



# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 15, 2023 – 11:33 AM EDT

PDB ID : 7UJK  
Title : Integrin alaphIIBbeta3 complex with lamifiban  
Authors : Lin, F.-Y.; Zhu, J.; Zhu, J.; Springer, T.A.  
Deposited on : 2022-03-30  
Resolution : 2.43 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>.

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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 : 2.36  
buster-report : 1.1.7 (2018)  
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) : 2.36

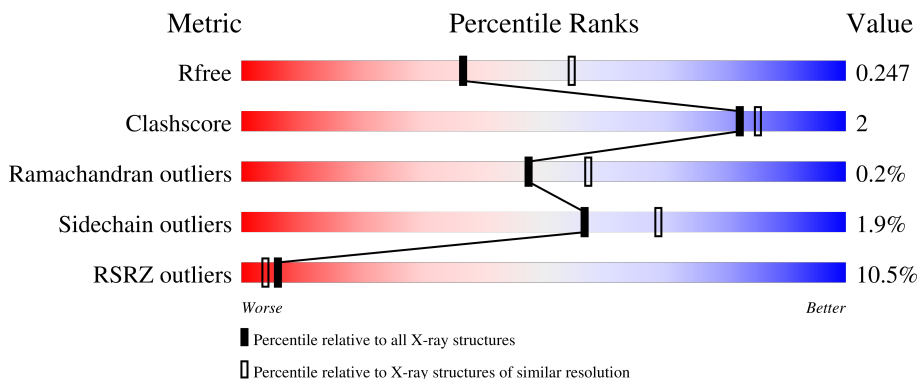
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.43 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	1564 (2.46-2.42)
Clashscore	141614	1631 (2.46-2.42)
Ramachandran outliers	138981	1617 (2.46-2.42)
Sidechain outliers	138945	1617 (2.46-2.42)
RSRZ outliers	127900	1547 (2.46-2.42)

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	457	
1	C	457	
2	B	472	
2	D	472	
3	E	221	

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Mol	Chain	Length	Quality of chain
3	H	221	<p>11% 91% 5% ..</p>
4	F	214	<p>32% 94% 6%</p>
4	L	214	<p>2% 93% 7%</p>
5	G	5	<p>60% 40%</p>
6	I	2	<p>100%</p>
6	K	2	<p>50% 50%</p>
7	J	4	<p>50% 50%</p>

## 2 Entry composition [i](#)

There are 15 unique types of molecules in this entry. The entry contains 22145 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 Integrin alpha-IIb heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	454	Total	C	N	O	S	0	8	0
			3532	2245	611	668	8			
1	C	453	Total	C	N	O	S	0	4	0
			3502	2224	604	666	8			

- Molecule 2 is a protein called Isoform Beta-3C of Integrin beta-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	466	Total	C	N	O	S	4	8	0
			3649	2273	622	720	34			
2	D	471	Total	C	N	O	S	3	2	0
			3642	2270	621	716	35			

- Molecule 3 is a protein called 10E5 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	E	214	Total	C	N	O	S	0	0	0
			1631	1035	264	326	6			
3	H	216	Total	C	N	O	S	0	0	0
			1642	1041	266	329	6			

- Molecule 4 is a protein called 10E5 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	F	214	Total	C	N	O	S	0	0	0
			1637	1019	268	341	9			
4	L	214	Total	C	N	O	S	0	0	0
			1637	1019	268	341	9			

- Molecule 5 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
			Total	C	N	O			
5	G	5	61	34	2	25	0	0	0

- Molecule 6 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
			Total	C	N	O			
6	I	2	28	16	2	10	0	0	0
6	K	2	28	16	2	10	0	0	0

- Molecule 7 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
			Total	C	N	O			
7	J	4	50	28	2	20	0	0	0

- Molecule 8 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total O S 5 4 1	0	0
8	A	1	Total O S 5 4 1	0	0
8	A	1	Total O S 5 4 1	0	0
8	C	1	Total O S 5 4 1	0	0
8	C	1	Total O S 5 4 1	0	0
8	C	1	Total O S 5 4 1	0	0
8	L	1	Total O S 5 4 1	0	0

- Molecule 9 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	1	Total	C O	0	0
			6	3 3		

- Molecule 10 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	4	Total	Ca	0	0
			4	4		
10	B	2	Total	Ca	0	0
			2	2		
10	C	4	Total	Ca	0	0
			4	4		
10	D	2	Total	Ca	0	0
			2	2		

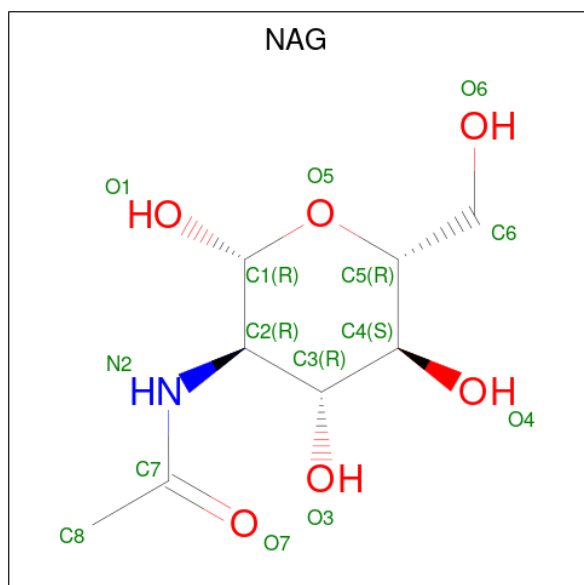
- Molecule 11 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	1	Total	Cl	0	0
			1	1		
11	C	2	Total	Cl	0	0
			2	2		

- Molecule 12 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	B	1	Total Mg 1 1	0	0
12	D	1	Total Mg 1 1	0	0

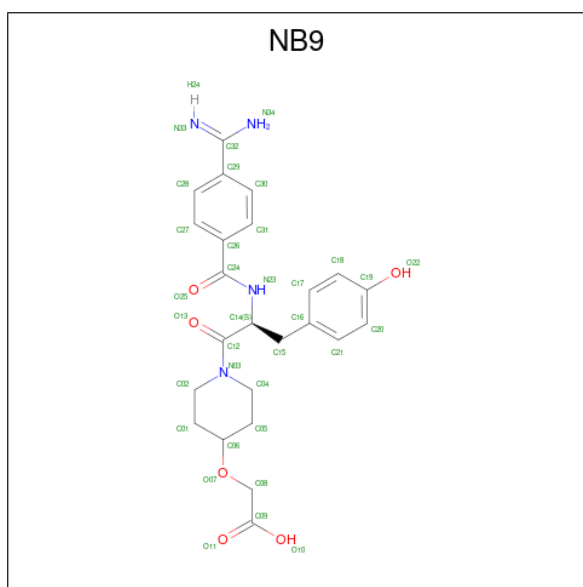
- Molecule 13 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	B	1	Total C N O 14 8 1 5	0	0
13	D	1	Total C N O 14 8 1 5	0	0

- Molecule 14 is Lamifiban (three-letter code: NB9) (formula: C<sub>24</sub>H<sub>28</sub>N<sub>4</sub>O<sub>6</sub>) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	
14	B	1	Total	C	N	O	0	0
			34	24	4	6		
14	D	1	Total	C	N	O	0	0
			34	24	4	6		

