



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 8, 2022 – 02:54 PM EDT

PDB ID : 7TMZ  
Title : Integrin  $\alpha$ IIb $\beta$ 3 complex with BMS compound 4  
Authors : Zhu, J.; Lin, F.-Y.; Zhu, J.; Springer, T.A.  
Deposited on : 2022-01-20  
Resolution : 2.20 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 : 2.29  
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) : 2.29

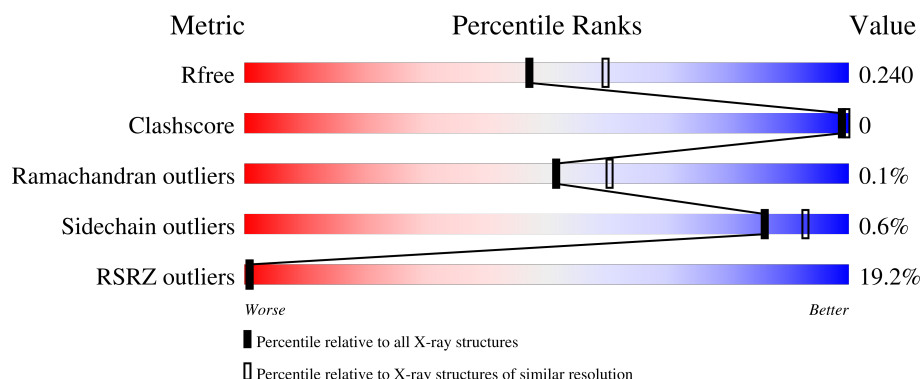
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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.



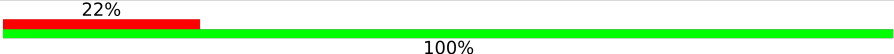
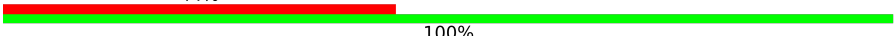
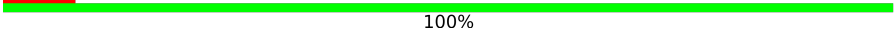
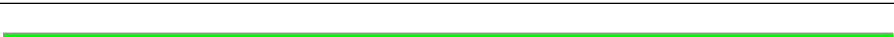
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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	454	<div> <div>11%</div> <div>98%</div> </div>
1	C	454	<div> <div>10%</div> <div>97%</div> </div>
2	B	471	<div> <div>17%</div> <div>97%</div> </div>
2	D	471	<div> <div>15%</div> <div>97%</div> </div>
3	E	216	<div> <div>54%</div> <div>98%</div> </div>

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Mol	Chain	Length	Quality of chain
3	H	216	 22%100%
4	F	214	 44%100%
4	L	214	 8%100%
5	G	5	 60%40%100%
6	I	2	 100%
6	K	2	 100%
7	J	4	 100%

## 2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 42485 atoms, of which 20311 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.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	454	Total	C	H	N	O	S	2	6	0
			6846	2226	3347	601	664	8			
1	C	453	Total	C	H	N	O	S	0	6	0
			6840	2224	3338	604	666	8			

- Molecule 2 is a protein called Integrin beta-3.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	466	Total	C	H	N	O	S	7	6	0
			7138	2245	3534	615	710	34			
2	D	471	Total	C	H	N	O	S	10	1	0
			7167	2255	3544	619	715	34			

- Molecule 3 is a protein called Fab heavy chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	E	214	Total	C	H	N	O	S	0	0	0
			3221	1035	1590	264	326	6			
3	H	216	Total	C	H	N	O	S	0	0	0
			3242	1041	1600	266	329	6			

- Molecule 4 is a protein called Fab light chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	F	214	Total	C	H	N	O	S	0	0	0
			3190	1019	1553	268	341	9			
4	L	214	Total	C	H	N	O	S	0	0	0
			3190	1019	1553	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
5	G	5	Total	C	H	N	O	0	0	0
			118	34	57	2	25			

- 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
6	I	2	Total	C	H	N	O	0	0	0
			55	16	27	2	10			
6	K	2	Total	C	H	N	O	0	0	0
			55	16	27	2	10			

- 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
7	J	4	Total	C	H	N	O	0	0	0
			97	28	47	2	20			

- 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	0	0
			5	4	1		
8	A	1	Total	O	S	0	0
			5	4	1		
8	A	1	Total	O	S	0	0
			5	4	1		
8	A	1	Total	O	S	0	0
			5	4	1		
8	A	1	Total	O	S	0	0
			5	4	1		
8	C	1	Total	O	S	0	0
			5	4	1		
8	C	1	Total	O	S	0	0
			5	4	1		
8	C	1	Total	O	S	0	0
			5	4	1		
8	C	1	Total	O	S	0	0
			5	4	1		
8	L	1	Total	O	S	0	0
			5	4	1		

- Molecule 9 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	4	Total	Ca	0	0
			4	4		
9	B	2	Total	Ca	0	0
			2	2		

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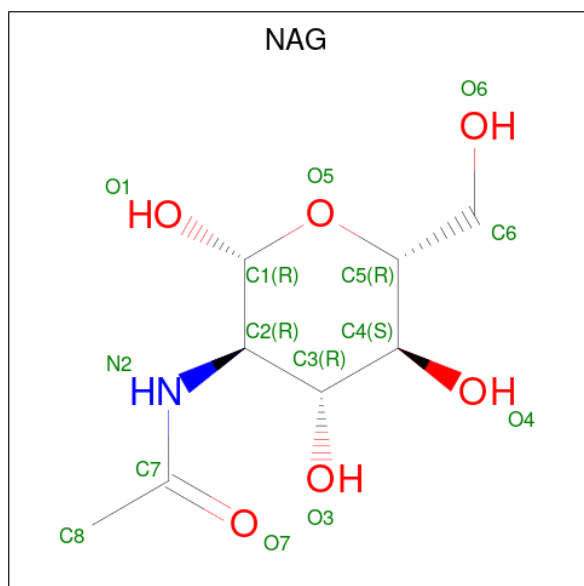
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	C	4	Total	Ca	0	0
			4	4		
9	D	2	Total	Ca	0	0
			2	2		

- Molecule 10 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

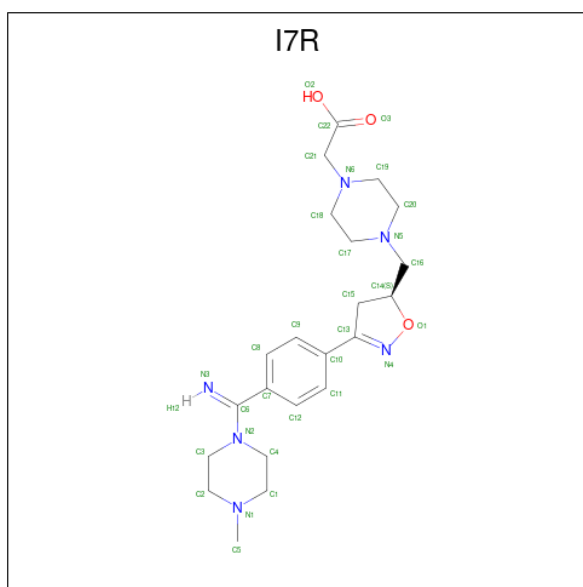
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	B	1	Total	Mg	0	0
			1	1		
10	D	1	Total	Mg	0	0
			1	1		

- Molecule 11 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
11	B	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
11	D	1	Total	C	H	N	O	0	0
			28	8	14	1	5		

- Molecule 12 is (4-{[(5S)-3-{4-[(E)-imino(4-methylpiperazin-1-yl)methyl]phenyl}-4,5-dihydro-1,2-oxazol-5-yl]methyl}piperazin-1-yl)acetic acid (three-letter code: I7R) (formula: C<sub>22</sub>H<sub>32</sub>N<sub>6</sub>O<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	B	1	Total	C	H	N	O	
			64	22	33	6	3	0
12	D	1	Total	C	H	N	O	
			64	22	33	6	3	0

