

# wwPDB X-ray Structure Validation Summary Report (i)

Jun 19, 2024 – 02:26 AM EDT

PDB ID	:	4G2Z
Title	:	Crystal Structure of C-lobe of Bovine lactoferrin Complexed with Mefenamic
		acid at 1.90 A Resolution
Authors	:	Shukla, P.K.; Gautam, L.; Sinha, M.; Kaur, P.; Sharma, S.; Singh, T.P.
Deposited on		
Resolution	:	1.90 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 A user guide is available at https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

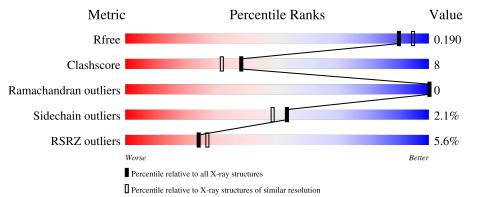
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as 543 be (2022)
Xtriage (Phenix)	:	1.20.1
$\mathrm{EDS}$	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:  $X\text{-}RAY \, DIFFRACTION$ 

The reported resolution of this entry is 1.90 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	$\begin{array}{c} \textbf{Whole archive} \\ (\#\textbf{Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
$R_{free}$	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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 >=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 <=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	А	335	4% 85%	14% •
2	В	6	67%	17%
3	С	2	50% 50%	
3	D	2	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
9	ID8	А	711	-	-	-	Х



# 2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 3009 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 Lactotransferrin.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
1	А	335	Total 2560	C 1593	N 448	O 499	S 20	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	565	LYS	ASN	conflict	UNP P24627
А	608	GLU	LYS	conflict	UNP P24627

• Molecule 2 is a protein called C-terminal peptide from Lactotransferrin.

Mol	Chain	Residues		Ato	oms			ZeroOcc	AltConf	Trace
2	В	6	Total 44	C 29	N 6	0 8	S 1	0	0	0

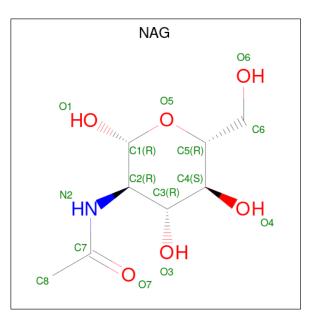
• Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-a cetamido-2-deoxy-beta-D-glucopyranose.



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

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





Mol	Chain	Residues	A	tor	ns		ZeroOcc	AltConf
4	А	1	Total	С	Ν	Ο	0	0
	11	1	14	8	1	5		Ŭ

• Molecule 5 is FE (III) ION (three-letter code: FE) (formula: Fe).

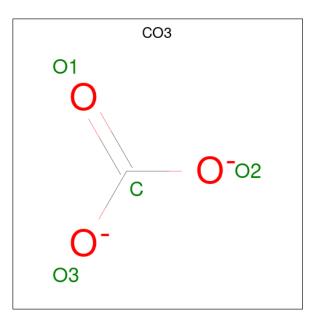
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	А	1	Total Fe 1 1	0	0

• Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

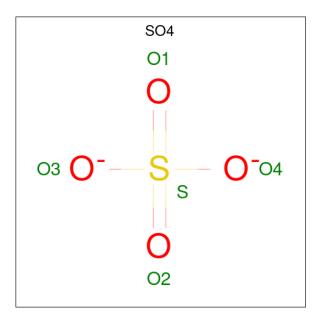
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	А	2	Total Zn 2 2	0	0

• Molecule 7 is CARBONATE ION (three-letter code: CO3) (formula: CO<sub>3</sub>).





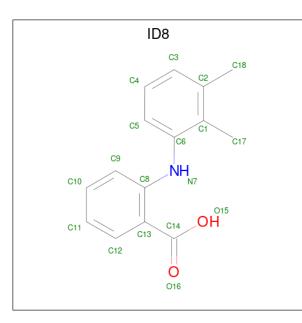
Mol	Chain	Residues	Ate	oms		ZeroOcc	AltConf
7	А	1	Total 4	С 1	O 3	0	0



Mol	Chain	Residues	Ato	oms		ZeroOcc	AltConf
8	А	1	Total 5	0 4	S 1	0	0

• Molecule 9 is 2-[(2,3-DIMETHYLPHENYL)AMINO]BENZOIC ACID (three-letter code: ID8) (formula:  $C_{15}H_{15}NO_2$ ).





