

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

### Sep 26, 2023 – 10:48 AM EDT

PDB ID	:	6C01
Title	:	Human ectonucleotide pyrophosphatase / phosphodiesterase 3 (ENPP3,
		NPP3, CD203c)
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Deposited on	:	2017-12-27
Resolution	:	2.30  Å(reported)

This is a Full wwPDB X-ray Structure Validation 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	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
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)	:	2.35.1

# 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 2.30 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.



Motria	Whole archive	Similar resolution
Metric	$(\# {\rm Entries})$	$(\# { m Entries},  { m resolution}  { m range}({ m \AA}))$
$R_{free}$	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575(2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	838	4% 95% · ·
1	В	838	3% 94% · ·
2	С	2	100%
2	K	2	100%
2	R	2	100%



Mol	Chain	Length	Quality of chain							
3	D	3	100%							
3	F	3	100%							
3	Ν	3	33% 67%	6						
4	Е	3	100%							
4	Н	3	100%							
4	J	3	67%	33%						
4	М	3	100%							
4	0	3	100%							
4	Q	3	67%	33%						
5	G	5	80%	20%						
6	Ι	4	50%	50%						
7	L	4	75%	25%						
8	Р	5	60%	40%						

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
4	FUC	J	3	-	-	-	Х
7	MAN	L	4	-	-	-	Х



# 2 Entry composition (i)

There are 13 unique types of molecules in this entry. The entry contains 27890 atoms, of which 13140 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 Ectonucleotide pyrophosphatase/phosphodiesterase family member 3.

Mol	Chain	Residues			Aton	ns	ZeroOcc	AltConf	Trace		
1	А	819	Total 12898	C 4202	Н 6290	N 1125	O 1224	${f S}\ 57$	0	0	0
1	В	807	Total 12712	C 4145	Н 6200	N 1106	O 1204	S 57	0	0	0

Chain	Residue	Modelled	Actual	Comment	Reference
А	38	ASP	-	expression tag	UNP 014638
А	39	ARG	-	expression tag	UNP O14638
А	40	HIS	-	expression tag	UNP O14638
А	41	HIS	-	expression tag	UNP O14638
А	42	HIS	-	expression tag	UNP 014638
А	43	HIS	-	expression tag	UNP 014638
А	44	HIS	-	expression tag	UNP 014638
А	45	HIS	-	expression tag	UNP 014638
А	46	LYS	-	expression tag	UNP O14638
А	47	LEU	-	expression tag	UNP 014638
В	38	ASP	-	expression tag	UNP 014638
В	39	ARG	-	expression tag	UNP 014638
В	40	HIS	-	expression tag	UNP 014638
В	41	HIS	-	expression tag	UNP 014638
В	42	HIS	-	expression tag	UNP 014638
В	43	HIS	-	expression tag	UNP 014638
В	44	HIS	-	expression tag	UNP 014638
В	45	HIS	-	expression tag	UNP 014638
В	46	LYS	-	expression tag	UNP 014638
B	47	LEU	-	expression tag	UNP 014638

There are 20 discrepancies between the modelled and reference sequences:

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





Mol	Chain	Residues		$\mathbf{At}$	$\mathbf{oms}$			ZeroOcc	AltConf	Trace
2	С	9	Total	С	Η	Ν	Ο	0	0	0
	C		55	16	27	2	10	0	0	0
0	K	n	Total	С	Η	Ν	0	0	0	0
	Γ	2	55	16	27	2	10	0	0	0
9	В	9	Total	С	Η	Ν	0	0	0	0
	п	2	55	16	27	2	10	0	U	0

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	3	Total 76	C 22	Н 37	N 2	0 15	0	0	0
3	F	3	Total 76	C 22	Н 37	N 2	0 15	0	0	0
3	Ν	3	Total 76	C 22	Н 37	N 2	0 15	0	0	0

• Molecule 4 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[al pha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
4	F	2	Total	С	Η	Ν	0	0	0	0
4	Ľ	ა	75	22	37	2	14	0		0
4	Ц	2	Total	С	Η	Ν	0	0	0	0
4	п	9	75	22	37	2	14	0		0
4	т	9	Total	С	Η	Ν	0	0	0	0
4	1	3	75	22	37	2	14	0	0	0
4	м	1 2	Total	С	Η	Ν	0	0	0	0
4 M	3	75	22	37	2	14	U	0	U	



