

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

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PDB ID	:	5 MJ6
Title	:	Ligand-induced conformational change of Insulin-regulated aminopeptidase:
		insights on catalytic mechanism and active site plasticity.
Authors	:	Mpakali, A.; Stratikos, E.; Saridakis, E.; Giastas, P.
Deposited on	:	2016-11-30
Resolution	:	2.53  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	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
$\mathrm{EDS}$	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

# 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 2.53 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.



Matria	Whole archive	Similar resolution
Metric	$(\# { m Entries})$	$(\# { m Entries},  { m resolution}  { m range}({ m \AA}))$
$R_{free}$	130704	5743 (2.54-2.50)
Clashscore	141614	6463 (2.54-2.50)
Ramachandran outliers	138981	6335 (2.54-2.50)
Sidechain outliers	138945	6337 (2.54-2.50)
RSRZ outliers	127900	5630(2.54-2.50)

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	881	2% <b>87%</b>	11% •
1	В	881	3% 86%	12% •
2	С	4	75%	25%
2	R	4	50%	50%
3	D	3	100%	



Mol	Chain	Length	Qualit	Quality of chain				
3	F	3	100%					
3	Κ	3	33%	67%				
3	N	3	33%	67%				
3	Р	3	67%	33%				
4	Е	2		100%				
4	Н	2		100%				
4	J	2		100%				
4	L	2	50%	50%				
4	М	2	50%	50%				
4	0	2	50%	50%				
4	Q	2		100%				
5	G	5	20%	80%				
5	Ι	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
3	BMA	D	3	-	-	-	Х
4	NAG	J	2	-	-	-	Х
4	NAG	L	2	-	-	-	Х
4	NAG	М	2	-	-	-	Х
4	NAG	Q	2	-	-	-	Х
5	MAN	Ι	4	-	-	-	Х
5	MAN	Ι	5	-	-	-	Х
6	NAG	А	1132	-	-	-	Х
6	NAG	В	1122	-	-	-	Х
6	NAG	B	1123	_	_	_	X



# 2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 15376 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 Leucyl-cystinyl aminopeptidase.
 Mol Chain Residues Atoms ZeroOcc Alt

Mol	Chain	Residues		Α	toms			ZeroOcc	AltConf	Trace
1	А	870	Total 7131	C 4607	N 1165	0 1331	S 28	0	12	0
1	В	866	Total 7115	C 4603	N 1161	0 1324	S 27	0	13	0

Chain	Residue	Modelled	Actual	Comment	Reference
А	1026	ARG	-	expression tag	UNP Q9UIQ6
А	1027	THR	-	expression tag	UNP Q9UIQ6
А	1028	GLU	-	expression tag	UNP Q9UIQ6
A	1029	THR	-	expression tag	UNP Q9UIQ6
А	1030	SER	-	expression tag	UNP Q9UIQ6
A	1031	GLN	-	expression tag	UNP Q9UIQ6
А	1032	VAL	-	expression tag	UNP Q9UIQ6
A	1033	ALA	-	expression tag	UNP Q9UIQ6
А	1034	PRO	-	expression tag	UNP Q9UIQ6
А	1035	ALA	-	expression tag	UNP Q9UIQ6
В	1026	ARG	-	expression tag	UNP Q9UIQ6
В	1027	THR	-	expression tag	UNP Q9UIQ6
В	1028	GLU	-	expression tag	UNP Q9UIQ6
В	1029	THR	-	expression tag	UNP Q9UIQ6
В	1030	SER	-	expression tag	UNP Q9UIQ6
В	1031	GLN	-	expression tag	UNP Q9UIQ6
В	1032	VAL	-	expression tag	UNP Q9UIQ6
В	1033	ALA	-	expression tag	UNP Q9UIQ6
B	1034	PRO	-	expression tag	UNP Q9UIQ6
B	1035	ALA	-	expression tag	UNP Q9UIQ6

There are 20 discrepancies between the modelled and reference sequences:

• Molecule 2 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	I	Aton	ns		ZeroOcc	AltConf	Trace
2	С	4	Total 50	C 28	N 2	O 20	0	0	0
2	R	4	Total 50	C 28	N 2	O 20	0	0	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         C         N         O           39         22         2         15	0	0	0
3	F	3	Total         C         N         O           39         22         2         15	0	0	0
3	K	3	Total         C         N         O           39         22         2         15	0	0	0
3	N	3	Total         C         N         O           39         22         2         15	0	0	0
3	Р	3	Total         C         N         O           39         22         2         15	0	0	0

• Molecule 4 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
4	Е	2	Total C 28 16	N O 2 10	0	0	0
4	Н	2	Total         C           28         16	N O 2 10	0	0	0
4	J	2	Total         C           28         16	N O 2 10	0	0	0



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
4	L	2	Total         C         N         O           28         16         2         10	0	0	0
4	М	2	Total         C         N         O           28         16         2         10	0	0	0
4	О	2	Total         C         N         O           28         16         2         10	0	0	0
4	Q	2	Total         C         N         O           28         16         2         10	0	0	0

• Molecule 5 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		
5	G	5	Total 61	С 34	N 2	O 25	0	0	0
5	Ι	5	Total 61	С 34	N 2	O 25	0	0	0

• Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).





Mol	Chain	Residues	A	ton	ns		ZeroOcc	AltConf
6	Δ	1	Total	С	Ν	0	0	0
0	A	L	14	8	1	5	0	0
6	Δ	1	Total	С	Ν	Ο	0	0
0	A	L	14	8	1	5	0	0
6	Λ	1	Total	С	Ν	0	0	0
0	A	L	14	8	1	5	0	0
6	Λ	1	Total	С	Ν	Ο	0	0
0	Л	T	14	8	1	5	0	0
6	В	1	Total	С	Ν	Ο	0	0
0	D	T	14	8	1	5	0	0
6	В	1	Total	С	Ν	Ο	0	0
0	D	T	14	8	1	5	0	0
6	В	1	Total	С	Ν	Ο	0	0
0	D	T	14	8	1	5	0	0
6	В	1	Total	С	Ν	Ο	0	0
0	D	T	14	8	1	5	0	0
6	В	1	Total	С	Ν	Ο	0	0
0	D	T	14	8	1	5	0	0
6	В	1	Total	С	Ν	Ο	0	0
0	D	T	14	8	1	5	0	0
6	B	1	Total	С	Ν	0	0	0
0		1	14	8	1	5		0
6	B	1	Total	С	Ν	0	0	0
0	D	L	14	8	1	5		0

• Molecule 7 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	А	1	Total Zn 1 1	0	0
7	В	1	Total Zn 1 1	0	0

• Molecule 8 is [(2 {S})-2-[[(2 {S})-1-azanyl-1-oxidanylidene-3-phenyl-propan-2-yl]carbamoyl ]-4,4-diphenyl-butyl]-[(1 {R})-1-azanyl-3-phenyl-propyl]phosphinic acid (three-letter code: 7O2) (formula:  $C_{35}H_{40}N_3O_4P$ ).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf			
0	Δ	1	Total	С	Ν	0	Р	0	0	
0		T	43	35	3	4	1	0	0	
0	Р	1	Total	С	Ν	0	Р	0	0	
8	D	D		43	35	3	4	1	U	0

• Molecule 9 is BROMIDE ION (three-letter code: BR) (formula: Br).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	А	15	Total Br 15 15	0	0
9	В	6	Total Br 6 6	0	0

• Molecule 10 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	А	152	Total O 152 152	0	0
10	В	88	Total         O           88         88	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: Leucyl-cystinyl aminopeptidase







 $\bullet \ Molecule \ 2: \ alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose$ 

$O_{1} \rightarrow O_{2}$		
Unam C:	75%	25%
onam o.	7370	23/0

#### NAG1 NAG2 BMA3 MAN4

 $\bullet \ Molecule \ 2: \ alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose \\ eta-D-glucopyranose \ (1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose \ (1-4)-2-acetamido-2-deoxy-beta-D-glucopyra$ 

