



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 20, 2026 – 07:57 PM UTC

PDB ID : 8DF1 / pdb\_00008df1  
Title : Chi3l1 bound by antibody C59  
Authors : Wrapp, D.; McLellan, J.S.  
Deposited on : 2022-06-21  
Resolution : 3.30 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

---

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

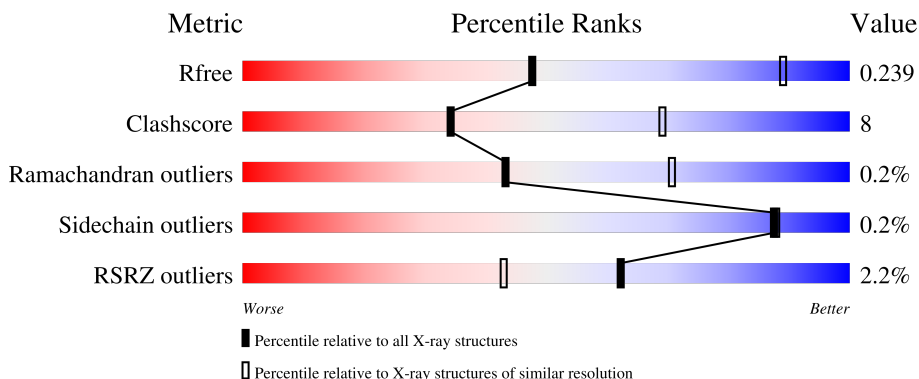
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.30 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))
$R_{free}$	180053	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	362	 82% 18%
1	B	362	 86% 14%
1	C	362	 84% 16%
1	D	362	 81% 19%
1	E	362	 % 83% 17%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	362	83% 17%
2	H	223	5% 79% 21%
2	M	223	4% 76% 23%
2	O	223	7% 83% 17%
2	Q	223	4% 79% 20%
2	S	223	4% 85% 14%
2	U	223	8% 81% 18%
3	L	214	2% 83% 17%
3	N	214	% 82% 18%
3	P	214	4% 79% 21%
3	R	214	% 81% 19%
3	T	214	85% 15%
3	V	214	5% 80% 20%
4	G	4	25% 50% 25%
4	W	4	25% 50% 25%
5	I	3	67% 33%
5	K	3	67% 33%
5	X	3	33% 33% 33%
6	J	5	80% 20%

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 36890 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 Chitinase-3-like protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	362	2860	1827	493	529	11	0	0	0
1	B	362	2860	1827	493	529	11	0	0	0
1	C	362	2860	1827	493	529	11	0	0	0
1	D	362	2860	1827	493	529	11	0	0	0
1	E	362	2860	1827	493	529	11	0	0	0
1	F	362	2860	1827	493	529	11	0	0	0

- Molecule 2 is a protein called C59 Fab Heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	M	223	1647	1042	267	327	11	0	0	0
2	H	223	1647	1042	267	327	11	0	0	0
2	O	223	1647	1042	267	327	11	0	0	0
2	Q	223	1647	1042	267	327	11	0	0	0
2	S	223	1647	1042	267	327	11	0	0	0
2	U	223	1647	1042	267	327	11	0	0	0

- Molecule 3 is a protein called C59 Fab Light chain.

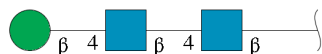
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	N	214	Total	C	N	O	S	0	0	0
			1595	999	257	332	7			
3	L	214	Total	C	N	O	S	0	0	0
			1595	999	257	332	7			
3	P	214	Total	C	N	O	S	0	0	0
			1595	999	257	332	7			
3	R	214	Total	C	N	O	S	0	0	0
			1595	999	257	332	7			
3	T	214	Total	C	N	O	S	0	0	0
			1595	999	257	332	7			
3	V	214	Total	C	N	O	S	0	0	0
			1595	999	257	332	7			

- Molecule 4 is an oligosaccharide called 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
4	G	4	Total	C	N	O	0	0	0
			50	28	2	20			
4	W	4	Total	C	N	O	0	0	0
			50	28	2	20			

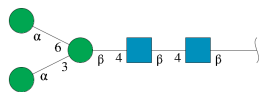
- Molecule 5 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



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

ose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

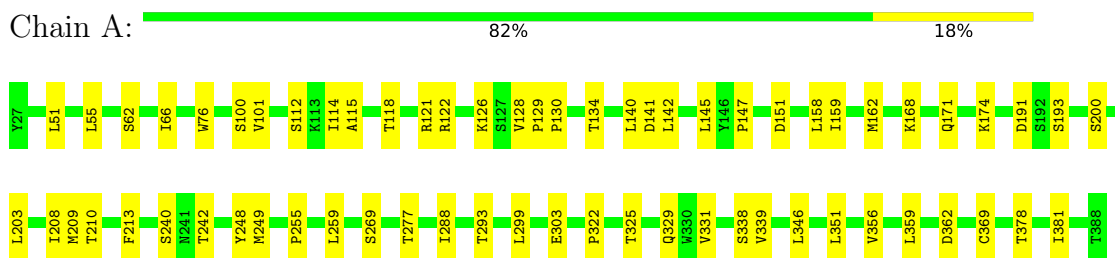


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
6	J	5	61	34	2	25	0	0	0

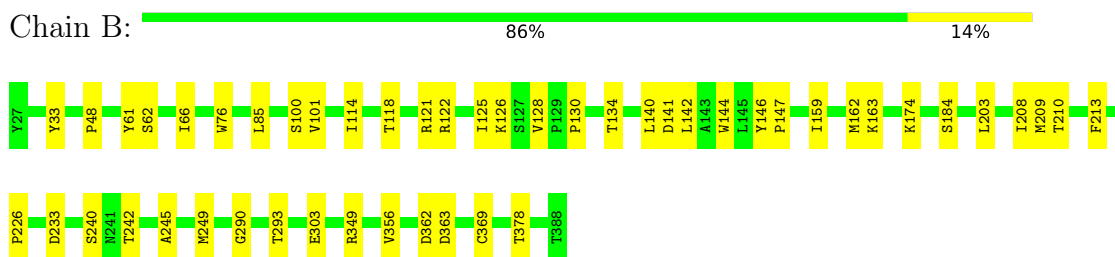
### 3 Residue-property plots

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.

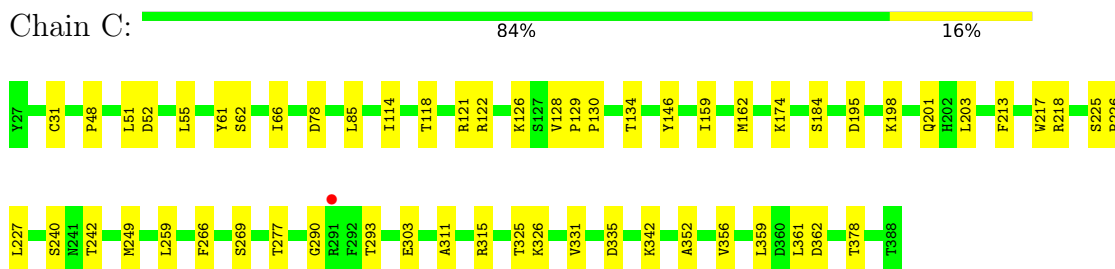
- Molecule 1: Chitinase-3-like protein 1



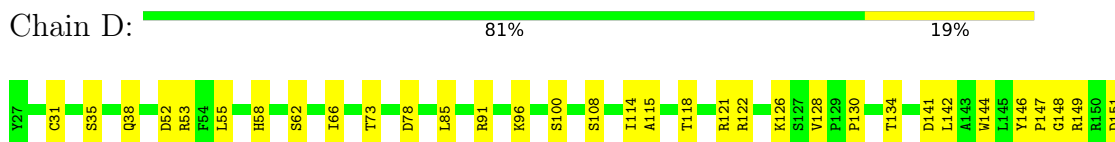
- Molecule 1: Chitinase-3-like protein 1

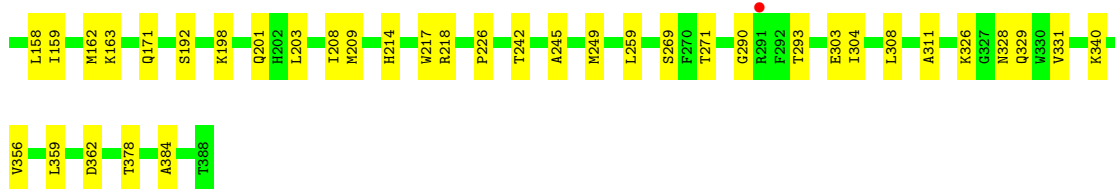


- Molecule 1: Chitinase-3-like protein 1

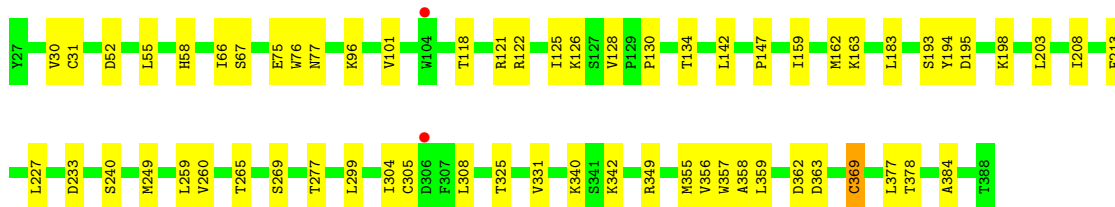
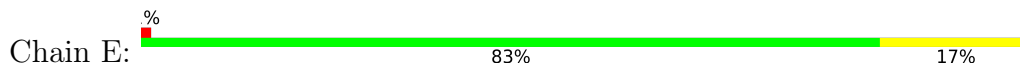


- Molecule 1: Chitinase-3-like protein 1

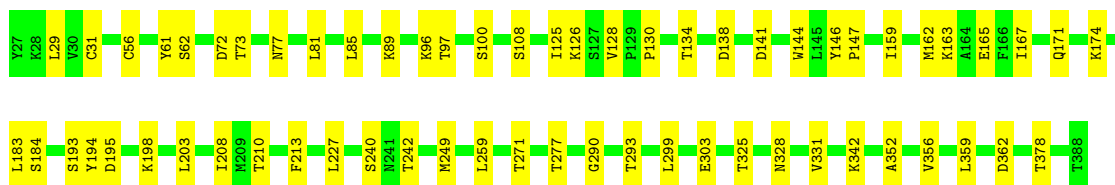
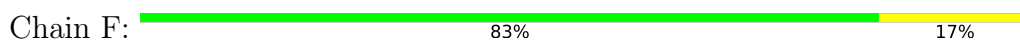