- Molecule 13 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	C	2	Total	Cl		
			2	2	0	0
13	D	1	Total	Cl		
			1	1	0	0

- Molecule 14 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	410	Total	O		
			410	410	0	0
14	B	230	Total	O		
			230	230	0	0
14	C	187	Total	O		
			187	187	0	0
14	D	150	Total	O		
			150	150	0	0
14	E	15	Total	O		
			15	15	0	0

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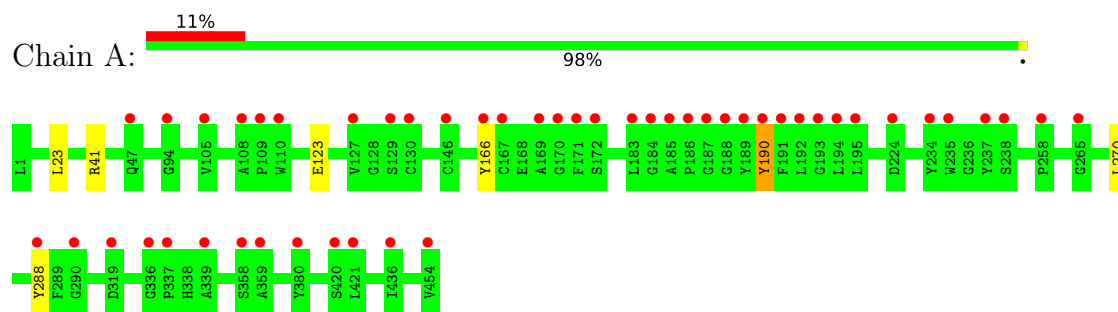
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	F	6	Total 6	O 6	0	0
14	H	33	Total 33	O 33	0	0
14	L	44	Total 44	O 44	0	0

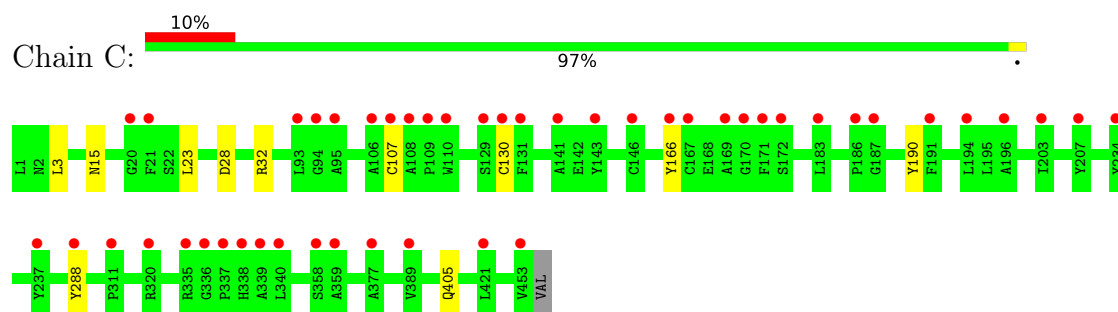
### 3 Residue-property plots [i](#)

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

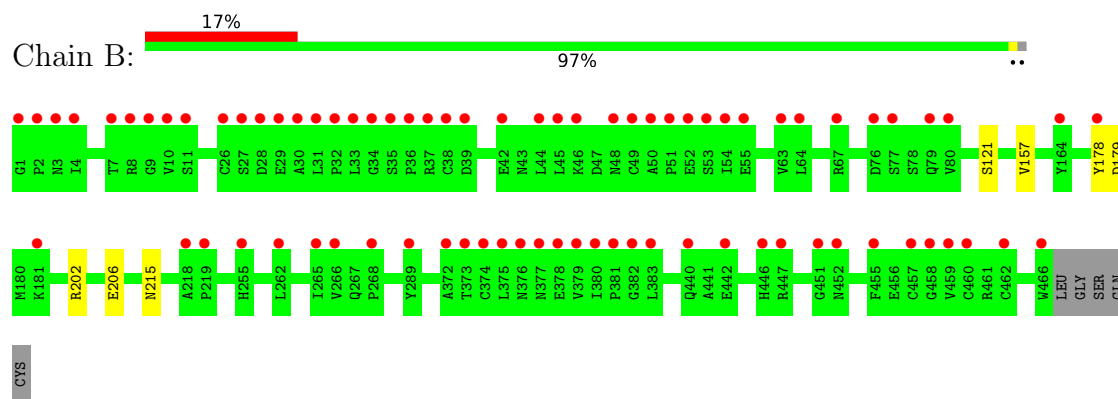
- Molecule 1: Integrin alpha-IIb



- Molecule 1: Integrin alpha-IIb



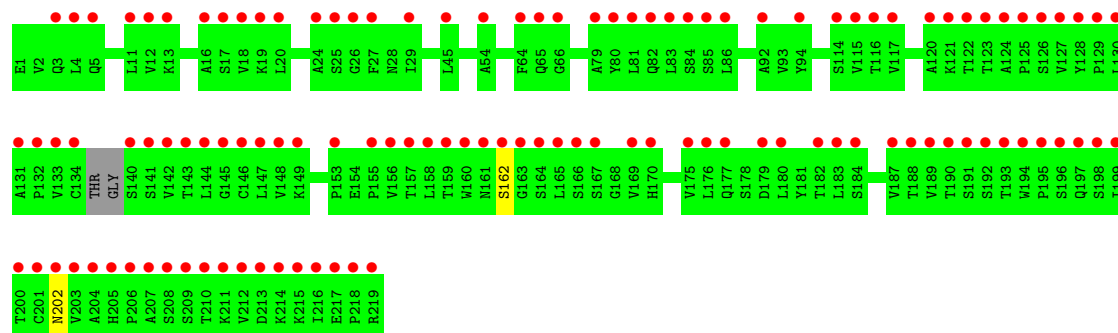
- Molecule 2: Integrin beta-3



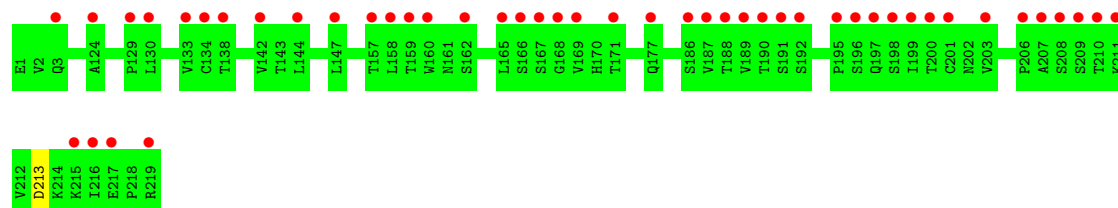
- Molecule 2: Integrin beta-3



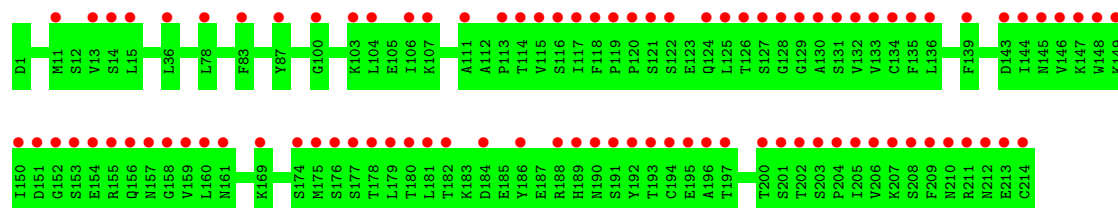
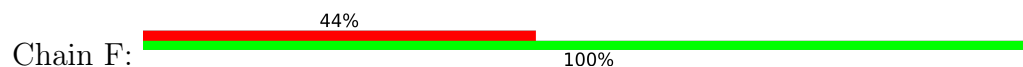
- Molecule 3: Fab heavy chain