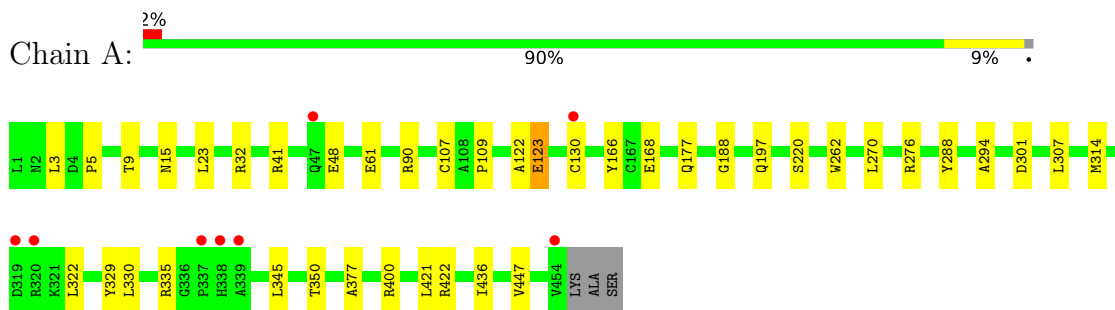
- Molecule 15 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	A	323	Total	O	0	0
			323	323		
15	B	214	Total	O	0	0
			214	214		
15	C	125	Total	O	0	0
			125	125		
15	D	118	Total	O	0	0
			118	118		
15	E	35	Total	O	0	0
			35	35		
15	F	35	Total	O	0	0
			35	35		
15	H	46	Total	O	0	0
			46	46		
15	L	56	Total	O	0	0
			56	56		

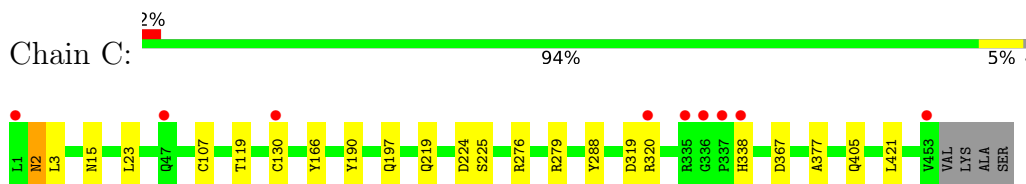
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

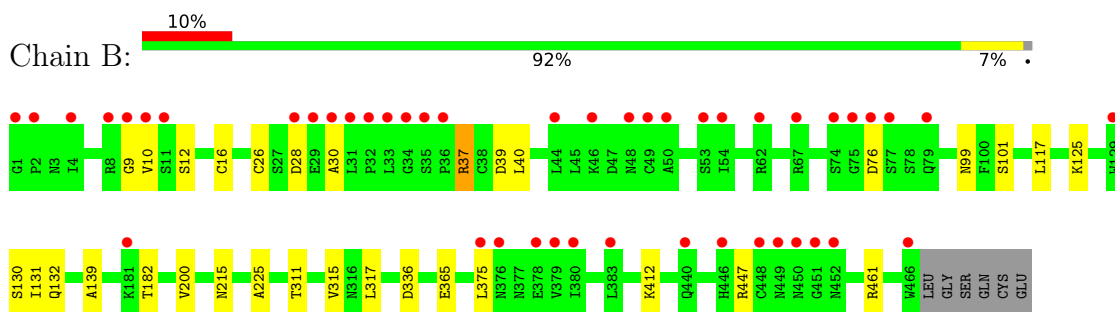
- Molecule 1: Integrin alpha-IIb heavy chain



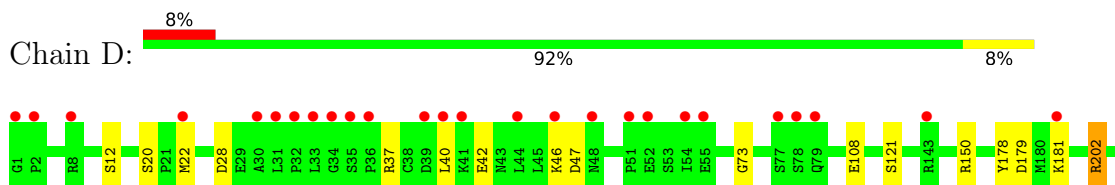
- Molecule 1: Integrin alpha-IIb heavy chain