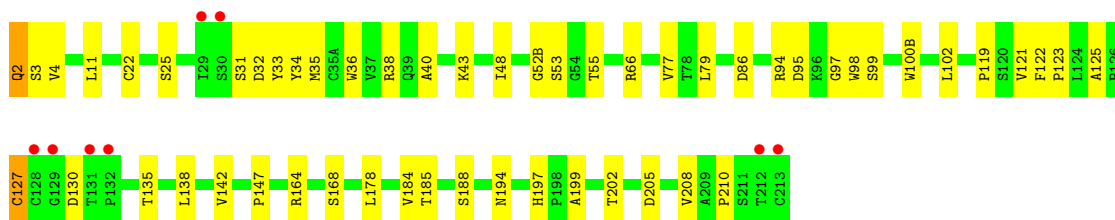
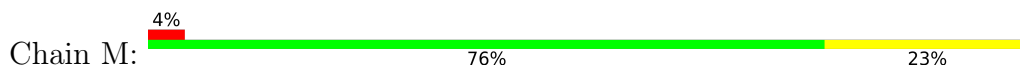
- Molecule 1: Chitinase-3-like protein 1



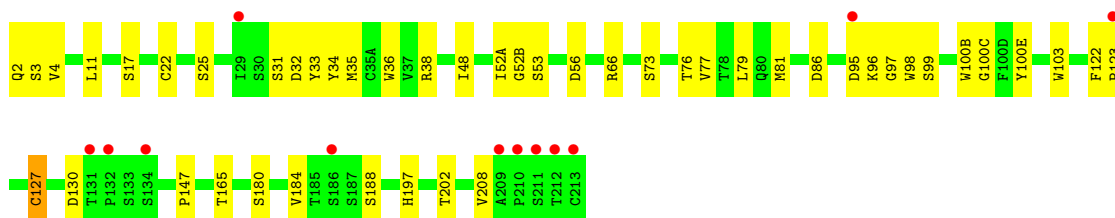
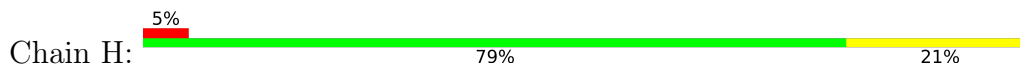
- Molecule 1: Chitinase-3-like protein 1



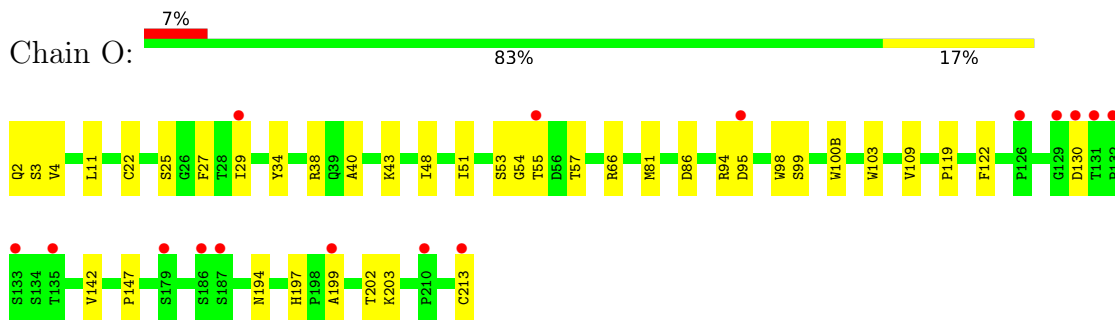
- Molecule 2: C59 Fab Heavy chain



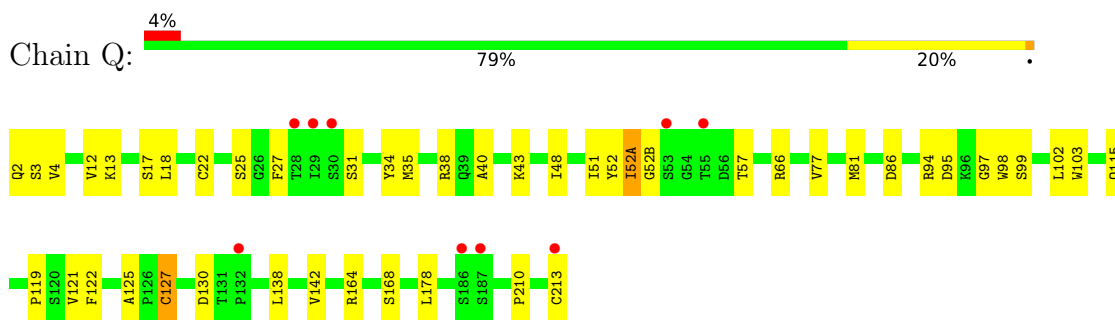
- Molecule 2: C59 Fab Heavy chain



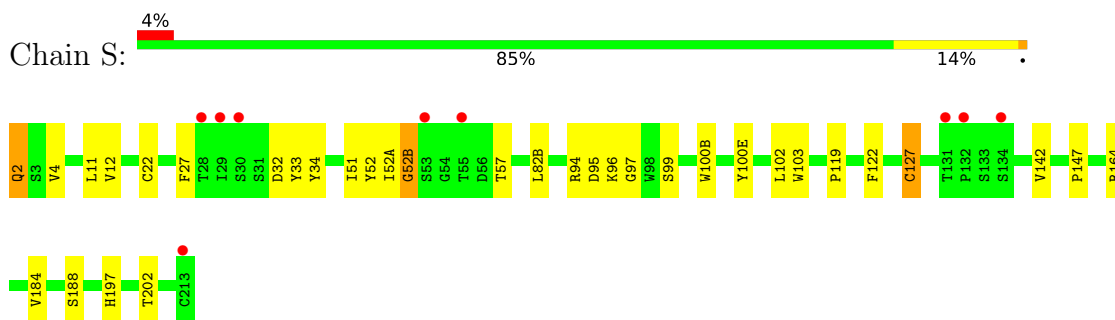
- Molecule 2: C59 Fab Heavy chain



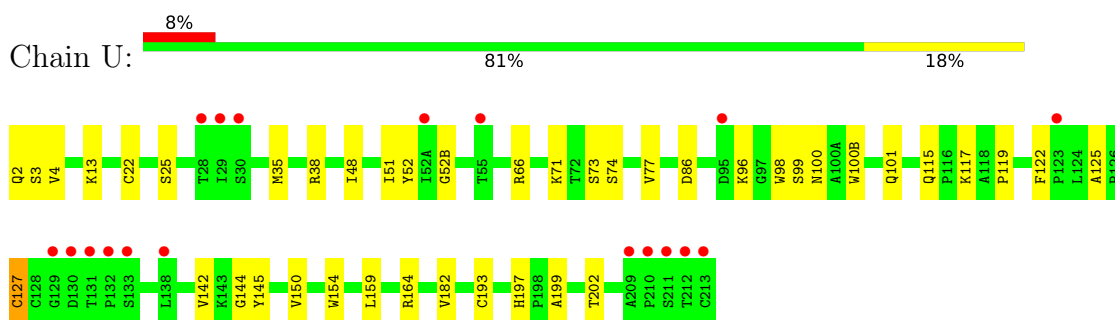
- Molecule 2: C59 Fab Heavy chain



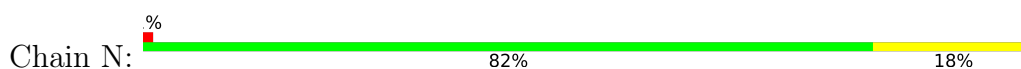
- Molecule 2: C59 Fab Heavy chain

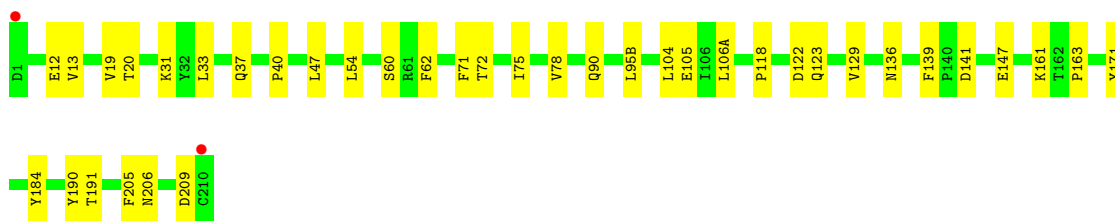


- Molecule 2: C59 Fab Heavy chain

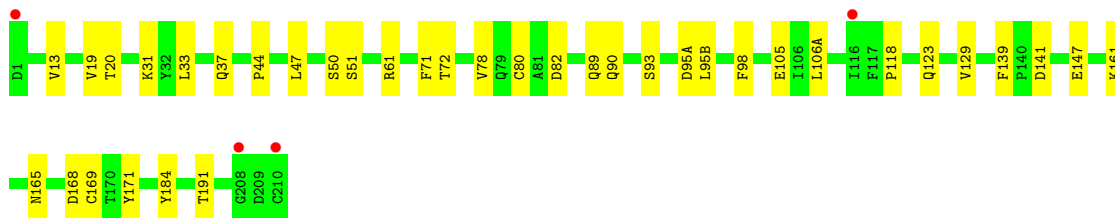
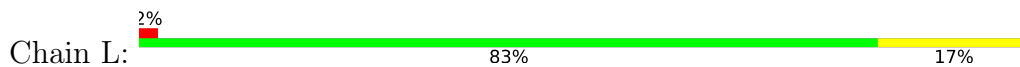


