



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 22, 2020 – 01:12 AM BST

PDB ID : 1NQ9  
Title : Crystal Structure of Antithrombin in the Pentasaccharide-Bound Intermediate State  
Authors : Huntington, J.A.; Johnson, D.J.D.  
Deposited on : 2003-01-21  
Resolution : 2.60 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13.1

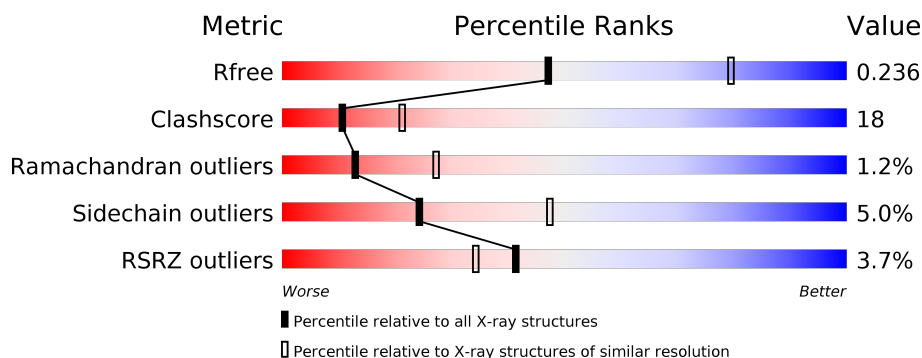
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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.



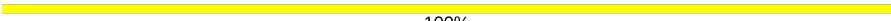
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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

Mol	Chain	Length	Quality of chain
1	I	432	<div> <div>4%</div> <div> <div></div> <div>60%</div> <div>31%</div> <div>• 6%</div> </div> </div>
1	L	432	<div> <div>3%</div> <div> <div></div> <div>69%</div> <div>23%</div> <div>• • •</div> </div> </div>
2	A	2	<div> <div></div> <div> <div>50%</div> <div>50%</div> </div> </div>
2	B	2	<div> <div></div> <div> <div>50%</div> <div>50%</div> </div> </div>
2	C	2	<div> <div></div> <div> <div>50%</div> <div>50%</div> </div> </div>
3	D	5	<div> <div></div> <div> <div>20%</div> <div>80%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
3	E	5	 100%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	B	2	-	-	-	X
4	NAG	I	801	-	-	-	X



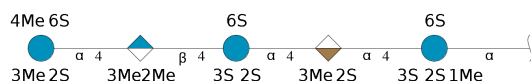
In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 2 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
2	A	2	Total 28	C 16	N 2	O 10	0	0	0
2	B	2	Total 28	C 16	N 2	O 10	0	0	0
2	C	2	Total 28	C 16	N 2	O 10	0	0	0

- Molecule 3 is an oligosaccharide called 3,4-di-O-methyl-2,6-di-O-sulfo-alpha-D-glucopyranose-(1-4)-2,3-di-O-methyl-beta-D-glucopyranuronic acid-(1-4)-2,3,6-tri-O-sulfo-alpha-D-glucopyranose-(1-4)-3-O-methyl-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-methyl 2,3,6-tri-O-sulfo-alpha-D-glucopyranoside.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	D	5	Total	C	O	S	0	0	0
			100	36	55	9			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	5	Total	C	O	S	0	0	0
			100	36	55	9			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	I	36	Total	O	0	0
			36	36		
5	L	53	Total	O	0	0
			53	53		



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

Chain A:  50% 50%

NA01  
NA02

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

Chain B:  50% 50%

NA01  
NA02

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

Chain C:  50% 50%

NA01  
NA02

- Molecule 3: 3,4-di-O-methyl-2,6-di-O-sulfo-alpha-D-glucopyranose-(1-4)-2,3-di-O-methyl-beta-D-glucopyranuronic acid-(1-4)-2,3,6-tri-O-sulfo-alpha-D-glucopyranose-(1-4)-3-O-methyl-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-methyl 2,3,6-tri-O-sulfo-alpha-D-glucopyranoside