Conti	nued fron	ı previous pa	ge							
Mol	Chain	Residues		At	$\mathbf{oms}$			ZeroOcc	AltConf	Trace
4	0	9	Total	С	Η	Ν	0	0	0	0
4	0	0	75	22	37	2	14	0	0	0
4	0	9	Total	С	Η	Ν	0	0	0	0
4	Q	0	75	22	37	2	14	0	0	0

• Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranos e-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acet amido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
5	G	5	Total 117	C 34	Н 57	N 2	O 24	0	0	0

• Molecule 6 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-beta-D-mannopyranos e-(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		
6	Ι	4	Total 97	C 28	Н 47	N 2	O 20	0	0	0

• Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranos e-(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	L	4	Total 97	C 28	Н 47	N 2	O 20	0	0	0



• Molecule 8 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyran ose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-a cetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
8	Р	5	Total 118	C 34	Н 57	N 2	O 25	0	0	0

• Molecule 9 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	А	2	Total Zn 2 2	0	0
9	В	2	Total Zn 2 2	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	А	1	Total Ca 1 1	0	0
10	В	1	Total Ca 1 1	0	0

• Molecule 11 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).







Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
11	Λ	1	Total	С	Η	Ν	Ο	0	0
	A	1	28	8	14	1	5	0	0
11	Р	1	Total	С	Η	Ν	Ο	0	0
11	D	T	28	8	14	1	5	0	0

• Molecule 12 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	А	1	Total Na 1 1	0	0
12	В	1	Total Na 1 1	0	0

• Molecule 13 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	А	527	Total O 527 527	0	0
13	В	417	Total         O           417         417	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: Ectonucleotide pyrophosphatase/phosphodiesterase family member 3



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

Chain C:

100%

NAG1 NAG2

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

Chain K:

100%

NAG1 NAG2



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

Chain R:

100%

### NAG1 NAG2

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

Chain D:	100%

#### NAG1 NAG2 BMA3

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

Chain F:	100%	
NAG1 NAG2 BMA3		

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

Chain N:	33%	67%
NAG1 NAG2 BMA3		

• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:

100%

#### NAG1 NAG2 FUC3

 • Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)] 2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:

100%

#### NAG1 NAG2 FUC3

 • Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)] 2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:

67%

33%



#### NAG1 NAG2 FUC3

 • Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)] 2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:	100	%	-
NAG1 NAG2 FUC3			
• Molecule 4: 2-acet tamido-2-deoxy-beta	amido-2-deoxy-beta-D- -D-glucopyranose	glucopyranose-(1-4)-[alpha-L-f	ucopyranose-(1-6)]2-ace
Chain O:	1009	%	-
NAG1 NAG2 FUC3			
• Molecule 4: 2-acet tamido-2-deoxy-beta	amido-2-deoxy-beta-D- -D-glucopyranose	glucopyranose-(1-4)-[alpha-L-f	ucopyranose-(1-6)]2-ace
Chain Q:	67%	33%	-
NA61 NAG2 FUG3			
• Molecule 5: alpha- eta-D-glucopyranose e	D-mannopyranose-(1-3 -(1-4)-[alpha-L-fucopyr	)-beta-D-mannopyranose-(1-4) anose-(1-6)]2-acetamido-2-deo:	-2-acetamido-2-deoxy-b xy-beta-D-glucopyranos
Chain G:	80%	20%	-
NAG1 NAG2 BMAG2 FUC5 FUC5			
• Molecule 6: alpha- eta-D-glucopyranose	D-mannopyranose-(1-6 -(1-4)-2-acetamido-2-de	)-beta-D-mannopyranose-(1-4) eoxy-beta-D-glucopyranose	-2-acetamido-2-deoxy-b
Chain I:	50%	50%	•
NAG1 NAG2 MAN4 MAN4			

 $\bullet \ {\rm Molecule \ 7: \ alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose} (1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose (1-4)-2-acetamido-2-deoxy-beta-D-glucopyrano$ 

Chain L:

75%

25%

NAG1 NAG2 BMA3 MAN4



 $\bullet$  Molecule 8: 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 nose

60%

Chain P:

40%

NAG1 NAG2 BMA3 MAN4 MAN5 MAN5



# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	96.18Å 133.64Å 167.43Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $90.00^{\circ}$	Depositor
Bosolution(A)	48.27 - 2.30	Depositor
Resolution (A)	48.27 - 2.30	EDS
% Data completeness	90.5 (48.27-2.30)	Depositor
(in resolution range)	83.3 (48.27-2.30)	EDS
$R_{merge}$	(Not available)	Depositor
R <sub>sym</sub>	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.40 (at 2.29 \text{\AA})$	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
B B.	0.174 , $0.214$	Depositor
II, II, <i>free</i>	0.176 , $0.216$	DCC
$R_{free}$ test set	1918 reflections $(2.20\%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	29.7	Xtriage
Anisotropy	0.112	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.36 , $43.0$	EDS
L-test for $twinning^2$	$ < L >=0.48, < L^2>=0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	27890	wwPDB-VP
Average B, all atoms $(Å^2)$	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The analyses of the Patterson function reveals a significant off-origin peak that is 49.99 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.8911e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.

<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: FUC, NAG, CA, MAN, ZN, BMA, NA

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).

Mal	Mal Chain		Bond lengths		angles
	Unam	RMSZ	# Z  > 5	RMSZ	# Z  > 5
1	А	0.30	0/6806	0.47	0/9255
1	В	0.29	0/6707	0.47	0/9119
All	All	0.30	0/13513	0.47	0/18374

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	А	6608	6290	6290	11	1
1	В	6512	6200	6199	10	0
2	С	28	27	25	0	0
2	Κ	28	27	25	0	0
2	R	28	27	25	0	0
3	D	39	37	34	0	0
3	F	39	37	34	0	0
3	Ν	39	37	34	0	0
4	Е	38	37	34	0	0
4	Н	38	37	34	0	0
4	J	38	37	34	0	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	М	38	37	34	0	0
4	0	38	37	34	0	0
4	Q	38	37	34	0	0
5	G	60	57	52	0	0
6	Ι	50	47	43	0	0
7	L	50	47	43	0	0
8	Р	61	57	52	0	1
9	А	2	0	0	0	0
9	В	2	0	0	0	0
10	А	1	0	0	0	0
10	В	1	0	0	0	0
11	А	14	14	13	0	0
11	В	14	14	13	1	0
12	А	1	0	0	0	0
12	В	1	0	0	0	0
13	A	527	0	0	2	1
13	В	417	0	0	3	1
All	All	14750	13140	13086	22	2

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 1.

All (22) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom 1	Atom 2	Interatomic	Clash
Atom-1 Atom-2		distance (Å)	overlap (Å)
1:A:70:ARG:NH2	13:A:1001:HOH:O	2.18	0.76
1:B:102:ARG:NH2	1:B:115:CYS:SG	2.60	0.73
1:B:170:ARG:NH2	13:B:1002:HOH:O	2.23	0.70
1:A:225:ASP:OD1	1:A:226:ASN:N	2.34	0.59
1:A:195:LYS:NZ	1:A:510:GLU:OE1	2.40	0.54
1:A:55:ARG:NH2	1:A:100:LYS:O	2.41	0.53
1:A:170:ARG:NH2	13:A:1009:HOH:O	2.40	0.51
1:B:650:GLN:HG3	1:B:738:THR:HA	1.95	0.48
1:B:92:SER:O	1:B:102:ARG:NH1	2.41	0.47
1:B:739:GLU:OE1	13:B:1001:HOH:O	2.20	0.47
1:B:72:ASP:OD2	1:B:78:ARG:NH1	2.48	0.47
11:B:929:NAG:H61	11:B:929:NAG:H2	1.99	0.45
1:A:145:ASP:OD2	1:A:363:ASN:ND2	2.45	0.44
1:A:404:PRO:HG2	1:A:461:LEU:HB2	1.98	0.44
1:A:218:PRO:HA	1:A:221:HIS:CE1	2.54	0.43
1:A:372:ASP:N	1:A:372:ASP:OD1	2.50	0.41



6C01
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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:269:TYR:O	1:B:270:PHE:HB2	2.18	0.41
1:B:159:PRO:HB3	1:B:364:CYS:O	2.20	0.41
1:A:146:THR:O	1:A:151:GLN:NE2	2.52	0.41
1:A:396:PHE:O	1:A:471:ARG:NH2	2.45	0.41
1:B:170:ARG:HG2	13:B:1119:HOH:O	2.21	0.40
1:B:218:PRO:HA	1:B:221:HIS:CE1	2.55	0.40

All (2) 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)
1:A:326:SER:O	8:P:5:MAN:O6[4_566]	2.08	0.12
13:A:1321:HOH:O	13:B:1126:HOH:O[4_476]	2.09	0.11

