



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 7, 2020 – 07:47 AM BST

PDB ID : 1DZH  
Title : P14-FLUORESCCEIN-N135Q-S380C-ANTITHROMBIN-III  
Authors : Mccoy, A.J.; Huntington, J.A.; Carrell, R.W.  
Deposited on : 2000-02-28  
Resolution : 2.85 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

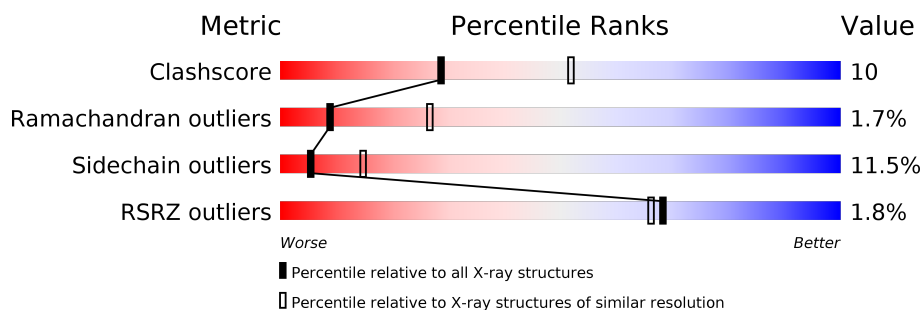
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.85 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))
Clashscore	141614	3438 (2.90-2.82)
Ramachandran outliers	138981	3348 (2.90-2.82)
Sidechain outliers	138945	3351 (2.90-2.82)
RSRZ outliers	127900	3103 (2.90-2.82)

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>68%</div> <div>25%</div> <div>• •</div> </div>
2	L	432	<div> <div>3%</div> <div>67%</div> <div>22%</div> <div>5% • 6%</div> </div>
3	A	2	<div> <div>100%</div> </div>
3	B	2	<div> <div>50%</div> <div>50%</div> </div>
4	C	4	<div> <div>50%</div> <div>50%</div> </div>

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
1	CYF	I	380	X	-	-	-
3	NAG	A	2	-	-	-	X
4	BMA	C	3	-	-	-	X
5	NAG	I	801	-	-	-	X

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 6609 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 ANTITHROMBIN-III.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	I	418	Total	C	N	O	S	0	0	0
			3302	2108	551	625	18			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	135	GLN	ASN	engineered mutation	UNP P01008
I	380	CYF	SER	engineered mutation	UNP P01008

- Molecule 2 is a protein called ANTITHROMBIN-III.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	407	Total	C	N	O	S	0	0	1
			3110	1988	522	583	17			

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



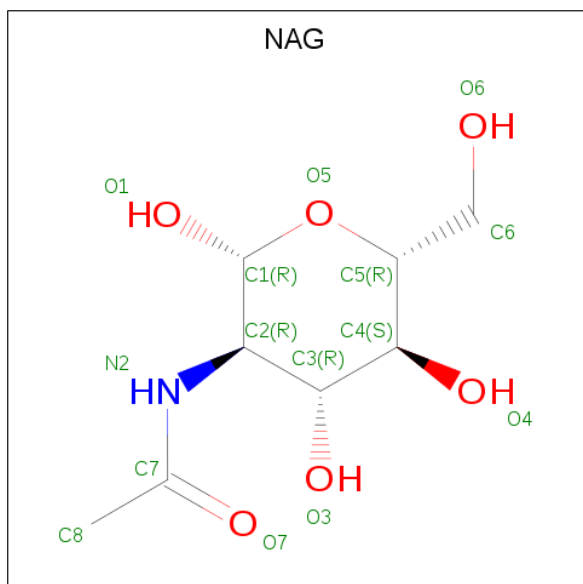
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	A	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	B	2	Total	C	N	O	0	0	0
			28	16	2	10			

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

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	I	1	Total	C	O	0	0
			6	3	3		
6	L	1	Total	C	O	0	0
			6	3	3		