Chain D:  20% 80%

Z9L1  
Z9K2  
G063  
G014  
Z9H5

- Molecule 3: 3,4-di-O-methyl-2,6-di-O-sulfo-alpha-D-glucopyranose-(1-4)-2,3-di-O-methyl-beta-D-glucopyranuronic acid-(1-4)-2,3,6-tri-O-sulfo-alpha-D-glucopyranose-(1-4)-3-O-methyl-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-methyl 2,3,6-tri-O-sulfo-alpha-D-glucopyranoside

Chain E:  100%

Z9L1  
Z9K2  
G063  
G014  
Z9H5

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	69.68 Å   86.76 Å   96.92 Å 90.00°   109.54°   90.00°	Depositor
Resolution (Å)	24.43 – 2.60 24.43 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.5 (24.43-2.60) 99.6 (24.43-2.60)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.95 (at 2.60 Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.209 , 0.250 0.199 , 0.236	Depositor DCC
$R_{free}$ test set	1666 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	47.3	Xtriage
Anisotropy	0.473	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 55.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.019 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	6779	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.35% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, Z9L, Z9K, Z9H, GU1, GU6

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	I	0.38	0/3226	0.60	0/4374
1	L	0.40	0/3279	0.65	0/4440
All	All	0.39	0/6505	0.63	0/8814

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

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	I	3162	0	3061	127	0
1	L	3216	0	3136	108	0
2	A	28	0	25	5	0
2	B	28	0	25	3	0
2	C	28	0	25	2	0
3	D	100	0	16	4	0
3	E	100	0	16	0	0
4	I	14	0	13	0	0
4	L	14	0	13	0	0
5	I	36	0	0	0	0
5	L	53	0	0	2	0
All	All	6779	0	6330	239	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 18.

The worst 5 of 239 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:263:VAL:HG12	1:L:264:ALA:H	1.07	1.12
1:L:428:ASN:HD21	1:L:430:CYS:HB2	1.27	0.97
1:L:263:VAL:HG12	1:L:264:ALA:N	1.82	0.93
1:L:263:VAL:CG1	1:L:264:ALA:H	1.83	0.91
1:L:428:ASN:ND2	1:L:430:CYS:H	1.70	0.90

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	I	399/432 (92%)	365 (92%)	31 (8%)	3 (1%)	19	39
1	L	405/432 (94%)	368 (91%)	30 (7%)	7 (2%)	9	18
All	All	804/864 (93%)	733 (91%)	61 (8%)	10 (1%)	13	27

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	38	GLN
1	L	361	ASP
1	I	141	VAL
1	L	418	ASN
1	I	14	ASP

### 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	I	338/383 (88%)	325 (96%)	13 (4%)	33	59
1	L	348/383 (91%)	327 (94%)	21 (6%)	19	39
All	All	686/766 (90%)	652 (95%)	34 (5%)	24	47

5 of 34 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	23	TYR
1	L	119	ILE
1	L	362	LEU
1	L	38	GLN
1	I	217	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	L	18	ASN
1	L	159	GLN
1	L	336	GLN
1	I	319	HIS
1	L	233	ASN