- Molecule 3: C59 Fab Light chain

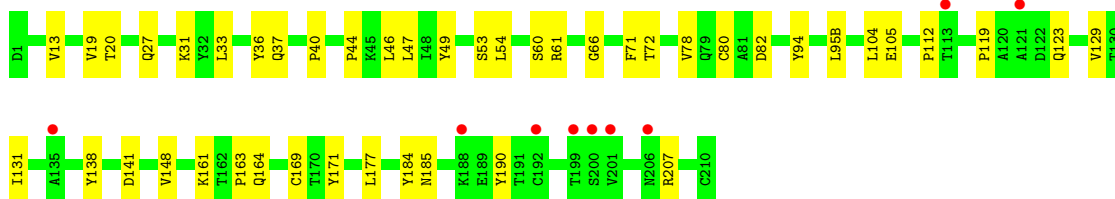
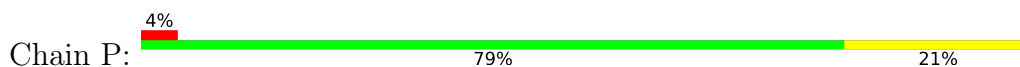




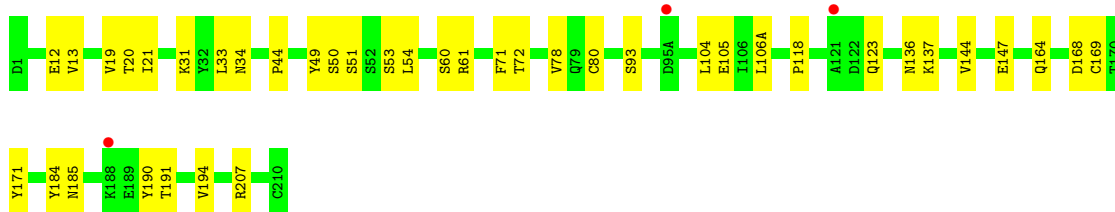
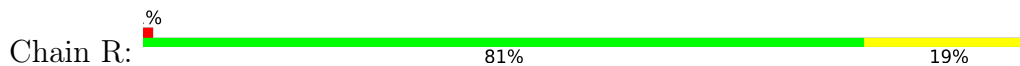
- Molecule 3: C59 Fab Light chain



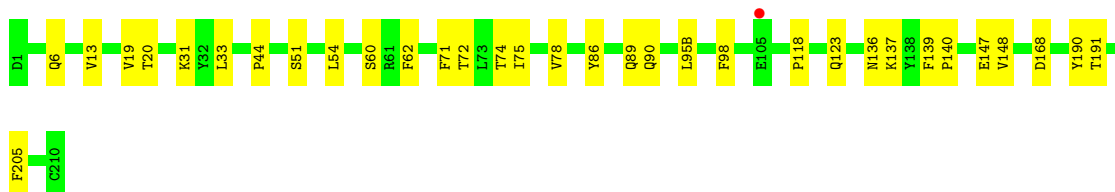
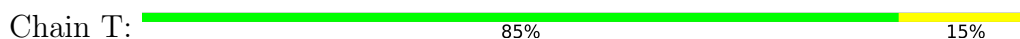
- Molecule 3: C59 Fab Light chain



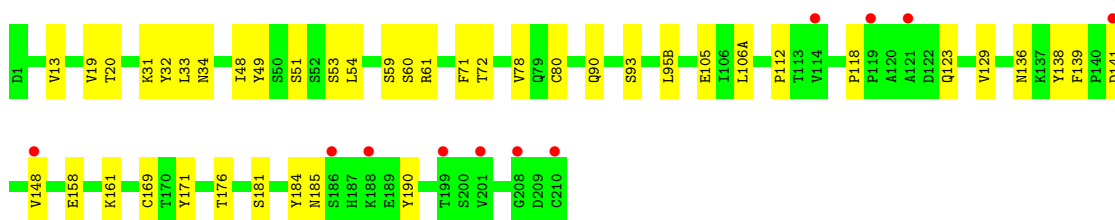
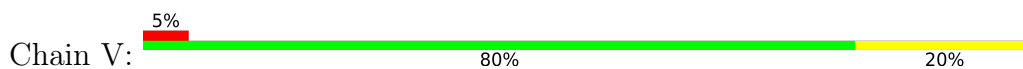
- Molecule 3: C59 Fab Light chain



- Molecule 3: C59 Fab Light chain



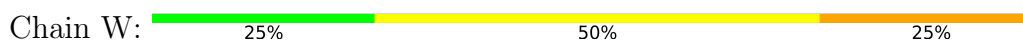
- Molecule 3: C59 Fab Light chain



- Molecule 4: 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



- Molecule 4: 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



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



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



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



- 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:



MAG1
MAG2
BMJ3
MAN4
MAN5

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	102.10Å 172.92Å 404.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	87.29 – 3.30 87.29 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.9 (87.29-3.30) 99.9 (87.29-3.30)	Depositor EDS
$R_{merge}$	0.80	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.94 (at 3.33Å)	Xtrriage
Refinement program	PHENIX 1.20.1-4487	Depositor
R, $R_{free}$	0.206 , 0.243 0.203 , 0.239	Depositor DCC
$R_{free}$ test set	5506 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	56.9	Xtrriage
Anisotropy	0.666	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 38.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	36890	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	71.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 19.46% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, BMA, MAN, PCA

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	0.35	0/2936	0.58	2/3978 (0.1%)
1	B	0.34	0/2936	0.57	2/3978 (0.1%)
1	C	0.34	0/2936	0.58	2/3978 (0.1%)
1	D	0.35	0/2936	0.61	2/3978 (0.1%)
1	E	0.34	0/2936	0.58	0/3978
1	F	0.36	0/2936	0.58	2/3978 (0.1%)
2	H	0.28	0/1684	0.51	0/2311
2	M	0.30	0/1684	0.54	0/2311
2	O	0.27	0/1684	0.50	0/2311
2	Q	0.27	0/1684	0.51	0/2311
2	S	0.27	0/1684	0.51	0/2311
2	U	0.31	0/1684	0.53	0/2311
3	L	0.30	0/1629	0.53	0/2231
3	N	0.32	0/1629	0.53	0/2231
3	P	0.28	0/1629	0.51	0/2231
3	R	0.30	0/1629	0.53	0/2231
3	T	0.28	0/1629	0.52	0/2231
3	V	0.30	0/1629	0.51	0/2231
All	All	0.32	0/37494	0.55	10/51120 (0.0%)

There are no bond length outliers.

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	62	SER	CA-C-N	6.30	133.03	121.70
1	B	62	SER	C-N-CA	6.30	133.03	121.70
1	F	62	SER	CA-C-N	5.81	132.16	121.70
1	F	62	SER	C-N-CA	5.81	132.16	121.70
1	C	62	SER	CA-C-N	5.78	132.10	121.70

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	2860	0	2781	45	0
1	B	2860	0	2781	36	2
1	C	2860	0	2781	39	0
1	D	2860	0	2781	47	0
1	E	2860	0	2781	45	2
1	F	2860	0	2781	39	0
2	H	1647	0	1597	31	0
2	M	1647	0	1597	37	0
2	O	1647	0	1597	28	0
2	Q	1647	0	1597	31	0
2	S	1647	0	1597	22	0
2	U	1647	0	1597	26	0
3	L	1595	0	1532	26	0
3	N	1595	0	1532	27	0
3	P	1595	0	1532	32	0
3	R	1595	0	1532	35	0
3	T	1595	0	1532	26	0
3	V	1595	0	1532	34	0
4	G	50	0	43	1	0
4	W	50	0	43	1	0
5	I	39	0	34	1	0
5	K	39	0	34	1	0
5	X	39	0	34	4	0
6	J	61	0	52	1	0
All	All	36890	0	35700	551	2

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 8.

The worst 5 of 551 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:L:13:VAL:HG21	3:L:19:VAL:HG22	1.46	0.98
3:N:13:VAL:HG21	3:N:19:VAL:HG22	1.55	0.89
3:T:13:VAL:HG21	3:T:19:VAL:HG22	1.57	0.87
2:M:164:ARG:NH2	3:N:136:ASN:OD1	2.08	0.86
3:P:13:VAL:HG21	3:P:19:VAL:HG22	1.56	0.86

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:349:ARG:NH2	1:E:233:ASP:OD2[1_655]	2.01	0.19
1:B:233:ASP:OD2	1:E:349:ARG:NH2[1_655]	2.14	0.06

## 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	360/362 (99%)	352 (98%)	8 (2%)	0	100	100
1	B	360/362 (99%)	351 (98%)	9 (2%)	0	100	100
1	C	360/362 (99%)	351 (98%)	9 (2%)	0	100	100
1	D	360/362 (99%)	353 (98%)	7 (2%)	0	100	100
1	E	360/362 (99%)	352 (98%)	8 (2%)	0	100	100
1	F	360/362 (99%)	350 (97%)	10 (3%)	0	100	100
2	H	221/223 (99%)	211 (96%)	9 (4%)	1 (0%)	24	55
2	M	221/223 (99%)	210 (95%)	10 (4%)	1 (0%)	24	55
2	O	221/223 (99%)	210 (95%)	10 (4%)	1 (0%)	24	55
2	Q	221/223 (99%)	209 (95%)	11 (5%)	1 (0%)	24	55
2	S	221/223 (99%)	209 (95%)	10 (4%)	2 (1%)	14	43
2	U	221/223 (99%)	211 (96%)	10 (4%)	0	100	100

*Continued on next page...*

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	L	212/214 (99%)	207 (98%)	4 (2%)	1 (0%)	24	55
3	N	212/214 (99%)	205 (97%)	7 (3%)	0	100	100
3	P	212/214 (99%)	206 (97%)	6 (3%)	0	100	100
3	R	212/214 (99%)	205 (97%)	6 (3%)	1 (0%)	24	55
3	T	212/214 (99%)	206 (97%)	6 (3%)	0	100	100
3	V	212/214 (99%)	205 (97%)	7 (3%)	0	100	100
All	All	4758/4794 (99%)	4603 (97%)	147 (3%)	8 (0%)	43	71

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	M	32	ASP
2	H	32	ASP
2	O	54	GLY
2	S	32	ASP
2	Q	52(A)	ILE