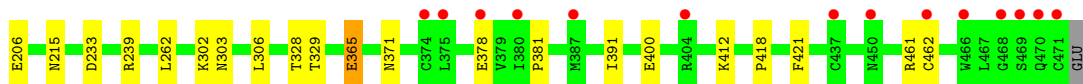


- Molecule 2: Isoform Beta-3C of Integrin beta-3

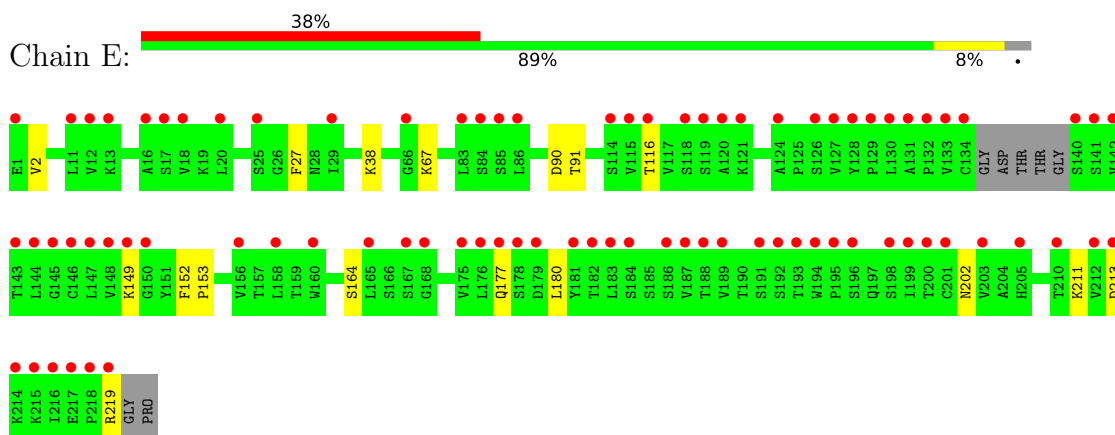


- Molecule 2: Isoform Beta-3C of Integrin beta-3

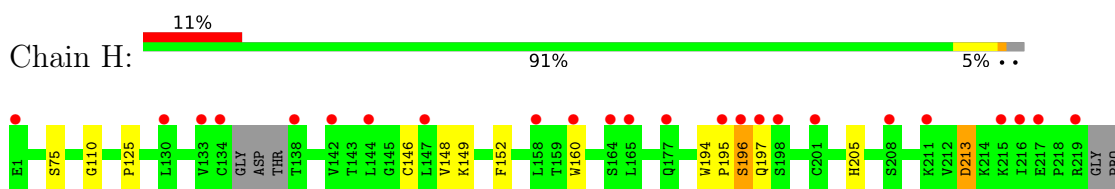




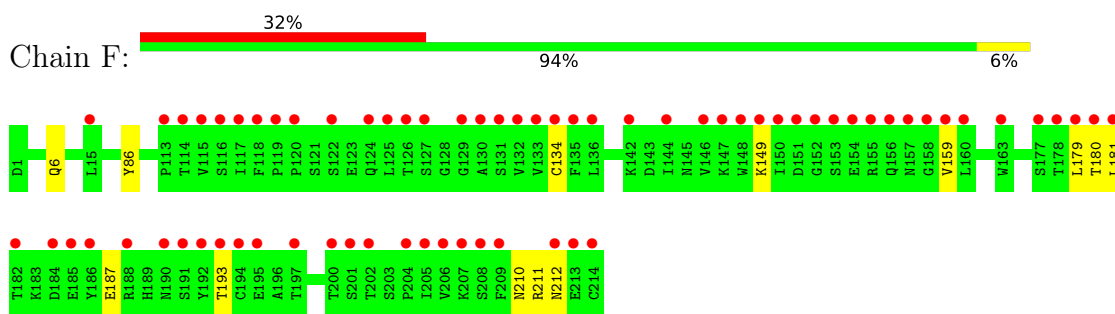
- Molecule 3: 10E5 Fab heavy chain



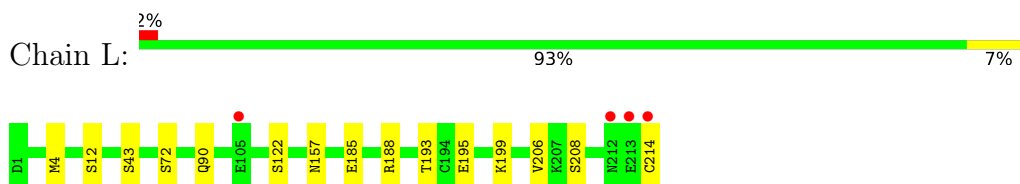
- Molecule 3: 10E5 Fab heavy chain



- Molecule 4: 10E5 Fab light chain



- Molecule 4: 10E5 Fab light chain



- Molecule 5: 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





- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:  100%



- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:  50% 50%



- Molecule 7: 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 J:  50% 50%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	259.38Å 145.25Å 105.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.78 – 2.43 48.78 – 2.43	Depositor EDS
% Data completeness (in resolution range)	96.8 (48.78-2.43) 86.6 (48.78-2.43)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.63 (at 2.42Å)	Xtrriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, $R_{free}$	0.221 , 0.247 0.221 , 0.247	Depositor DCC
$R_{free}$ test set	1981 reflections (1.36%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	39.6	Xtrriage
Anisotropy	0.317	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 39.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	22145	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	68.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.00% 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: CA, CL, MG, GOL, NB9, MAN, BMA, SO4, NAG

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	0/3647	0.47	0/4969
1	C	0.25	0/3605	0.45	0/4912
2	B	0.25	0/3725	0.44	0/5049
2	D	0.24	0/3714	0.44	0/5036
3	E	0.24	0/1673	0.45	0/2290
3	H	0.24	0/1684	0.46	0/2305
4	F	0.26	0/1673	0.45	0/2269
4	L	0.25	0/1673	0.46	0/2269
All	All	0.25	0/21394	0.45	0/29099

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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	3532	0	3383	29	0
1	C	3502	0	3334	8	0
2	B	3649	0	3571	15	0
2	D	3642	0	3558	19	0
3	E	1631	0	1590	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	H	1642	0	1600	10	0
4	F	1637	0	1553	7	0
4	L	1637	0	1553	7	0
5	G	61	0	52	0	0
6	I	28	0	25	0	0
6	K	28	0	25	2	0
7	J	50	0	43	0	0
8	A	15	0	0	1	0
8	C	15	0	0	0	0
8	L	5	0	0	0	0
9	A	6	0	8	0	0
10	A	4	0	0	0	0
10	B	2	0	0	0	0
10	C	4	0	0	0	0
10	D	2	0	0	0	0
11	A	1	0	0	0	0
11	C	2	0	0	0	0
12	B	1	0	0	0	0
12	D	1	0	0	0	0
13	B	14	0	13	1	0
13	D	14	0	13	0	0
14	B	34	0	0	0	0
14	D	34	0	0	2	0
15	A	323	0	0	18	0
15	B	214	0	0	3	0
15	C	125	0	0	1	0
15	D	118	0	0	3	0
15	E	35	0	0	2	0
15	F	35	0	0	2	0
15	H	46	0	0	6	0
15	L	56	0	0	1	0
All	All	22145	0	20321	103	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

The worst 5 of 103 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)
2:D:181:LYS:NZ	15:D:2101:HOH:O	2.20	0.75
1:A:48:GLU:OE2	1:A:90[B]:ARG:NH1	2.20	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:H:333:HOH:O	4:L:214:CYS:SG	2.45	0.73
2:B:365:GLU:OE2	2:B:412:LYS:NZ	2.22	0.72
1:A:436:ILE:O	15:A:601:HOH:O	2.13	0.66

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	460/457 (101%)	444 (96%)	15 (3%)	1 (0%)	47	57
1	C	455/457 (100%)	437 (96%)	18 (4%)	0	100	100
2	B	472/472 (100%)	451 (96%)	18 (4%)	3 (1%)	25	29
2	D	471/472 (100%)	445 (94%)	26 (6%)	0	100	100
3	E	210/221 (95%)	191 (91%)	18 (9%)	1 (0%)	29	34
3	H	212/221 (96%)	195 (92%)	17 (8%)	0	100	100
4	F	212/214 (99%)	193 (91%)	18 (8%)	1 (0%)	29	34
4	L	212/214 (99%)	204 (96%)	8 (4%)	0	100	100
All	All	2704/2728 (99%)	2560 (95%)	138 (5%)	6 (0%)	47	57

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	E	164	SER
1	A	123	GLU
2	B	9	GLY
2	B	76	ASP
2	B	375	LEU



### 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	370/364 (102%)	361 (98%)	9 (2%)	49	61
1	C	365/364 (100%)	354 (97%)	11 (3%)	41	53
2	B	420/417 (101%)	415 (99%)	5 (1%)	71	81
2	D	418/417 (100%)	409 (98%)	9 (2%)	52	64
3	E	186/190 (98%)	185 (100%)	1 (0%)	88	93
3	H	187/190 (98%)	184 (98%)	3 (2%)	62	74
4	F	188/188 (100%)	186 (99%)	2 (1%)	73	83
4	L	188/188 (100%)	183 (97%)	5 (3%)	44	57
All	All	2322/2318 (100%)	2277 (98%)	45 (2%)	57	69

5 of 45 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	215	ASN
4	F	134	CYS
2	D	262	LEU
2	D	378	GLU
3	H	75	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	452	ASN
4	F	138	ASN
4	L	27	GLN
2	D	280	HIS
1	C	372	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

13 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	G	1	2,5	14,14,15	0.29	0	17,19,21	0.60	0
5	NAG	G	2	5	14,14,15	0.34	0	17,19,21	0.41	0
5	BMA	G	3	5	11,11,12	0.62	0	15,15,17	0.81	0
5	MAN	G	4	5	11,11,12	0.61	0	15,15,17	1.01	2 (13%)
5	MAN	G	5	5	11,11,12	0.65	0	15,15,17	0.96	2 (13%)
6	NAG	I	1	6,2	14,14,15	0.32	0	17,19,21	0.43	0
6	NAG	I	2	6	14,14,15	0.26	0	17,19,21	0.38	0
7	NAG	J	1	7,2	14,14,15	0.31	0	17,19,21	0.61	1 (5%)
7	NAG	J	2	7	14,14,15	0.27	0	17,19,21	0.47	0
7	BMA	J	3	7	11,11,12	0.56	0	15,15,17	0.92	0
7	MAN	J	4	7	11,11,12	0.70	0	15,15,17	1.01	2 (13%)
6	NAG	K	1	6,2	14,14,15	0.29	0	17,19,21	0.54	0
6	NAG	K	2	6	14,14,15	0.37	0	17,19,21	0.75	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
5	NAG	G	1	2,5	-	0/6/23/26	0/1/1/1
5	NAG	G	2	5	-	0/6/23/26	0/1/1/1
5	BMA	G	3	5	-	0/2/19/22	0/1/1/1
5	MAN	G	4	5	-	0/2/19/22	0/1/1/1
5	MAN	G	5	5	-	1/2/19/22	0/1/1/1
6	NAG	I	1	6,2	-	1/6/23/26	0/1/1/1

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

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	G	4	MAN	C1-O5-C5	2.65	115.78	112.19
7	J	4	MAN	C1-O5-C5	2.34	115.36	112.19
6	K	2	NAG	C1-O5-C5	2.22	115.20	112.19
5	G	4	MAN	O2-C2-C3	-2.18	105.77	110.14
7	J	4	MAN	O2-C2-C3	-2.17	105.79	110.14