Mol	Chain	Residues	A	ton	ns		ZeroOcc	AltConf
0	Δ	1	Total	С	Ν	0	0	0
9	Л	1	18	15	1	2	0	0

• Molecule 10 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	А	302	Total O 302 302	0	0
10	В	3	Total O 3 3	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.

Chain A:	85%	14% •	
Y342           T343           T343           M347           M347           G364           G365           G367           G368           G369           G369           G369           G369           G369	Y398 R415 S417 S417 S417 S421 F423 F423 F423 F423 F423 F423 F423 F423	D513 K514 C515 C515 K520 K520 K565 R566 R566 R566 F569 F569 F569	
V681 N594 H595 N600 S601 S601 S601 S602 N603 H506 K503 N621 ●	P5.05 D6.27 K6.39 F6.39 F6.39 E6.46 E6.46 E6.46 E6.46 E6.46 F6.63 E6.46 F6.63 F6.64 F6.65 F6.65 F6.65 F6.65 F6.65 F6.65 F6.65 F6.65 F6.65 F6.65 F6.75		
• Molecule 2: C-ter	minal peptide from Lactotransfe	errin	
	67%	_	
Chain B:	83%	17%	
L681 E682 A683 A685 F686 F686			
• Molecule 3: 2-ace opyranose	tamido-2-deoxy-beta-D-glucopy	ranose-(1-4)-2-acetamido-2-deoxy-beta-D	)-gluo
Chain C:	50%	50%	

• Molecule 1: Lactotransferrin

#### NAG1 NAG2

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

Chain D:

100%

NAG1 NAG2



# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	62.39Å 49.83Å 65.32Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $107.05^{\circ}$ $90.00^{\circ}$	Depositor
Resolution (Å)	19.92 - 1.90	Depositor
nesolution (A)	19.92 - 1.90	EDS
% Data completeness	99.7 (19.92-1.90)	Depositor
(in resolution range)	99.8 (19.92 - 1.90)	EDS
R <sub>merge</sub>	(Not available)	Depositor
R <sub>sym</sub>	0.04	Depositor
$< I/\sigma(I) > 1$	$11.30 (at 1.90 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
D D.	0.148 , $0.191$	Depositor
$R, R_{free}$	0.149 , $0.190$	DCC
$R_{free}$ test set	1537 reflections $(5.04\%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	18.0	Xtriage
Anisotropy	0.080	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.40 , $53.1$	EDS
L-test for twinning <sup>2</sup>	$<  L  > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.017 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	3009	wwPDB-VP
Average B, all atoms $(Å^2)$	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 6.53% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;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.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

# 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: FE, SO4, CO3, ID8, ZN, 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	Bo	nd lengths	Bond angles		
IVIOI	Chain	RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	А	1.17	6/2608~(0.2%)	1.06	7/3533~(0.2%)	
2	В	0.84	0/44	0.74	0/58	
All	All	1.17	6/2652~(0.2%)	1.06	7/3591~(0.2%)	

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\mathrm{Ideal}(\mathrm{\AA})$
1	А	601	SER	CB-OG	-6.25	1.34	1.42
1	А	448	TRP	CD2-CE2	5.54	1.48	1.41
1	А	523	TYR	CE1-CZ	5.17	1.45	1.38
1	А	467	TRP	CD2-CE2	5.08	1.47	1.41
1	А	569	PHE	CG-CD1	5.05	1.46	1.38

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$\mathbf{Ideal}(^{o})$
1	А	600	ARG	NE-CZ-NH2	8.45	124.52	120.30
1	А	415	ARG	NE-CZ-NH2	-8.39	116.11	120.30
1	А	600	ARG	NE-CZ-NH1	-7.97	116.31	120.30
1	А	526	TYR	CB-CG-CD2	-6.17	117.30	121.00
1	А	643	ASP	CB-CG-OD1	5.68	123.41	118.30