## 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	817/838~(98%)	793~(97%)	23~(3%)	1 (0%)	51	64
1	В	801/838~(96%)	773~(96%)	28~(4%)	0	100	100
All	All	1618/1676~(96%)	1566 (97%)	51 (3%)	1 (0%)	51	64

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	662	PRO

### 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	americ Outliers		Percentiles		
1	А	740/758~(98%)	735~(99%)	5 (1%)	84	92		
1	В	730/758~(96%)	726 (100%)	4 (0%)	88	95		
All	All	1470/1516~(97%)	1461 (99%)	9 (1%)	86	94		

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	$\mathbf{Res}$	Type
1	А	164	PHE
1	А	228	MET
1	А	370	LEU
1	А	462	PHE
1	А	808	ILE
1	В	164	PHE
1	В	221	HIS
1	В	228	MET
1	В	370	LEU

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such side chains are listed below:

Mol	Chain	Res	Type
1	В	499	HIS

### 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)

51 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).

Mal	<b>T</b>	Chain	Dec	T :1-	Bond lengths		Bond angles			
	Type	Chain	Res	Link	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NAG	С	1	2,1	14,14,15	0.30	0	17,19,21	0.58	0
2	NAG	С	2	2	14,14,15	0.23	0	17,19,21	0.50	0
3	NAG	D	1	3,1	14,14,15	0.39	0	17,19,21	0.48	0
3	NAG	D	2	3	14,14,15	0.49	0	17,19,21	0.49	0
3	BMA	D	3	3	$11,\!11,\!12$	0.92	0	$15,\!15,\!17$	0.79	0
4	NAG	Е	1	4,1	$14,\!14,\!15$	0.30	0	$17,\!19,\!21$	0.59	0
4	NAG	Е	2	4	14,14,15	0.42	0	17,19,21	0.39	0
4	FUC	Е	3	4	10,10,11	0.89	0	14,14,16	0.83	0
3	NAG	F	1	3,1	$14,\!14,\!15$	0.19	0	17,19,21	0.68	0
3	NAG	F	2	3	14,14,15	0.49	0	17,19,21	0.45	0
3	BMA	F	3	3	11,11,12	0.76	0	$15,\!15,\!17$	0.70	0
5	NAG	G	1	5,1	14,14,15	0.26	0	17,19,21	0.42	0
5	NAG	G	2	5	14,14,15	0.26	0	17,19,21	0.38	0
5	BMA	G	3	5	11,11,12	0.64	0	$15,\!15,\!17$	0.89	0
5	MAN	G	4	5	11,11,12	0.96	0	$15,\!15,\!17$	1.22	1 (6%)
5	FUC	G	5	5	10,10,11	0.62	0	14,14,16	0.71	0
4	NAG	Н	1	4,1	14,14,15	0.39	0	17,19,21	0.58	0
4	NAG	Н	2	4	$14,\!14,\!15$	0.24	0	$17,\!19,\!21$	0.48	0
4	FUC	Н	3	4	10,10,11	0.81	0	$14,\!14,\!16$	0.80	0
6	NAG	Ι	1	6,1	14,14,15	0.46	0	17,19,21	0.49	0
6	NAG	Ι	2	6	14,14,15	0.23	0	17,19,21	0.50	0
6	BMA	Ι	3	6	11,11,12	1.11	1 (9%)	$15,\!15,\!17$	0.79	0
6	MAN	Ι	4	6	11,11,12	1.14	2 (18%)	$15,\!15,\!17$	1.12	2 (13%)
4	NAG	J	1	4,1	14,14,15	0.35	0	17,19,21	0.38	0
4	NAG	J	2	4	14,14,15	0.25	0	17,19,21	0.46	0
4	FUC	J	3	4	10,10,11	1.44	2 (20%)	$14,\!14,\!16$	1.42	1 (7%)
2	NAG	K	1	2,1	14,14,15	0.22	0	17,19,21	0.51	0
2	NAG	K	2	2	14,14,15	0.23	0	17,19,21	0.58	0
7	NAG	L	1	7,1	14,14,15	0.29	0	17,19,21	0.49	0
7	NAG	L	2	7	14,14,15	0.37	0	17,19,21	0.42	0
7	BMA	L	3	7	11,11,12	0.80	0	$15,\!15,\!17$	0.67	0
7	MAN	L	4	7	11,11,12	0.88	1 (9%)	$15,\!15,\!17$	1.21	1 (6%)
4	NAG	М	1	4,1	14,14,15	0.29	0	17,19,21	0.45	0
4	NAG	М	2	4	14,14,15	0.27	0	17,19,21	0.65	0
4	FUC	М	3	4	10,10,11	0.89	0	14,14,16	0.83	0
3	NAG	N	1	3,1	14,14,15	0.32	0	17,19,21	0.62	0



