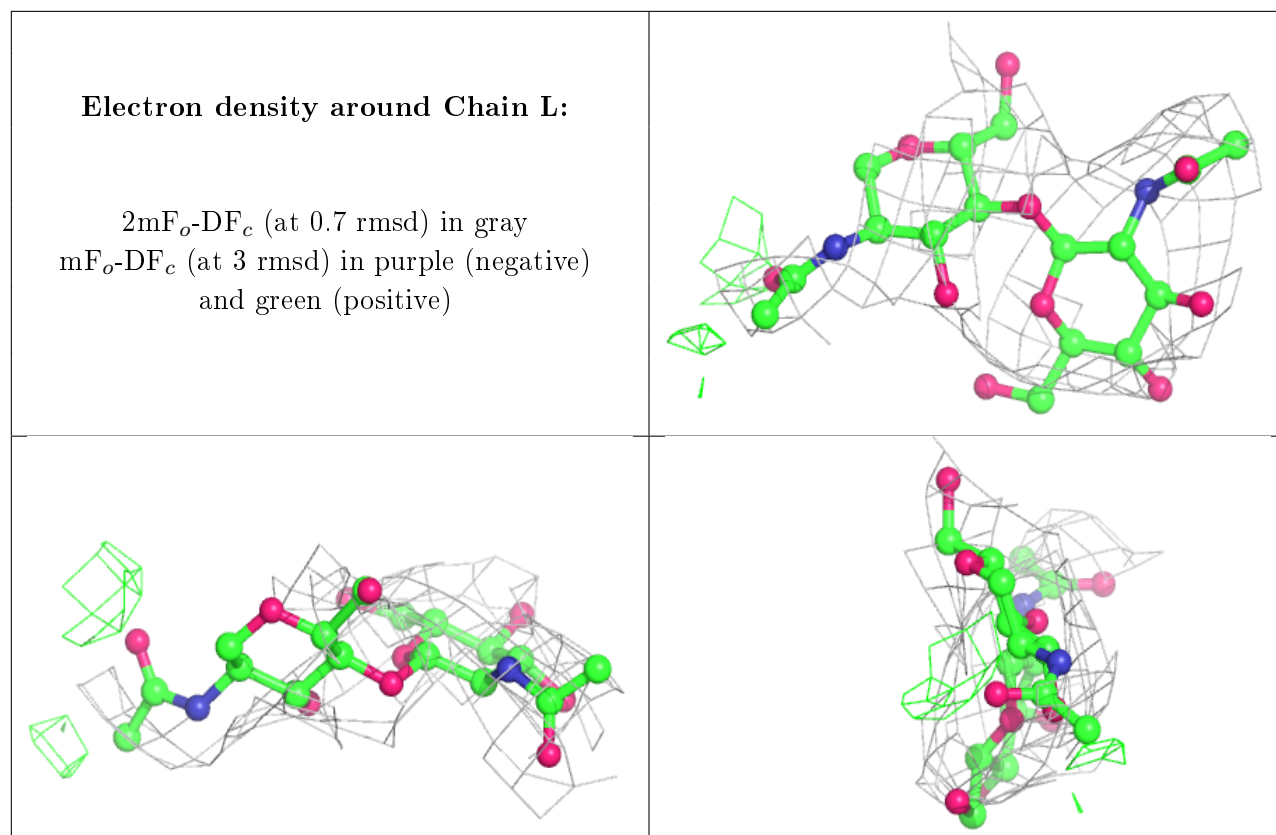
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around Chain K:**

$2mF_o-DF_c$  (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
8	NAG	E	905	14/15	0.64	0.35	197,219,232,234	0
8	NAG	A	901	14/15	0.83	0.20	125,133,142,148	0
8	NAG	A	902	14/15	0.83	0.21	20,63,79,79	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.