### 5.3.2 Protein sidechains [i](#)

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	302/302 (100%)	301 (100%)	1 (0%)	86	86
1	B	302/302 (100%)	302 (100%)	0	100	100
1	C	302/302 (100%)	302 (100%)	0	100	100
1	D	302/302 (100%)	302 (100%)	0	100	100
1	E	302/302 (100%)	301 (100%)	1 (0%)	86	86
1	F	302/302 (100%)	302 (100%)	0	100	100
2	H	186/186 (100%)	185 (100%)	1 (0%)	81	83
2	M	186/186 (100%)	185 (100%)	1 (0%)	81	83
2	O	186/186 (100%)	186 (100%)	0	100	100
2	Q	186/186 (100%)	185 (100%)	1 (0%)	81	83

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	S	186/186 (100%)	185 (100%)	1 (0%)	81	83
2	U	186/186 (100%)	185 (100%)	1 (0%)	81	83
3	L	182/182 (100%)	182 (100%)	0	100	100
3	N	182/182 (100%)	182 (100%)	0	100	100
3	P	182/182 (100%)	182 (100%)	0	100	100
3	R	182/182 (100%)	182 (100%)	0	100	100
3	T	182/182 (100%)	182 (100%)	0	100	100
3	V	182/182 (100%)	182 (100%)	0	100	100
All	All	4020/4020 (100%)	4013 (100%)	7 (0%)	87	88

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	127	CYS
2	Q	127	CYS
2	U	127	CYS
2	S	127	CYS
2	M	127	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 33 such sidechains are listed below:

Mol	Chain	Res	Type
3	R	153	GLN
3	R	187	HIS
3	V	159	ASN
1	E	379	ASN
1	E	319	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

6 non-standard protein/DNA/RNA residues 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
2	PCA	M	2	2	7,8,9	1.96	1 (14%)	9,10,12	2.69	5 (55%)
2	PCA	U	2	2	7,8,9	1.85	1 (14%)	9,10,12	2.23	5 (55%)
2	PCA	H	2	2	7,8,9	1.86	1 (14%)	9,10,12	2.30	5 (55%)
2	PCA	O	2	2	7,8,9	1.95	1 (14%)	9,10,12	2.54	5 (55%)
2	PCA	Q	2	2	7,8,9	1.90	1 (14%)	9,10,12	2.00	4 (44%)
2	PCA	S	2	2	7,8,9	1.90	1 (14%)	9,10,12	2.46	5 (55%)

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
2	PCA	M	2	2	-	0/0/11/13	0/1/1/1
2	PCA	U	2	2	-	0/0/11/13	0/1/1/1
2	PCA	H	2	2	-	0/0/11/13	0/1/1/1
2	PCA	O	2	2	-	0/0/11/13	0/1/1/1
2	PCA	Q	2	2	-	0/0/11/13	0/1/1/1
2	PCA	S	2	2	-	0/0/11/13	0/1/1/1

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	M	2	PCA	CD-N	5.03	1.47	1.34
2	O	2	PCA	CD-N	4.94	1.46	1.34
2	Q	2	PCA	CD-N	4.92	1.46	1.34
2	S	2	PCA	CD-N	4.87	1.46	1.34
2	H	2	PCA	CD-N	4.74	1.46	1.34

The worst 5 of 29 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	2	PCA	CB-CA-C	-4.42	106.59	112.66
2	M	2	PCA	OE-CD-CG	-3.82	119.91	126.72
2	O	2	PCA	OE-CD-CG	-3.57	120.35	126.72

*Continued on next page...*

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	2	PCA	CB-CA-C	-3.47	107.89	112.66
2	S	2	PCA	CB-CA-C	-3.31	108.12	112.66

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	M	2	PCA	1	0
2	S	2	PCA	1	0

## 5.5 Carbohydrates [i](#)

22 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	G	1	1,4	14,14,15	0.51	0	17,19,21	1.24	1 (5%)
4	NAG	G	2	4	14,14,15	0.49	0	17,19,21	0.57	0
4	BMA	G	3	4	11,11,12	1.25	1 (9%)	15,15,17	0.96	1 (6%)
4	MAN	G	4	4	11,11,12	1.24	2 (18%)	15,15,17	1.00	1 (6%)
5	NAG	I	1	1,5	14,14,15	0.46	0	17,19,21	1.45	2 (11%)
5	NAG	I	2	5	14,14,15	0.38	0	17,19,21	0.44	0
5	BMA	I	3	5	11,11,12	0.87	0	15,15,17	0.87	0
6	NAG	J	1	1,6	14,14,15	0.38	0	17,19,21	1.40	2 (11%)
6	NAG	J	2	6	14,14,15	0.62	1 (7%)	17,19,21	0.58	0
6	BMA	J	3	6	11,11,12	0.88	0	15,15,17	0.90	1 (6%)
6	MAN	J	4	6	11,11,12	1.34	1 (9%)	15,15,17	0.98	1 (6%)
6	MAN	J	5	6	11,11,12	0.99	0	15,15,17	0.82	1 (6%)
5	NAG	K	1	1,5	14,14,15	0.58	0	17,19,21	1.26	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	NAG	K	2	5	14,14,15	0.79	1 (7%)	17,19,21	0.42	0
5	BMA	K	3	5	11,11,12	1.04	1 (9%)	15,15,17	0.83	0
4	NAG	W	1	1,4	14,14,15	0.61	1 (7%)	17,19,21	0.57	0
4	NAG	W	2	4	14,14,15	0.33	0	17,19,21	0.41	0
4	BMA	W	3	4	11,11,12	0.97	0	15,15,17	1.02	1 (6%)
4	MAN	W	4	4	11,11,12	1.45	2 (18%)	15,15,17	1.31	1 (6%)
5	NAG	X	1	1,5	14,14,15	0.81	1 (7%)	17,19,21	1.34	1 (5%)
5	NAG	X	2	5	14,14,15	0.46	0	17,19,21	0.52	0
5	BMA	X	3	5	11,11,12	1.14	1 (9%)	15,15,17	0.77	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
4	NAG	G	1	1,4	-	4/6/23/26	0/1/1/1
4	NAG	G	2	4	-	1/6/23/26	0/1/1/1
4	BMA	G	3	4	-	0/2/19/22	0/1/1/1
4	MAN	G	4	4	-	0/2/19/22	0/1/1/1
5	NAG	I	1	1,5	-	4/6/23/26	0/1/1/1
5	NAG	I	2	5	-	1/6/23/26	0/1/1/1
5	BMA	I	3	5	-	0/2/19/22	0/1/1/1
6	NAG	J	1	1,6	-	4/6/23/26	0/1/1/1
6	NAG	J	2	6	-	1/6/23/26	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
5	NAG	K	1	1,5	-	4/6/23/26	0/1/1/1
5	NAG	K	2	5	-	1/6/23/26	0/1/1/1
5	BMA	K	3	5	-	0/2/19/22	0/1/1/1
4	NAG	W	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	W	2	4	-	1/6/23/26	0/1/1/1
4	BMA	W	3	4	-	0/2/19/22	0/1/1/1
4	MAN	W	4	4	-	2/2/19/22	0/1/1/1
5	NAG	X	1	1,5	-	3/6/23/26	0/1/1/1
5	NAG	X	2	5	-	1/6/23/26	0/1/1/1
5	BMA	X	3	5	-	0/2/19/22	0/1/1/1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	J	4	MAN	C2-C3	3.05	1.57	1.52
4	W	4	MAN	C1-C2	3.03	1.59	1.52
5	K	2	NAG	O5-C1	-2.89	1.38	1.43
5	X	1	NAG	C1-C2	-2.70	1.48	1.52
4	G	4	MAN	C4-C5	2.40	1.58	1.53

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	W	4	MAN	C1-O5-C5	4.17	117.77	112.19
5	I	1	NAG	C2-N2-C7	3.93	128.16	122.90
5	X	1	NAG	C2-N2-C7	3.84	128.05	122.90
4	G	1	NAG	C2-N2-C7	3.81	128.01	122.90
5	K	1	NAG	C2-N2-C7	3.75	127.93	122.90

There are no chirality outliers.

5 of 29 torsion outliers are listed below:

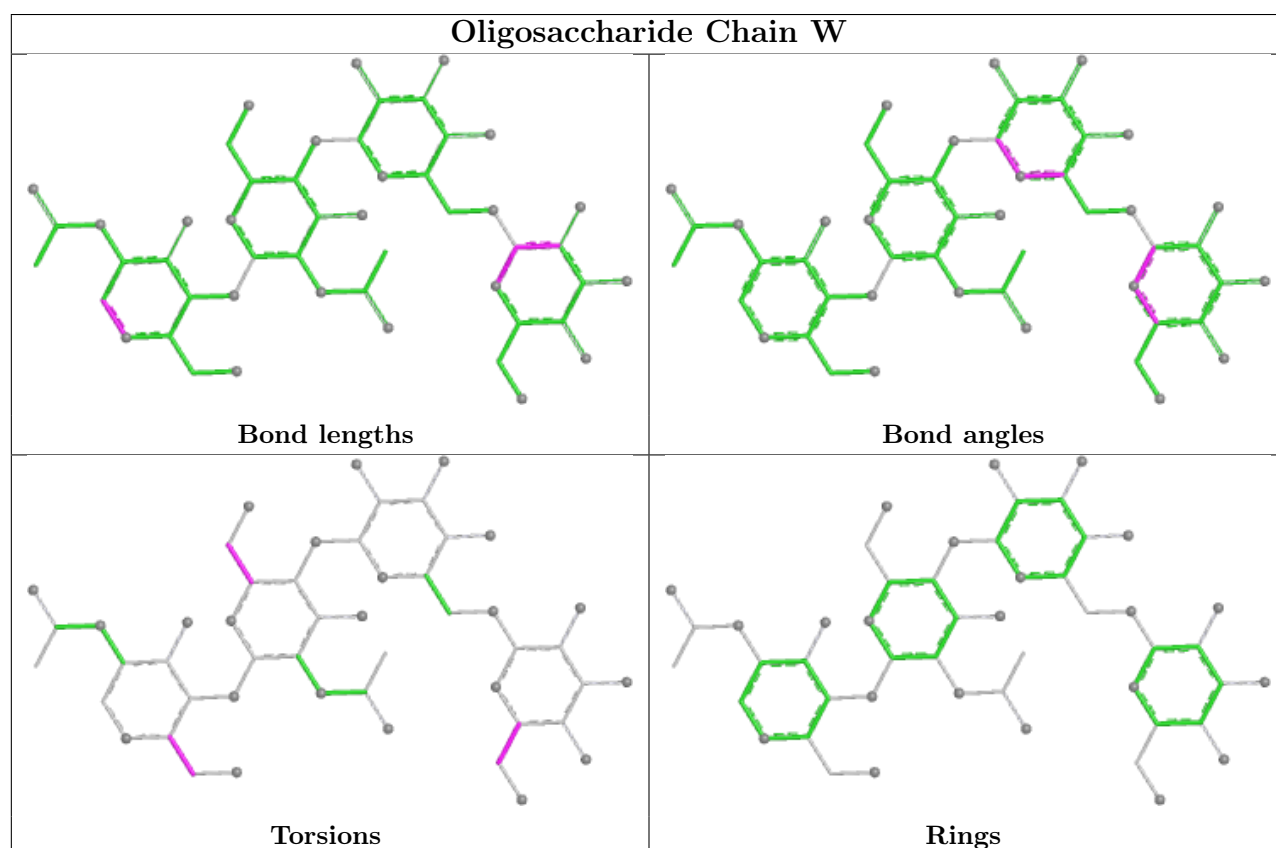
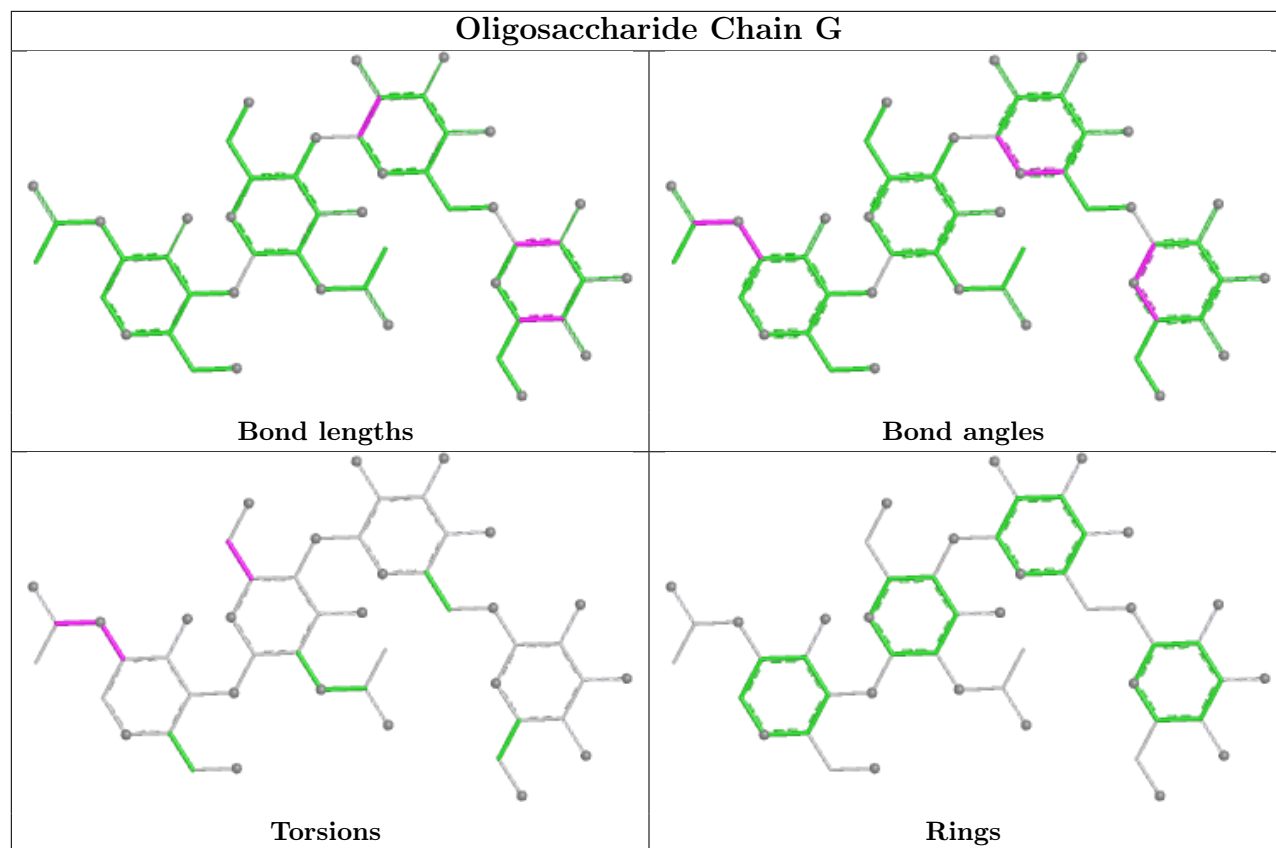
Mol	Chain	Res	Type	Atoms
4	G	1	NAG	C8-C7-N2-C2
4	G	1	NAG	O7-C7-N2-C2
5	I	1	NAG	C8-C7-N2-C2
5	I	1	NAG	O7-C7-N2-C2
5	K	1	NAG	C8-C7-N2-C2

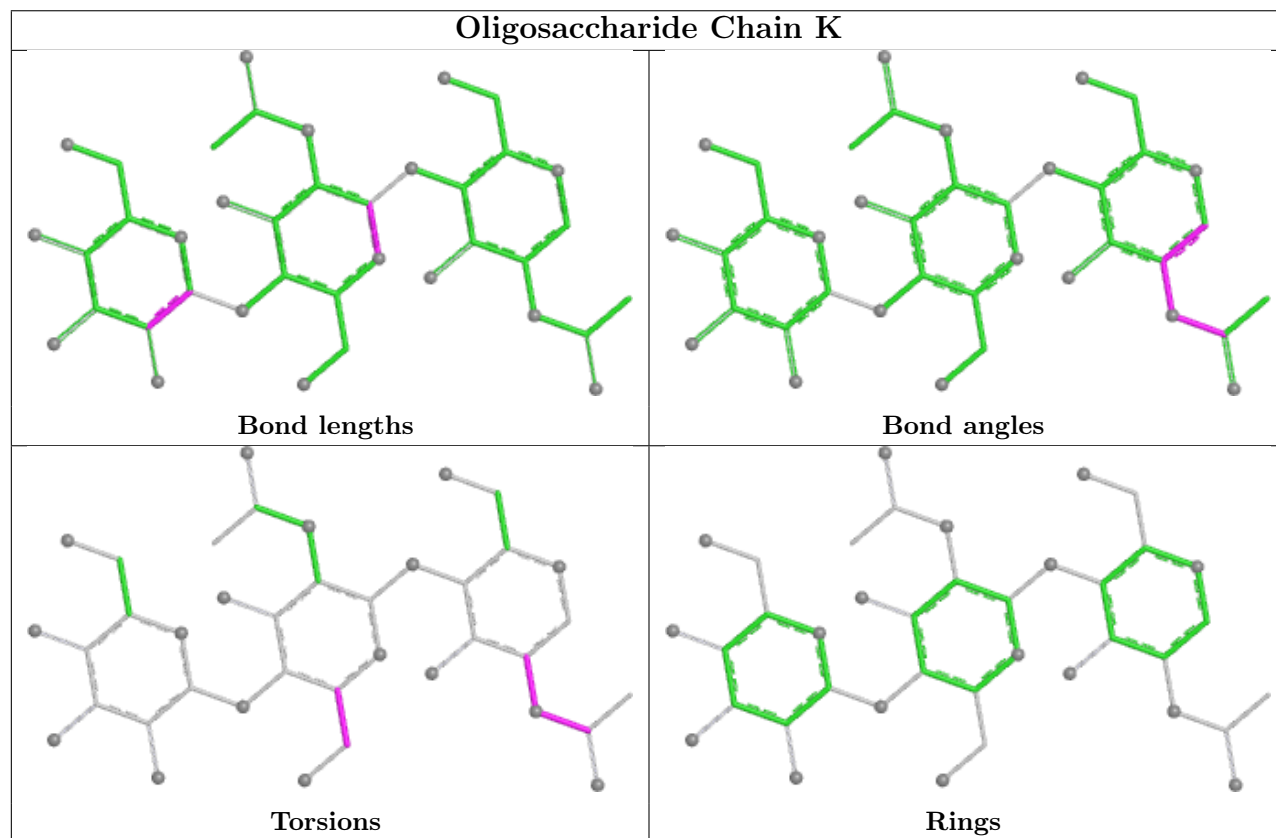
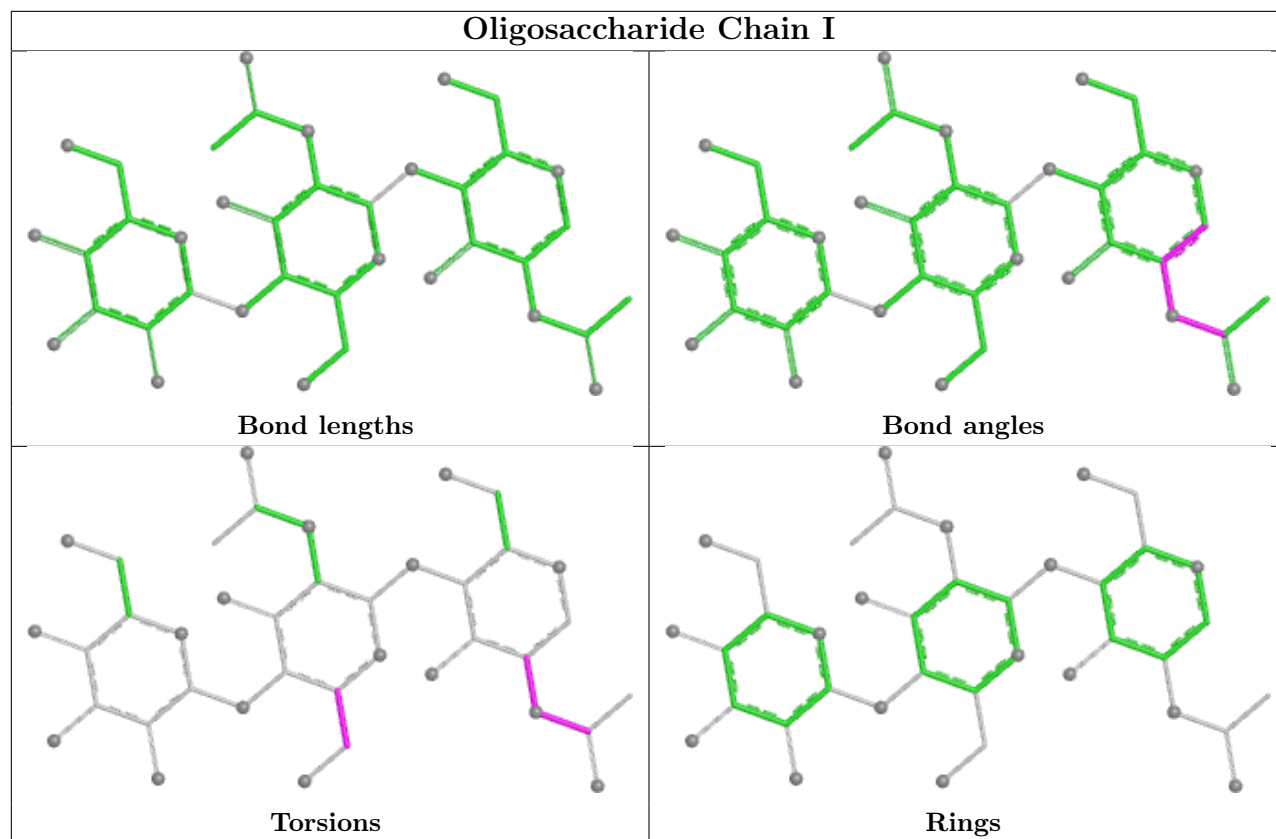
There are no ring outliers.