Mal	Mol Type	Chain	Dog	Link	Bo	ond leng	$_{\rm sths}$	B	ond ang	les
IVIOI	туре	Ullalli	nes		Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NAG	Ν	2	3	$14,\!14,\!15$	0.60	1 (7%)	17,19,21	0.74	0
3	BMA	Ν	3	3	11,11,12	1.12	1 (9%)	$15,\!15,\!17$	0.89	1 (6%)
4	NAG	0	1	4,1	14,14,15	0.34	0	17,19,21	0.55	0
4	NAG	0	2	4	14,14,15	0.34	0	17,19,21	0.39	0
4	FUC	0	3	4	10,10,11	0.56	0	14,14,16	0.85	0
8	NAG	Р	1	8,1	14,14,15	0.36	0	17,19,21	0.49	0
8	NAG	Р	2	8	14,14,15	0.18	0	17,19,21	0.50	0
8	BMA	Р	3	8	11,11,12	0.43	0	15,15,17	0.72	0
8	MAN	Р	4	8	11,11,12	0.87	0	15,15,17	1.08	1 (6%)
8	MAN	Р	5	8	11,11,12	0.94	0	15,15,17	0.90	0
4	NAG	Q	1	4,1	14,14,15	0.31	0	17,19,21	0.43	0
4	NAG	Q	2	4	14,14,15	0.38	0	17,19,21	0.48	0
4	FUC	Q	3	4	10,10,11	0.77	0	14,14,16	1.03	1 (7%)
2	NAG	R	1	2,1	14,14,15	0.39	0	17,19,21	0.78	0
2	NAG	R	2	2	14,14,15	0.32	0	17,19,21	0.40	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
2	NAG	С	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	С	2	2	-	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	-	2/6/23/26	0/1/1/1
3	BMA	D	3	3	-	0/2/19/22	0/1/1/1
4	NAG	Е	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	Е	2	4	-	2/6/23/26	0/1/1/1
4	FUC	Е	3	4	-	-	0/1/1/1
3	NAG	F	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	F	2	3	-	2/6/23/26	0/1/1/1
3	BMA	F	3	3	-	2/2/19/22	0/1/1/1
5	NAG	G	1	5,1	-	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	FUC	G	5	5	-	-	0/1/1/1
4	NAG	Н	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	Н	2	4	-	2/6/23/26	0/1/1/1



Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	FUC	Н	3	4	-	-	0/1/1/1
6	NAG	Ι	1	6,1	-	1/6/23/26	0/1/1/1
6	NAG	Ι	2	6	-	0/6/23/26	0/1/1/1
6	BMA	Ι	3	6	-	2/2/19/22	0/1/1/1
6	MAN	Ι	4	6	-	0/2/19/22	0/1/1/1
4	NAG	J	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	J	2	4	-	2/6/23/26	0/1/1/1
4	FUC	J	3	4	-	-	0/1/1/1
2	NAG	K	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	K	2	2	-	0/6/23/26	0/1/1/1
7	NAG	L	1	7,1	-	0/6/23/26	0/1/1/1
7	NAG	L	2	7	-	2/6/23/26	0/1/1/1
7	BMA	L	3	7	-	2/2/19/22	0/1/1/1
7	MAN	L	4	7	-	0/2/19/22	0/1/1/1
4	NAG	М	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	М	2	4	-	2/6/23/26	0/1/1/1
4	FUC	М	3	4	-	-	0/1/1/1
3	NAG	N	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	N	2	3	-	2/6/23/26	0/1/1/1
3	BMA	Ν	3	3	-	2/2/19/22	0/1/1/1
4	NAG	0	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	0	2	4	-	2/6/23/26	0/1/1/1
4	FUC	0	3	4	-	-	0/1/1/1
8	NAG	Р	1	8,1	-	2/6/23/26	0/1/1/1
8	NAG	Р	2	8	-	0/6/23/26	0/1/1/1
8	BMA	Р	3	8	-	0/2/19/22	0/1/1/1
8	MAN	Р	4	8	-	1/2/19/22	0/1/1/1
8	MAN	Р	5	8	-	2/2/19/22	0/1/1/1
4	NAG	Q	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	Q	2	4	-	0/6/23/26	0/1/1/1
4	FUC	Q	3	4	-	-	0/1/1/1
2	NAG	R	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	R	2	2	-	1/6/23/26	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	J	3	FUC	C1-C2	3.84	1.61	1.52
6	Ι	3	BMA	C1-C2	2.60	1.58	1.52
3	Ν	3	BMA	C4-C5	2.35	1.58	1.53