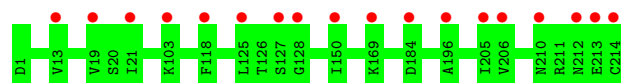
- Molecule 3: Fab heavy chain



- Molecule 4: Fab light chain



- Molecule 4: 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

Chain G:  60% 40%

MAG1  
MAG2  
EMJ3  
MAN4  
MAN5

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

Chain I:  100%

MAG1  
MAG2

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

Chain K:  100%

MAG1  
MAG2

- 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:  100%

MAG1  
MAG2  
EMJ3  
MAN4

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	258.89Å 144.21Å 105.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.38 – 2.20 49.38 – 2.20	Depositor EDS
% Data completeness (in resolution range)	95.1 (49.38-2.20) 98.9 (49.38-2.20)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.37 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.11.1 _2575	Depositor
R, $R_{free}$	0.214 , 0.241 0.214 , 0.240	Depositor DCC
$R_{free}$ test set	2000 reflections (1.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	51.2	Xtriage
Anisotropy	0.233	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 47.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	42485	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	66.0	wwPDB-VP

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

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

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, SO4, MAN, I7R, CA, MG, NAG, CL

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	0.29	0/3620	0.47	0/4935
1	C	0.26	0/3618	0.42	0/4930
2	B	0.26	0/3710	0.43	0/5030
2	D	0.24	0/3702	0.40	0/5019
3	E	0.22	0/1673	0.38	0/2290
3	H	0.23	0/1684	0.40	0/2305
4	F	0.22	0/1673	0.37	0/2269
4	L	0.23	0/1673	0.39	0/2269
All	All	0.25	0/21353	0.42	0/29047

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	3499	3347	3331	2	0
1	C	3502	3338	3320	3	0
2	B	3604	3534	3495	3	0
2	D	3623	3544	3532	5	0
3	E	1631	1590	1590	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	H	1642	1600	1600	1	0
4	F	1637	1553	1553	0	0
4	L	1637	1553	1553	0	0
5	G	61	57	52	0	0
6	I	28	27	25	0	0
6	K	28	27	25	1	0
7	J	50	47	43	0	0
8	A	25	0	0	0	0
8	C	20	0	0	0	0
8	L	5	0	0	0	0
9	A	4	0	0	0	0
9	B	2	0	0	0	0
9	C	4	0	0	0	0
9	D	2	0	0	0	0
10	B	1	0	0	0	0
10	D	1	0	0	0	0
11	B	14	14	13	0	0
11	D	14	14	13	0	0
12	B	31	33	0	2	0
12	D	31	33	0	1	0
13	C	2	0	0	0	0
13	D	1	0	0	0	0
14	A	410	0	0	1	1
14	B	230	0	0	0	0
14	C	187	0	0	0	0
14	D	150	0	0	1	1
14	E	15	0	0	0	0
14	F	6	0	0	0	0
14	H	33	0	0	0	0
14	L	44	0	0	0	0
All	All	22174	20311	20145	17	1

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 0.

The worst 5 of 17 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:456:GLU:OE2	2:D:461:ARG:NH1	2.30	0.64
6:K:1:NAG:O4	6:K:2:NAG:H83	2.02	0.60
1:C:3:LEU:O	1:C:405:GLN:NE2	2.35	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:182:THR:OG1	2:D:183:THR:N	2.41	0.54
1:A:41:ARG:NH1	14:A:609:HOH:O	2.39	0.51

All (1) 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)
14:A:894:HOH:O	14:D:2175:HOH:O[1_554]	2.16	0.04

## 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	458/454 (101%)	442 (96%)	15 (3%)	1 (0%)	47	55
1	C	457/454 (101%)	439 (96%)	18 (4%)	0	100	100
2	B	470/471 (100%)	455 (97%)	14 (3%)	1 (0%)	47	55
2	D	470/471 (100%)	452 (96%)	17 (4%)	1 (0%)	47	55
3	E	210/216 (97%)	194 (92%)	16 (8%)	0	100	100
3	H	212/216 (98%)	201 (95%)	11 (5%)	0	100	100
4	F	212/214 (99%)	199 (94%)	13 (6%)	0	100	100
4	L	212/214 (99%)	207 (98%)	5 (2%)	0	100	100
All	All	2701/2710 (100%)	2589 (96%)	109 (4%)	3 (0%)	51	60

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	123	GLU
2	B	157	VAL
2	D	157	VAL



### 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	367/362 (101%)	362 (99%)	5 (1%)	67	80
1	C	366/362 (101%)	361 (99%)	5 (1%)	67	80
2	B	418/416 (100%)	417 (100%)	1 (0%)	93	97
2	D	417/416 (100%)	414 (99%)	3 (1%)	84	91
3	E	186/187 (100%)	186 (100%)	0	100	100
3	H	187/187 (100%)	187 (100%)	0	100	100
4	F	188/188 (100%)	188 (100%)	0	100	100
4	L	188/188 (100%)	188 (100%)	0	100	100
All	All	2317/2306 (100%)	2303 (99%)	14 (1%)	86	93

5 of 14 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	23	LEU
1	C	166	TYR
2	D	365	GLU
2	D	143	ARG
2	D	215	ASN

Sometimes 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 [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	5,2	14,14,15	0.20	0	17,19,21	0.44	0
5	NAG	G	2	5	14,14,15	0.30	0	17,19,21	0.37	0
5	BMA	G	3	5	11,11,12	0.78	0	15,15,17	0.78	0
5	MAN	G	4	5	11,11,12	0.90	0	15,15,17	1.08	2 (13%)
5	MAN	G	5	5	11,11,12	1.05	1 (9%)	15,15,17	1.22	1 (6%)
6	NAG	I	1	6,2	14,14,15	0.37	0	17,19,21	0.37	0
6	NAG	I	2	6	14,14,15	0.20	0	17,19,21	0.48	0
7	NAG	J	1	2,7	14,14,15	0.35	0	17,19,21	0.70	0
7	NAG	J	2	7	14,14,15	0.33	0	17,19,21	0.66	0
7	BMA	J	3	7	11,11,12	0.30	0	15,15,17	0.69	0
7	MAN	J	4	7	11,11,12	0.27	0	15,15,17	0.63	0
6	NAG	K	1	6,2	14,14,15	0.35	0	17,19,21	0.69	0
6	NAG	K	2	6	14,14,15	0.25	0	17,19,21	0.74	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
5	NAG	G	1	5,2	-	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	-	2/2/19/22	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	-	0/6/23/26	0/1/1/1
6	NAG	I	2	6	-	3/6/23/26	0/1/1/1
7	NAG	J	1	2,7	-	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	G	5	MAN	C4-C5	2.18	1.57	1.53

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	G	5	MAN	C1-O5-C5	3.57	117.03	112.19
5	G	4	MAN	C1-O5-C5	2.33	115.35	112.19
5	G	4	MAN	O2-C2-C3	-2.03	106.08	110.14