### 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 ⓘ

16 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$
2	NAG	A	1	1,2	14,14,15	0.60	0	17,19,21	0.69	0
2	NAG	A	2	2	14,14,15	0.56	0	17,19,21	0.71	1 (5%)
2	NAG	B	1	1,2	14,14,15	0.68	0	17,19,21	1.18	1 (5%)
2	NAG	B	2	2	14,14,15	0.60	0	17,19,21	0.52	0
2	NAG	C	1	1,2	14,14,15	0.58	0	17,19,21	0.97	1 (5%)
2	NAG	C	2	2	14,14,15	0.62	0	17,19,21	0.56	0
3	Z9L	D	1	3	25,25,25	1.35	3 (12%)	30,39,39	0.97	2 (6%)
3	Z9K	D	2	3	14,17,18	1.48	1 (7%)	15,25,27	1.34	4 (26%)
3	GU6	D	3	3	23,23,24	1.42	3 (13%)	25,36,38	1.18	2 (8%)
3	GU1	D	4	3	11,14,15	1.62	3 (27%)	13,19,21	0.91	0
3	Z9H	D	5	3	21,21,22	1.10	0	25,31,33	1.35	3 (12%)
3	Z9L	E	1	3	25,25,25	1.27	2 (8%)	30,39,39	1.04	4 (13%)
3	Z9K	E	2	3	14,17,18	1.35	2 (14%)	15,25,27	1.43	2 (13%)
3	GU6	E	3	3	23,23,24	1.55	3 (13%)	25,36,38	1.03	1 (4%)
3	GU1	E	4	3	11,14,15	1.50	3 (27%)	13,19,21	0.87	0
3	Z9H	E	5	3	21,21,22	1.29	3 (14%)	25,31,33	1.39	3 (12%)

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	NAG	A	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	A	2	2	-	4/6/23/26	0/1/1/1
2	NAG	B	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	B	2	2	-	6/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	C	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	C	2	2	-	4/6/23/26	0/1/1/1
3	Z9L	D	1	3	-	7/18/38/38	0/1/1/1
3	Z9K	D	2	3	-	0/7/28/31	0/1/1/1
3	GU6	D	3	3	-	2/16/33/36	0/1/1/1
3	GU1	D	4	3	-	2/4/25/28	0/1/1/1
3	Z9H	D	5	3	-	5/15/32/35	0/1/1/1
3	Z9L	E	1	3	-	3/18/38/38	0/1/1/1
3	Z9K	E	2	3	-	0/7/28/31	0/1/1/1
3	GU6	E	3	3	-	5/16/33/36	0/1/1/1
3	GU1	E	4	3	-	2/4/25/28	0/1/1/1
3	Z9H	E	5	3	-	5/15/32/35	0/1/1/1

The worst 5 of 23 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	3	GU6	C1-C2	4.05	1.58	1.51
3	D	2	Z9K	C1-C2	3.78	1.57	1.51
3	D	3	GU6	C1-C2	3.55	1.57	1.51
3	D	4	GU1	C1-C2	3.24	1.56	1.51
3	E	4	GU1	C1-C2	3.06	1.56	1.51

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	5	Z9H	O2-C2-C3	4.25	111.36	106.65
3	D	5	Z9H	O2-C2-C3	4.02	111.10	106.65
3	E	2	Z9K	C1-O5-C5	3.63	118.57	112.17
3	D	3	GU6	O2-C2-C3	3.43	110.45	106.65
2	B	1	NAG	C4-C3-C2	3.14	115.63	111.02

There are no chirality outliers.

5 of 53 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	1	Z9L	C6-O6-S1-O11
3	D	1	Z9L	C6-O6-S1-O15
3	E	5	Z9H	C4-C5-C6-O6
3	E	5	Z9H	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	E	5	Z9H	C6-O6-S1-O7