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

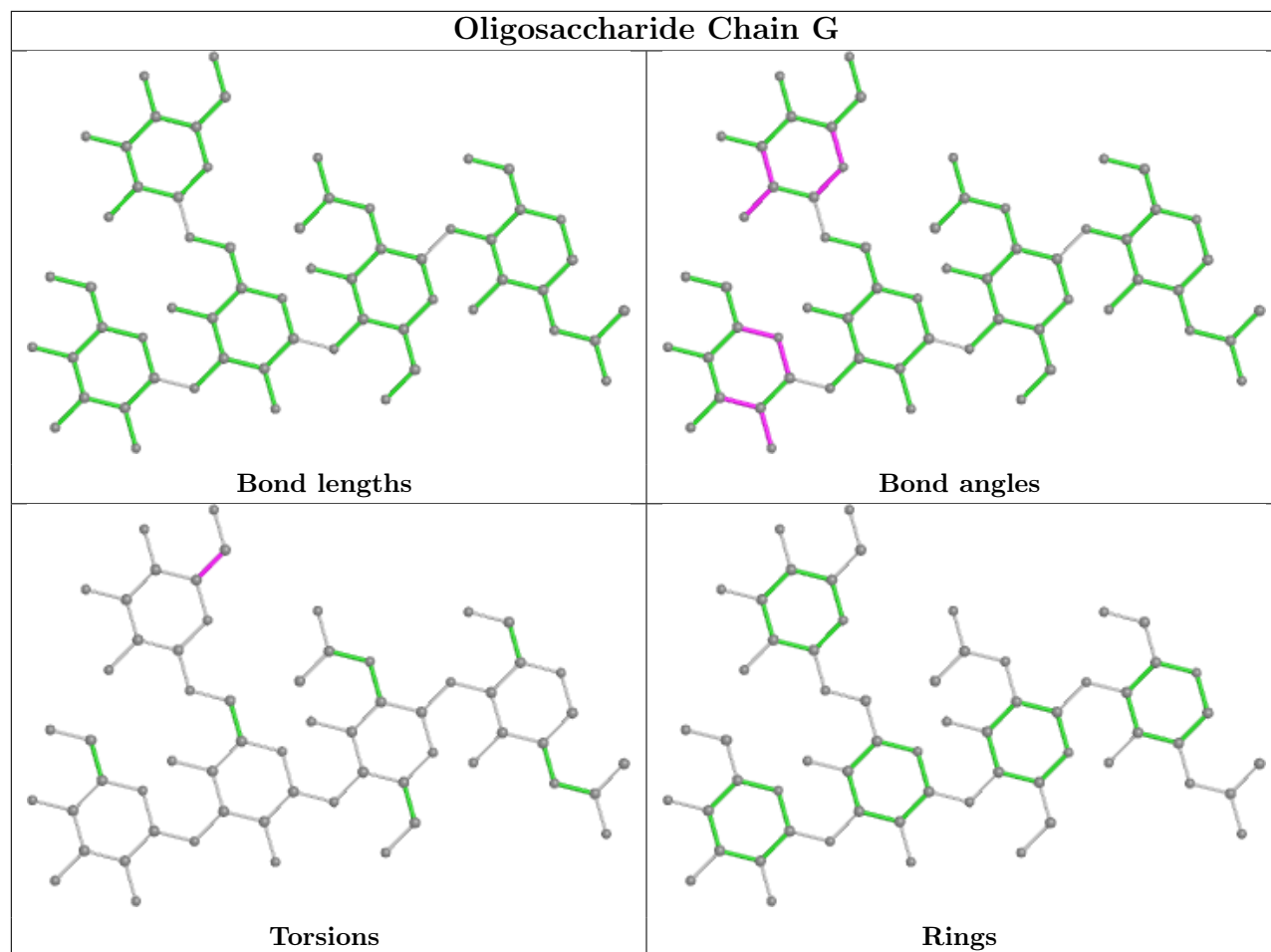
Mol	Chain	Res	Type	Atoms
6	I	2	NAG	C8-C7-N2-C2
6	I	2	NAG	O7-C7-N2-C2
6	K	2	NAG	C8-C7-N2-C2
6	K	2	NAG	O7-C7-N2-C2
7	J	4	MAN	O5-C5-C6-O6

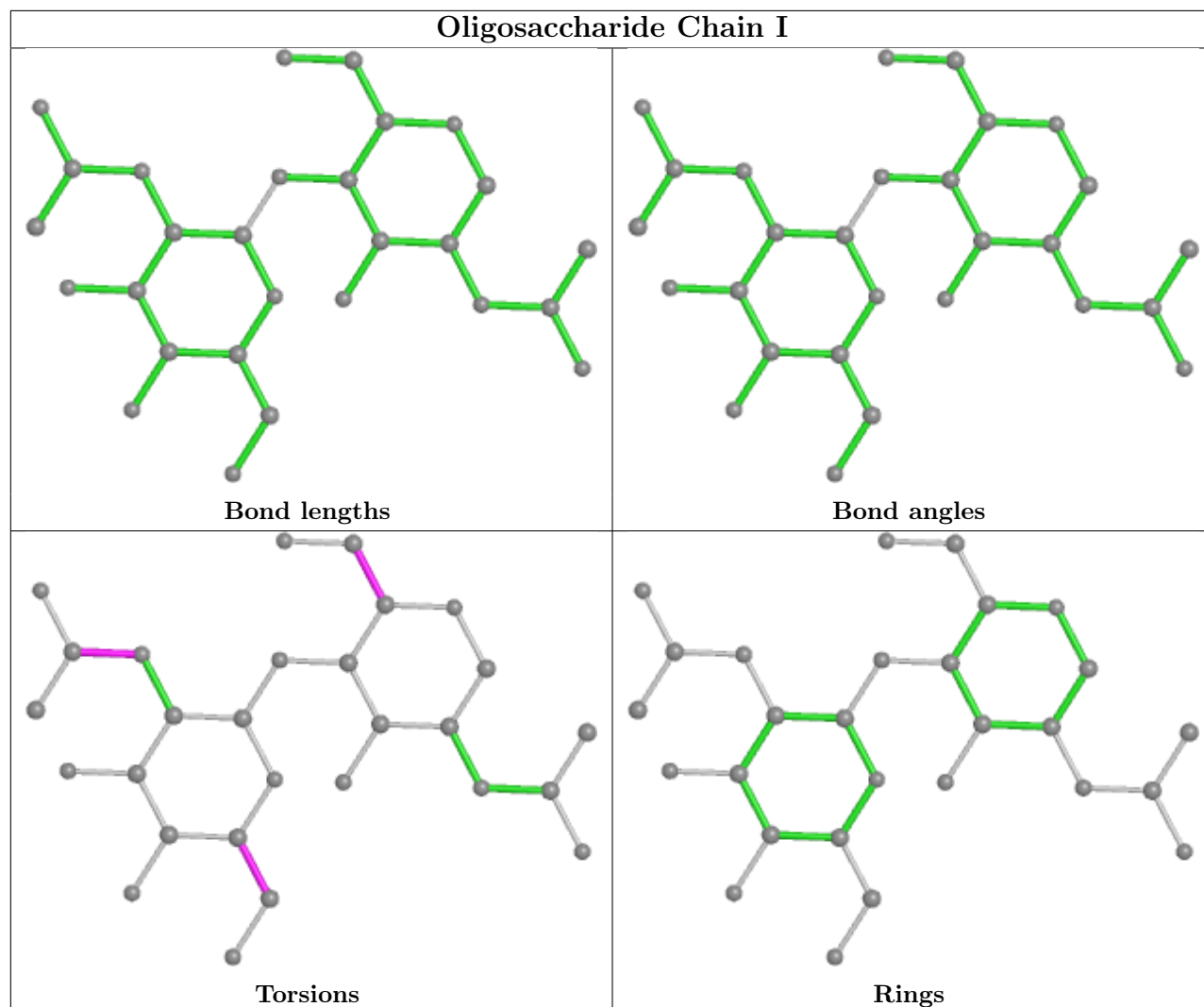
There are no ring outliers.