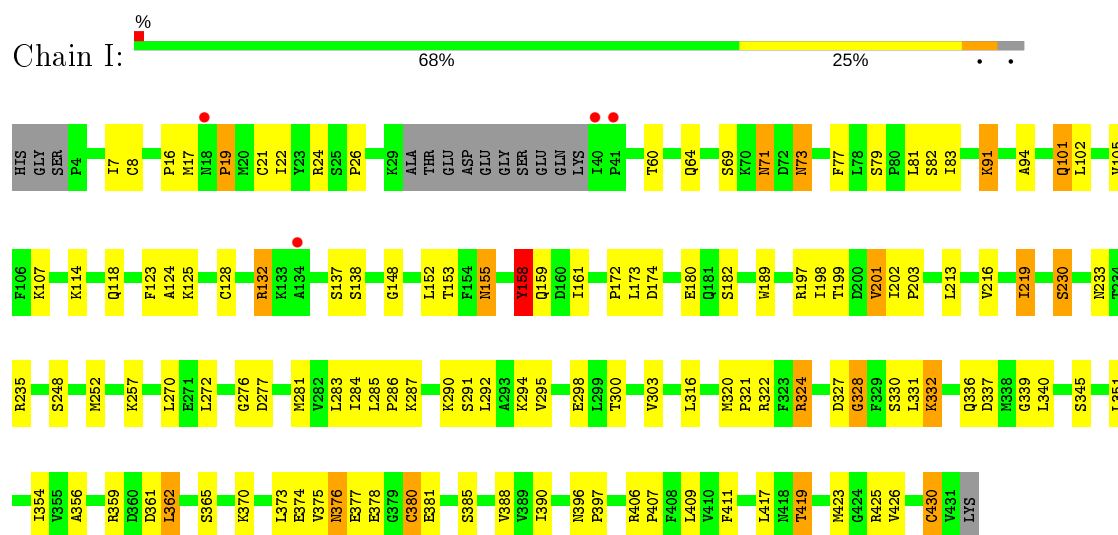
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	I	28	Total	O	0	0
			28	28		
7	L	9	Total	O	0	0
			9	9		

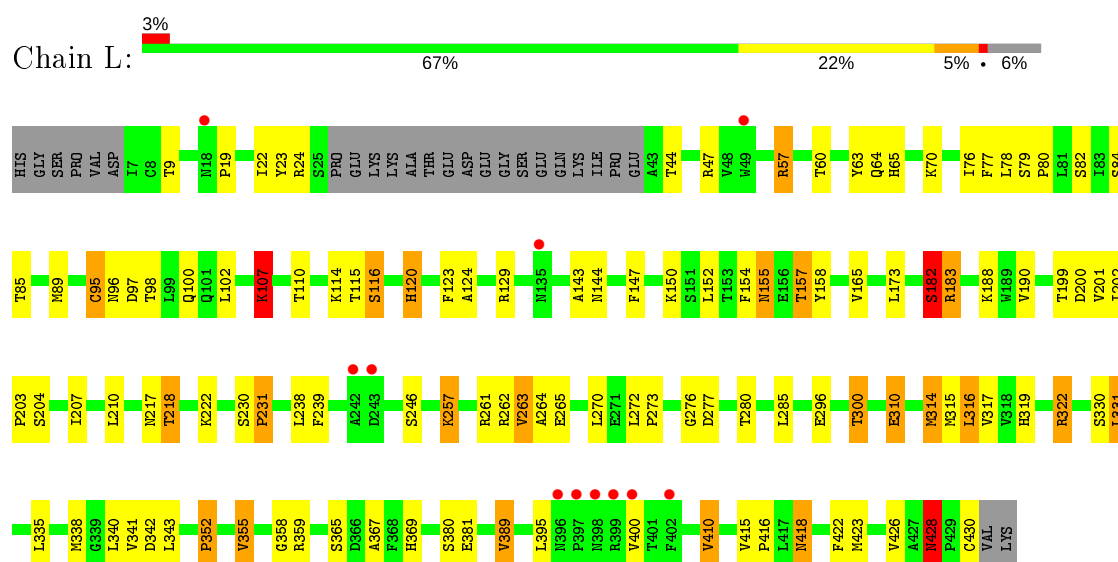
### 3 Residue-property plots [i](#)

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: ANTITHROMBIN-III



- Molecule 2: ANTITHROMBIN-III




- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain A:  100%

MA1  
MA2

- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain B:  50% 50%

MA1  
MA2

- Molecule 4: beta-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 C:  50% 50%