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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)			
3	Ν	2	NAG	O5-C1	-2.14	1.40	1.43			
4	J	3	FUC	C2-C3	2.13	1.55	1.52			
6	Ι	4	MAN	O5-C1	-2.10	1.40	1.43			
7	L	4	MAN	C1-C2	2.03	1.56	1.52			
6	Ι	4	MAN	C4-C3	2.02	1.57	1.52			

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
4	J	3	FUC	C1-C2-C3	4.20	114.83	109.67
5	G	4	MAN	C1-O5-C5	3.72	117.23	112.19
7	L	4	MAN	C1-O5-C5	3.50	116.93	112.19
8	Р	4	MAN	C1-O5-C5	2.86	116.07	112.19
4	Q	3	FUC	C1-C2-C3	2.83	113.14	109.67
3	Ν	3	BMA	C3-C4-C5	2.25	114.25	110.24
6	Ι	4	MAN	O2-C2-C3	-2.21	105.71	110.14
6	Ι	4	MAN	C1-O5-C5	2.01	114.92	112.19

There are no chirality outliers.

All (39) torsion outliers are listed below:

Mol	Chain	$\mathbf{Res}$	Type	Atoms
3	F	3	BMA	O5-C5-C6-O6
3	N	2	NAG	O5-C5-C6-O6
2	С	1	NAG	O5-C5-C6-O6
8	Р	5	MAN	O5-C5-C6-O6
2	С	1	NAG	C4-C5-C6-O6
4	Н	2	NAG	C4-C5-C6-O6
8	Р	5	MAN	C4-C5-C6-O6
4	0	2	NAG	O5-C5-C6-O6
4	Н	2	NAG	O5-C5-C6-O6
5	G	3	BMA	O5-C5-C6-O6
3	F	3	BMA	C4-C5-C6-O6
7	L	3	BMA	C4-C5-C6-O6
3	Ν	2	NAG	C4-C5-C6-O6
4	J	2	NAG	C4-C5-C6-O6
3	F	2	NAG	O5-C5-C6-O6
8	Р	1	NAG	O5-C5-C6-O6
4	0	2	NAG	C4-C5-C6-O6
5	G	3	BMA	C4-C5-C6-O6
3	D	2	NAG	O5-C5-C6-O6
4	М	2	NAG	O5-C5-C6-O6



6C01	

Mol	Chain	Res	Tvpe	Atoms
1	T	2002	$-JP^{\circ}$	O5 C5 C6 O6
4	J	2	NAG	03-03-00-00
3	<u> </u>	2	NAG	C4-C5-C6-O6
4	М	2	NAG	C4-C5-C6-O6
3	D	2	NAG	C4-C5-C6-O6
6	Ι	3	BMA	C4-C5-C6-O6
8	Р	1	NAG	C4-C5-C6-O6
7	L	3	BMA	O5-C5-C6-O6
2	K	1	NAG	O5-C5-C6-O6
6	Ι	3	BMA	O5-C5-C6-O6
2	R	2	NAG	O5-C5-C6-O6
3	N	3	BMA	C4-C5-C6-O6
3	N	3	BMA	O5-C5-C6-O6
4	Е	2	NAG	C4-C5-C6-O6
4	Е	2	NAG	O5-C5-C6-O6
7	L	2	NAG	C4-C5-C6-O6
7	L	2	NAG	O5-C5-C6-O6
8	Р	4	MAN	C4-C5-C6-O6
6	Ι	1	NAG	C4-C5-C6-O6
2	K	1	NAG	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	Р	5	MAN	0	1

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 10 ligands modelled in this entry, 8 are monoatomic - leaving 2 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).