Chain R:	50%	50%
IAG1 IAG2 IAN4 IAN4		

• 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 K:	33%	67%

#### 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%





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

33%

67%

Chain P:

#### NAG1 NAG2 BMA3

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

Chain E:	100%	
NAG1 NAG2		
• Molecule 4: opyranose	2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamid	.o-2-deoxy-beta-D-gluc

Chain H:	100%	
NAG1 NAG2		
• Molecule 4: opyranose	eq:2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-a	luc
Chain J:	100%	
NAG1 NAG2		

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

50%

Chain L:

#### NAG1 NAG2

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

Chain M:	50%	50%

50%

#### NAG1 NAG2

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

Chain O:	50%	50%



#### NAG1 NAG2

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

100%

Chain Q:

#### NAG1 NAG2

 • Molecule 5: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)] beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:	20%	80%	
NAG1 NAG2 BMA3 MAN4 MAN4 MAN5			

 • Molecule 5: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)] beta-D-mannopyrano<br/> se-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I: 60% 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	112.24Å 143.17Å 148.99Å	Deperitor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $90.00^{\circ}$	Depositor
$\mathbf{P}_{\text{assolution}}(\hat{\mathbf{A}})$	40.80 - 2.53	Depositor
Resolution (A)	40.80 - 2.53	EDS
% Data completeness	100.0 (40.80-2.53)	Depositor
(in resolution range)	$100.0 \ (40.80-2.53)$	EDS
R <sub>merge</sub>	0.20	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.73 (at 2.54 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.8.4_1496	Depositor
D D	0.174 , $0.229$	Depositor
$\Lambda, \Lambda_{free}$	0.176 , $0.230$	DCC
$R_{free}$ test set	3983 reflections $(4.94%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	52.1	Xtriage
Anisotropy	0.097	Xtriage
Bulk solvent $k_{sol}(e/A^3), B_{sol}(A^2)$	0.32 , $43.9$	EDS
L-test for twinning <sup>2</sup>	$< L >=0.48, < L^2>=0.31$	Xtriage
Estimated twinning fraction	0.018 for -h,l,k	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	15376	wwPDB-VP
Average B, all atoms $(Å^2)$	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.78% 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: MAN, BMA, BR, NAG, ZN, 702

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	Chain	Bo	nd lengths	Bo	ond angles
1VIOI	Chain	RMSZ	# Z  > 5	RMSZ	# Z  > 5
1	А	0.50	0/7339	0.62	3/9945~(0.0%)
1	В	0.47	2/7328~(0.0%)	0.60	2/9934~(0.0%)
All	All	0.49	2/14667~(0.0%)	0.61	5/19879~(0.0%)

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	А	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\mathrm{Ideal}(\mathrm{\AA})$
1	В	282	GLU	CD-OE1	5.61	1.31	1.25
1	В	282	GLU	CD-OE2	5.05	1.31	1.25

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	А	433	TRP	CA-CB-CG	7.80	128.53	113.70
1	В	477	MET	CA-CB-CG	-5.43	104.08	113.30
1	В	958	LEU	CA-CB-CG	5.38	127.69	115.30
1	А	209	LEU	CB-CG-CD1	-5.17	102.22	111.00
1	А	804	GLN	N-CA-C	5.15	124.90	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:



Mol	Chain	Res	Type	Group
1	А	598	ASN	Sidechain

### 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	7131	0	7052	72	0
1	В	7115	0	7039	74	0
2	С	50	0	43	1	0
2	R	50	0	43	0	0
3	D	39	0	34	0	0
3	F	39	0	34	1	0
3	K	39	0	34	0	0
3	N	39	0	34	0	0
3	Р	39	0	34	0	0
4	Е	28	0	25	0	0
4	Н	28	0	25	0	0
4	J	28	0	25	0	0
4	L	28	0	25	3	0
4	М	28	0	25	1	0
4	0	28	0	25	0	0
4	Q	28	0	25	0	0
5	G	61	0	52	0	0
5	Ι	61	0	52	2	0
6	А	56	0	52	1	0
6	В	112	0	104	1	0
7	А	1	0	0	0	0
7	В	1	0	0	0	0
8	A	43	0	0	1	0
8	В	43	0	0	0	0
9	A	15	0	0	2	0
9	В	6	0	0	0	0
10	A	152	0	0	4	0
10	В	88	0	0	3	0
All	All	15376	0	14782	149	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 5.

All (149) 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:B:472:GLY:HA2	1:B:486:ASN:HD22	1.29	0.98
1:B:219:VAL:HG21	1:B:234:ILE:HG13	1.63	0.80
1:A:230:LYS:N	1:A:230:LYS:HD3	1.99	0.77
1:B:701:ILE:HG23	1:B:734:ASN:HD22	1.51	0.75
1:B:234:ILE:HD11	1:B:245:ILE:HD13	1.69	0.75
1:B:621:VAL:HG22	1:B:630:ILE:HG22	1.67	0.74
1:A:659:VAL:HG23	1:A:669:GLN:HB3	1.76	0.68
9:A:1152:BR:BR	10:A:1349:HOH:O	2.66	0.67
1:A:281:ASP:HB3	1:A:283:SER:H	1.58	0.67
1:A:226:SER:HG	1:A:228:GLN:HE21	1.40	0.67
1:B:575:TYR:OH	1:B:584:ILE:HD13	1.95	0.66
1:A:638:ASN:OD1	1:A:639:MET:N	2.27	0.65
1:B:521:LYS:NZ	1:B:964:GLN:OE1	2.28	0.65
1:B:472:GLY:HA2	1:B:486:ASN:ND2	2.08	0.65
1:A:857:THR:HG22	1:A:860:MET:HE2	1.78	0.65
1:B:621:VAL:HG21	1:B:692:VAL:HG21	1.80	0.64
1:A:228:GLN:HG3	1:A:230:LYS:HE2	1.81	0.63
1:A:597:THR:HG21	1:A:601:LEU:O	1.98	0.63
1:A:191[A]:ARG:NH2	10:A:1202:HOH:O	2.31	0.63
1:B:955:LYS:NZ	10:B:1203:HOH:O	2.32	0.62
1:B:637:LEU:HB2	1:B:741:LEU:HD22	1.82	0.62
1:A:515:ARG:HD3	1:A:554:SER:HB3	1.84	0.60
1:B:992:GLU:HG3	1:B:996:ARG:HG2	1.84	0.59
1:B:339:LEU:HD11	1:B:345:GLN:HB2	1.85	0.59
1:A:796:PHE:HB2	1:A:832:LEU:HD13	1.84	0.58
1:B:709[B]:TRP:CH2	1:B:713:ILE:HD12	2.38	0.58
1:B:369:LEU:HD23	1:B:394:LEU:HD22	1.85	0.58
1:B:219:VAL:HG21	1:B:234:ILE:CG1	2.34	0.57
1:A:800:GLN:HG3	1:A:804:GLN:OE1	2.05	0.57
1:A:478:LYS:HG2	1:A:583:SER:HB3	1.87	0.57
1:A:847:MET:HE2	1:A:872:LYS:HE2	1.87	0.56
1:A:159:LYS:O	1:A:159:LYS:HG2	2.06	0.56
1:A:321:ARG:NH1	1:A:346:ASP:OD2	2.38	0.56
1:B:485:LEU:HD13	1:B:584:ILE:HD12	1.88	0.55
1:A:223:SER:HB2	1:A:226:SER:HB3	1.87	0.55
1:A:794:ARG:NE	1:A:1028:GLU:OE1	2.37	0.55
1:A:870:THR:HG21	10:A:1345:HOH:O	2.07	0.55
1:B:492:PHE:HZ	1:B:560:LYS:HD3	1.72	0.55
1:B:934:HIS:HE1	10:B:1246:HOH:O	1.90	0.54
1:A:282:GLU:HG3	1:A:385:GLU:OE1	2.08	0.53
1:B:209:LEU:HD21	1:B:306:PHE:CE1	2.44	0.53