MA1  
MA2  
BM3  
BM4



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	69.17Å 99.86Å 89.42Å 90.00° 105.63° 90.00°	Depositor
Resolution (Å)	20.00 – 2.85 20.01 – 2.85	Depositor EDS
% Data completeness (in resolution range)	99.7 (20.00-2.85) 100.0 (20.01-2.85)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.47 (at 2.83Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.207 , 0.258 0.206 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	63.4	Xtriage
Anisotropy	0.568	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 67.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	6609	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.99% 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: GOL, BMA, NAG, CYF

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	0.51	0/3332	1.00	2/4507 (0.0%)
2	L	0.50	0/3173	1.00	4/4305 (0.1%)
All	All	0.51	0/6505	1.00	6/8812 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	I	1	8
2	L	0	10
All	All	1	18

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	322	ARG	NE-CZ-NH1	9.84	125.22	120.30
2	L	322	ARG	CD-NE-CZ	5.66	131.52	123.60
1	I	132	ARG	NE-CZ-NH1	5.57	123.09	120.30
2	L	316	LEU	CA-CB-CG	5.35	127.60	115.30
2	L	322	ARG	NE-CZ-NH2	-5.25	117.67	120.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	I	380	CYF	C10

5 of 18 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	I	107	LYS	Mainchain
1	I	155	ASN	Mainchain
1	I	180	GLU	Mainchain
1	I	189	TRP	Mainchain
1	I	71	ASN	Mainchain

## 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	3302	0	3213	66	0
2	L	3110	0	2984	59	0
3	A	28	0	25	2	0
3	B	28	0	25	1	0
4	C	50	0	43	1	0
5	I	28	0	26	0	0
5	L	14	0	13	0	0
6	I	6	0	8	0	0
6	L	6	0	8	0	0
7	I	28	0	0	1	0
7	L	9	0	0	0	0
All	All	6609	0	6345	125	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 10.

The worst 5 of 125 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:I:105:VAL:HG21	1:I:340:LEU:HB2	1.61	0.83
2:L:222:LYS:HE2	2:L:381:GLU:HG3	1.62	0.81
1:I:213:LEU:HD11	1:I:354:ILE:HD13	1.65	0.78
1:I:91:LYS:HB2	1:I:102:LEU:HD13	1.67	0.76
2:L:331:LEU:HD21	2:L:369:HIS:HB2	1.71	0.73

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	413/432 (96%)	364 (88%)	40 (10%)	9 (2%)	6	21
2	L	403/432 (93%)	349 (87%)	49 (12%)	5 (1%)	13	35
All	All	816/864 (94%)	713 (87%)	89 (11%)	14 (2%)	9	27

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	I	174	ASP
1	I	362	LEU
1	I	19	PRO
1	I	159	GLN
2	L	418	ASN

### 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	I	353/382 (92%)	320 (91%)	33 (9%)	9	24
2	L	323/383 (84%)	278 (86%)	45 (14%)	3	9
All	All	676/765 (88%)	598 (88%)	78 (12%)	5	15

5 of 78 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	L	44	THR

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Mol	Chain	Res	Type
2	L	115	THR
2	L	389	VAL
2	L	47	ARG
2	L	84	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
1	I	418	ASN
2	L	71	ASN
2	L	336	GLN
1	I	376	ASN
2	L	369	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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
1	CYF	I	380	1	35,38,39	3.15	9 (25%)	43,54,56	2.24	13 (30%)

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
1	CYF	I	380	1	1/1/4/6	1/14/32/34	0/4/4/4

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	380	CYF	C14-C10	-8.46	1.41	1.53
1	I	380	CYF	C19-C20	-8.17	1.39	1.47
1	I	380	CYF	C9-C10	-8.14	1.38	1.52
1	I	380	CYF	C11-C10	-6.47	1.41	1.52
1	I	380	CYF	O1-C1	-5.39	1.24	1.37

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	380	CYF	C11-C10-C9	8.97	119.20	105.83
1	I	380	CYF	CAL-CL-NL	4.19	120.15	114.41
1	I	380	CYF	OL-CL-CAL	-4.13	114.45	121.58
1	I	380	CYF	C4-O2-C3	-3.65	110.58	118.58
1	I	380	CYF	O2-C4-C9	3.58	127.31	122.38

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	I	380	CYF	C10

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	I	380	CYF	SG-CAL-CL-NL

There are no ring outliers.