Mal	Trune	Chain	Dec	Timle	Bo	ond leng	$\mathbf{ths}$	В	ond ang	les
INIOI	туре	Chain	nes	LIIIK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z  > 2
11	NAG	В	929	1	14,14,15	0.79	1 (7%)	17,19,21	1.51	1 (5%)
11	NAG	А	930	1	14,14,15	0.23	0	17,19,21	0.42	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	В	929	1	-	0/6/23/26	0/1/1/1
11	NAG	А	930	1	-	2/6/23/26	0/1/1/1

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	Ideal(Å)
11	В	929	NAG	O5-C1	2.79	1.48	1.43

All (1) bond length outliers are listed below:

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
11	В	929	NAG	C1-O5-C5	5.77	120.00	112.19

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	А	930	NAG	O5-C5-C6-O6
11	А	930	NAG	C4-C5-C6-O6

There are no ring outliers.



1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	В	929	NAG	1	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	< <b>RSRZ</b> >	#RSRZ>2	$OWAB(Å^2)$	Q<0.9
1	А	819/838~(97%)	-0.04	33 (4%) 38 45	20, 36, 79, 139	0
1	В	807/838~(96%)	0.02	29 (3%) 42 49	21, 40, 88, 150	0
All	All	1626/1676~(97%)	-0.01	62 (3%) 40 47	20, 38, 83, 150	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	А	66	LEU	9.0
1	А	68	ASN	9.0
1	В	74	ALA	8.7
1	В	73	VAL	8.3
1	В	62	SER	7.7
1	В	652	GLY	7.0
1	А	67	GLU	6.4
1	В	78	ARG	6.3
1	В	121	GLN	6.1
1	А	64	ARG	5.9
1	А	63	PHE	5.4
1	А	62	SER	5.4
1	В	59	PHE	5.2
1	В	77	ASP	5.0
1	А	69	CYS	4.9
1	В	653	ASP	4.7
1	А	150	SER	4.3
1	А	121	GLN	4.2
1	А	65	GLY	4.0
1	В	392	ARG	3.6
1	A	149	GLN	3.5
1	А	61	ALA	3.4
1	В	60	ASP	3.4
1	А	60	ASP	3.4



Mol	Chain	Res	Type	RSRZ
1	А	80	ASP	3.2
1	А	73	VAL	3.2
1	В	80	ASP	3.1
1	В	86	GLU	3.0
1	А	146	THR	3.0
1	А	82	CYS	2.9
1	В	70	ARG	2.8
1	В	581	GLN	2.8
1	А	81	CYS	2.8
1	А	392	ARG	2.7
1	В	391	PRO	2.6
1	В	110	ALA	2.6
1	А	654	THR	2.6
1	А	151	GLN	2.5
1	А	79	GLY	2.5
1	А	662	PRO	2.5
1	А	53	SER	2.4
1	В	89	CYS	2.4
1	В	71	CYS	2.4
1	А	240	SER	2.4
1	В	654	THR	2.4
1	А	83	TRP	2.3
1	В	657	LEU	2.3
1	А	59	PHE	2.3
1	В	76	LYS	2.3
1	В	651	LEU	2.3
1	А	84	ASP	2.3
1	В	57	LYS	2.3
1	В	154	GLU	2.2
1	А	391	PRO	2.2
1	В	656	PRO	2.2
1	А	117	ASP	2.2
1	А	71	CYS	2.2
1	А	70	ARG	2.1
1	В	83	TRP	2.1
1	А	56	LYS	2.0
1	В	61	ALA	2.0
1	В	79	GLY	2.0