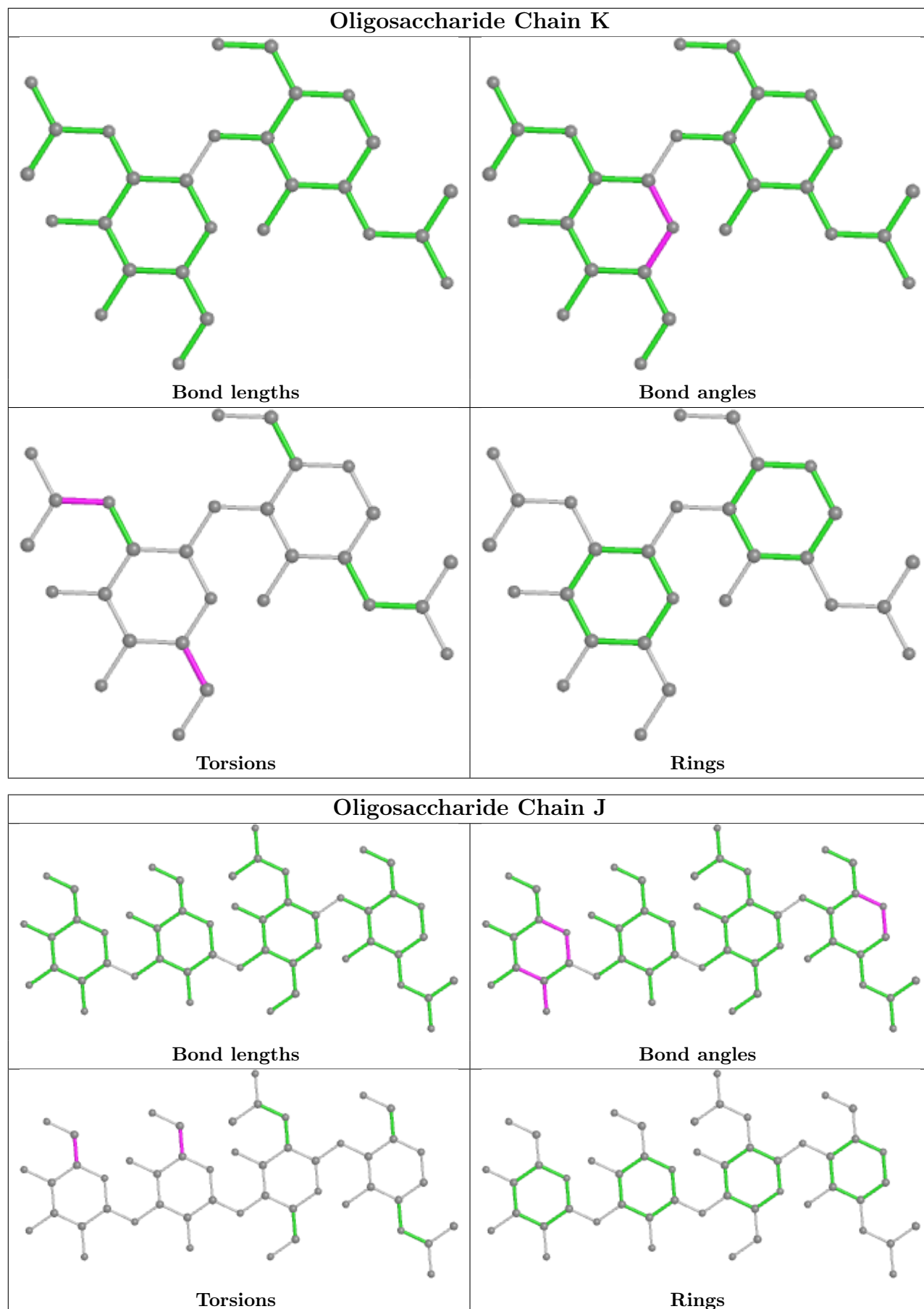
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	K	2	NAG	1	0
6	K	1	NAG	2	0

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







## 5.6 Ligand geometry [i](#)

Of 29 ligands modelled in this entry, 17 are monoatomic - leaving 12 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
13	NAG	D	2004	2	14,14,15	0.51	0	17,19,21	0.37	0
8	SO4	C	501	-	4,4,4	0.14	0	6,6,6	0.05	0
14	NB9	B	2005	12	36,36,36	2.60	9 (25%)	44,49,49	1.51	3 (6%)
8	SO4	A	508	-	4,4,4	0.17	0	6,6,6	0.19	0
8	SO4	L	301	-	4,4,4	0.14	0	6,6,6	0.05	0
13	NAG	B	2004	2	14,14,15	0.39	0	17,19,21	0.47	0
8	SO4	C	503	-	4,4,4	0.14	0	6,6,6	0.04	0
9	GOL	A	503	-	5,5,5	0.36	0	5,5,5	0.38	0
8	SO4	A	501	-	4,4,4	0.14	0	6,6,6	0.05	0
14	NB9	D	2005	12	36,36,36	2.62	9 (25%)	44,49,49	1.28	3 (6%)
8	SO4	A	502	-	4,4,4	0.14	0	6,6,6	0.05	0
8	SO4	C	502	-	4,4,4	0.14	0	6,6,6	0.05	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	NAG	D	2004	2	-	2/6/23/26	0/1/1/1
14	NB9	B	2005	12	-	1/29/39/39	0/3/3/3
13	NAG	B	2004	2	-	1/6/23/26	0/1/1/1
9	GOL	A	503	-	-	2/4/4/4	-
14	NB9	D	2005	12	-	2/29/39/39	0/3/3/3

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	D	2005	NB9	C12-N03	10.56	1.50	1.34
14	B	2005	NB9	C12-N03	10.47	1.49	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	2005	NB9	C24-N23	7.08	1.49	1.34
14	D	2005	NB9	C24-N23	7.07	1.49	1.34
14	B	2005	NB9	O13-C12	-4.52	1.14	1.22

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	2005	NB9	C02-C01-C06	5.86	116.77	110.32
14	B	2005	NB9	C04-C05-C06	5.01	115.83	110.32
14	D	2005	NB9	C02-C01-C06	4.51	115.28	110.32
14	D	2005	NB9	C04-C05-C06	3.79	114.49	110.32
14	B	2005	NB9	C05-C06-C01	3.25	118.02	111.74

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	D	2004	NAG	C4-C5-C6-O6
13	D	2004	NAG	O5-C5-C6-O6
9	A	503	GOL	O1-C1-C2-C3
13	B	2004	NAG	O5-C5-C6-O6
9	A	503	GOL	O1-C1-C2-O2

There are no ring outliers.