1 monomer is involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	I	380	CYF	7	0

## 5.5 Carbohydrates

8 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	$\# Z  > 2$
3	NAG	A	1	1,3	14,14,15	1.23	1 (7%)	17,19,21	0.87	1 (5%)
3	NAG	A	2	3	14,14,15	1.21	1 (7%)	17,19,21	0.80	0
3	NAG	B	1	3,2	14,14,15	1.50	4 (28%)	17,19,21	1.42	3 (17%)
3	NAG	B	2	3	14,14,15	1.46	2 (14%)	17,19,21	1.85	3 (17%)
4	NAG	C	1	2,4	14,14,15	1.33	2 (14%)	17,19,21	0.98	1 (5%)
4	NAG	C	2	4	14,14,15	1.33	1 (7%)	17,19,21	1.92	4 (23%)
4	BMA	C	3	4	11,11,12	0.99	1 (9%)	15,15,17	1.79	2 (13%)
4	BMA	C	4	4	11,11,12	1.43	2 (18%)	15,15,17	3.48	2 (13%)

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
3	NAG	A	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	2	3	-	2/6/23/26	0/1/1/1
3	NAG	B	1	3,2	-	2/6/23/26	0/1/1/1
3	NAG	B	2	3	-	2/6/23/26	0/1/1/1
4	NAG	C	1	2,4	-	0/6/23/26	0/1/1/1
4	NAG	C	2	4	-	3/6/23/26	0/1/1/1
4	BMA	C	3	4	-	2/2/19/22	0/1/1/1
4	BMA	C	4	4	-	2/2/19/22	0/1/1/1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	1	NAG	O7-C7	-3.75	1.14	1.23
4	C	2	NAG	O7-C7	-3.74	1.14	1.23
3	B	1	NAG	O7-C7	-3.74	1.14	1.23
4	C	4	BMA	O5-C1	-3.66	1.37	1.43
3	B	2	NAG	O7-C7	-3.66	1.15	1.23

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

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
4	C	4	BMA	C1-O5-C5	12.30	128.85	112.19
4	C	2	NAG	C1-O5-C5	5.46	119.59	112.19
4	C	3	BMA	C1-O5-C5	5.01	118.98	112.19
3	B	2	NAG	O5-C1-C2	-4.59	104.04	111.29
3	B	2	NAG	C4-C3-C2	-4.44	104.51	111.02

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	2	NAG	O5-C5-C6-O6
4	C	3	BMA	O5-C5-C6-O6
3	B	1	NAG	O5-C5-C6-O6
4	C	4	BMA	C4-C5-C6-O6
4	C	2	NAG	O5-C5-C6-O6

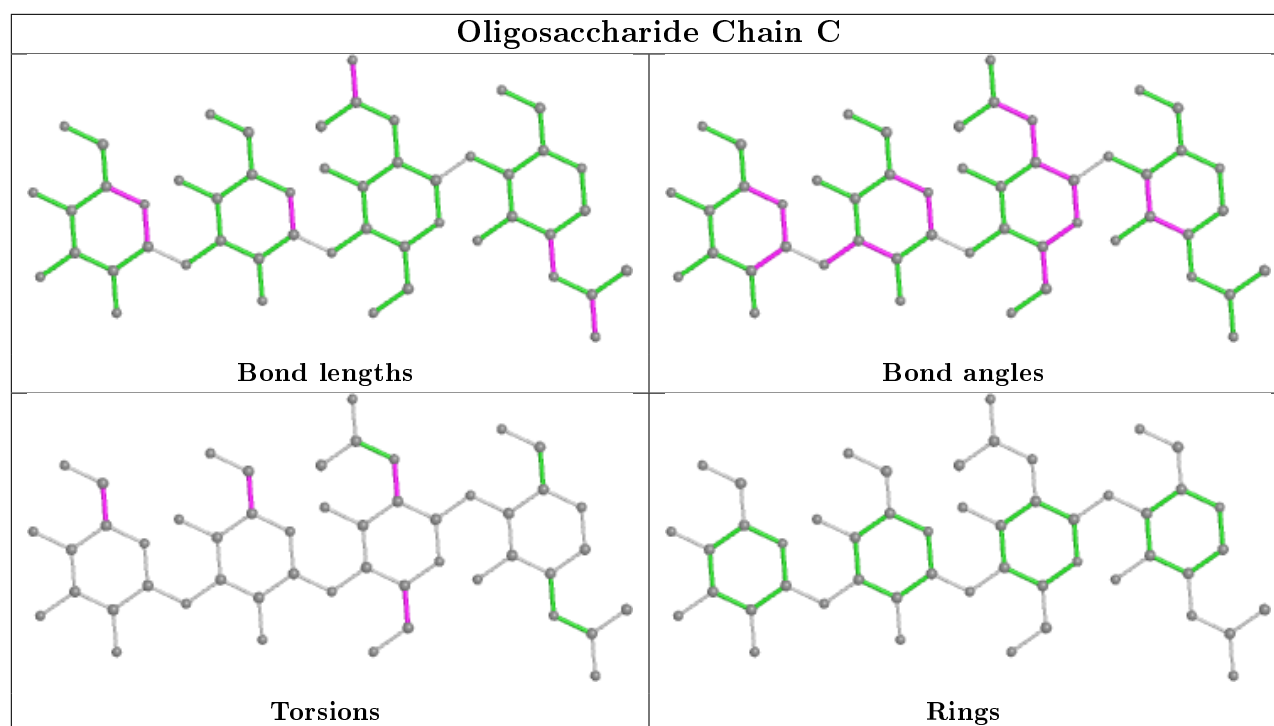
There are no ring outliers.