		Interatomic	Clash		
Atom-1	Atom-2	distance (Å)	overlap (Å)		
1:B:665:TYR:HD1	1:B:665:TYR:N	2.07	0.52		
1:A:891:ASN:OD1	1:A:923:LYS:NZ	2.39	0.52		
1:A:226:SER:OG	1:A:228:GLN:NE2	2.30	0.52		
1:A:492:PHE:HZ	1:A:560:LYS:HD3	1.75	0.51		
1:A:496:PHE:HE1	1:A:560:LYS:HE3	1.75	0.51		
1:A:561:THR:HG22	9:A:1138:BR:BR	2.65	0.51		
1:A:870:THR:HG22	1:A:872:LYS:H	1.75	0.51		
1:B:501:ILE:HG13	1:B:502:PHE:CD1	2.46	0.51		
1:B:740:GLY:O	1:B:741:LEU:HD23	2.11	0.51		
1:B:205:TRP:CE2	1:B:250:ALA:HB2	2.45	0.50		
1:A:741:LEU:HD22	1:A:743:LYS:HG2	1.93	0.50		
1:B:895:GLU:HB2	1:B:926:PHE:HZ	1.76	0.50		
1:B:294:PHE:HA	1:B:298:ALA:HB3	1.93	0.50		
1:B:934:HIS:CE1	10:B:1246:HOH:O	2.65	0.50		
1:B:777:ASN:O	1:B:781:LYS:HG2	2.12	0.49		
1:A:228:GLN:HB2	1:A:230:LYS:NZ	2.27	0.49		
1:A:785:MET:HB3	1:B:904[B]:ARG:HH22	1.77	0.49		
1:B:1014:MET:HE3	1:B:1018:LEU:HD13	1.94	0.49		
1:A:476:THR:O	1:A:583:SER:HA	2.12	0.49		
1:A:482:ASP:HB3	1:A:485:LEU:HD12	1.95	0.49		
1:A:750:PHE:HD1	1:A:753:ILE:HD11	1.78	0.49		
1:B:865:LYS:HE3	1:B:895:GLU:HG2	1.95	0.49		
1:B:381:TYR:HB2	1:B:420:VAL:HG22	1.94	0.49		
1:A:374:ASN:HD22	5:I:1:NAG:H83	1.78	0.48		
1:B:441:GLU:CD	1:B:891:ASN:HD21	2.17	0.48		
1:B:665:TYR:N	1:B:665:TYR:CD1	2.80	0.48		
1:B:685:GLU:HB3	6:B:1117:NAG:H62	1.95	0.48		
1:B:181:LEU:HB2	1:B:319:ILE:HD13	1.95	0.48		
1:A:817:ARG:HB3	1:A:858:ASP:OD2	2.14	0.48		
1:A:228:GLN:HG3	1:A:230:LYS:CE	2.44	0.47		
1:A:639:MET:HG2	1:A:1012:GLN:HE22	1.79	0.47		
1:A:415:LYS:H	1:A:415:LYS:HG3	1.53	0.47		
1:A:433:TRP:CE2	1:A:473:ASN:HB3	2.50	0.47		
1:A:281:ASP:HB3	1:A:283:SER:N	2.27	0.47		
1:A:804:GLN:HE21	4:L:2:NAG:H62	1.80	0.47		
1:B:343:LEU:HD22	4:M:1:NAG:H83	1.97	0.46		
1:B:477:MET:HG3	1:B:477:MET:O	2.15	0.46		
1:B:871:ASP:OD1	1:B:905:LYS:NZ	2.41	0.46		
1:A:496:PHE:CE1	1:A:560:LYS:HE3	2.50	0.46		
1:B:205:TRP:CZ2	1:B:250:ALA:HB2	2.50	0.46		
1:B:796:PHE:HB2	1:B:832:LEU:HD13	1.96	0.46		



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		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:B:495:TYR:CD1	1:B:511:PHE:HB2	2.51	0.46	
1:A:747:LYS:HE3	1:A:747:LYS:HB3	1.79	0.46	
1:B:391:HIS:O	1:B:395:GLU:HG3	2.16	0.46	
1:B:209:LEU:HD23	1:B:209:LEU:HA	1.71	0.46	
4:L:2:NAG:H3	4:L:2:NAG:C8	2.45	0.46	
1:A:658:TYR:CZ	1:A:670:SER:HB3	2.50	0.45	
1:B:747:LYS:HB2	1:B:747:LYS:HE3	1.74	0.45	
1:A:631:GLN:HG2	1:A:678:SER:HB3	1.98	0.45	
1:A:789:SER:OG	1:A:1031:GLN:HB2	2.17	0.45	
8:A:1137:7O2:C30	8:A:1137:7O2:C24	2.93	0.45	
1:A:446:ASP:OD1	6:A:1132:NAG:H82	2.17	0.45	
1:B:975:SER:OG	1:B:1010:ASN:HB3	2.17	0.45	
1:A:657:SER:HB2	1:A:694:ILE:HD12	1.99	0.45	
1:B:760:ASN:N	1:B:760:ASN:OD1	2.50	0.45	
1:B:857:THR:HG22	1:B:860:MET:HE1	1.99	0.45	
1:A:562:TYR:CZ	1:A:673:LEU:HD12	2.52	0.44	
1:A:322:ASP:OD1	2:C:2:NAG:H61	2.18	0.44	
1:A:874:TRP:CE2	1:A:905:LYS:HD3	2.53	0.44	
1:B:504:GLU:H	1:B:504:GLU:CD	2.21	0.44	
1:B:990:GLN:O	1:B:991:SER:HB3	2.18	0.44	
1:B:384:PRO:O	1:B:387:ILE:HG22	2.18	0.44	
1:B:564:SER:HB3	1:B:567:VAL:HG23	2.00	0.44	
1:B:599:GLN:C	1:B:601:LEU:H	2.20	0.44	
1:A:628:LEU:HD11	1:A:690:VAL:HG21	2.00	0.44	
1:B:599:GLN:C	1:B:601:LEU:N	2.72	0.44	
1:A:874:TRP:CD2	1:A:905:LYS:HD3	2.52	0.44	
1:B:1014:MET:HE3	1:B:1018:LEU:HD22	2.00	0.44	
1:A:412:TYR:CE2	1:A:414:LEU:HB2	2.53	0.43	
1:B:621:VAL:HG13	1:B:628:LEU:HD11	1.99	0.43	
1:B:530:ILE:HG22	1:B:611:THR:HA	2.00	0.43	
1:B:596:VAL:HG12	1:B:596:VAL:O	2.19	0.43	
1:A:777:ASN:O	1:A:781:LYS:HG2	2.18	0.43	
1:B:415:LYS:HA	1:B:415:LYS:HD3	1.77	0.43	
1:B:476:THR:O	1:B:583:SER:HA	2.17	0.43	
1:A:422:ILE:HA	1:A:423:PRO:HD3	1.86	0.43	
1:B:180:SER:HA	1:B:318:LYS:HB2	2.01	0.43	
1:B:362:ILE:HD12	1:B:435:LEU:HD21	2.00	0.43	
4:L:2:NAG:C8	4:L:2:NAG:C3	2.97	0.43	
1:A:506:SER:O	1:A:509:GLU:HG3	2.19	0.43	
1:A:601:LEU:HD12	10:A:1203:HOH:O	2.18	0.43	
1:A:958:LEU:HA	1:A:959:GLY:HA2	1.86	0.43	