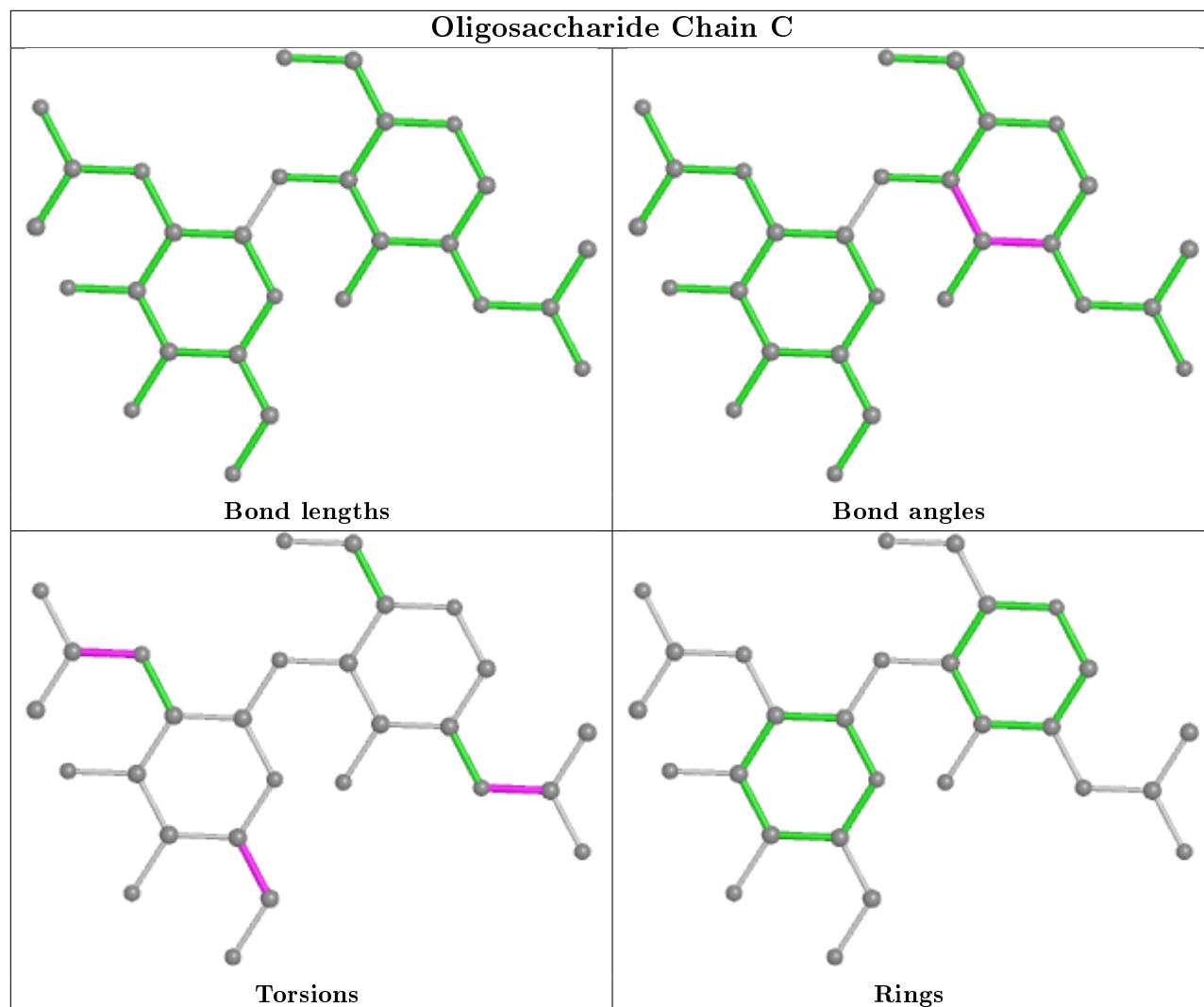
There are no ring outliers.

10 monomers are involved in 14 short contacts:

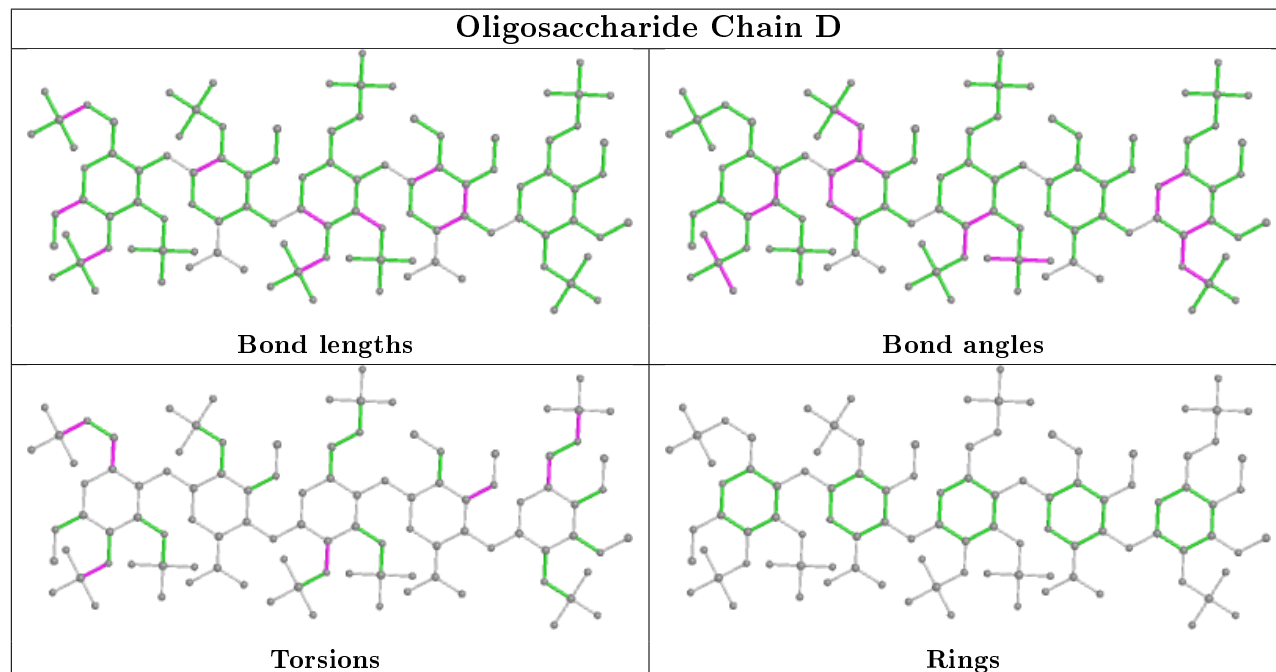
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	1	Z9L	1	0
2	B	2	NAG	3	0
3	D	2	Z9K	1	0
2	C	2	NAG	2	0
2	A	2	NAG	4	0
3	D	4	GU1	1	0
3	D	3	GU6	2	0
2	C	1	NAG	2	0
2	A	1	NAG	2	0
2	B	1	NAG	1	0