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

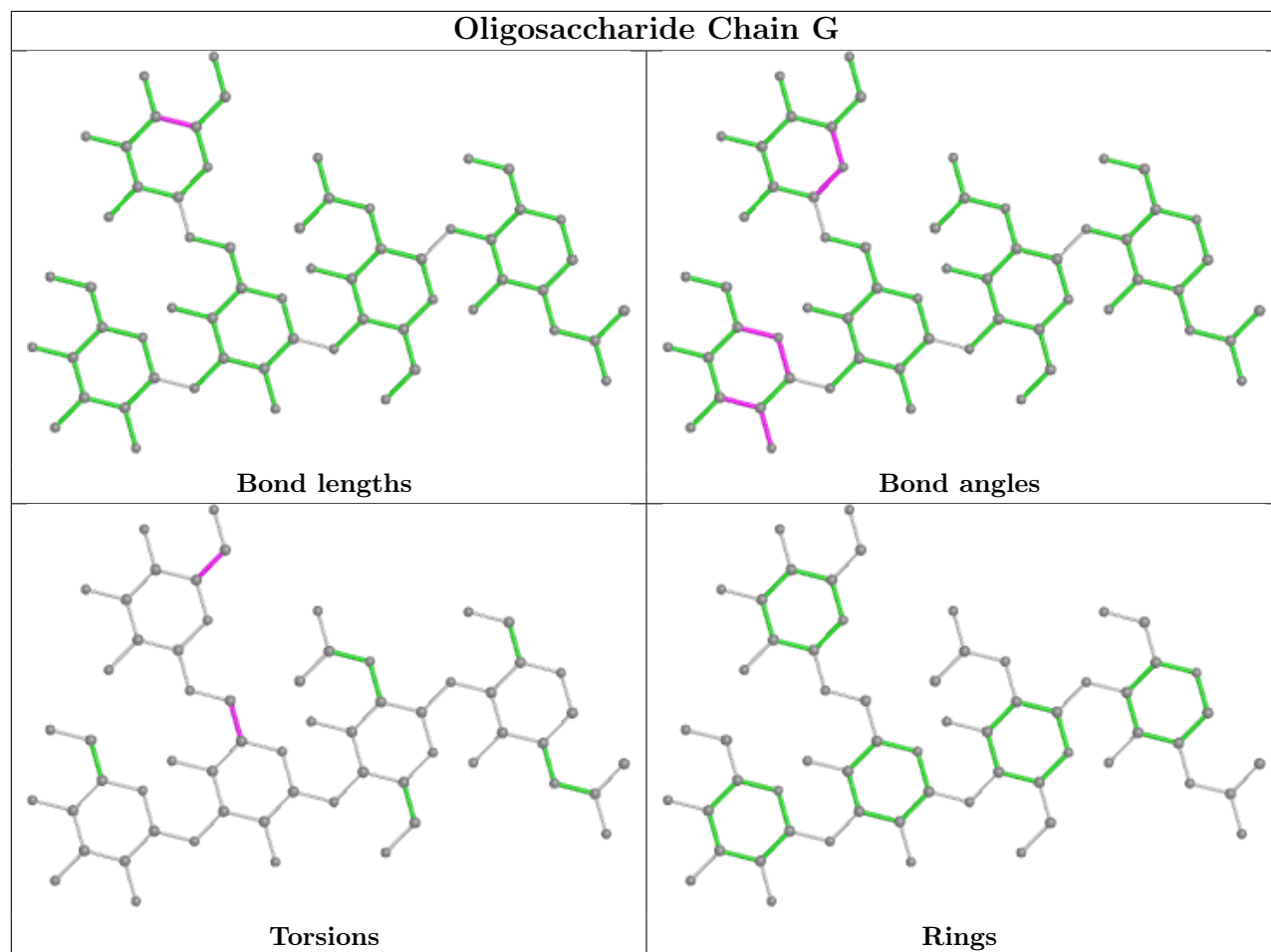
Mol	Chain	Res	Type	Atoms
7	J	4	MAN	O5-C5-C6-O6
7	J	3	BMA	O5-C5-C6-O6
5	G	3	BMA	C4-C5-C6-O6
7	J	3	BMA	C4-C5-C6-O6
6	I	2	NAG	C8-C7-N2-C2

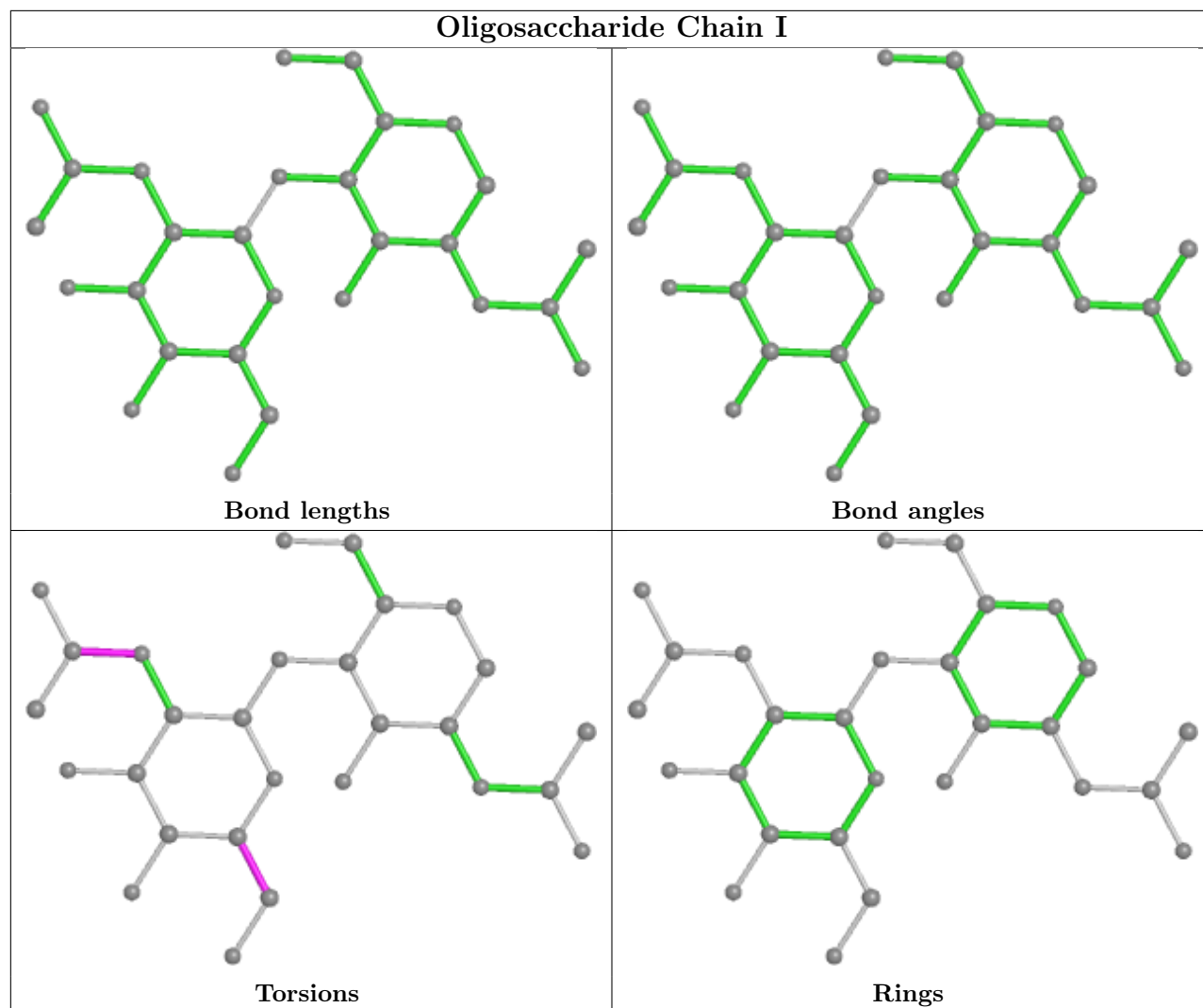
There are no ring outliers.