Atom 1	Atom 2	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:B:1019:LYS:HD3	1:B:1019:LYS:HA	1.63	0.43	
1:A:332:PRO:HG2	1:A:415:LYS:HD2	2.00	0.43	
1:A:494:GLU:O	1:A:498:LEU:HG	2.19	0.43	
1:B:228:GLN:HG2	1:B:229:GLU:N	2.34	0.43	
1:B:739:ALA:HB1	1:B:746:LEU:HA	2.00	0.42	
1:A:750:PHE:CD1	1:A:753:ILE:HD11	2.55	0.42	
1:B:339:LEU:HD11	1:B:345:GLN:CB	2.48	0.42	
1:B:559:LEU:HD12	1:B:559:LEU:HA	1.86	0.42	
1:A:237:TYR:CE1	1:A:239:TYR:HB3	2.54	0.42	
1:B:373:VAL:HG21	1:B:401:LEU:HD23	2.02	0.42	
1:A:480:TRP:HB2	1:A:534:VAL:HG21	2.02	0.41	
1:A:719:ASN:OD1	3:F:2:NAG:H81	2.20	0.41	
1:A:800:GLN:O	1:A:804:GLN:HB2	2.20	0.41	
1:B:599:GLN:O	1:B:601:LEU:N	2.53	0.41	
1:A:636:PHE:HE2	1:A:638:ASN:HB2	1.85	0.41	
1:A:870:THR:HG22	1:A:872:LYS:N	2.34	0.41	
1:B:730:ASN:O	1:B:734:ASN:OD1	2.38	0.41	
1:B:590:TRP:CZ3	1:B:607:MET:HG3	2.55	0.41	
1:B:207:ILE:HB	1:B:245:ILE:HB	2.03	0.41	
1:A:720:PRO:HG2	1:A:721:TYR:CE2	2.55	0.41	
1:A:471:PHE:CE1	1:A:489:PHE:CD2	3.09	0.40	
1:B:660:THR:HG22	1:B:690:VAL:HG22	2.03	0.40	
1:A:272:TYR:OH	1:A:296:PRO:HD2	2.21	0.40	
1:A:605:ARG:HD3	1:A:605:ARG:HA	1.84	0.40	
1:B:297:LEU:HD21	1:B:540:ILE:HD13	2.02	0.40	
1:A:577:HIS:HD2	5:I:4:MAN:H4	1.86	0.40	

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	Percei	ntiles
1	А	878/881~(100%)	839~(96%)	37 (4%)	2(0%)	47	67
1	В	875/881 (99%)	849~(97%)	24 (3%)	2(0%)	47	67
All	All	1753/1762~(100%)	1688 (96%)	61 (4%)	4 (0%)	47	67

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	В	991	SER
1	А	917	ASP
1	В	747	LYS
1	А	563	LEU

### 5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain 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	А	790/788~(100%)	787 (100%)	3~(0%)	91	97	
1	В	788/788~(100%)	782~(99%)	6 (1%)	81	92	
All	All	1578/1576~(100%)	1569 (99%)	9(1%)	88	94	

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

Mol	Chain	$\operatorname{Res}$	Type
1	А	284	ASN
1	А	598	ASN
1	А	964	GLN
1	В	234	ILE
1	В	272[A]	TYR
1	В	272[B]	TYR
1	В	535[A]	GLN
1	В	535[B]	GLN
1	В	782	LEU

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such side chains are listed below:



Mol	Chain	Res	Type
1	А	228	GLN
1	А	486	ASN
1	А	1012	GLN
1	В	730	ASN
1	В	734	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)

47 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	Mol Type Chain Res		Dog	Link	Bo	Bond lengths			Bond angles		
WIOI	туре	Ullalli	nes		Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2	
2	NAG	С	1	2,1	14,14,15	0.71	1 (7%)	17,19,21	0.83	1 (5%)	
2	NAG	С	2	2	14,14,15	1.17	1 (7%)	17,19,21	1.28	2 (11%)	
2	BMA	С	3	2	11,11,12	0.79	0	15,15,17	1.99	4 (26%)	
2	MAN	С	4	2	11,11,12	1.58	4 (36%)	15,15,17	1.25	2 (13%)	
3	NAG	D	1	1,3	14,14,15	0.81	1 (7%)	17,19,21	0.59	0	
3	NAG	D	2	3	14,14,15	0.62	0	17,19,21	1.02	1 (5%)	
3	BMA	D	3	3	11,11,12	2.58	3 (27%)	15,15,17	2.79	6 (40%)	
4	NAG	Е	1	4,1	14,14,15	0.38	0	17,19,21	1.59	3 (17%)	
4	NAG	Е	2	4	14,14,15	1.05	1 (7%)	17,19,21	0.85	1 (5%)	
3	NAG	F	1	1,3	14,14,15	0.24	0	17,19,21	0.76	1 (5%)	
3	NAG	F	2	3	14,14,15	0.51	0	17,19,21	0.55	0	
3	BMA	F	3	3	11,11,12	1.17	1 (9%)	15,15,17	0.91	0	



Mal	<b>T</b>	Chain	Dag	T : 1-	Bond lengths		Bond angles			
IVIOI	Type	Chain	Res	LINK	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z >2
5	NAG	G	1	1,5	14,14,15	0.52	0	17,19,21	0.57	0
5	NAG	G	2	5	14,14,15	0.80	1 (7%)	$17,\!19,\!21$	0.45	0
5	BMA	G	3	5	11,11,12	0.79	0	$15,\!15,\!17$	1.28	2 (13%)
5	MAN	G	4	5	11,11,12	1.24	2 (18%)	$15,\!15,\!17$	1.38	3 (20%)
5	MAN	G	5	5	11,11,12	1.52	4 (36%)	$15,\!15,\!17$	1.46	3 (20%)
4	NAG	Н	1	4,1	14,14,15	0.42	0	17,19,21	0.51	0
4	NAG	Н	2	4	14,14,15	0.40	0	17,19,21	0.39	0
5	NAG	Ι	1	1,5	14,14,15	0.34	0	17,19,21	1.36	2 (11%)
5	NAG	Ι	2	5	14,14,15	0.71	1 (7%)	17,19,21	0.68	0
5	BMA	Ι	3	5	11,11,12	1.68	4 (36%)	$15,\!15,\!17$	2.82	4 (26%)
5	MAN	Ι	4	5	11,11,12	2.26	4 (36%)	$15,\!15,\!17$	2.13	3 (20%)
5	MAN	Ι	5	5	11,11,12	2.88	6 (54%)	$15,\!15,\!17$	2.20	6 (40%)
4	NAG	J	1	4,1	14,14,15	0.82	1 (7%)	17,19,21	0.94	1 (5%)
4	NAG	J	2	4	14,14,15	0.98	1 (7%)	17,19,21	1.14	2 (11%)
3	NAG	K	1	1,3	14,14,15	0.95	1 (7%)	17,19,21	1.00	1 (5%)
3	NAG	K	2	3	14,14,15	0.56	0	17,19,21	0.53	0
3	BMA	K	3	3	11,11,12	1.20	1 (9%)	$15,\!15,\!17$	1.18	1 (6%)
4	NAG	L	1	4,1	14,14,15	0.48	0	17,19,21	0.78	1 (5%)
4	NAG	L	2	4	14,14,15	1.09	1 (7%)	17,19,21	2.12	4 (23%)
4	NAG	М	1	4,1	14,14,15	0.27	0	17,19,21	0.66	0
4	NAG	М	2	4	14,14,15	0.40	0	17,19,21	0.56	0
3	NAG	Ν	1	1,3	14,14,15	0.26	0	$17,\!19,\!21$	0.77	1 (5%)
3	NAG	N	2	3	14,14,15	0.29	0	17,19,21	0.51	0
3	BMA	Ν	3	3	11,11,12	1.33	1 (9%)	$15,\!15,\!17$	1.00	0
4	NAG	Ο	1	4,1	14,14,15	0.64	1 (7%)	$17,\!19,\!21$	0.58	0
4	NAG	0	2	4	14,14,15	0.45	0	17,19,21	0.58	0
3	NAG	Р	1	1,3	14,14,15	0.51	0	17,19,21	0.59	0
3	NAG	Р	2	3	14,14,15	0.79	0	17,19,21	0.88	0
3	BMA	Р	3	3	11,11,12	2.03	5 (45%)	$15,\!15,\!17$	2.10	3 (20%)
4	NAG	Q	1	4,1	14,14,15	0.24	0	$17,\!19,\!21$	0.62	0
4	NAG	Q	2	4	14,14,15	0.34	0	17,19,21	0.43	0
2	NAG	R	1	2,1	14,14,15	0.60	0	17,19,21	0.60	0
2	NAG	R	2	2	14,14,15	0.50	0	17,19,21	0.72	0
2	BMA	R	3	2	11,11,12	1.01	1 (9%)	15,15,17	2.74	6 (40%)
2	MAN	R	4	2	11,11,12	2.27	3 (27%)	$15,\!15,\!17$	2.32	8 (53%)