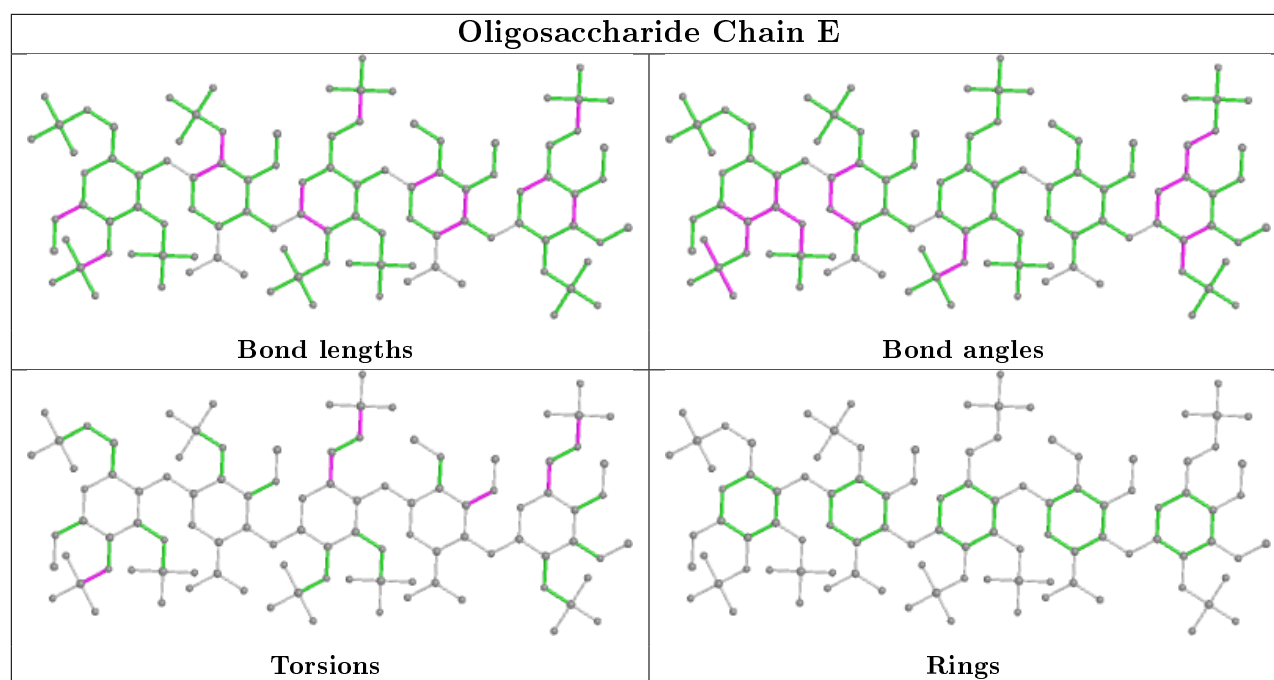
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

## Oligosaccharide Chain C



## Oligosaccharide Chain D





## 5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
4	NAG	L	801	1	14,14,15	0.54	0	17,19,21	0.72	0
4	NAG	I	801	1	14,14,15	0.64	0	17,19,21	0.66	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
4	NAG	L	801	1	-	2/6/23/26	0/1/1/1
4	NAG	I	801	1	-	3/6/23/26	0/1/1/1

There are no bond length outliers.



There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	I	801	NAG	C3-C2-N2-C7
4	L	801	NAG	C8-C7-N2-C2
4	L	801	NAG	O7-C7-N2-C2
4	I	801	NAG	C8-C7-N2-C2
4	I	801	NAG	O7-C7-N2-C2

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [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	I	406/432 (93%)	0.10	18 (4%) 34 27	24, 52, 85, 95	0
1	L	413/432 (95%)	-0.04	12 (2%) 51 45	15, 40, 71, 94	0
All	All	819/864 (94%)	0.03	30 (3%) 41 34	15, 46, 82, 95	0

The worst 5 of 30 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	398	ASN	4.7
1	I	384	ALA	4.2
1	I	14	ASP	4.0
1	L	26	PRO	3.5
1	L	38	GLN	3.4