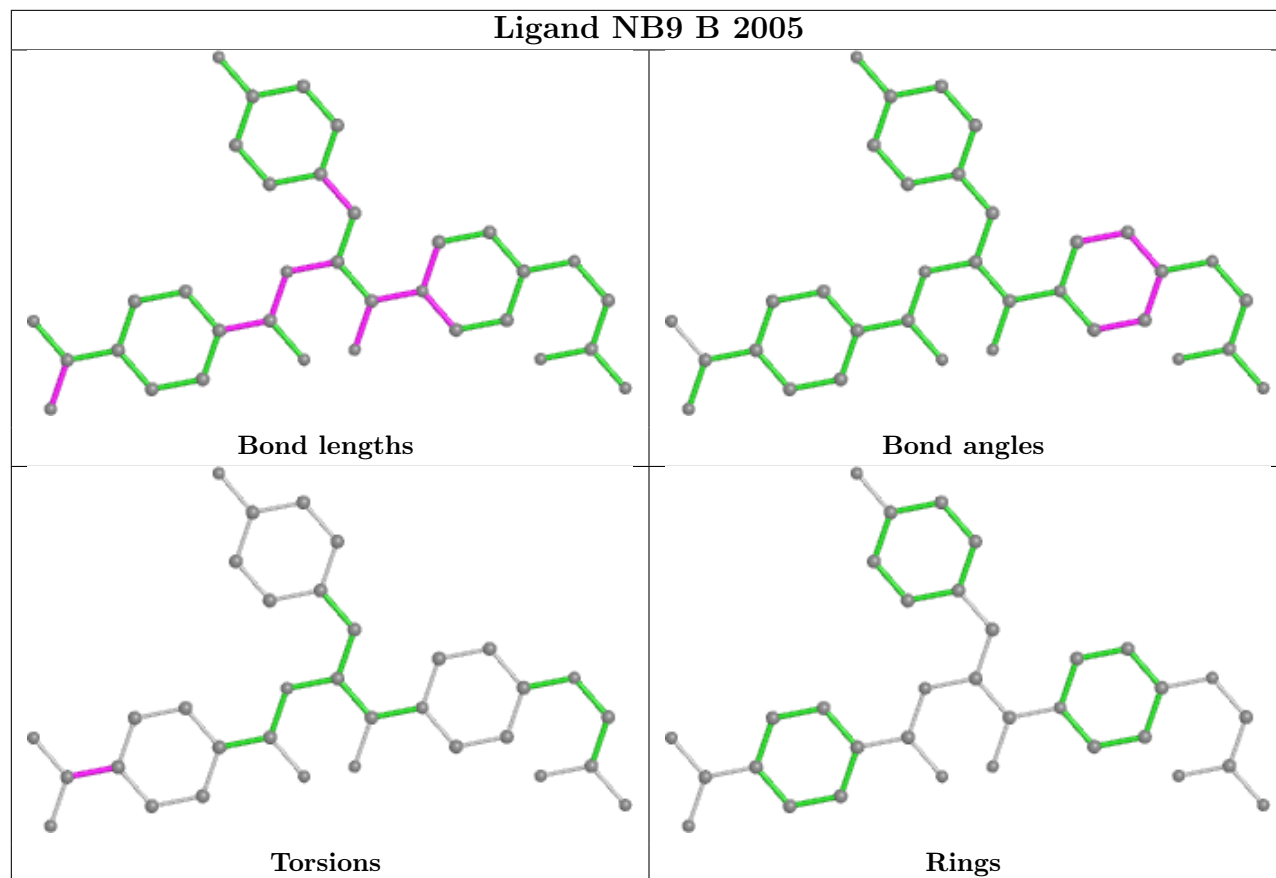
3 monomers are involved in 4 short contacts:

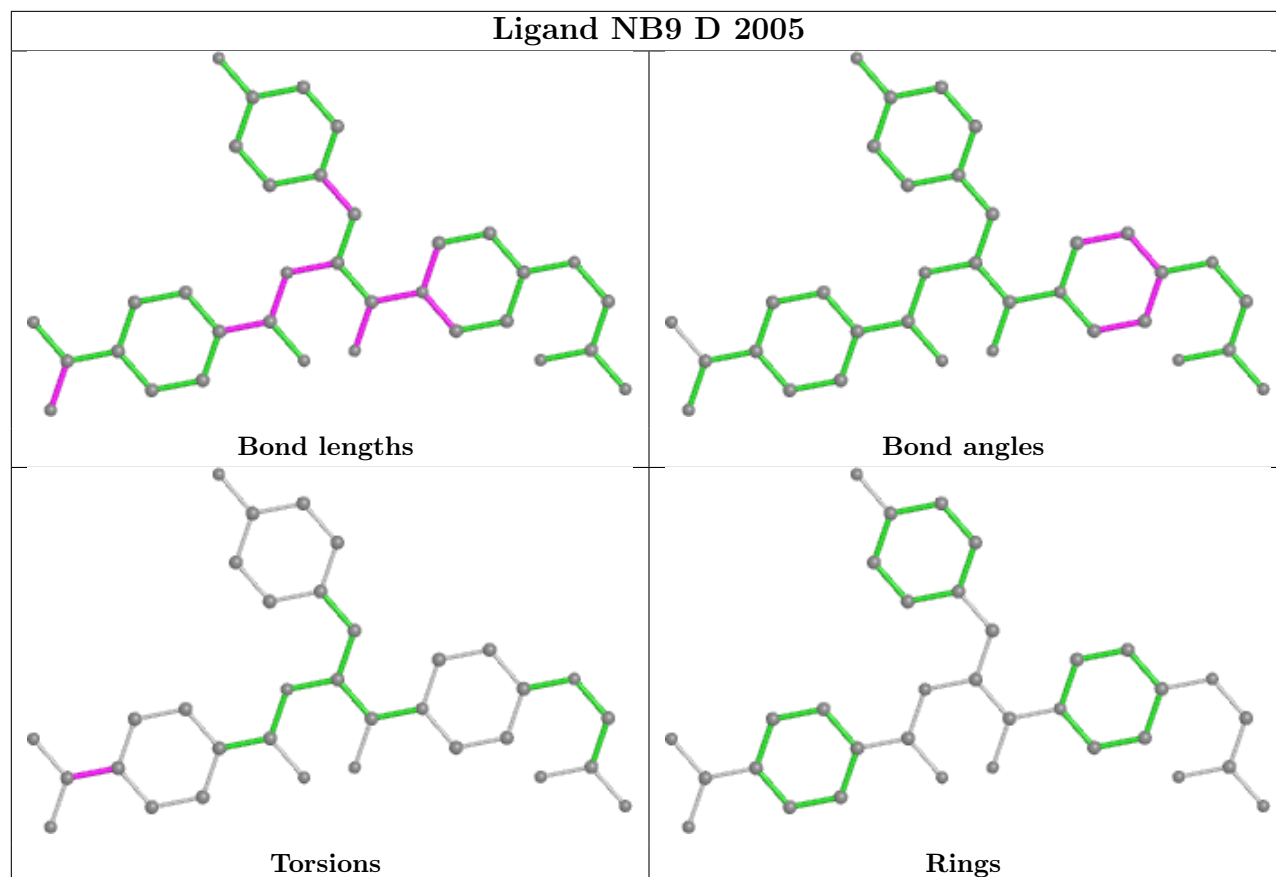
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	B	2004	NAG	1	0
14	D	2005	NB9	2	0
8	A	502	SO4	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient



equivalents in the CSD to analyse the geometry.





## 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	454/457 (99%)	0.33	8 (1%) 68 64	30, 39, 55, 71	0
1	C	453/457 (99%)	0.23	9 (1%) 65 61	35, 50, 68, 86	0
2	B	466/472 (98%)	0.59	46 (9%) 7 5	31, 59, 114, 132	1 (0%)
2	D	471/472 (99%)	0.50	40 (8%) 10 8	38, 67, 106, 119	1 (0%)
3	E	214/221 (96%)	2.04	83 (38%) 0 0	67, 107, 157, 163	0
3	H	216/221 (97%)	0.66	24 (11%) 5 3	50, 86, 115, 120	0
4	F	214/214 (100%)	1.71	69 (32%) 0 0	69, 112, 150, 158	0
4	L	214/214 (100%)	0.29	4 (1%) 66 63	53, 78, 91, 109	0
All	All	2702/2728 (99%)	0.66	283 (10%) 6 4	30, 63, 135, 163	2 (0%)

The worst 5 of 283 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	E	212	VAL	12.7
4	F	214	CYS	11.3
3	E	216	ILE	10.7
3	E	133	VAL	10.4
3	E	134	CYS	10.4