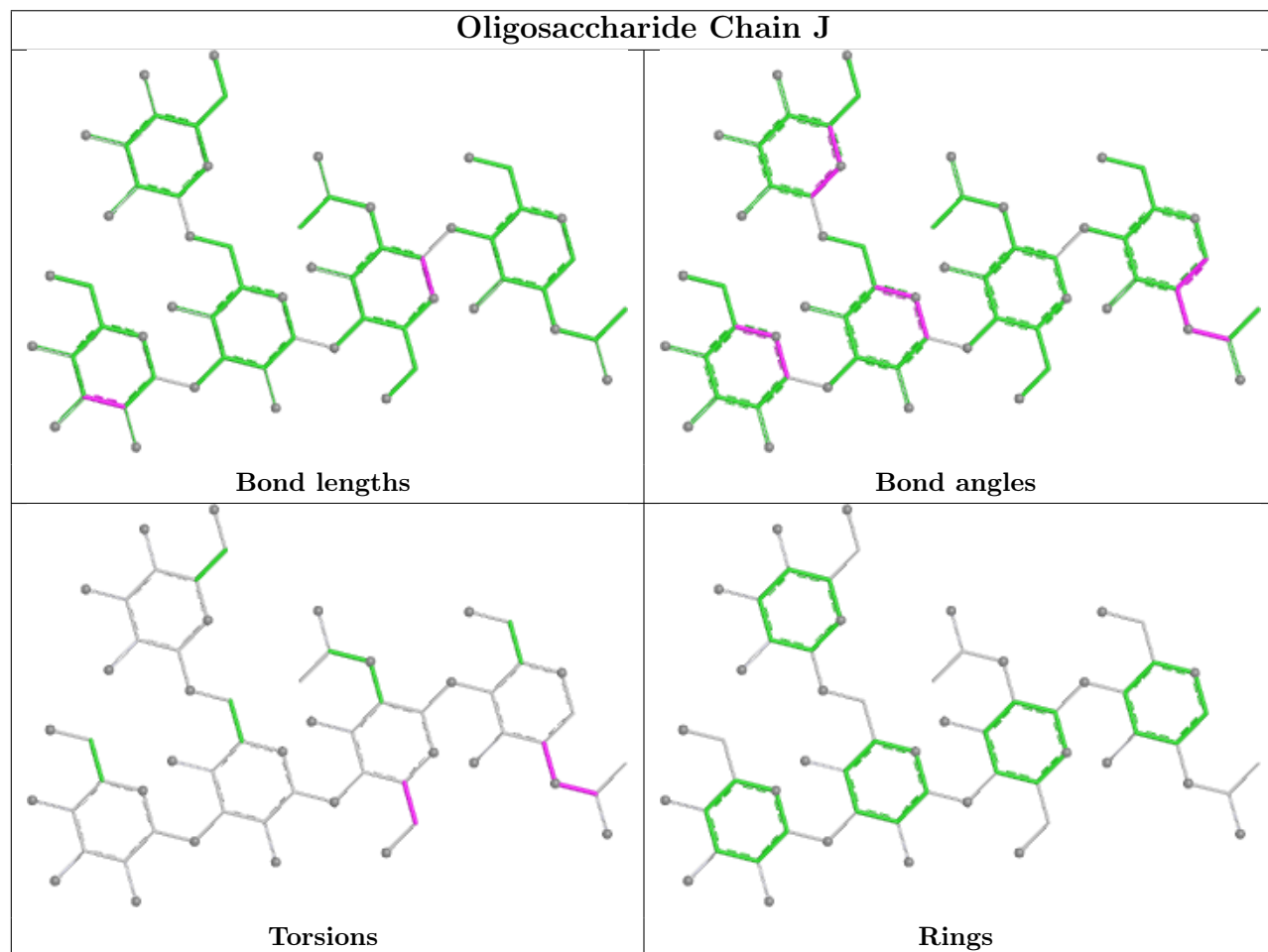
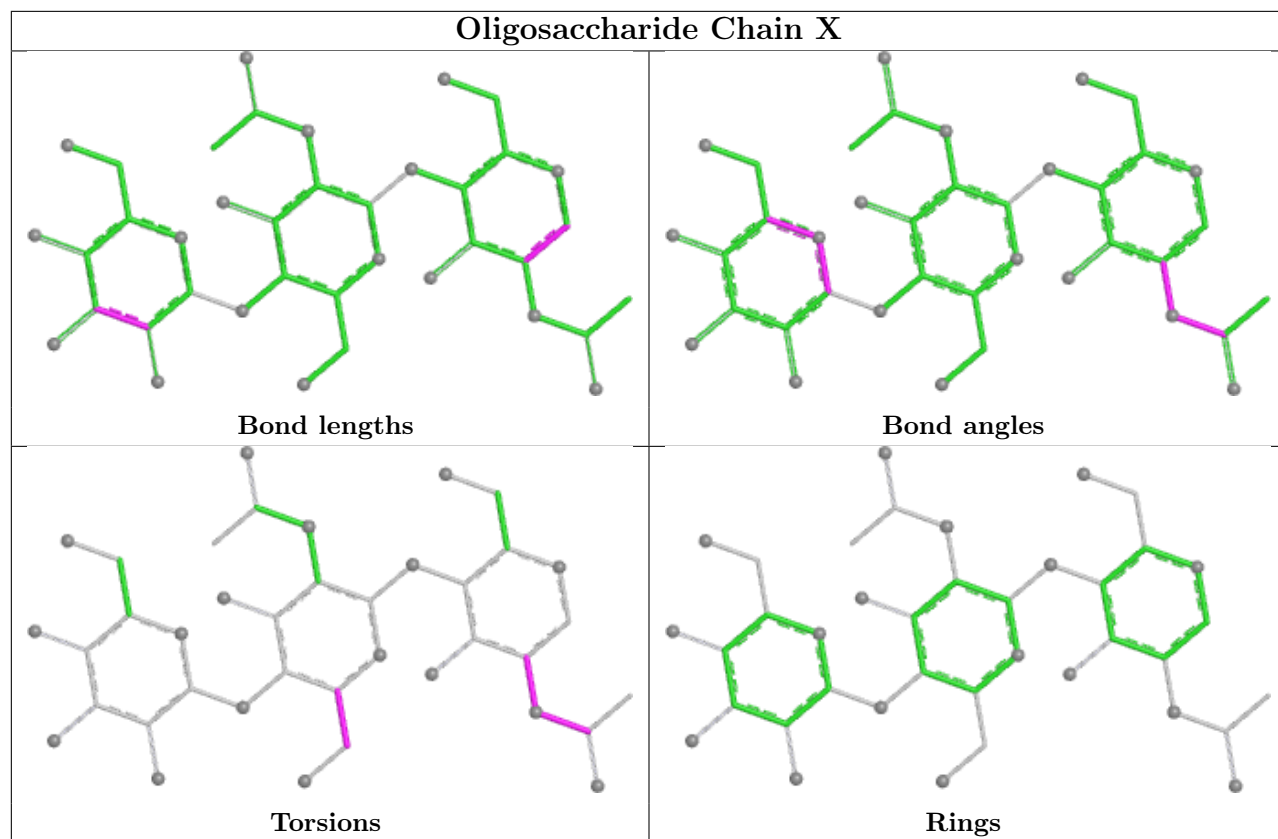
6 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	1	NAG	1	0
4	W	1	NAG	1	0
6	J	1	NAG	1	0
5	X	1	NAG	4	0
5	K	1	NAG	1	0
5	I	1	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](#)

There are no ligands in this entry.