2 monomers are involved in 1 short contact:

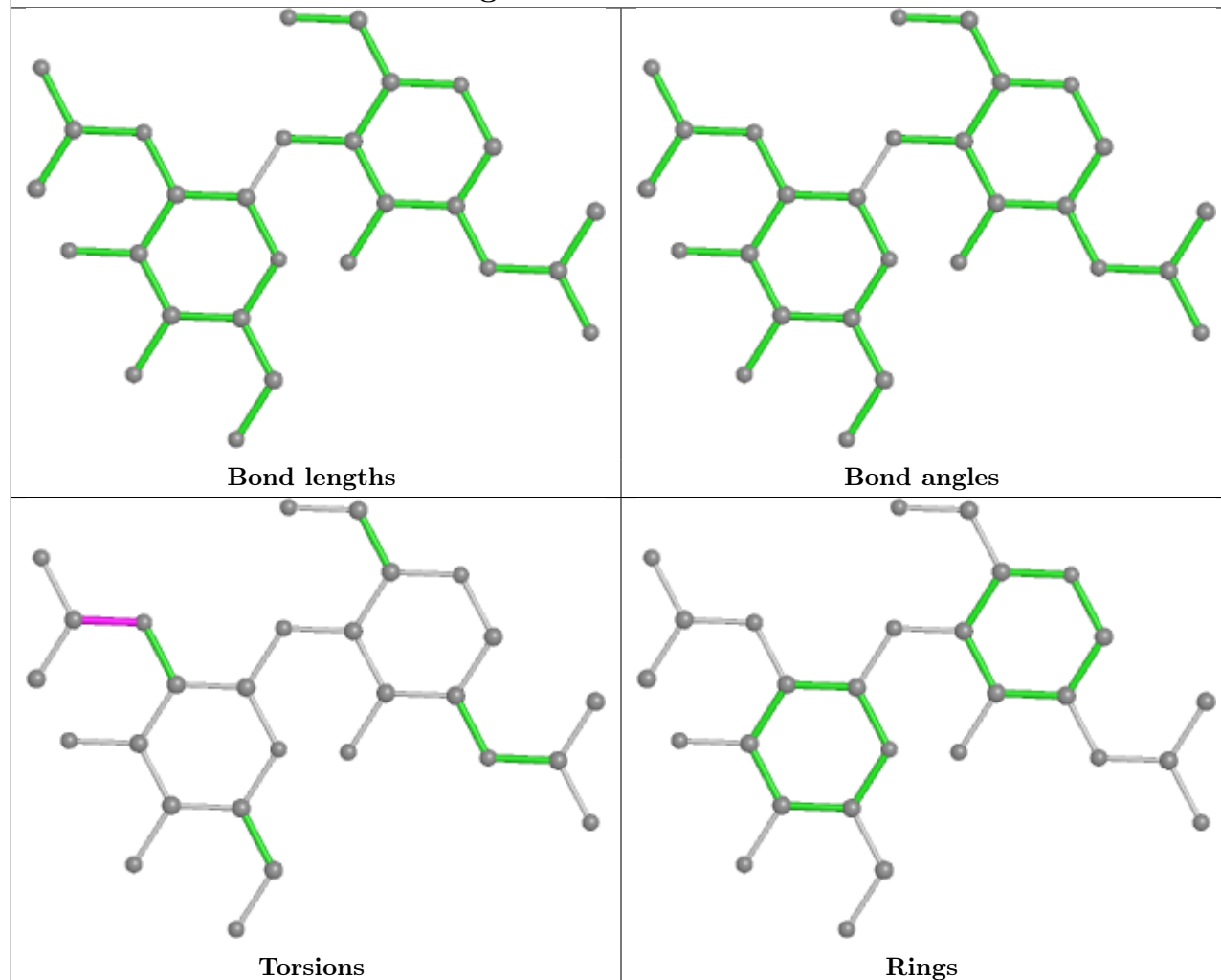
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	K	2	NAG	1	0
6	K	1	NAG	1	0

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

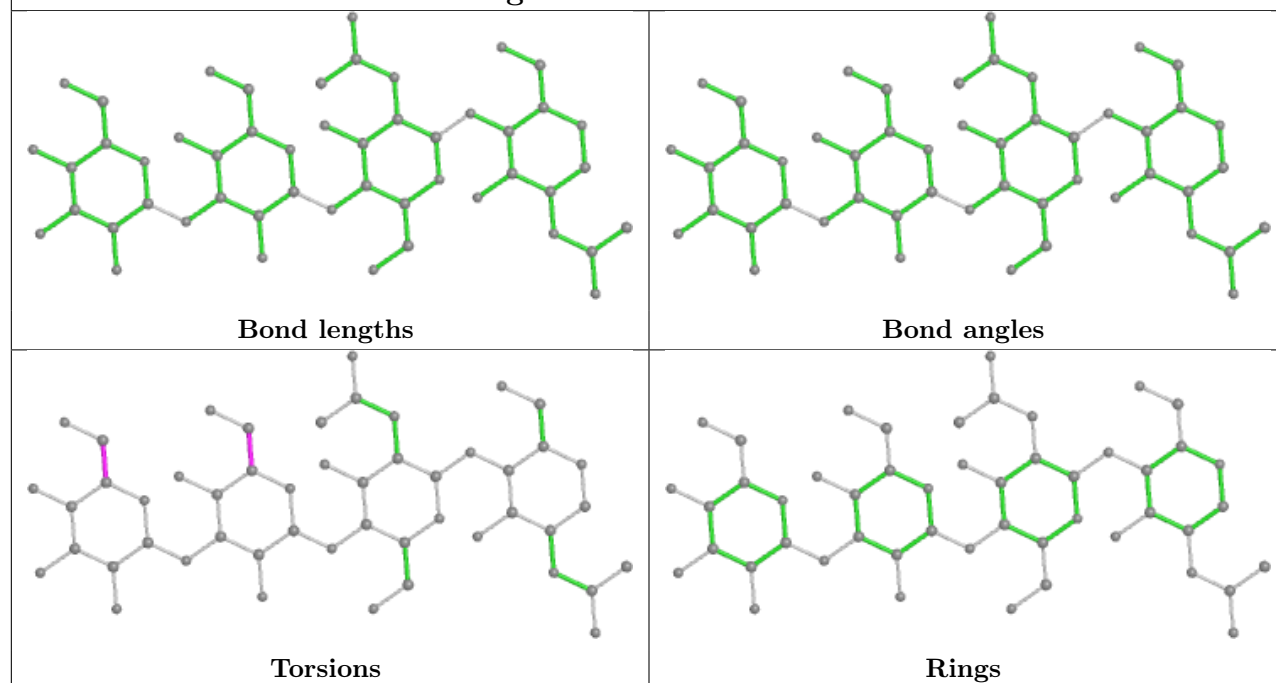




## Oligosaccharide Chain K



## Oligosaccharide Chain J



## 5.6 Ligand geometry

Of 31 ligands modelled in this entry, 17 are monoatomic - leaving 14 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
11	NAG	D	2004	2	14,14,15	0.39	0	17,19,21	0.46	0
8	SO4	C	502	-	4,4,4	0.14	0	6,6,6	0.06	0
12	I7R	B	2005	10	34,34,34	1.06	2 (5%)	44,47,47	0.93	1 (2%)
11	NAG	B	2004	2	14,14,15	0.20	0	17,19,21	0.53	0
8	SO4	A	509	-	4,4,4	0.15	0	6,6,6	0.12	0
8	SO4	C	501	-	4,4,4	0.14	0	6,6,6	0.07	0
8	SO4	A	508	-	4,4,4	0.14	0	6,6,6	0.06	0
8	SO4	C	503	-	4,4,4	0.14	0	6,6,6	0.05	0
12	I7R	D	2006	10	34,34,34	1.24	4 (11%)	44,47,47	1.06	3 (6%)
8	SO4	A	502	-	4,4,4	0.14	0	6,6,6	0.08	0
8	SO4	C	510	-	4,4,4	0.14	0	6,6,6	0.07	0
8	SO4	A	501	-	4,4,4	0.14	0	6,6,6	0.07	0
8	SO4	L	301	-	4,4,4	0.14	0	6,6,6	0.05	0
8	SO4	A	507	-	4,4,4	0.15	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
11	NAG	D	2004	2	-	0/6/23/26	0/1/1/1
11	NAG	B	2004	2	-	2/6/23/26	0/1/1/1
12	I7R	B	2005	10	-	5/18/49/49	0/4/4/4
12	I7R	D	2006	10	-	6/18/49/49	0/4/4/4