### 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.

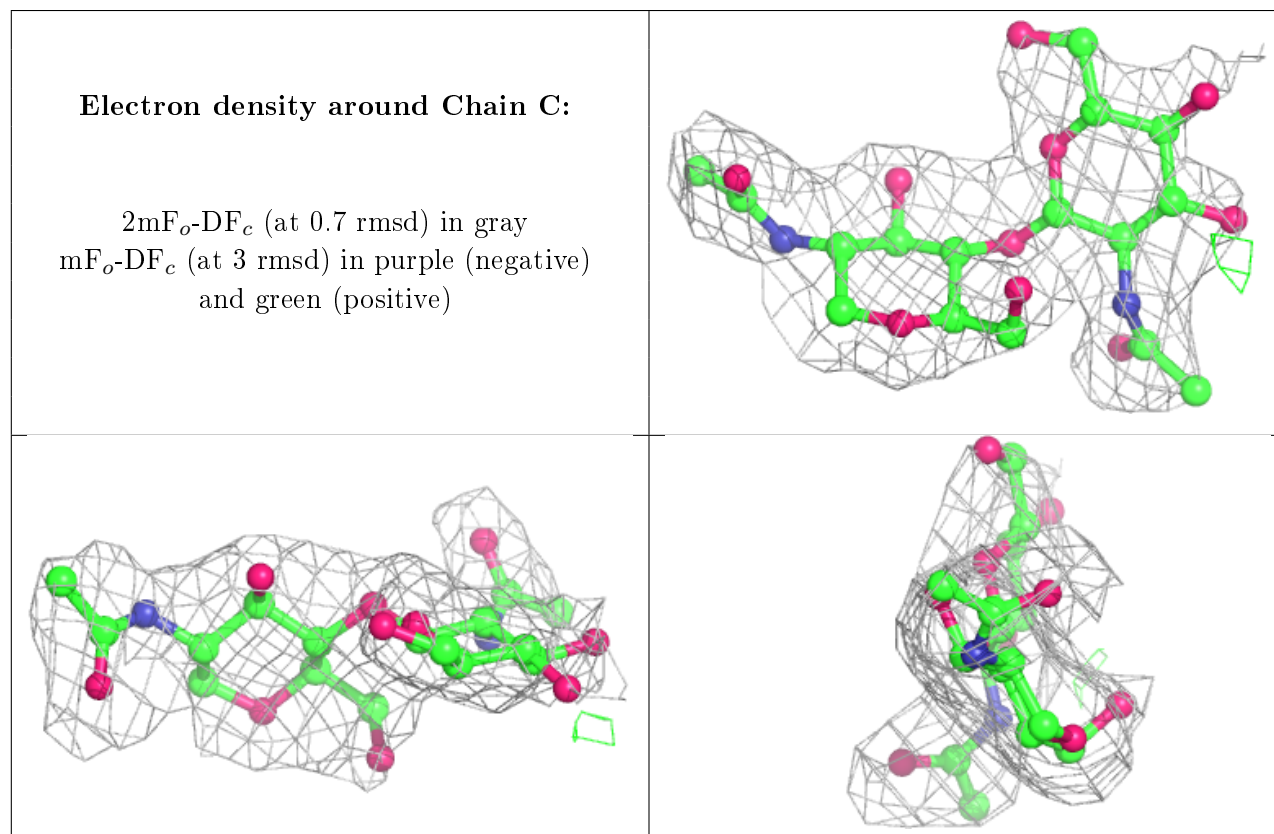
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	NAG	B	2	14/15	0.78	0.44	84,88,90,91	0
2	NAG	A	1	14/15	0.83	0.26	82,86,91,94	0
2	NAG	A	2	14/15	0.84	0.47	98,101,102,103	0
2	NAG	C	2	14/15	0.87	0.40	76,78,80,81	0
3	Z9H	D	5	21/22	0.91	0.17	72,77,83,84	0