## 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	362/362 (100%)	-0.25	0 <span style="border: 1px solid blue; padding: 0 2px;">100</span> <span style="border: 1px solid blue; padding: 0 2px;">100</span>	35, 52, 81, 133	0
1	B	362/362 (100%)	-0.25	0 <span style="border: 1px solid blue; padding: 0 2px;">100</span> <span style="border: 1px solid blue; padding: 0 2px;">100</span>	35, 53, 82, 133	0
1	C	362/362 (100%)	-0.26	1 (0%) <span style="border: 1px solid blue; padding: 0 2px;">90</span> <span style="border: 1px solid blue; padding: 0 2px;">82</span>	40, 55, 86, 143	0
1	D	362/362 (100%)	-0.21	1 (0%) <span style="border: 1px solid blue; padding: 0 2px;">90</span> <span style="border: 1px solid blue; padding: 0 2px;">82</span>	39, 52, 80, 133	0
1	E	362/362 (100%)	-0.20	2 (0%) <span style="border: 1px solid blue; padding: 0 2px;">85</span> <span style="border: 1px solid blue; padding: 0 2px;">73</span>	39, 55, 84, 124	0
1	F	362/362 (100%)	-0.32	0 <span style="border: 1px solid blue; padding: 0 2px;">100</span> <span style="border: 1px solid blue; padding: 0 2px;">100</span>	33, 48, 84, 133	0
2	H	222/223 (99%)	0.22	12 (5%) <span style="border: 1px solid red; padding: 0 2px;">31</span> <span style="border: 1px solid red; padding: 0 2px;">21</span>	42, 76, 159, 211	0
2	M	222/223 (99%)	-0.01	8 (3%) <span style="border: 1px solid red; padding: 0 2px;">46</span> <span style="border: 1px solid red; padding: 0 2px;">31</span>	37, 66, 132, 187	0
2	O	222/223 (99%)	0.43	16 (7%) <span style="border: 1px solid red; padding: 0 2px;">21</span> <span style="border: 1px solid red; padding: 0 2px;">15</span>	48, 84, 191, 218	0
2	Q	222/223 (99%)	0.33	9 (4%) <span style="border: 1px solid red; padding: 0 2px;">41</span> <span style="border: 1px solid red; padding: 0 2px;">27</span>	48, 84, 152, 212	0
2	S	222/223 (99%)	0.24	9 (4%) <span style="border: 1px solid red; padding: 0 2px;">41</span> <span style="border: 1px solid red; padding: 0 2px;">27</span>	51, 80, 140, 189	0
2	U	222/223 (99%)	0.26	18 (8%) <span style="border: 1px solid red; padding: 0 2px;">18</span> <span style="border: 1px solid red; padding: 0 2px;">13</span>	43, 69, 178, 235	0
3	L	214/214 (100%)	0.07	4 (1%) <span style="border: 1px solid blue; padding: 0 2px;">66</span> <span style="border: 1px solid blue; padding: 0 2px;">48</span>	37, 69, 150, 178	0
3	N	214/214 (100%)	-0.14	2 (0%) <span style="border: 1px solid blue; padding: 0 2px;">81</span> <span style="border: 1px solid blue; padding: 0 2px;">65</span>	34, 59, 114, 155	0
3	P	214/214 (100%)	0.33	9 (4%) <span style="border: 1px solid red; padding: 0 2px;">40</span> <span style="border: 1px solid red; padding: 0 2px;">26</span>	44, 79, 181, 233	0
3	R	214/214 (100%)	0.05	3 (1%) <span style="border: 1px solid blue; padding: 0 2px;">73</span> <span style="border: 1px solid blue; padding: 0 2px;">55</span>	43, 69, 144, 163	0
3	T	214/214 (100%)	-0.07	1 (0%) <span style="border: 1px solid blue; padding: 0 2px;">87</span> <span style="border: 1px solid blue; padding: 0 2px;">76</span>	44, 68, 108, 128	0
3	V	214/214 (100%)	0.32	11 (5%) <span style="border: 1px solid red; padding: 0 2px;">33</span> <span style="border: 1px solid red; padding: 0 2px;">22</span>	39, 75, 165, 199	0
All	All	4788/4794 (99%)	-0.02	106 (2%) <span style="border: 1px solid blue; padding: 0 2px;">62</span> <span style="border: 1px solid blue; padding: 0 2px;">43</span>	33, 59, 148, 235	0

The worst 5 of 106 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	S	53	SER	4.4
2	O	132	PRO	4.1
2	O	131	THR	4.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	U	55	THR	4.0
2	S	132	PRO	4.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [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
2	PCA	H	2	8/9	0.86	0.12	62,67,70,72	0
2	PCA	S	2	8/9	0.87	0.14	64,69,73,74	0
2	PCA	U	2	8/9	0.90	0.11	63,64,66,67	0
2	PCA	M	2	8/9	0.92	0.10	57,62,64,66	0
2	PCA	O	2	8/9	0.92	0.10	66,68,70,72	0
2	PCA	Q	2	8/9	0.93	0.09	63,65,69,71	0

## 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.

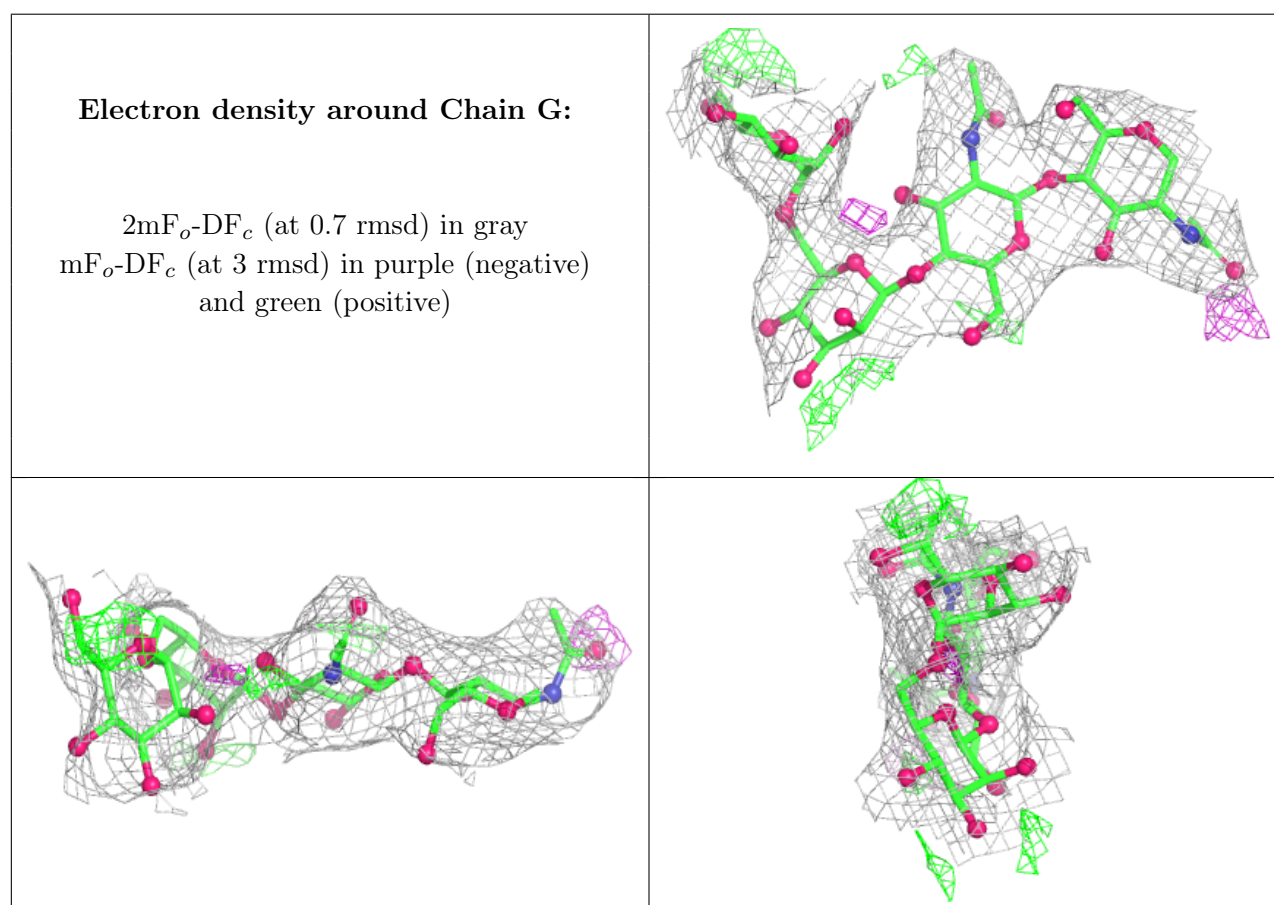
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	NAG	G	1	14/15	-	-	50,54,62,70	0
4	NAG	G	2	14/15	-	-	72,77,95,99	0
4	BMA	G	3	11/12	-	-	109,117,120,123	0
4	MAN	G	4	11/12	-	-	114,121,125,126	0
4	MAN	W	4	11/12	0.26	0.15	122,124,128,131	0
4	BMA	W	3	11/12	0.32	0.15	142,149,154,156	0
5	BMA	X	3	11/12	0.34	0.15	129,138,143,143	0
5	NAG	X	2	14/15	0.80	0.12	84,90,107,116	0
5	NAG	I	1	14/15	-	-	49,56,65,75	0
5	NAG	I	2	14/15	-	-	83,85,100,100	0
5	BMA	I	3	11/12	-	-	99,101,102,102	0
5	NAG	K	1	14/15	-	-	56,61,74,88	0
5	NAG	K	2	14/15	-	-	104,108,126,130	0
5	BMA	K	3	11/12	-	-	132,134,136,136	0
4	NAG	W	2	14/15	0.80	0.11	92,102,117,124	0

*Continued on next page...*

Continued from previous page...

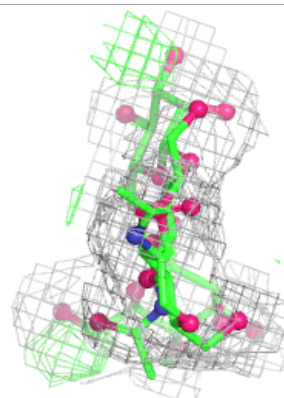
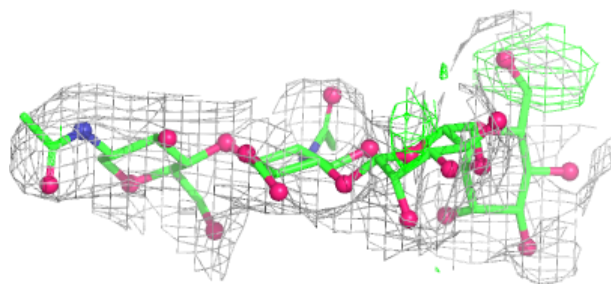
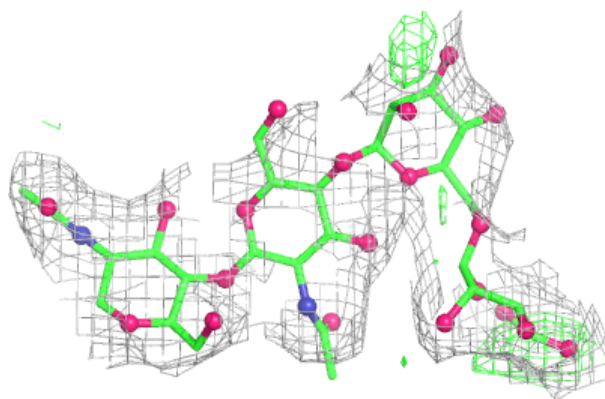
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	NAG	X	1	14/15	0.87	0.13	51,55,66,77	0
4	NAG	W	1	14/15	0.91	0.10	59,67,77,86	0
6	NAG	J	1	14/15	-	-	60,67,76,84	0
6	NAG	J	2	14/15	-	-	87,95,120,129	0
6	BMA	J	3	11/12	-	-	164,169,177,178	0
6	MAN	J	4	11/12	-	-	151,159,161,162	0
6	MAN	J	5	11/12	-	-	132,141,145,147	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.