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	D	2006	I7R	O1-C14	-4.05	1.41	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	2005	I7R	C6-N3	2.84	1.34	1.27
12	B	2005	I7R	O1-C14	-2.74	1.42	1.46
12	D	2006	I7R	O2-C22	-2.57	1.22	1.30
12	D	2006	I7R	C6-N3	2.42	1.33	1.27

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	D	2006	I7R	C4-C1-N1	-2.86	107.58	110.80
12	D	2006	I7R	C17-C18-N6	2.43	115.64	110.64
12	D	2006	I7R	C14-C15-C13	2.16	102.83	100.85
12	B	2005	I7R	C14-C15-C13	2.04	102.72	100.85

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	B	2005	I7R	C15-C14-C16-N5
12	B	2005	I7R	O1-C14-C16-N5
12	D	2006	I7R	C15-C14-C16-N5
12	D	2006	I7R	O1-C14-C16-N5
11	B	2004	NAG	O5-C5-C6-O6

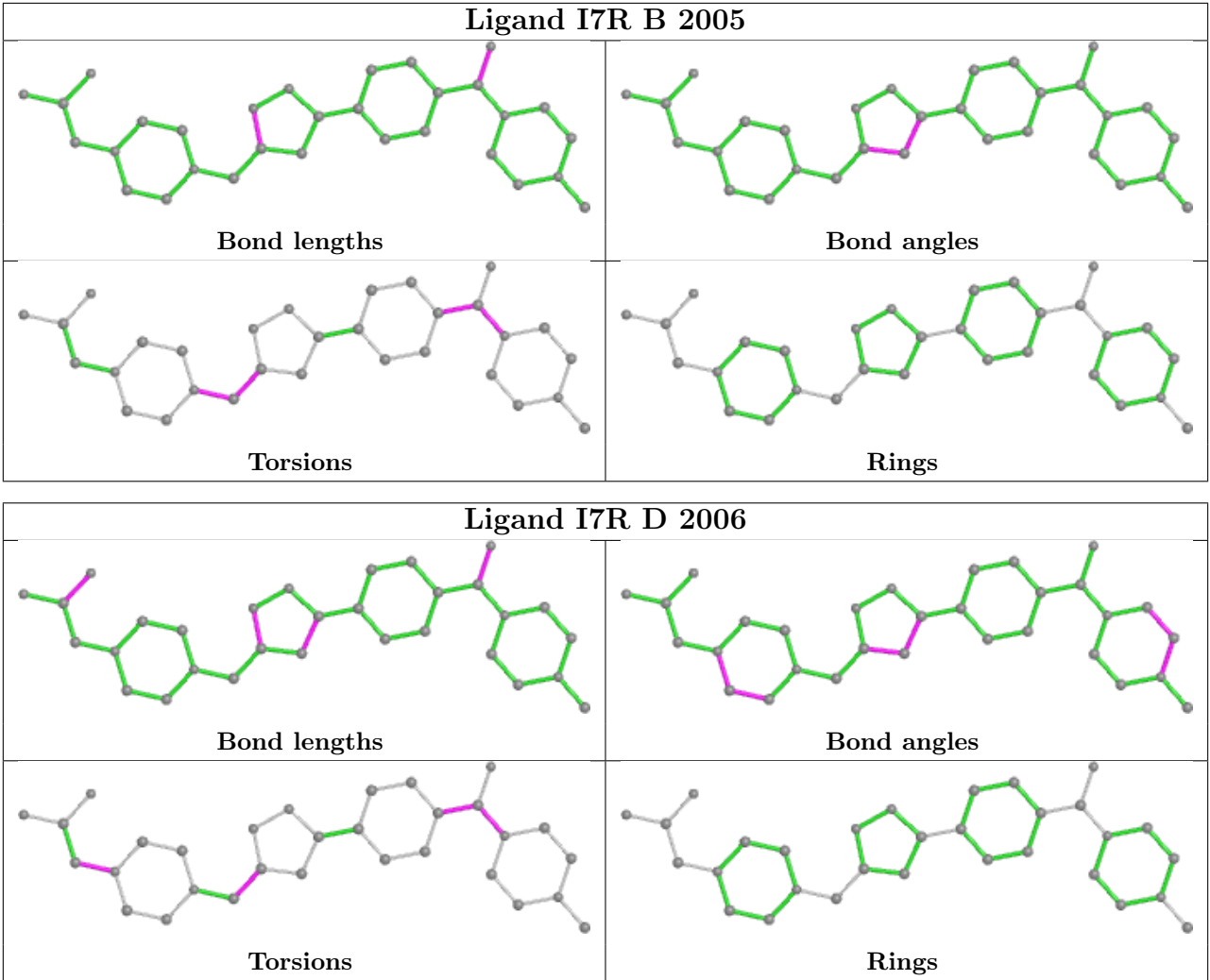
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	B	2005	I7R	2	0
12	D	2006	I7R	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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	H	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	H	134:CYS	C	138:THR	N	7.08

## 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	454/454 (100%)	0.93	49 (10%) 5 5	34, 48, 78, 125	0
1	C	453/454 (99%)	0.77	47 (10%) 6 5	44, 66, 98, 131	0
2	B	466/471 (98%)	1.03	78 (16%) 1 1	34, 72, 153, 182	1 (0%)
2	D	471/471 (100%)	0.92	69 (14%) 2 2	45, 84, 140, 166	1 (0%)
3	E	214/216 (99%)	3.18	117 (54%) 0 0	81, 137, 218, 228	0
3	H	216/216 (100%)	1.16	47 (21%) 0 0	57, 105, 163, 181	0
4	F	214/214 (100%)	2.53	94 (43%) 0 0	82, 131, 196, 218	0
4	L	214/214 (100%)	0.69	18 (8%) 11 9	61, 96, 124, 158	0
All	All	2702/2710 (99%)	1.22	519 (19%) 1 1	34, 81, 171, 228	2 (0%)

The worst 5 of 519 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	E	201	CYS	15.8
3	E	212	VAL	14.8
3	E	165	LEU	13.9
3	E	142	VAL	12.7
2	B	33	LEU	12.5