5 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	2	NAG	1	0
3	A	1	NAG	2	0
3	A	2	NAG	2	0
4	C	3	BMA	1	0
3	B	2	NAG	1	0

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





## 5.6 Ligand geometry [i](#)

5 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$
5	NAG	I	801	1	14,14,15	1.21	1 (7%)	17,19,21	1.06	1 (5%)
6	GOL	I	805	-	5,5,5	0.69	0	5,5,5	0.53	0
6	GOL	L	808	-	5,5,5	0.75	0	5,5,5	0.70	0
5	NAG	L	801	2	14,14,15	1.27	1 (7%)	17,19,21	1.27	2 (11%)
5	NAG	I	804	1	14,14,15	1.25	1 (7%)	17,19,21	1.55	2 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	I	801	1	-	3/6/23/26	0/1/1/1
6	GOL	I	805	-	-	0/4/4/4	-
6	GOL	L	808	-	-	2/4/4/4	-
5	NAG	L	801	2	-	3/6/23/26	0/1/1/1
5	NAG	I	804	1	-	2/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	L	801	NAG	O7-C7	-3.75	1.14	1.23
5	I	801	NAG	O7-C7	-3.67	1.14	1.23
5	I	804	NAG	O7-C7	-3.64	1.15	1.23

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	I	804	NAG	C1-O5-C5	5.11	119.12	112.19
5	L	801	NAG	C1-C2-N2	3.08	115.75	110.49
5	L	801	NAG	C2-N2-C7	2.64	126.66	122.90
5	I	801	NAG	C1-O5-C5	2.26	115.26	112.19
5	I	804	NAG	C6-C5-C4	-2.10	108.09	113.00

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	L	808	GOL	O1-C1-C2-C3
5	I	801	NAG	C4-C5-C6-O6
5	L	801	NAG	O5-C5-C6-O6
5	L	801	NAG	C4-C5-C6-O6
5	I	801	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

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	417/432 (96%)	-0.44	4 (0%) 82 81	27, 57, 100, 148	0
2	L	407/432 (94%)	-0.29	11 (2%) 54 50	28, 59, 123, 148	0
All	All	824/864 (95%)	-0.37	15 (1%) 68 66	27, 58, 115, 148	0

The worst 5 of 15 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	L	135	ASN	4.0
2	L	398	ASN	3.9
2	L	402	PHE	3.8
2	L	242	ALA	3.4
2	L	400	VAL	3.2