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



Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	С	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	С	2	2	-	2/6/23/26	0/1/1/1
2	BMA	С	3	2	-	0/2/19/22	0/1/1/1
2	MAN	С	4	2	-	1/2/19/22	0/1/1/1
3	NAG	D	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	D	2	3	-	2/6/23/26	0/1/1/1
3	BMA	D	3	3	-	2/2/19/22	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
3	NAG	F	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	F	2	3	-	2/6/23/26	0/1/1/1
3	BMA	F	3	3	-	0/2/19/22	0/1/1/1
5	NAG	G	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	G	2	5	-	0/6/23/26	0/1/1/1
5	BMA	G	3	5	-	0/2/19/22	0/1/1/1
5	MAN	G	4	5	-	1/2/19/22	0/1/1/1
5	MAN	G	5	5	-	2/2/19/22	0/1/1/1
4	NAG	Н	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	Н	2	4	-	0/6/23/26	0/1/1/1
5	NAG	Ι	1	1,5	-	4/6/23/26	0/1/1/1
5	NAG	Ι	2	5	-	2/6/23/26	0/1/1/1
5	BMA	Ι	3	5	-	2/2/19/22	0/1/1/1
5	MAN	Ι	4	5	-	2/2/19/22	0/1/1/1
5	MAN	Ι	5	5	-	1/2/19/22	0/1/1/1
4	NAG	J	1	4,1	-	1/6/23/26	0/1/1/1
4	NAG	J	2	4	-	2/6/23/26	0/1/1/1
3	NAG	K	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	K	2	3	-	2/6/23/26	0/1/1/1
3	BMA	K	3	3	-	2/2/19/22	0/1/1/1
4	NAG	L	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	L	2	4	-	3/6/23/26	0/1/1/1
4	NAG	М	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	М	2	4	-	1/6/23/26	0/1/1/1
3	NAG	N	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	N	2	3	-	2/6/23/26	0/1/1/1
3	BMA	N	3	3	-	0/2/19/22	0/1/1/1

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.



5MJ6
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1	Mal	Tuno	Chain	Doc	Tink	Chirola	Torgiong	Dinge
	IVIOI	Type	Chain	nes	LIIIK	Unirais	TOPSIONS	nings
	4	NAG	Ο	1	4,1	-	2/6/23/26	0/1/1/1
	4	NAG	0	2	4	-	4/6/23/26	0/1/1/1
	3	NAG	Р	1	1,3	-	2/6/23/26	0/1/1/1
	3	NAG	Р	2	3	-	2/6/23/26	0/1/1/1
	3	BMA	Р	3	3	-	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	-	1/6/23/26	0/1/1/1
	2	NAG	R	1	2,1	-	2/6/23/26	0/1/1/1
	2	NAG	R	2	2	-	2/6/23/26	0/1/1/1
	2	BMA	R	3	2	-	2/2/19/22	0/1/1/1
	2	MAN	R	4	2	-	0/2/19/22	1/1/1/1

All (50) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	Ι	5	MAN	C1-C2	5.85	1.65	1.52
2	R	4	MAN	C4-C3	5.39	1.66	1.52
5	Ι	4	MAN	C4-C3	5.35	1.65	1.52
3	D	3	BMA	O5-C1	-5.05	1.35	1.43
3	D	3	BMA	C4-C5	4.93	1.63	1.53
2	С	2	NAG	O5-C1	-4.31	1.36	1.43
5	Ι	5	MAN	O5-C5	-4.20	1.35	1.43
3	D	3	BMA	C4-C3	4.19	1.63	1.52
2	R	4	MAN	O5-C1	-3.82	1.37	1.43
4	L	2	NAG	O5-C1	3.77	1.49	1.43
5	Ι	4	MAN	C4-C5	3.70	1.60	1.53
3	Р	3	BMA	C1-C2	3.69	1.60	1.52
4	Е	2	NAG	O5-C1	-3.60	1.38	1.43
3	Р	3	BMA	C2-C3	3.48	1.57	1.52
4	J	2	NAG	O5-C1	-3.45	1.38	1.43
5	Ι	5	MAN	O5-C1	-3.28	1.38	1.43
5	Ι	3	BMA	C6-C5	-3.19	1.41	1.51
5	Ι	5	MAN	C2-C3	3.12	1.57	1.52
3	D	1	NAG	O5-C1	-2.95	1.39	1.43
4	J	1	NAG	O5-C1	-2.86	1.39	1.43
3	Κ	1	NAG	O5-C1	-2.75	1.39	1.43
5	G	2	NAG	O5-C1	-2.69	1.39	1.43
5	Ι	5	MAN	O3-C3	2.66	1.49	1.43
5	G	5	MAN	C1-C2	2.59	1.58	1.52
5	G	4	MAN	O5-C5	2.51	1.48	1.43



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	Р	3	BMA	O2-C2	-2.51	1.38	1.43
2	R	3	BMA	O3-C3	-2.45	1.37	1.43
3	Ν	3	BMA	C1-C2	2.39	1.57	1.52
5	G	5	MAN	O5-C1	-2.37	1.39	1.43
5	Ι	3	BMA	C4-C3	-2.35	1.46	1.52
2	С	1	NAG	O5-C1	-2.35	1.40	1.43
2	С	4	MAN	C4-C3	2.35	1.58	1.52
2	С	4	MAN	O5-C1	-2.35	1.40	1.43
2	С	4	MAN	C4-C5	2.33	1.57	1.53
5	Ι	3	BMA	C2-C3	-2.32	1.49	1.52
3	Р	3	BMA	O5-C1	-2.28	1.40	1.43
5	Ι	5	MAN	O2-C2	2.25	1.48	1.43
5	Ι	2	NAG	O5-C1	-2.24	1.40	1.43
5	G	4	MAN	O5-C1	-2.21	1.40	1.43
5	Ι	3	BMA	O5-C5	2.19	1.47	1.43
5	Ι	4	MAN	C1-C2	-2.18	1.47	1.52
3	F	3	BMA	C4-C5	2.12	1.57	1.53
5	G	5	MAN	C4-C5	2.11	1.57	1.53
4	0	1	NAG	O5-C1	-2.10	1.40	1.43
3	Κ	3	BMA	C4-C3	2.10	1.57	1.52
5	Ι	4	MAN	O5-C1	-2.07	1.40	1.43
3	Р	3	BMA	O5-C5	2.05	1.47	1.43
2	С	4	MAN	C2-C3	2.05	1.55	1.52
5	G	5	MAN	O5-C5	2.01	1.47	1.43
2	R	4	MAN	C1-C2	2.00	1.56	1.52

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
5	Ι	3	BMA	C1-C2-C3	-8.49	99.24	109.67
3	D	3	BMA	C1-C2-C3	-8.04	99.78	109.67
4	L	2	NAG	C2-N2-C7	7.24	133.22	122.90
2	R	3	BMA	O3-C3-C2	-6.31	97.92	109.99
3	Р	3	BMA	C1-O5-C5	-5.15	105.22	112.19
5	Ι	4	MAN	C1-C2-C3	-4.97	103.56	109.67
5	Ι	3	BMA	O3-C3-C2	4.85	119.28	109.99
2	С	3	BMA	C1-C2-C3	-4.71	103.88	109.67
5	Ι	4	MAN	C1-O5-C5	-4.71	105.82	112.19
2	R	3	BMA	C1-C2-C3	4.60	115.32	109.67
2	R	4	MAN	C1-O5-C5	4.58	118.39	112.19
5	Ι	5	MAN	C2-C3-C4	4.44	118.57	110.89
2	R	3	BMA	O2-C2-C3	-4.34	101.44	110.14