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

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

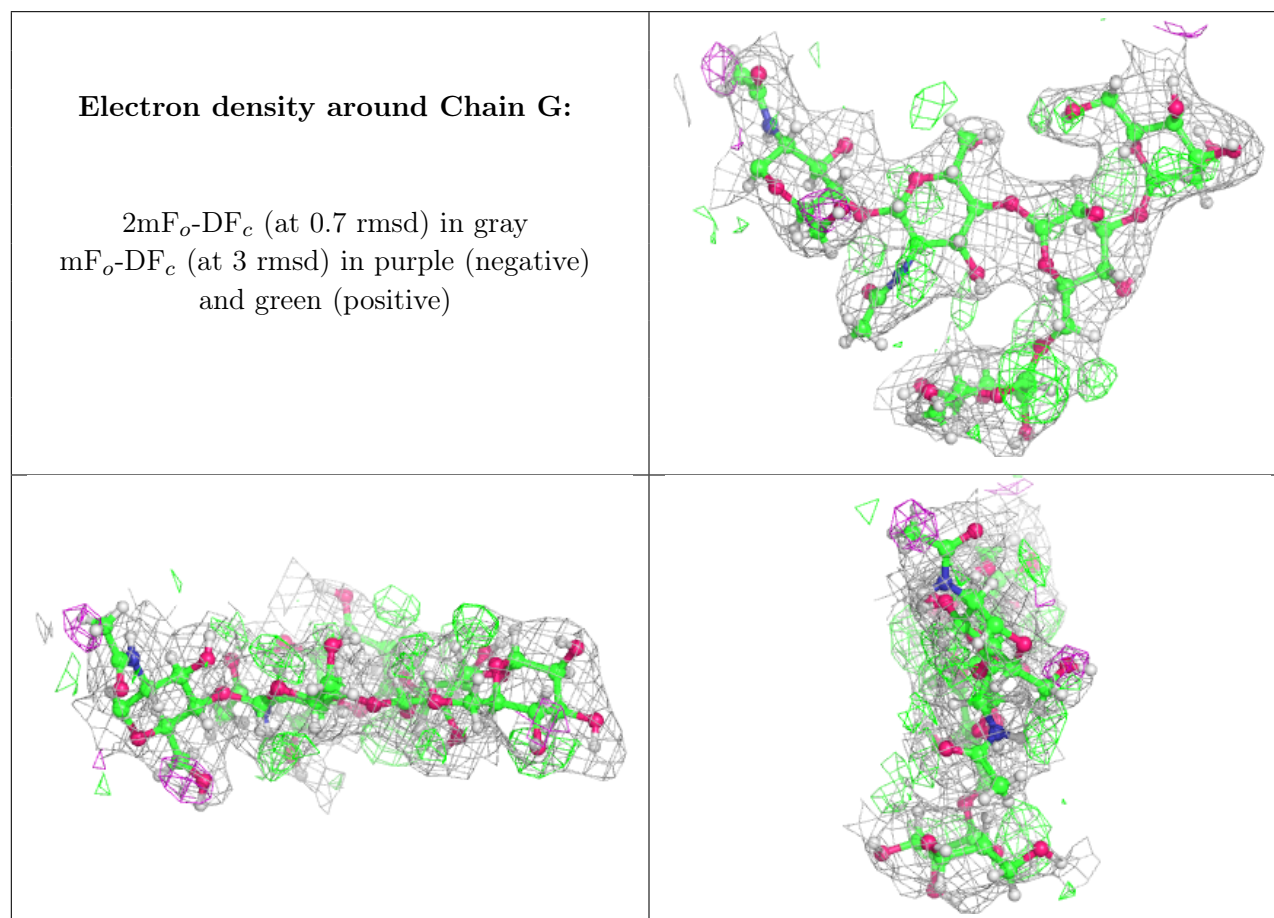
### 6.3 Carbohydrates [i](#)

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.

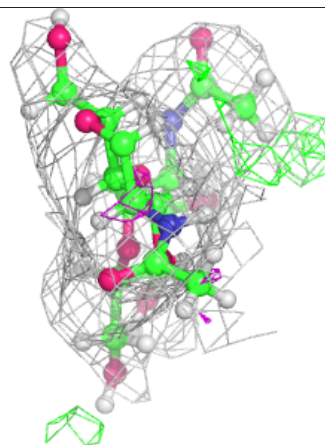
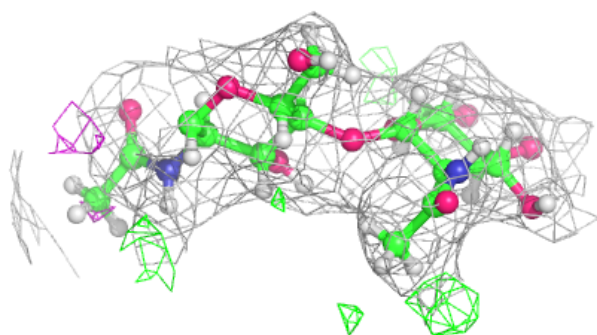
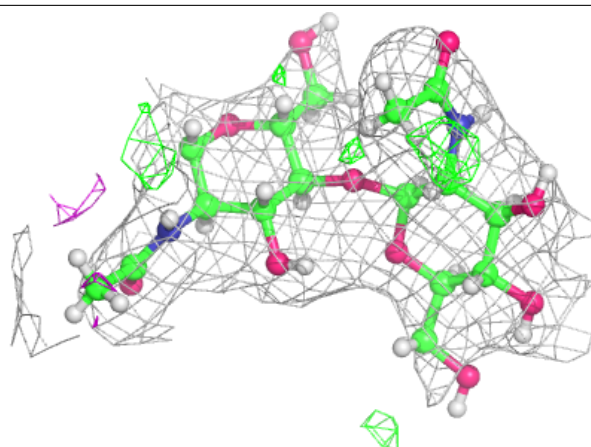
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
6	NAG	K	1	14/15	0.71	0.20	45,45,118,118	0
5	BMA	G	3	11/12	0.75	0.14	45,97,97,97	0
6	NAG	I	1	14/15	0.76	0.25	45,45,113,113	0
5	MAN	G	5	11/12	0.77	0.19	45,45,106,106	0
7	BMA	J	3	11/12	0.77	0.30	45,45,109,109	0
5	MAN	G	4	11/12	0.81	0.12	45,45,94,94	0
7	MAN	J	4	11/12	0.81	0.29	45,45,111,111	0
6	NAG	K	2	14/15	0.83	0.26	45,45,124,124	0
7	NAG	J	2	14/15	0.86	0.22	45,45,89,89	0
5	NAG	G	2	14/15	0.87	0.12	45,45,73,73	0
6	NAG	I	2	14/15	0.87	0.22	45,45,119,119	0
7	NAG	J	1	14/15	0.87	0.13	45,45,72,72	0
5	NAG	G	1	14/15	0.89	0.17	45,45,54,54	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.



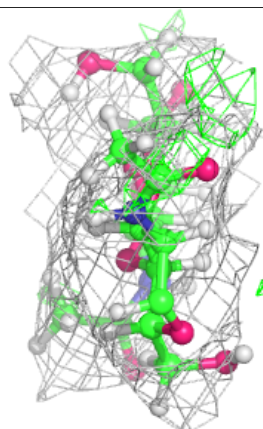
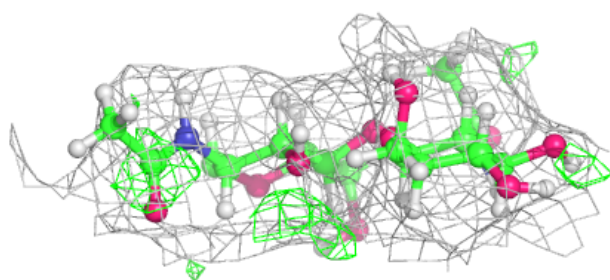
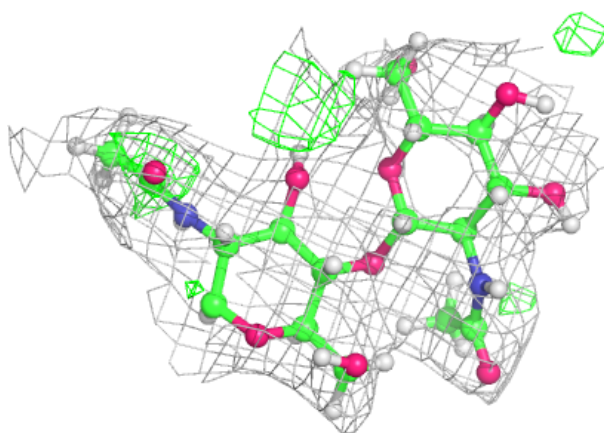
**Electron density around Chain I:**