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

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

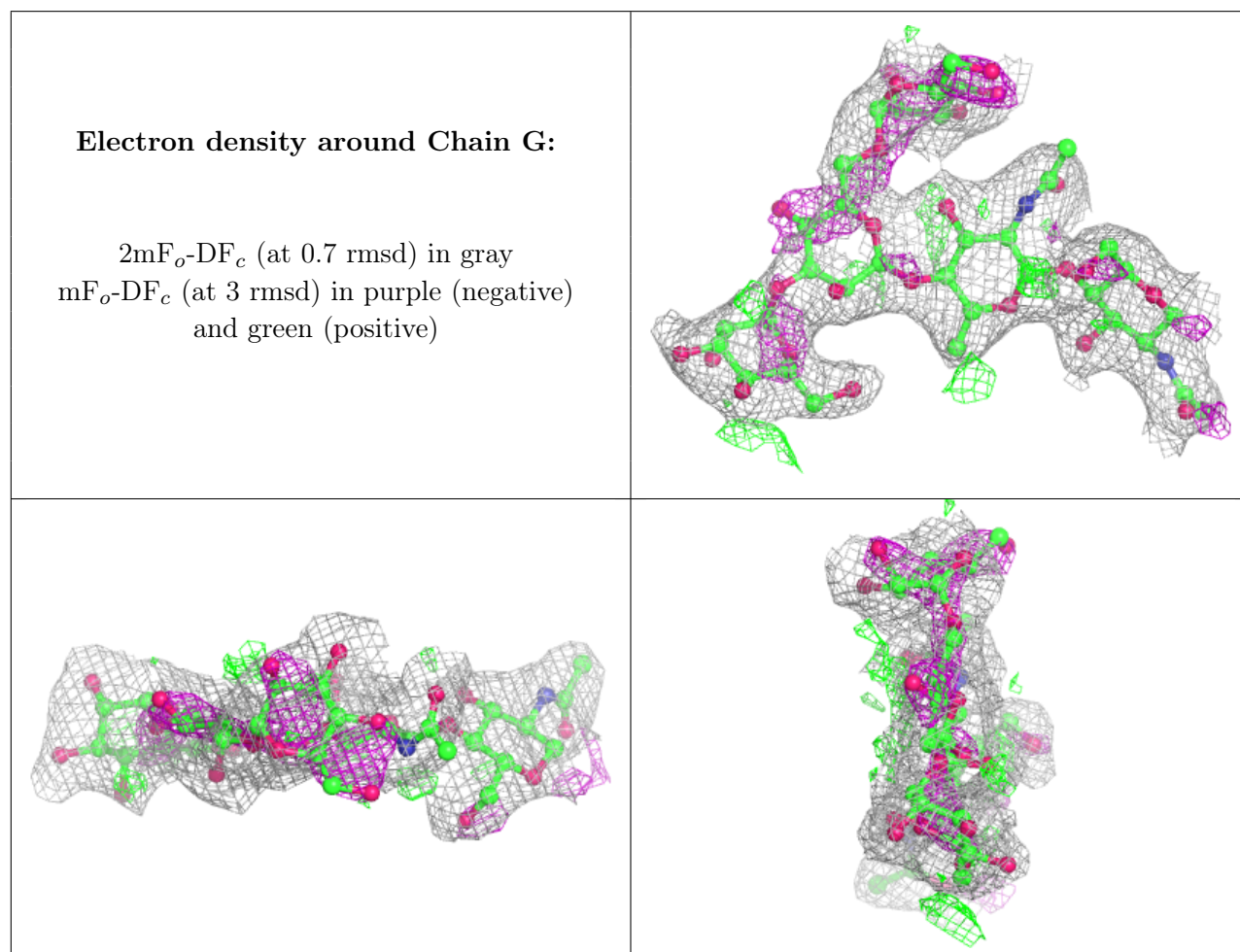
### 6.3 Carbohydrates [i](#)

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.

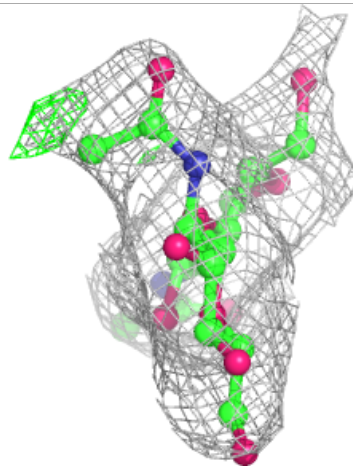
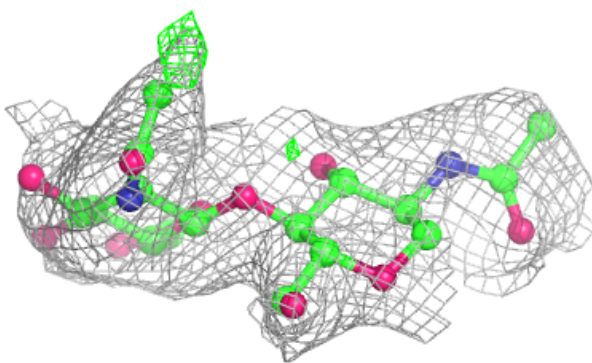
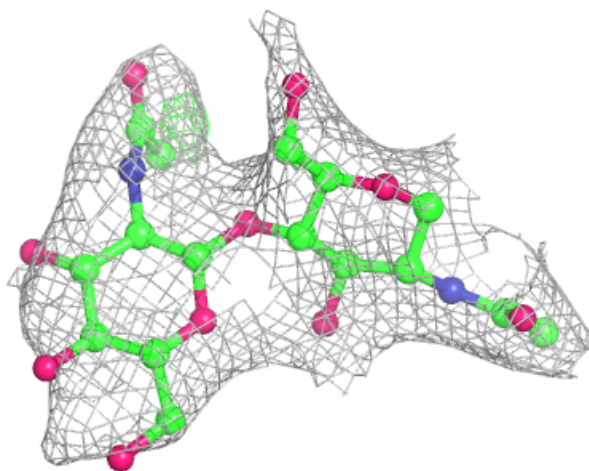
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
5	BMA	G	3	11/12	0.64	0.27	70,70,70,70	0
5	MAN	G	5	11/12	0.68	0.39	75,75,75,75	0
7	BMA	J	3	11/12	0.70	0.34	76,76,76,76	0
7	MAN	J	4	11/12	0.77	0.29	76,76,76,76	0
5	MAN	G	4	11/12	0.81	0.21	68,68,68,68	0
6	NAG	K	2	14/15	0.82	0.32	94,94,94,94	0
5	NAG	G	2	14/15	0.84	0.16	61,61,61,61	0
7	NAG	J	2	14/15	0.84	0.27	69,69,69,69	0
6	NAG	K	1	14/15	0.86	0.27	89,89,89,89	0
6	NAG	I	2	14/15	0.89	0.24	85,85,85,85	0
6	NAG	I	1	14/15	0.89	0.22	83,83,83,83	0
5	NAG	G	1	14/15	0.90	0.14	48,48,48,48	0
7	NAG	J	1	14/15	0.94	0.12	58,58,58,58	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.



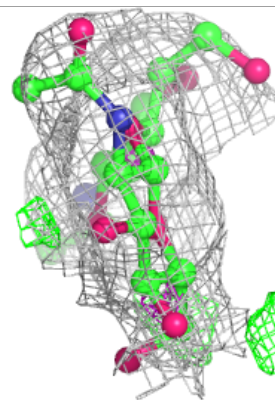
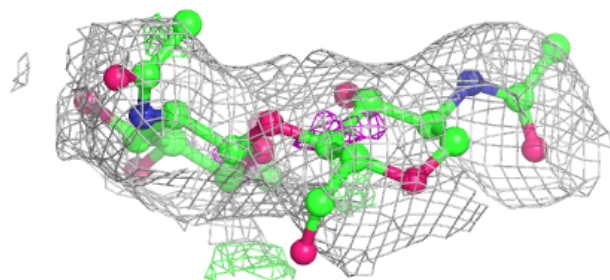
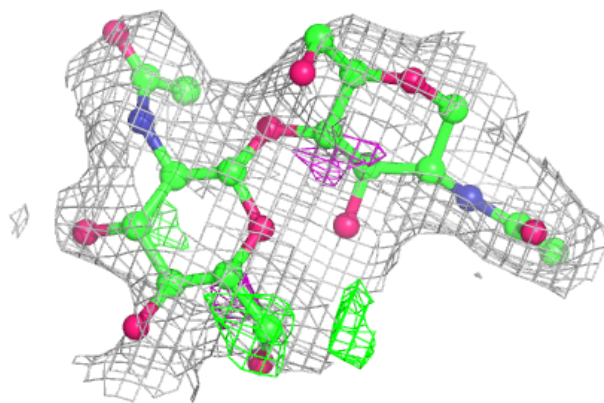
**Electron density around Chain I:**