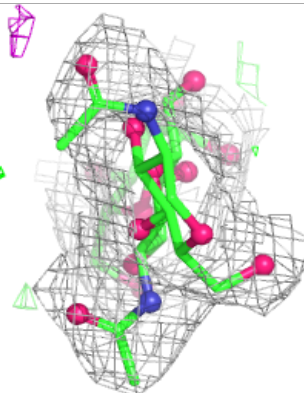
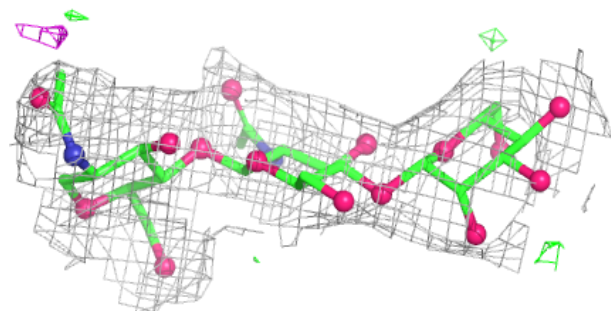
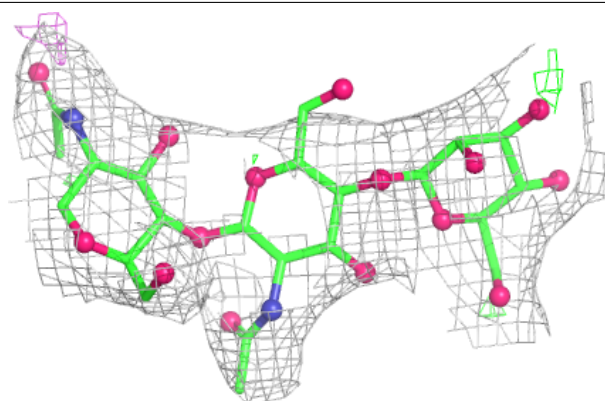


**Electron density around Chain W:**

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

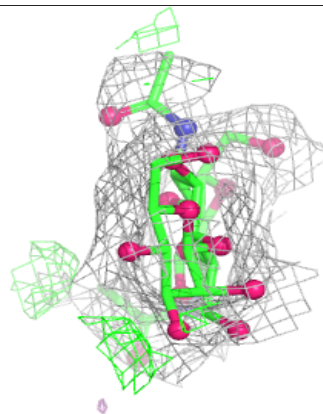
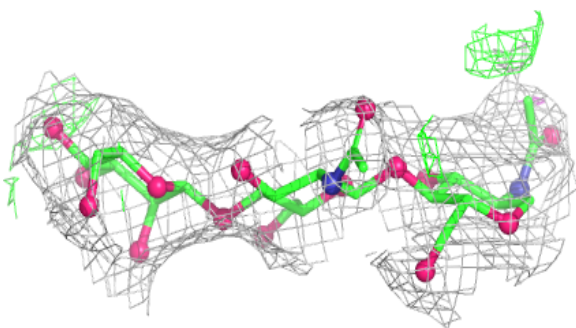
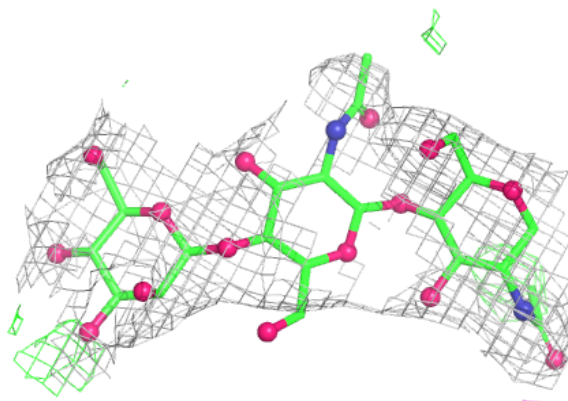
**Electron density around Chain I:**

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

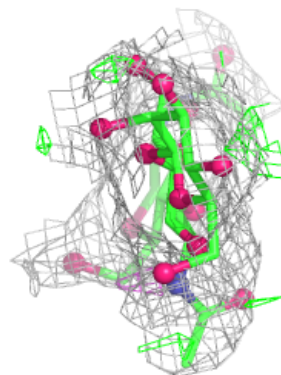
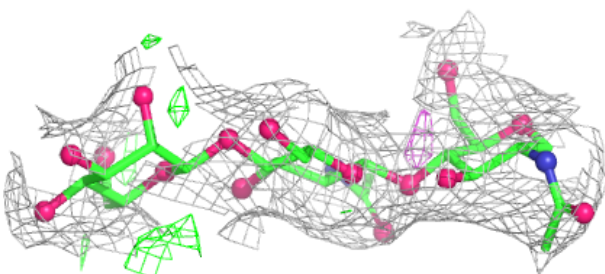
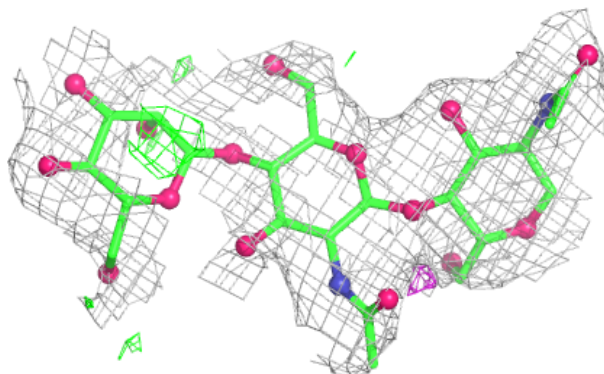


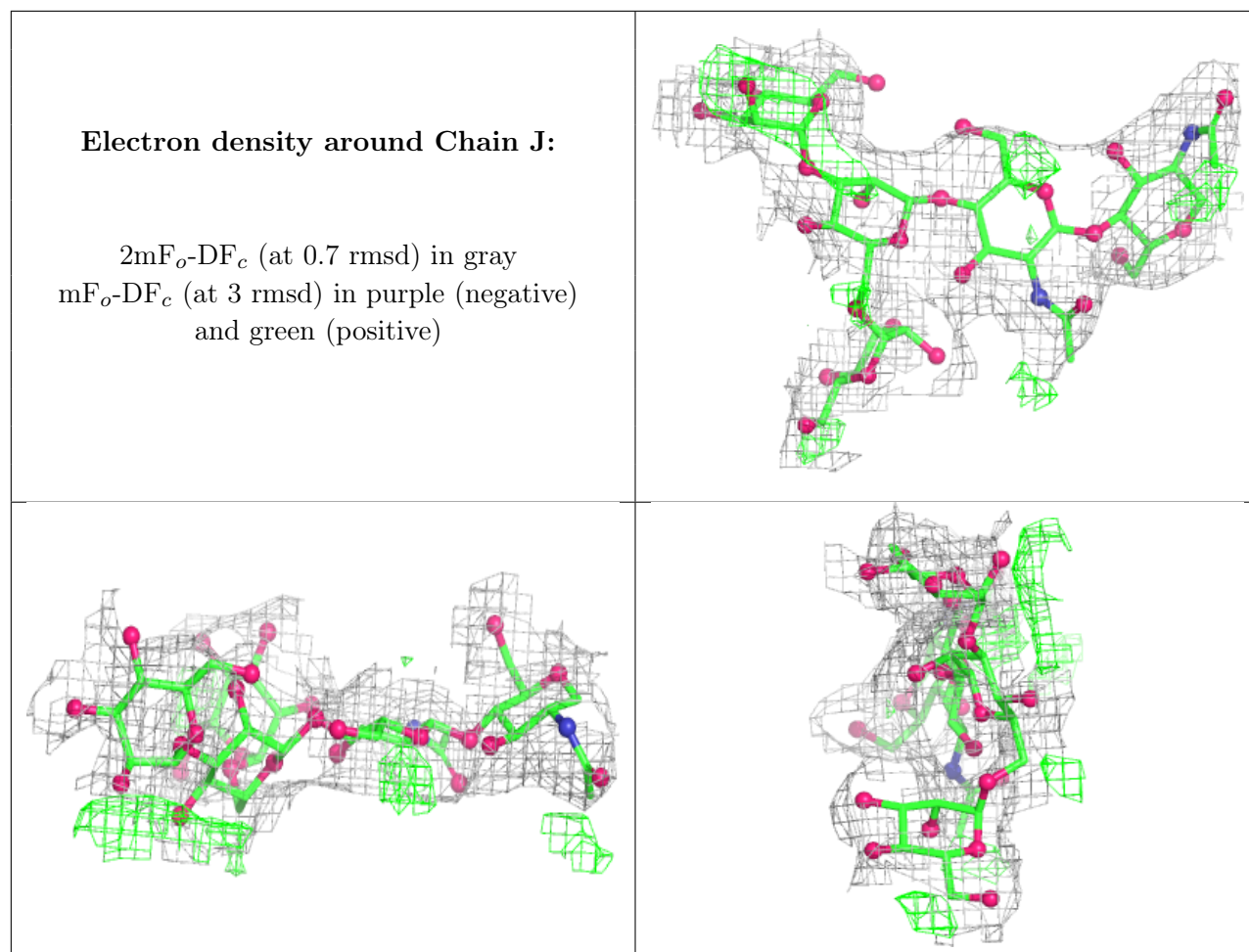
**Electron density around Chain K:**

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

**Electron density around Chain X:**

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





## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.