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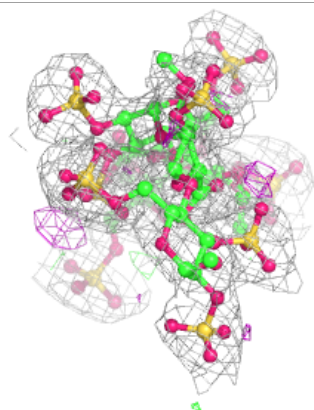
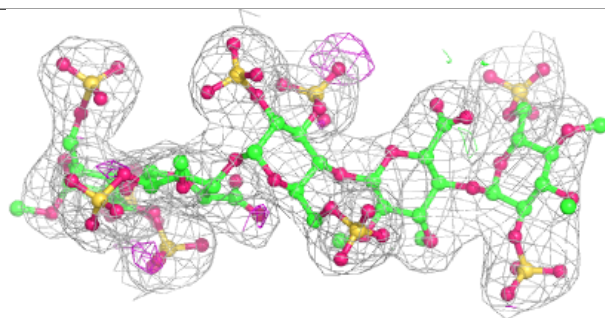
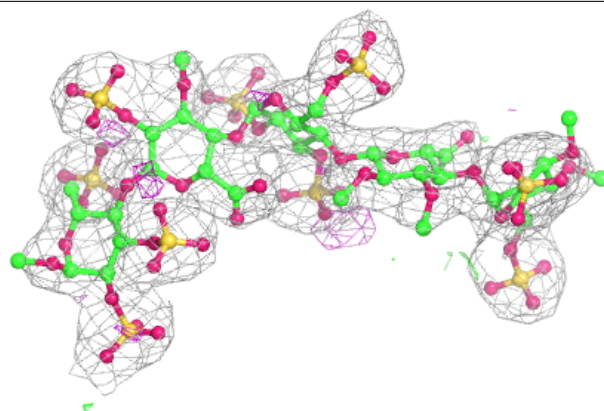
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	Z9H	E	5	21/22	0.91	0.16	57,67,70,72	0
2	NAG	B	1	14/15	0.91	0.23	60,66,69,77	0
3	Z9K	D	2	17/18	0.92	0.15	63,65,66,66	0
2	NAG	C	1	14/15	0.92	0.23	58,61,66,71	0
3	GU1	D	4	14/15	0.93	0.15	53,60,62,67	0
3	GU1	E	4	14/15	0.94	0.18	55,59,67,68	0
3	Z9L	D	1	25/25	0.95	0.17	66,69,72,73	0
3	GU6	D	3	23/24	0.95	0.15	58,64,70,70	0
3	Z9K	E	2	17/18	0.96	0.15	52,53,56,57	0
3	Z9L	E	1	25/25	0.96	0.14	49,52,60,61	0
3	GU6	E	3	23/24	0.96	0.12	45,54,63,64	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.

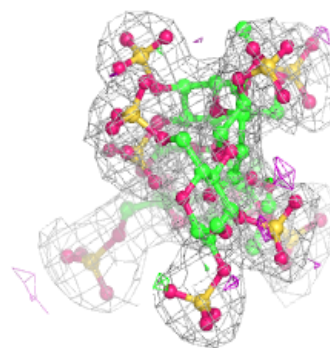
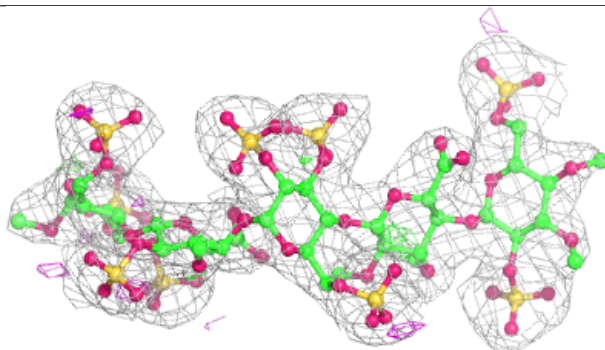
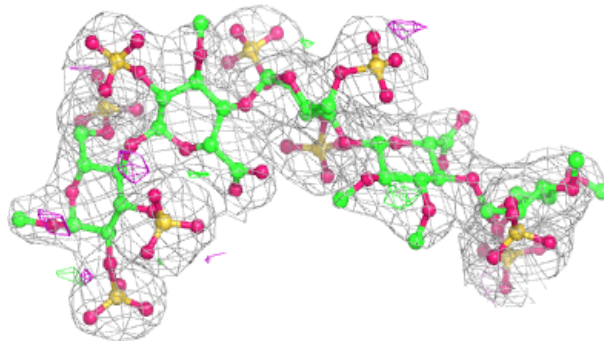


**Electron density around Chain D:**

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

**Electron density around Chain E:**

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



## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	NAG	I	801	14/15	0.74	0.46	77,79,81,81	0
4	NAG	L	801	14/15	0.87	0.27	66,68,70,71	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.