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
3	Р	3	BMA	O5-C5-C6	4.29	113.92	107.20
2	R	3	BMA	O3-C3-C4	-4.11	100.85	110.35
3	D	3	BMA	C1-O5-C5	-4.09	106.64	112.19
4	Е	1	NAG	C1-O5-C5	4.02	117.63	112.19
5	Ι	5	MAN	O5-C5-C4	-3.95	101.21	110.83
2	С	3	BMA	O3-C3-C2	3.95	117.56	109.99
5	Ι	1	NAG	C1-O5-C5	3.86	117.42	112.19
5	Ι	4	MAN	O5-C5-C6	-3.55	101.64	107.20
2	R	4	MAN	O5-C5-C6	-3.49	101.74	107.20
5	Ι	5	MAN	O5-C1-C2	3.36	115.96	110.77
2	R	4	MAN	C3-C4-C5	-3.26	104.42	110.24
4	Е	1	NAG	O4-C4-C5	3.24	117.34	109.30
5	Ι	5	MAN	C6-C5-C4	3.10	120.28	113.00
5	G	4	MAN	C1-O5-C5	3.10	116.39	112.19
4	Е	1	NAG	O4-C4-C3	-3.05	103.30	110.35
2	С	2	NAG	C1-O5-C5	3.01	116.27	112.19
3	D	3	BMA	C3-C4-C5	2.97	115.54	110.24
5	G	3	BMA	O2-C2-C3	-2.92	104.29	110.14
2	С	4	MAN	C1-O5-C5	-2.91	108.25	112.19
4	J	2	NAG	C3-C4-C5	2.82	115.28	110.24
5	Ι	5	MAN	O3-C3-C2	-2.77	104.69	109.99
5	Ι	3	BMA	O5-C1-C2	2.76	115.03	110.77
2	R	4	MAN	O3-C3-C2	2.76	115.27	109.99
5	G	3	BMA	C1-O5-C5	2.73	115.90	112.19
2	R	3	BMA	O5-C1-C2	2.69	114.93	110.77
2	R	4	MAN	C6-C5-C4	2.65	119.20	113.00
4	Ε	2	NAG	C3-C4-C5	2.65	114.96	110.24
4	J	2	NAG	C1-O5-C5	-2.62	108.64	112.19
3	F	1	NAG	C1-O5-C5	2.61	115.73	112.19
2	С	3	BMA	O3-C3-C4	2.59	116.34	110.35
4	J	1	NAG	O4-C4-C3	-2.57	104.41	110.35
2	R	4	MAN	O2-C2-C1	2.54	114.34	109.15
5	G	4	MAN	O2-C2-C3	-2.53	105.07	110.14
2	С	2	NAG	C3-C4-C5	2.47	114.65	110.24
2	R	4	MAN	O3-C3-C4	2.45	116.01	110.35
5	Ι	1	NAG	O3-C3-C2	2.45	114.53	109.47
5	G	5	MAN	O2-C2-C3	-2.43	105.27	110.14
5	G	5	MAN	O3-C3-C2	$2.4\overline{2}$	114.62	109.99
3	Κ	1	NAG	C1-O5-C5	-2.42	108.92	112.19
4	L	1	NAG	C1-O5-C5	2.39	115.44	112.19
3	D	3	BMA	O2-C2-C3	-2.37	105.39	110.14
5	G	5	MAN	C1-O5-C5	2.34	115.37	112.19



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	С	4	MAN	O5-C1-C2	2.34	114.38	110.77
2	С	1	NAG	O4-C4-C5	-2.28	103.62	109.30
3	D	3	BMA	O3-C3-C2	2.24	114.29	109.99
4	L	2	NAG	C1-O5-C5	2.19	115.16	112.19
5	Ι	5	MAN	O6-C6-C5	-2.16	103.89	111.29
4	L	2	NAG	O3-C3-C2	2.16	113.93	109.47
3	Ν	1	NAG	C1-O5-C5	2.14	115.09	112.19
3	Р	3	BMA	O2-C2-C3	-2.11	105.92	110.14
2	С	3	BMA	C1-O5-C5	2.10	115.04	112.19
5	G	4	MAN	C1-C2-C3	-2.10	107.08	109.67
4	L	2	NAG	C8-C7-N2	2.09	119.64	116.10
2	R	4	MAN	O5-C1-C2	2.08	113.97	110.77
2	R	3	BMA	C3-C4-C5	2.07	113.94	110.24
3	K	3	BMA	C1-O5-C5	2.07	115.00	112.19
5	Ι	3	BMA	C6-C5-C4	-2.02	108.26	113.00
3	D	3	BMA	O5-C5-C6	2.02	110.37	107.20
3	D	2	NAG	C1-O5-C5	2.02	114.93	112.19

There are no chirality outliers.

All (	(73)	) torsion	outliers	are	listed	below:
		/				

Mol	Chain	Res	Type	Atoms
4	L	2	NAG	C3-C2-N2-C7
3	Р	2	NAG	O5-C5-C6-O6
3	Κ	3	BMA	C4-C5-C6-O6
3	Ν	2	NAG	C4-C5-C6-O6
3	F	2	NAG	O5-C5-C6-O6
3	D	2	NAG	C4-C5-C6-O6
3	Κ	3	BMA	O5-C5-C6-O6
4	Н	1	NAG	O5-C5-C6-O6
3	Р	3	BMA	O5-C5-C6-O6
5	Ι	4	MAN	O5-C5-C6-O6
3	Р	2	NAG	C4-C5-C6-O6
2	С	2	NAG	O5-C5-C6-O6
4	L	1	NAG	O5-C5-C6-O6
3	D	3	BMA	C4-C5-C6-O6
5	G	1	NAG	C4-C5-C6-O6
4	М	1	NAG	C4-C5-C6-O6
4	L	1	NAG	C4-C5-C6-O6
5	G	5	MAN	O5-C5-C6-O6
3	D	1	NAG	C8-C7-N2-C2
3	D	1	NAG	O7-C7-N2-C2



Mol	Chain	Res	Type	Atoms
4	L	2	NAG	C8-C7-N2-C2
4	L	2	NAG	O7-C7-N2-C2
4	0	2	NAG	C8-C7-N2-C2
4	0	2	NAG	O7-C7-N2-C2
5	Ι	1	NAG	C8-C7-N2-C2
5	Ι	1	NAG	O7-C7-N2-C2
2	R	2	NAG	O5-C5-C6-O6
2	С	2	NAG	C4-C5-C6-O6
3	F	2	NAG	C4-C5-C6-O6
3	D	2	NAG	O5-C5-C6-O6
3	Ν	2	NAG	O5-C5-C6-O6
2	R	1	NAG	O5-C5-C6-O6
4	0	2	NAG	O5-C5-C6-O6
4	Н	1	NAG	C4-C5-C6-O6
5	G	1	NAG	O5-C5-C6-O6
4	М	1	NAG	O5-C5-C6-O6
5	Ι	2	NAG	O5-C5-C6-O6
4	Ο	1	NAG	O5-C5-C6-O6
5	Ι	1	NAG	O5-C5-C6-O6
2	R	1	NAG	C4-C5-C6-O6
5	Ι	2	NAG	C4-C5-C6-O6
5	Ι	1	NAG	C4-C5-C6-O6
4	Е	2	NAG	C4-C5-C6-O6
3	D	1	NAG	O5-C5-C6-O6
4	J	2	NAG	C1-C2-N2-C7
5	G	5	MAN	C4-C5-C6-O6
5	Ι	3	BMA	O5-C5-C6-O6
3	F	1	NAG	O5-C5-C6-O6
4	Е	2	NAG	O5-C5-C6-O6
4	0	1	NAG	C4-C5-C6-O6
3	F	1	NAG	C4-C5-C6-O6
2	R	2	NAG	C4-C5-C6-O6
3	D	3	BMA	O5-C5-C6-O6
4	М	2	NAG	O5-C5-C6-O6
3	Р	1	NAG	O5-C5-C6-O6
5	Ι	4	MAN	C4-C5-C6-O6
5	Ι	3	BMA	C4-C5-C6-O6
3	K	1	NAG	C4-C5-C6-O6
2	R	3	BMA	C4-C5-C6-O6
3	Р	1	NAG	C4-C5-C6-O6
5	Ι	5	MAN	O5-C5-C6-O6
4	Q	2	NAG	O5-C5-C6-O6

Continued from previous page...