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



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	А	2560	0	2480	38	0
2	В	44	0	39	0	0
3	С	28	0	25	1	0
3	D	28	0	25	0	0
4	А	14	0	13	1	0
5	А	1	0	0	0	0
6	А	2	0	0	0	0
7	А	4	0	0	0	0
8	А	5	0	0	0	0
9	А	18	0	14	5	0
10	А	302	0	0	3	0
10	В	3	0	0	0	0
All	All	3009	0	2596	40	0

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.

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

The worst 5 of 40 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:A:342:TYR:HD2	1:A:342:TYR:O	1.55	0.89
1:A:342:TYR:C	1:A:342:TYR:CD2	2.47	0.86
1:A:342:TYR:O	1:A:342:TYR:CD2	2.30	0.85
1:A:565:LYS:HE3	1:A:567:GLU:H	1.47	0.79
1:A:662:GLY:CA	9:A:711:ID8:H173	2.13	0.78

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	Perce	ntiles
1	А	333/335~(99%)	323~(97%)	10 (3%)	0	100	100
2	В	4/6~(67%)	3~(75%)	1 (25%)	0	100	100
All	All	337/341~(99%)	326~(97%)	11 (3%)	0	100	100

There are no Ramachandran outliers to report.

#### 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 side chain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	А	278/278~(100%)	273~(98%)	5(2%)	59 55
2	В	4/4~(100%)	3~(75%)	1 (25%)	0 0
All	All	282/282~(100%)	276~(98%)	6(2%)	53 48

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	559	ASP
1	А	621	ASN
2	В	681	LEU
1	А	419	LYS
1	А	342	TYR

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such side chains are listed below:

Mol	Chain	Res	Type
1	А	360	GLN
1	А	489	GLN
1	А	551	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)

4 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	Trune	ype Chain Re	Dec	Link	Bo	Bond lengths			Bond angles		
	туре		nes	LIIIK	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2	
3	NAG	С	1	$^{3,1}$	14,14,15	0.89	0	17,19,21	1.63	4 (23%)	
3	NAG	С	2	3	14,14,15	0.75	0	17,19,21	1.72	5 (29%)	
3	NAG	D	1	3,1	14,14,15	1.15	2 (14%)	17,19,21	1.65	5 (29%)	
3	NAG	D	2	3	14,14,15	0.81	0	17,19,21	1.75	3 (17%)	

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	С	1	$^{3,1}$	-	2/6/23/26	0/1/1/1
3	NAG	С	2	3	-	0/6/23/26	0/1/1/1
3	NAG	D	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	D	2	3	-	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mo	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1	NAG	C1-C2	2.16	1.55	1.52
3	D	1	NAG	C4-C5	2.14	1.57	1.53

The worst 5 of 17 bond angle outliers are listed below:



Mol	Chain	Res	Type Atoms		Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
3	D	2	NAG	C3-C4-C5	-4.45	102.17	110.23
3	D	1	NAG	C1-O5-C5	3.97	117.51	112.19
3	С	2	NAG	O4-C4-C5	3.80	118.69	109.32
3	С	1	NAG	C1-C2-N2	-3.65	104.68	110.43
3	С	2	NAG	C2-N2-C7	3.16	127.13	122.90

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	С	1	NAG	C8-C7-N2-C2
3	С	1	NAG	O7-C7-N2-C2

There are no ring outliers.