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

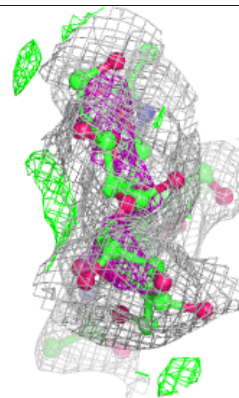
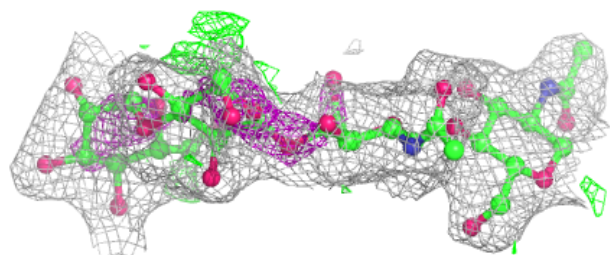
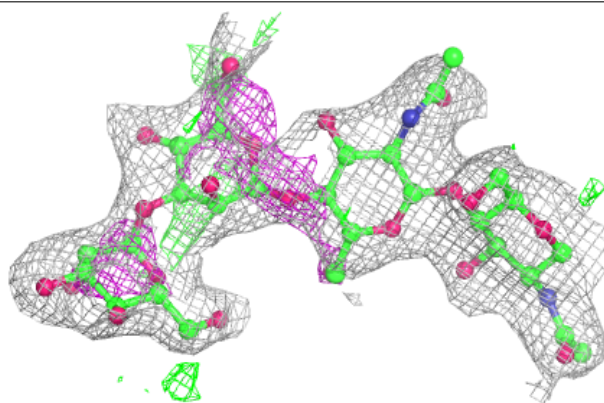


**Electron density around Chain K:**

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

**Electron density around Chain J:**

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



## 6.4 Ligands i

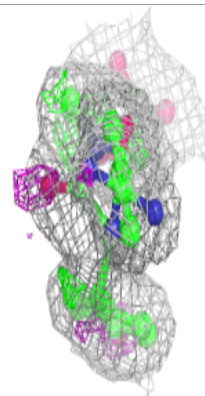
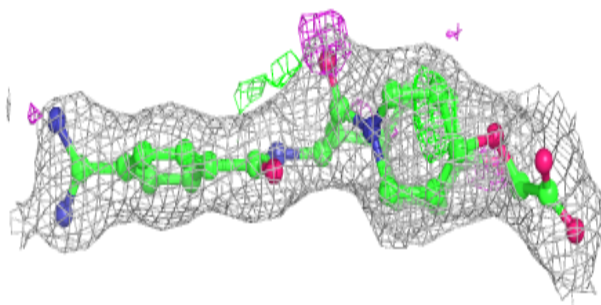
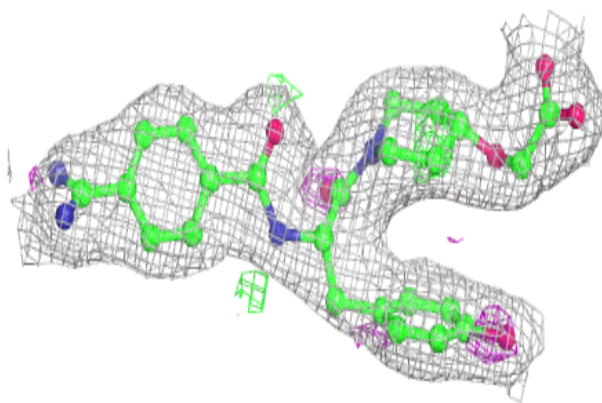
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
13	NAG	B	2004	14/15	0.78	0.34	86,86,86,86	0
13	NAG	D	2004	14/15	0.80	0.30	85,85,85,85	0
8	SO4	A	508	5/5	0.84	0.19	52,52,52,52	0
8	SO4	C	502	5/5	0.86	0.23	70,70,70,70	0
8	SO4	C	501	5/5	0.87	0.24	65,65,65,65	0
11	CL	C	504	1/1	0.88	0.07	56,56,56,56	0
11	CL	C	505	1/1	0.88	0.30	67,67,67,67	0
9	GOL	A	503	6/6	0.89	0.20	48,48,48,48	0
10	CA	C	506	1/1	0.89	0.05	64,64,64,64	0
10	CA	D	2002	1/1	0.90	0.10	53,53,53,53	0
8	SO4	L	301	5/5	0.91	0.26	71,71,71,71	0
8	SO4	A	501	5/5	0.91	0.31	61,61,61,61	0
14	NB9	B	2005	34/34	0.93	0.18	38,38,38,38	0
14	NB9	D	2005	34/34	0.93	0.18	48,48,48,48	0
10	CA	B	2002	1/1	0.94	0.04	52,52,52,52	0
11	CL	A	509	1/1	0.94	0.18	53,53,53,53	0
10	CA	A	504	1/1	0.95	0.05	48,48,48,48	0
12	MG	D	2001	1/1	0.95	0.20	40,40,40,40	0
10	CA	A	506	1/1	0.96	0.18	36,36,36,36	0
10	CA	A	507	1/1	0.96	0.17	36,36,36,36	0
10	CA	C	508	1/1	0.96	0.12	51,51,51,51	0
8	SO4	C	503	5/5	0.97	0.14	61,61,61,61	5
10	CA	C	507	1/1	0.97	0.07	56,56,56,56	0
10	CA	A	505	1/1	0.98	0.12	38,38,38,38	0
10	CA	D	2003	1/1	0.98	0.16	42,42,42,42	0
12	MG	B	2001	1/1	0.98	0.24	28,28,28,28	0
10	CA	C	509	1/1	0.98	0.12	49,49,49,49	0
10	CA	B	2003	1/1	0.99	0.18	33,33,33,33	0
8	SO4	A	502	5/5	0.99	0.07	50,50,50,50	0

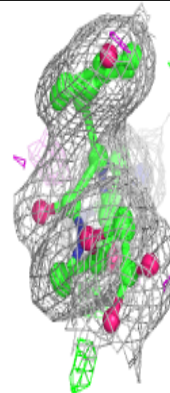
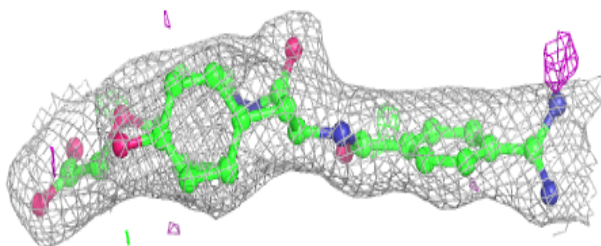
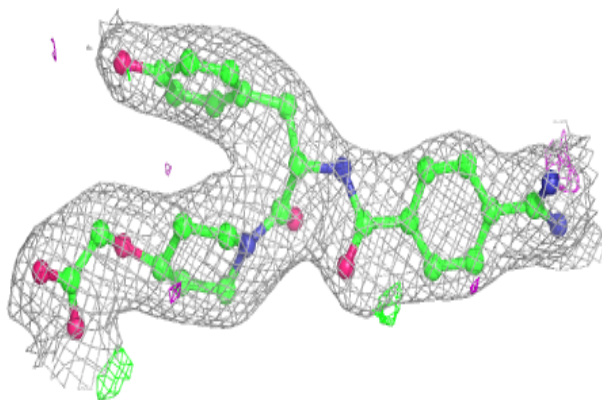
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around NB9 B 2005:**

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

**Electron density around NB9 D 2005:**

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





## 6.5 Other polymers [i](#)

There are no such residues in this entry.