Mol	Chain	Res	Type	Atoms
4	0	2	NAG	C4-C5-C6-O6
4	J	1	NAG	O5-C5-C6-O6
5	G	4	MAN	C4-C5-C6-O6
3	K	1	NAG	O5-C5-C6-O6
3	K	2	NAG	C4-C5-C6-O6
2	R	3	BMA	O5-C5-C6-O6
3	Р	3	BMA	C4-C5-C6-O6
3	D	1	NAG	C4-C5-C6-O6
3	K	2	NAG	O5-C5-C6-O6
2	С	4	MAN	O5-C5-C6-O6
4	J	2	NAG	C3-C2-N2-C7

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	R	4	MAN	C1-C2-C3-C4-C5-O5

6 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	М	1	NAG	1	0
5	Ι	1	NAG	1	0
4	L	2	NAG	3	0
2	С	2	NAG	1	0
3	F	2	NAG	1	0
5	Ι	4	MAN	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 37 ligands modelled in this entry, 23 are monoatomic - leaving 14 for Mogul analysis.

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

Mal	Mol Type Chain		Dec	Link	Bo	Bond lengths			Bond angles		
INIOI	туре	Unam	nes		Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2	
6	NAG	А	1134	1	14,14,15	0.48	0	17,19,21	0.82	1 (5%)	
6	NAG	В	1109	1	14,14,15	0.17	0	17,19,21	0.69	1 (5%)	
6	NAG	А	1133	1	14,14,15	0.22	0	17,19,21	0.53	0	
6	NAG	В	1102	1	14,14,15	0.45	0	17,19,21	0.40	0	
8	702	А	1137	7	42,46,46	0.89	1 (2%)	48,62,62	0.99	2 (4%)	
8	702	В	1127	7	42,46,46	0.89	1 (2%)	48,62,62	0.65	0	



Mal	Mol Type Chain Bes		Dec	Tink	Bo	ond leng	$_{\rm ths}$	Bond angles		
INIOI	туре	Unam	nes	LIIIK	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	NAG	А	1135	1	$14,\!14,\!15$	0.68	0	17,19,21	0.55	0
6	NAG	В	1122	1	14,14,15	0.67	0	17,19,21	0.81	1 (5%)
6	NAG	В	1123	1	14,14,15	1.35	1 (7%)	17,19,21	0.71	0
6	NAG	А	1132	1	14,14,15	0.60	0	17,19,21	0.66	1 (5%)
6	NAG	В	1108	1	14,14,15	0.35	0	17,19,21	0.46	0
6	NAG	В	1125	1	14,14,15	1.25	1 (7%)	17,19,21	1.67	2 (11%)
6	NAG	В	1117	1	14,14,15	0.63	0	17,19,21	0.61	0
6	NAG	В	1124	1	14,14,15	0.18	0	17,19,21	0.41	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
6	NAG	А	1134	1	-	4/6/23/26	0/1/1/1
6	NAG	В	1109	1	-	1/6/23/26	0/1/1/1
6	NAG	А	1133	1	-	2/6/23/26	0/1/1/1
6	NAG	В	1102	1	-	2/6/23/26	0/1/1/1
8	702	А	1137	7	-	6/38/44/44	0/4/4/4
8	702	В	1127	7	-	7/38/44/44	0/4/4/4
6	NAG	А	1135	1	-	0/6/23/26	0/1/1/1
6	NAG	В	1122	1	-	0/6/23/26	0/1/1/1
6	NAG	В	1123	1	-	0/6/23/26	0/1/1/1
6	NAG	А	1132	1	-	2/6/23/26	0/1/1/1
6	NAG	В	1108	1	-	2/6/23/26	0/1/1/1
6	NAG	В	1125	1	-	3/6/23/26	0/1/1/1
6	NAG	В	1117	1	-	0/6/23/26	0/1/1/1
6	NAG	В	1124	1	-	0/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	В	1125	NAG	C1-C2	4.54	1.59	1.52
6	В	1123	NAG	O5-C1	-4.50	1.36	1.43
8	А	1137	702	C42-N43	3.74	1.42	1.32
8	В	1127	702	C42-N43	3.46	1.41	1.32

All (8) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$\operatorname{Ideal}(^{o})$
6	В	1125	NAG	C1-O5-C5	4.57	118.38	112.19
6	В	1125	NAG	C4-C3-C2	-3.76	105.51	111.02
8	А	1137	702	C25-C18-C19	-3.13	102.24	111.84
6	А	1134	NAG	C1-O5-C5	2.61	115.72	112.19
6	В	1109	NAG	C1-O5-C5	2.36	115.39	112.19
6	А	1132	NAG	C1-O5-C5	2.34	115.36	112.19
6	В	1122	NAG	O5-C5-C4	-2.12	105.68	110.83
8	А	1137	702	C27-C26-C25	-2.10	118.05	120.65

There are no chirality outliers.

Mol	Chain	$\operatorname{Res}$	Type	Atoms
6	В	1125	NAG	C8-C7-N2-C2
6	В	1125	NAG	O7-C7-N2-C2
8	А	1137	702	C16-C15-P12-O13
8	А	1137	702	C16-C15-P12-O14
8	В	1127	702	C2-C1-P12-O14
8	В	1127	702	P12-C15-C16-C31
8	В	1127	702	C16-C15-P12-O13
8	В	1127	702	C16-C15-P12-O14
6	А	1132	NAG	O5-C5-C6-O6
6	А	1133	NAG	O5-C5-C6-O6
6	А	1134	NAG	O5-C5-C6-O6
6	А	1132	NAG	C4-C5-C6-O6
6	А	1133	NAG	C4-C5-C6-O6
6	В	1102	NAG	O5-C5-C6-O6
6	В	1102	NAG	C4-C5-C6-O6
6	А	1134	NAG	C8-C7-N2-C2
6	А	1134	NAG	O7-C7-N2-C2
6	В	1108	NAG	O5-C5-C6-O6
6	В	1108	NAG	C4-C5-C6-O6
6	В	1109	NAG	O5-C5-C6-O6
6	А	1134	NAG	C4-C5-C6-O6
6	В	1125	NAG	O5-C5-C6-O6
8	А	1137	702	P12-C15-C16-C17
8	В	1127	702	P12-C15-C16-C17
8	А	1137	702	P12-C15-C16-C31
8	A	1137	702	C2-C3-C4-C9
8	В	1127	702	C2-C3-C4-C9
8	A	1137	702	C2-C3-C4-C5
8	В	1127	702	C2-C3-C4-C5

All (29) torsion outliers are listed below:



There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	А	1137	702	1	0
6	А	1132	NAG	1	0
6	В	1117	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 all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and sufficient the outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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## 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	$OWAB(Å^2)$	$Q{<}0.9$
1	А	870/881~(98%)	-0.18	17 (1%) 65 68	30, 45, 71, 115	0
1	В	866/881~(98%)	-0.01	25 (2%) 51 55	32, 52, 77, 109	0
All	All	1736/1762~(98%)	-0.10	42 (2%) 59 62	30, 48, 75, 115	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	А	1035	ALA	6.7
1	В	340	ASP	5.3
1	В	649	SER	5.1
1	А	1033	ALA	4.8
1	А	224	ALA	4.4
1	А	225	VAL	3.7
1	В	341	ASP	3.6
1	В	272[A]	TYR	3.4
1	А	157	ASN	3.3
1	А	1032	VAL	3.3
1	В	1035	ALA	3.2
1	В	599	GLN	3.1
1	В	343	LEU	3.0
1	В	535[A]	GLN	2.9
1	А	992	GLU	2.9
1	В	225	VAL	2.9
1	В	336	SER	2.8
1	В	337	VAL	2.8
1	В	428	GLY	2.6
1	A	598	ASN	2.6
1	В	1033	ALA	2.5
1	А	226	SER	2.5
1	A	227	SER	2.4
1	В	357	TYR	2.4