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

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

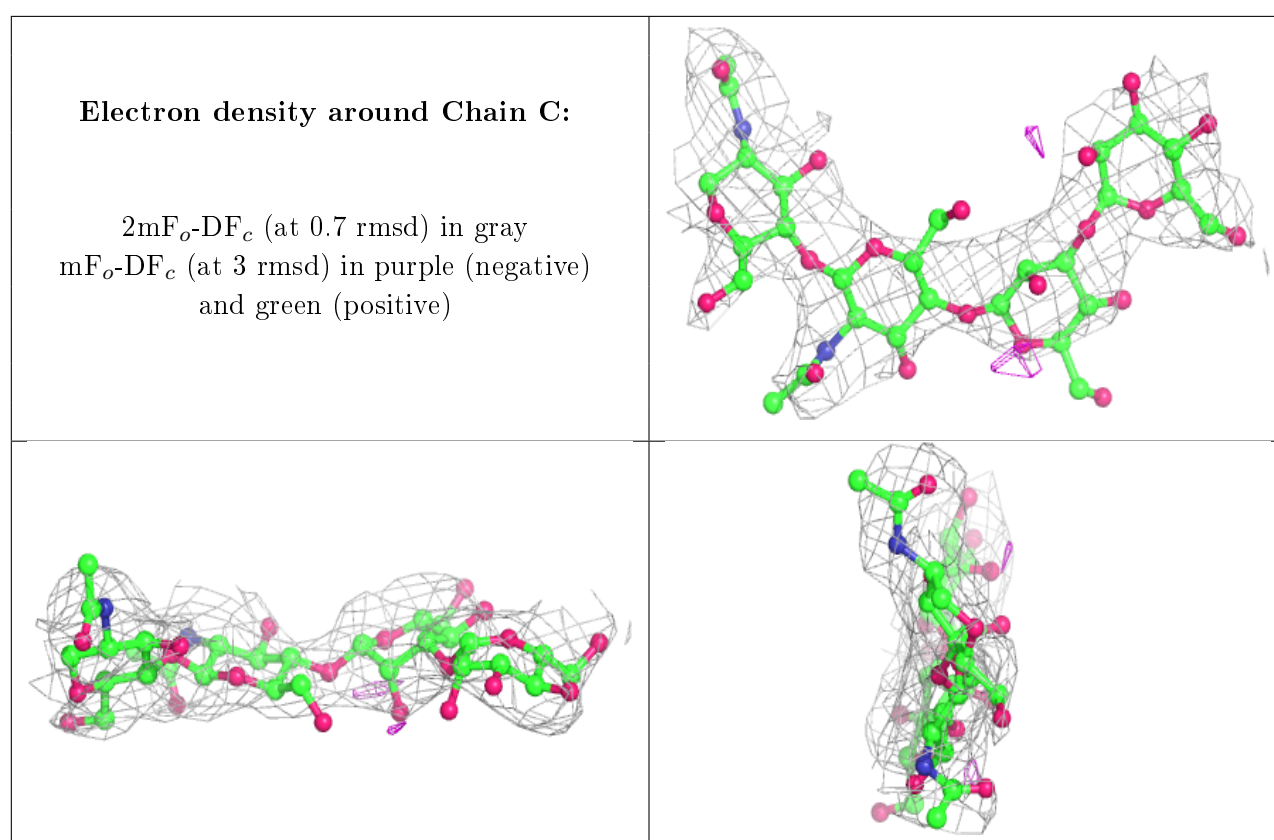
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
1	CYF	I	380	35/36	0.89	0.21	36,65,77,82	0

### 6.3 Carbohydrates [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	NAG	A	2	14/15	0.70	0.45	107,118,125,125	0
3	NAG	B	2	14/15	0.76	0.35	120,126,132,133	0
4	BMA	C	4	11/12	0.77	0.33	140,141,143,143	0
4	BMA	C	3	11/12	0.79	0.44	137,139,145,148	0
4	NAG	C	1	14/15	0.84	0.32	93,101,109,116	0
4	NAG	C	2	14/15	0.86	0.45	124,128,133,135	0
3	NAG	A	1	14/15	0.93	0.21	78,82,92,100	0
3	NAG	B	1	14/15	0.93	0.21	70,88,103,109	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.



## 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
5	NAG	L	801	14/15	0.73	0.29	110,115,122,123	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	NAG	I	801	14/15	0.79	0.41	121,128,135,138	0
5	NAG	I	804	14/15	0.81	0.43	112,118,121,124	0
6	GOL	I	805	6/6	0.92	0.21	50,52,56,58	0
6	GOL	L	808	6/6	0.94	0.15	61,65,69,70	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.