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# 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	$B-factors(Å^2)$	Q<0.9
4	NAG	E	2	14/15	0.60	0.34	87,94,111,113	0
4	NAG	Н	2	14/15	0.63	0.36	100,108,128,129	0
4	FUC	J	3	10/11	0.66	0.43	81,90,104,108	0
2	NAG	R	1	14/15	0.67	0.27	62,74,86,90	0
5	MAN	G	4	11/12	0.70	0.28	82,86,101,102	0
3	BMA	D	3	11/12	0.72	0.20	69,75,88,90	0
3	BMA	F	3	11/12	0.73	0.23	77,86,100,103	0
3	BMA	N	3	11/12	0.74	0.24	78,83,100,100	0
4	NAG	М	2	14/15	0.75	0.27	81,85,101,102	0
4	NAG	Н	1	14/15	0.75	0.20	72,88,106,106	0
2	NAG	R	2	14/15	0.76	0.38	86,92,109,111	0
4	FUC	Е	3	10/11	0.76	0.40	87,90,108,109	0
4	NAG	J	1	14/15	0.76	0.20	56,72,86,86	0
4	NAG	0	2	14/15	0.77	0.33	95,104,124,125	0
4	FUC	Н	3	10/11	0.78	0.21	91,94,113,113	0
4	FUC	М	3	10/11	0.78	0.36	78,81,97,98	0
6	BMA	Ι	3	11/12	0.79	0.15	52,63,75,76	0
7	BMA	L	3	11/12	0.79	0.19	72,80,95,96	0
4	NAG	J	2	14/15	0.80	0.28	89,97,115,116	0
7	MAN	L	4	11/12	0.80	0.46	91,97,115,116	0
4	FUC	0	3	10/11	0.81	0.20	84,87,104,105	0
2	NAG	K	2	14/15	0.82	0.30	$67,\!81,\!96,\!101$	0
5	BMA	G	3	11/12	0.82	0.23	77,82,98,98	0
6	NAG	Ι	1	14/15	0.83	0.12	43,61,76,77	0
4	NAG	0	1	14/15	0.84	0.21	63,80,93,96	0
8	MAN	Р	4	11/12	0.87	0.13	$52,\!59,\!69,\!71$	0
2	NAG	С	2	14/15	0.88	0.34	$65,\!77,\!92,\!93$	0
3	NAG	D	2	14/15	0.89	0.14	$47,\!57,\!68,\!71$	0
6	MAN	Ι	4	11/12	0.89	0.17	$56,\!65,\!76,\!79$	0
7	NAG	L	2	14/15	0.89	0.14	46,56,67,71	0
4	NAG	Q	2	14/15	0.90	0.20	73,79,95,95	0
6	NAG	Ι	2	14/15	0.90	0.17	67,73,88,90	0
4	NAG	М	1	14/15	0.90	0.18	51,68,80,82	0
2	NAG	С	1	14/15	0.90	0.13	41,52,62,65	0
3	NAG	N	2	14/15	0.91	0.15	41,55,71,72	0
4	FUC	Q	3	10/11	0.91	0.14	69,74,85,89	0
8	NAG	Р	1	14/15	0.91	0.10	38,47,55,57	0



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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
8	NAG	Р	2	14/15	0.91	0.14	48,56,69,69	0
4	NAG	Е	1	14/15	0.91	0.20	50,66,84,87	0
2	NAG	K	1	14/15	0.92	0.15	39,51,61,68	0
3	NAG	F	2	14/15	0.92	0.14	43,54,66,71	0
8	MAN	Р	5	11/12	0.92	0.14	$52,\!57,\!69,\!69$	0
5	NAG	G	2	14/15	0.93	0.10	$59,\!68,\!79,\!82$	0
8	BMA	Р	3	11/12	0.93	0.09	45,50,59,61	0
5	NAG	G	1	14/15	0.94	0.10	$36,\!47,\!54,\!57$	0
4	NAG	Q	1	14/15	0.95	0.10	$52,\!64,\!75,\!77$	0
5	FUC	G	5	10/11	0.95	0.10	$44,\!48,\!57,\!58$	0
3	NAG	D	1	14/15	0.95	0.12	28,42,52,53	0
7	NAG	L	1	14/15	0.95	0.12	$25,\!39,\!47,\!52$	0
3	NAG	N	1	14/15	0.97	0.15	18,27,32,35	0
3	NAG	F	1	14/15	0.98	0.14	22,29,36,36	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	$\mathbf{B} ext{-factors}(\mathbf{A}^2)$	Q < 0.9
11	NAG	В	929	14/15	0.73	0.36	74,85,101,102	0
11	NAG	А	930	14/15	0.76	0.38	72,85,101,102	0
12	NA	В	930	1/1	0.91	0.12	56, 56, 56, 56	0
12	NA	А	931	1/1	0.94	0.16	58, 58, 58, 58	0
9	ZN	А	902	1/1	0.99	0.16	34,34,34,34	0
9	ZN	В	902	1/1	0.99	0.15	33,33,33,33	0
9	ZN	А	901	1/1	0.99	0.16	28,28,28,28	0
10	CA	А	903	1/1	1.00	0.12	28,28,28,28	0
10	CA	В	903	1/1	1.00	0.14	27,27,27,27	0
9	ZN	В	901	1/1	1.00	0.14	29,29,29,29	0



# 6.5 Other polymers (i)

There are no such residues in this entry.