Mol	Chain	Res	Type	RSRZ	
1	В	429	ALA	2.3	
1	В	854	SER	2.3	
1	В	1032	VAL	2.3	
1	А	1029	THR	2.3	
1	А	639	MET	2.3	
1	В	358	LEU	2.2	
1	В	339	LEU	2.2	
1	В	342	GLY	2.2	
1	В	360	ALA	2.2	
1	А	638	ASN	2.2	
1	А	650	TYR	2.2	
1	В	853	GLN	2.1	
1	А	429	ALA	2.1	
1	А	433	TRP	2.0	
1	В	427	ALA	2.0	
1	В	852	THR	2.0	
1	В	322	ASP	2.0	
1	А	229	GLU	2.0	

## 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
2	BMA	R	3	11/12	0.45	0.31	91,124,128,130	0
3	BMA	D	3	11/12	0.58	0.47	122,134,141,145	0
4	NAG	М	2	14/15	0.64	0.45	97,116,120,123	0
3	BMA	K	3	11/12	0.67	0.38	96,104,113,114	0
2	MAN	R	4	11/12	0.67	0.34	102,112,122,125	0
3	NAG	D	2	14/15	0.70	0.36	93,113,125,133	0
5	MAN	Ι	4	11/12	0.70	0.44	84,97,112,120	0
5	MAN	Ι	5	11/12	0.71	0.44	98,108,118,122	0
2	BMA	С	3	11/12	0.73	0.24	96,105,112,115	0
4	NAG	L	2	14/15	0.74	0.60	84,106,109,109	0



Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	NAG	Q	2	14/15	0.75	0.43	90,103,114,115	0
2	MAN	C	4	11/12	0.75	0.40	100,109,119,123	0
4	NAG	Е	2	14/15	0.75	0.31	65,92,99,101	0
4	NAG	L	1	14/15	0.76	0.40	88,104,110,111	0
4	NAG	J	2	14/15	0.78	0.52	108,120,131,138	0
5	BMA	Ι	3	11/12	0.78	0.39	99,107,118,121	0
4	NAG	Н	2	14/15	0.78	0.36	92,111,116,120	0
4	NAG	0	2	14/15	0.78	0.40	103,115,124,128	0
5	NAG	Ι	2	14/15	0.80	0.36	94,103,110,114	0
2	NAG	R	2	14/15	0.80	0.38	111,121,127,128	0
3	BMA	Р	3	11/12	0.81	0.24	103,112,120,124	0
3	NAG	F	2	14/15	0.82	0.25	68,93,100,103	0
3	BMA	N	3	11/12	0.83	0.27	79,95,103,105	0
5	MAN	G	5	11/12	0.83	0.16	75,81,86,90	0
2	NAG	R	1	14/15	0.85	0.24	82,99,114,123	0
4	NAG	0	1	14/15	0.85	0.20	66,79,96,111	0
3	BMA	F	3	11/12	0.85	0.16	$79,\!91,\!103,\!104$	0
2	NAG	С	2	14/15	0.86	0.43	$80,\!95,\!107,\!108$	0
4	NAG	J	1	14/15	0.87	0.21	84,91,105,114	0
3	NAG	K	1	14/15	0.88	0.28	$62,\!79,\!87,\!92$	0
4	NAG	Н	1	14/15	0.90	0.29	91,99,104,105	0
5	NAG	Ι	1	14/15	0.92	0.22	80,84,94,94	0
3	NAG	K	2	14/15	0.92	0.42	77,88,97,99	0
3	NAG	Р	2	14/15	0.92	0.20	64,84,93,105	0
5	BMA	G	3	11/12	0.92	0.14	61,71,79,80	0
3	NAG	D	1	14/15	0.92	0.15	58,75,91,103	0
3	NAG	N	1	14/15	0.93	0.17	60,79,85,86	0
4	NAG	Q	1	14/15	0.93	0.25	81,86,91,101	0
4	NAG	M	1	14/15	0.93	0.26	68,84,97,106	0
3	NAG	F	1	14/15	0.93	0.26	58,72,82,84	0
4	NAG	E	1	14/15	0.93	0.14	48,58,68,68	0
2	NAG	C	1	14/15	0.94	0.15	44,56,67,68	0
3	NAG	N	2	14/15	0.94	0.16	70,79,87,95	0
5	MAN	G	4	11/12	0.94	0.09	57,64,72,80	0
3	NAG	P	1	14/15	0.95	0.15	57,72,82,86	0
5	NAG	G	1	14/15	0.96	0.11	41,53,57,67	0
5	NAG	G	2	14/15	0.97	0.12	$52,\!57,\!69,\!70$	0

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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	$\mathbf{B} extsf{-}\mathbf{B} extsf{-}\mathbf{factors}(\mathbf{A}^2)$	Q<0.9
9	BR	В	1132	1/1	0.10	0.26	151,151,151,151	0
9	BR	В	1131	1/1	0.60	0.17	149,149,149,149	0
6	NAG	В	1125	14/15	0.61	0.27	91,102,108,122	0
6	NAG	В	1123	14/15	0.66	0.52	94,111,121,122	0
9	BR	А	1150	1/1	0.68	0.26	158,158,158,158	0
6	NAG	В	1122	14/15	0.69	0.41	110,114,120,122	0
6	NAG	А	1132	14/15	0.74	0.42	93,106,113,115	0
6	NAG	В	1117	14/15	0.76	0.33	97,108,114,114	0
6	NAG	А	1134	14/15	0.76	0.39	61,89,103,105	0
9	BR	А	1144	1/1	0.76	0.12	126,126,126,126	0
6	NAG	А	1135	14/15	0.78	0.32	84,99,106,106	0



Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
9	BR	А	1143	1/1	0.79	0.17	109,109,109,109	0
6	NAG	В	1102	14/15	0.81	0.39	100,117,122,123	0
9	BR	А	1149	1/1	0.82	0.25	143,143,143,143	0
6	NAG	В	1124	14/15	0.83	0.55	113,127,133,134	0
6	NAG	А	1133	14/15	0.86	0.21	70,89,96,103	0
6	NAG	В	1109	14/15	0.87	0.21	62,83,91,99	0
9	BR	В	1130	1/1	0.90	0.12	119,119,119,119	0
6	NAG	В	1108	14/15	0.90	0.34	91,100,104,109	0
9	BR	А	1151	1/1	0.90	0.14	140,140,140,140	0
9	BR	В	1101	1/1	0.91	0.13	106,106,106,106	0
9	BR	В	1129	1/1	0.93	0.10	99,99,99,99	0
9	BR	А	1146	1/1	0.93	0.26	$151,\!151,\!151,\!151$	0
9	BR	А	1152	1/1	0.95	0.14	106,106,106,106	0
9	BR	А	1141	1/1	0.96	0.12	$105,\!105,\!105,\!105$	0
8	702	В	1127	43/43	0.96	0.23	37,46,54,63	0
9	BR	А	1139	1/1	0.96	0.06	94,94,94,94	0
9	BR	В	1128	1/1	0.96	0.05	94,94,94,94	0
8	702	А	1137	43/43	0.97	0.20	$31,\!39,\!48,\!53$	0
9	BR	А	1147	1/1	0.97	0.06	66,66,66,66	0
9	BR	А	1142	1/1	0.97	0.04	74, 74, 74, 74	0
9	BR	А	1145	1/1	0.97	0.06	83,83,83,83	0
9	BR	А	1138	1/1	0.98	0.06	71,71,71,71	0
9	BR	А	1148	1/1	0.98	0.10	76,76,76,76	0
9	BR	A	1140	1/1	0.98	0.08	107, 107, 107, 107, 107	0
7	ZN	В	1126	1/1	0.99	0.17	36,36,36,36	0
7	ZN	А	1136	1/1	1.00	0.16	$31,\!31,\!31,\!31$	0

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The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.









# 6.5 Other polymers (i)

There are no such residues in this entry.