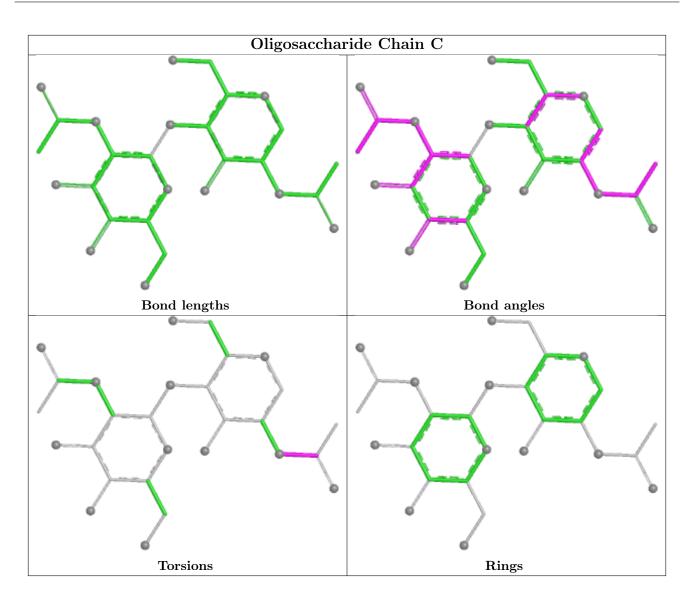
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	С	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.

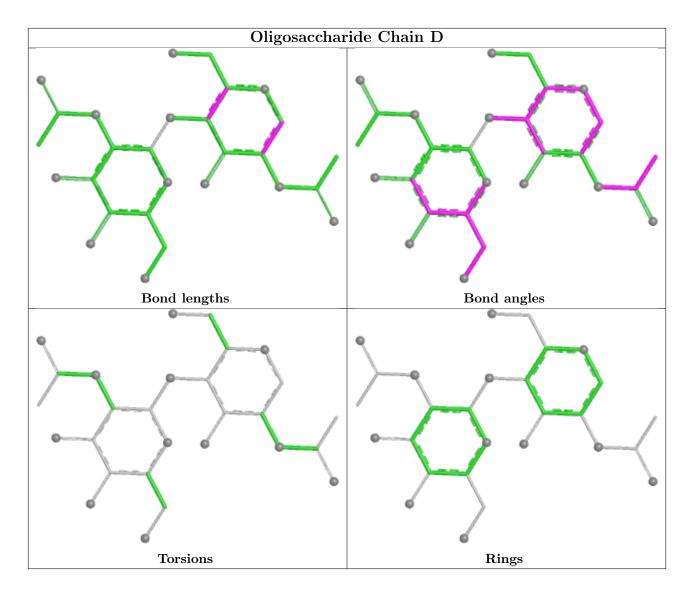












### 5.6 Ligand geometry (i)

Of 7 ligands modelled in this entry, 3 are monoatomic - leaving 4 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		
	туре	Ullaili	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z  > 2
4	NAG	А	701	1	14,14,15	1.12	2 (14%)	17,19,21	1.99	5 (29%)
9	ID8	А	711	-	19,19,19	0.96	0	26,26,26	2.56	7 (26%)
7	CO3	А	709	5	3,3,3	0.76	0	2,3,3	1.62	0



Mol	Mol Type Chain Res		Tink	Bond lengths			Bond angles			
	Type	Unam	nes	Link	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z  > 2
8	SO4	А	710	-	4,4,4	0.60	0	$6,\!6,\!6$	0.45	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	А	701	1	-	0/6/23/26	0/1/1/1
9	ID8	А	711	-	-	6/8/8/8	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	А	701	NAG	O7-C7	2.80	1.29	1.23
4	А	701	NAG	O5-C1	-2.22	1.40	1.43

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

Mol	Chain	Res	Type	Atoms	Ζ	$Observed(^{o})$	$Ideal(^{o})$
9	А	711	ID8	C8-C13-C14	6.95	129.46	121.72
9	А	711	ID8	C13-C8-N7	6.60	132.03	120.50
9	А	711	ID8	C9-C8-N7	-6.34	108.65	121.32
4	А	701	NAG	C8-C7-N2	-3.88	109.69	116.12
4	А	701	NAG	C2-N2-C7	3.75	127.92	122.90

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	А	711	ID8	C13-C8-N7-C6
9	А	711	ID8	C9-C8-N7-C6
9	А	711	ID8	C8-C13-C14-O15
9	А	711	ID8	C8-C13-C14-O16
9	А	711	ID8	C12-C13-C14-O15

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	А	701	NAG	1	0

Continued on next page...



Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	А	711	ID8	5	0

#### 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,  $95^{th}$  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	$\langle RSRZ \rangle$	# RSRZ > 2	$\mathbf{OWAB}(\mathbf{\mathring{A}}^2)$	Q < 0.9
1	А	335/335~(100%)	-0.23	15 (4%) 33 36	9, 18, 45, 95	1 (0%)
2	В	6/6~(100%)	4.82	4 (66%) 0 0	37, 39, 100, 107	0
All	All	341/341~(100%)	-0.14	19 (5%) 24 27	9, 18, 45, 107	1 (0%)

The worst 5 of 19 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	В	681	LEU	14.0
1	А	342	TYR	10.3
1	А	420	HIS	7.3
2	В	682	GLU	7.3
1	А	422	SER	6.4

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

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

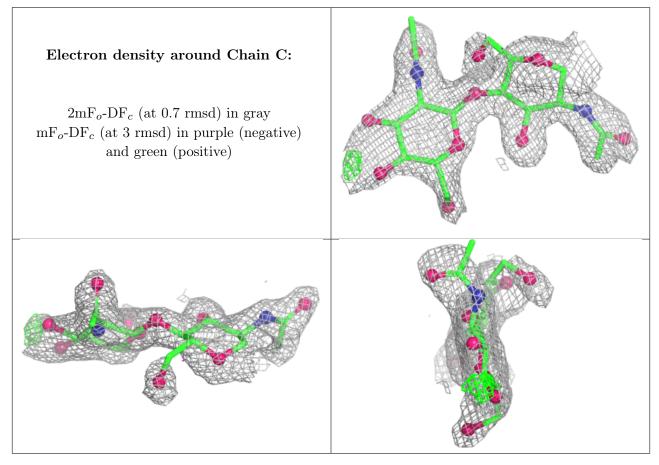
### 6.3 Carbohydrates (i)

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,  $95^{th}$  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.

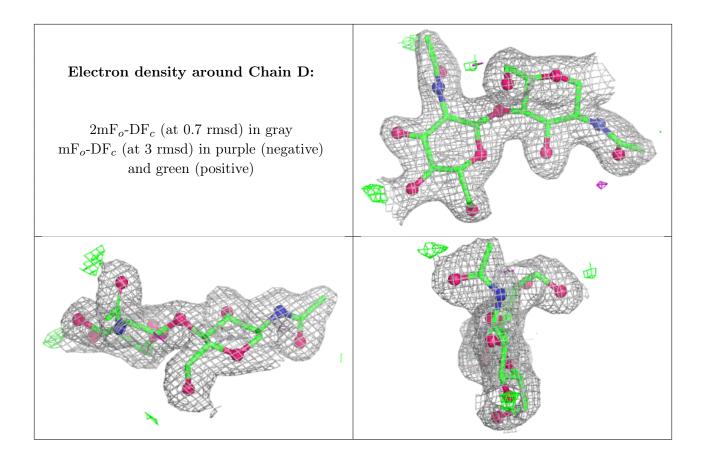
Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	Q < 0.9
3	NAG	С	1	14/15	0.85	0.17	$30,\!42,\!53,\!55$	0
3	NAG	С	2	14/15	0.87	0.30	47,56,62,62	0
3	NAG	D	2	14/15	0.91	0.20	34,38,45,54	0
3	NAG	D	1	14/15	0.94	0.09	21,27,31,32	0



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 (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,  $95^{th}$  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	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	Q<0.9
9	ID8	А	711	18/18	0.54	0.51	45,62,66,67	18
8	SO4	А	710	5/5	0.80	0.35	57,70,78,86	0
4	NAG	А	701	14/15	0.80	0.27	33,48,55,57	0
6	ZN	А	708	1/1	0.98	0.04	23,23,23,23	0
6	ZN	А	707	1/1	0.99	0.05	17,17,17,17	0
7	CO3	А	709	4/4	0.99	0.04	10,10,10,11	0
5	FE	А	706	1/1	1.00	0.04	9,9,9,9	0

### 6.5 Other polymers (i)

There are no such residues in this entry.