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

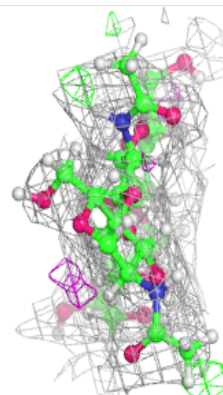
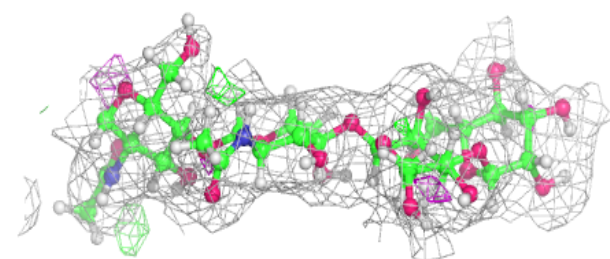
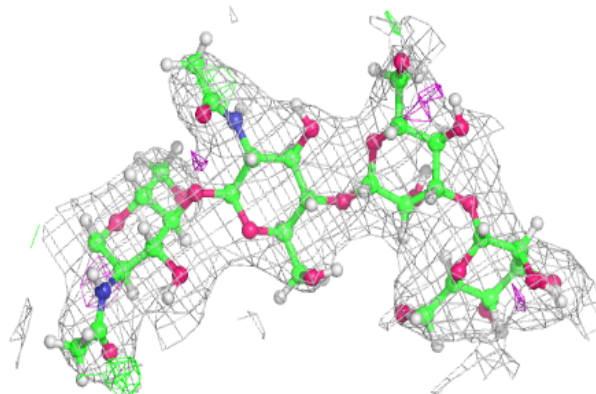


**Electron density around Chain K:**

$2mF_o-DF_c$  (at 0.7 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)



## 6.4 Ligands

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

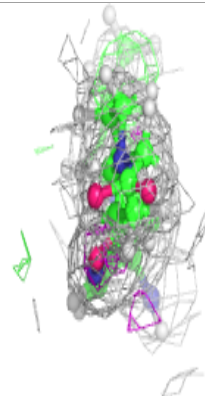
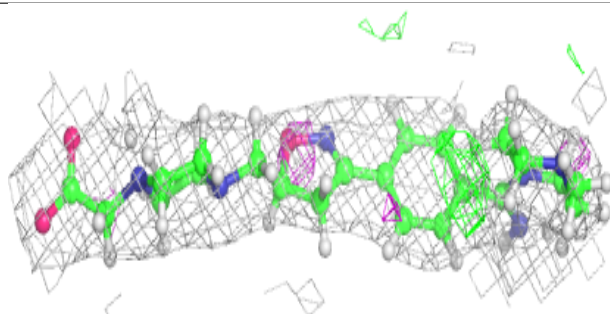
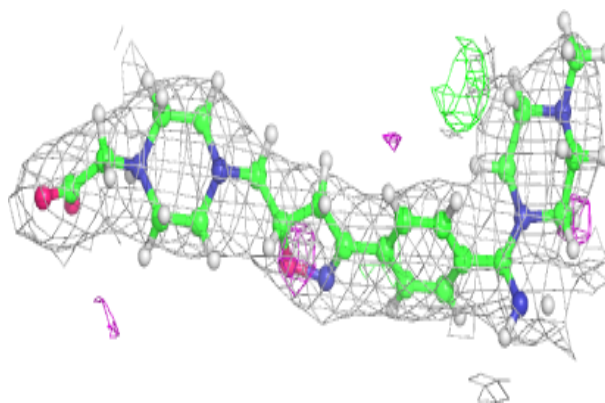
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
13	CL	C	505	1/1	0.66	0.16	98,98,98,98	0
11	NAG	D	2004	14/15	0.77	0.24	45,45,114,114	0
8	SO4	A	507	5/5	0.80	0.17	97,97,97,97	0
8	SO4	A	508	5/5	0.81	0.17	101,101,101,101	0
11	NAG	B	2004	14/15	0.81	0.30	45,45,120,120	0
13	CL	D	2005	1/1	0.82	0.26	99,99,99,99	0
8	SO4	C	502	5/5	0.87	0.15	110,110,110,110	0
12	I7R	D	2006	31/31	0.87	0.17	45,45,68,68	0
8	SO4	C	510	5/5	0.88	0.17	107,107,107,107	0
12	I7R	B	2005	31/31	0.90	0.23	45,45,54,54	0
13	CL	C	504	1/1	0.90	0.44	78,78,78,78	0
8	SO4	C	501	5/5	0.92	0.14	102,102,102,102	0
8	SO4	C	503	5/5	0.92	0.13	110,110,110,110	0
8	SO4	A	501	5/5	0.93	0.13	81,81,81,81	0
9	CA	C	506	1/1	0.94	0.05	89,89,89,89	0
9	CA	A	503	1/1	0.94	0.11	56,56,56,56	0
9	CA	D	2003	1/1	0.95	0.20	51,51,51,51	0
8	SO4	A	509	5/5	0.95	0.18	75,75,75,75	0
9	CA	C	507	1/1	0.95	0.07	71,71,71,71	0
9	CA	C	509	1/1	0.95	0.15	58,58,58,58	0
10	MG	D	2001	1/1	0.96	0.16	44,44,44,44	0
8	SO4	L	301	5/5	0.96	0.17	100,100,100,100	0
9	CA	C	508	1/1	0.97	0.14	59,59,59,59	0
9	CA	A	504	1/1	0.98	0.15	45,45,45,45	0
10	MG	B	2001	1/1	0.98	0.25	26,26,26,26	0
8	SO4	A	502	5/5	0.99	0.16	68,68,68,68	0
9	CA	A	505	1/1	0.99	0.21	38,38,38,38	0
9	CA	A	506	1/1	0.99	0.19	43,43,43,43	0
9	CA	B	2002	1/1	0.99	0.17	55,55,55,55	0
9	CA	D	2002	1/1	0.99	0.21	62,62,62,62	0
9	CA	B	2003	1/1	1.00	0.23	41,41,41,41	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.

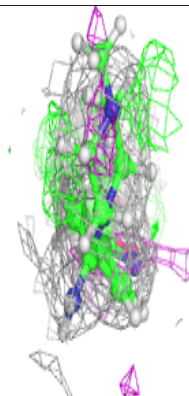
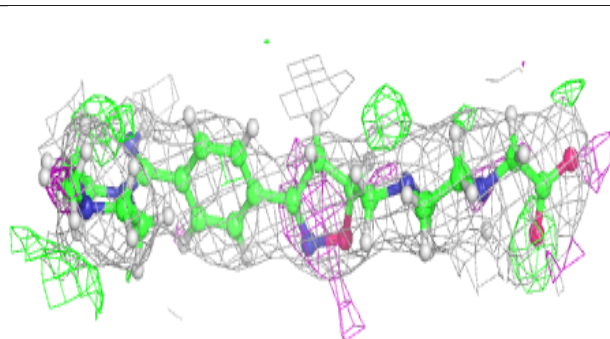
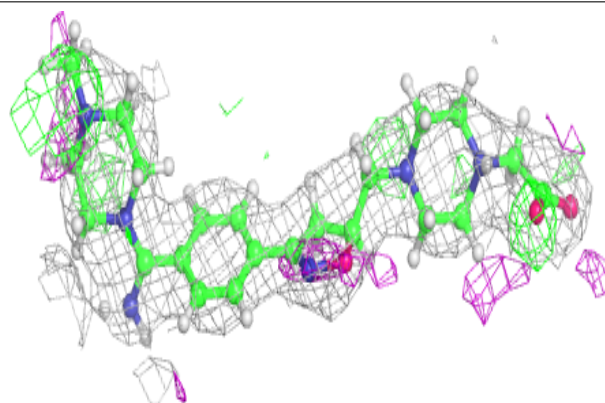


**Electron density around I7R D 2006:**

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

**Electron density around I7R 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)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.