

Full wwPDB X-ray Structure Validation Report (i)

Apr 30, 2024 – 08:14 PM JST

Title : Crystal structure of GH97 glucodextranase mutant E509Q from	Flavobac-
terium johnsoniae in complex with panose	
Authors : Kurata, R.; Nakamura, S.; Miyazaki, T.	
Deposited on : $2023-09-20$	
Resolution : 2.34 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	:	2.36.2
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)	:	2.36.2

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 2.34 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R_{free}	130704	2096 (2.36-2.32)
Clashscore	141614	2193 (2.36-2.32)
Ramachandran outliers	138981	2159 (2.36-2.32)
Sidechain outliers	138945	2160 (2.36-2.32)
RSRZ outliers	127900	2067 (2.36-2.32)

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	685	89%	9%
1	В	685	% 90%	9% •
1	С	685	91%	9%
1	D	685	90%	9%
2	Е	3	100%	
2	F	3	100%	





Mol	Chain	Length	Quality of chain
2	G	3	100%
2	Н	3	100%



8WG1

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 22517 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Δ	682	Total	С	Ν	Ο	S	0	0 1	0
1	A	082	5476	3490	919	1048	19	0		0
1	р	682	Total	С	Ν	Ο	S	0	0	0
	D	082	5471	3487	918	1047	19	0		0
1	C	699	Total	С	Ν	Ο	S	0	1	0
	082	5476	3490	919	1048	19	0		0	
1 D	685	Total	С	Ν	Ο	S	0	1	0	
	085	5495	3501	921	1054	19			0	

• Molecule 1 is a protein called Candidate alpha-glucosidase Glycoside hydrolase family 97.

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	20	SER	-	expression tag	UNP A5FBI0
А	509	GLN	GLU	engineered mutation	UNP A5FBI0
В	20	SER	-	expression tag	UNP A5FBI0
В	509	GLN	GLU	engineered mutation	UNP A5FBI0
С	20	SER	-	expression tag	UNP A5FBI0
С	509	GLN	GLU	engineered mutation	UNP A5FBI0
D	20	SER	-	expression tag	UNP A5FBI0
D	509	GLN	GLU	engineered mutation	UNP A5FBI0

• Molecule 2 is an oligosaccharide called alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose-(1-4)-beta-D-glucopyranose.



Mol	Chain	Residues	At	\mathbf{oms}		ZeroOcc	AltConf	Trace
2	Е	3	Total 34	C 18	0 16	0	0	0



Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace	
2	2 F	3	Total	C	0	0	0	0
			34	18	16			
2	G	3	Total	С	O	0	0	0
	ŭ		34	18	16			
2 H	п	2	Total	С	0	0	0	0
	П	9	34	18	16			

• Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	1	Total Ca 1 1	0	0
3	В	1	Total Ca 1 1	0	0
3	С	1	Total Ca 1 1	0	0
3	D	1	Total Ca 1 1	0	0

• Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
4	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0



Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	В	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
4	С	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
4	С	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
4	D	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0

• Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	А	1	Total Mg 1 1	0	0
5	С	2	Total Mg 2 2	0	0

• Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	А	130	Total O 130 130	0	0
6	В	89	Total O 89 89	0	0
6	С	121	Total O 121 121	0	0
6	D	92	Total O 92 92	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: Candidate alpha-glucosidase Glycoside hydrolase family 97





• Molecule 1: Candidate alpha-glucosidase Glycoside hydrolase family 97

Chain D:	90%	9%
220 L35 L35 S56 D72 D72 D72 T75 L175 H91 R91 B115 R16 R16 R16 R115 R146 K146 K146	Y161 D168 D168 E171 T207 T207 T207 C214 P1222 H222 H222 C23 R267	R276 P290 8291 R351 R351 R352 R356 R356
W374 W374 H405 A420 Y435 Y435 P441 H468 M482 M482 M482 M482 M482 M482 M482 M48	N518 1526 P527 M545 M545 M545 M545 P579 P579 P579 P579 P579 P579 P578 P579 P578 P578 P578 P578 P578 P578 P578 P578	8637 1639 1639 864 8652 K664 K674
K682 1683 8696 A703 A703		
• Molecule 2: alpha-D-glucopyrance	ose-(1-6)-alpha-D-glucopyranc	se-(1-4)-beta-D-glucopyranos
Chain E:	100%	
BGC1 GLC3 GLC3		
• Molecule 2: alpha-D-glucopyrance	ose-(1-6)-alpha-D-glucopyranc	se-(1-4)-beta-D-glucopyranos
Chain F:	100%	
BGC1 CLC2 CLC2 CLC2		
• Molecule 2: alpha-D-glucopyrance	ose-(1-6)-alpha-D-glucopyranc	ose-(1-4)-beta-D-glucopyranos
Chain G:	100%	
BGC1 GLC2 GLC3		
• Molecule 2: alpha-D-glucopyrance	ose-(1-6)-alpha-D-glucopyranc	se-(1-4)-beta-D-glucopyranos
Chain H:	100%	
BGC1 GLC2 GLC3		



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants	290.69Å 102.71Å 104.53Å	Deperitor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
$\mathbf{P}_{\text{assolution}}(\hat{\mathbf{A}})$	49.23 - 2.34	Depositor
Resolution (A)	49.18 - 2.34	EDS
% Data completeness	99.9 (49.23-2.34)	Depositor
(in resolution range)	99.9(49.18-2.34)	EDS
R _{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$2.50 (at 2.34 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.8.0419	Depositor
P. P.	0.208 , 0.254	Depositor
Π, Π_{free}	0.213 , 0.259	DCC
R_{free} test set	6575 reflections $(4.96%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	32.0	Xtriage
Anisotropy	0.265	Xtriage
Bulk solvent $k_{sol}(e/A^3), B_{sol}(A^2)$	0.32 , 22.6	EDS
L-test for $twinning^2$	$< L > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.006 for -h,l,k	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	22517	wwPDB-VP
Average B, all atoms $(Å^2)$	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 14.63% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



¹Intensities 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: MG, EDO, CA, GLC, BGC

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	Bond angles	
Moi Chain		RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.65	0/5623	1.09	13/7626~(0.2%)
1	В	0.63	1/5615~(0.0%)	1.08	13/7615~(0.2%)
1	С	0.66	0/5623	1.10	9/7626~(0.1%)
1	D	0.64	1/5642~(0.0%)	1.10	13/7652~(0.2%)
All	All	0.64	2/22503~(0.0%)	1.09	48/30519~(0.2%)

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	4
1	В	0	3
1	С	0	4
1	D	0	4
All	All	0	15

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\operatorname{Ideal}(\operatorname{\AA})$
1	D	171	GLU	CD-OE1	-5.90	1.19	1.25
1	В	372	GLU	CD-OE2	-5.75	1.19	1.25

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	D	579	GLU	CB-CA-C	-10.29	89.82	110.40
1	А	98	ARG	NE-CZ-NH1	9.78	125.19	120.30
1	С	115	ARG	NE-CZ-NH1	-9.62	115.49	120.30



8	V	V	G	1
U	v	v	U	Τ.

	Chain	Res	Type	Atoms	7.	Observed $(^{o})$	Ideal(°)
1	B	570	CIII		0.60	01.20	110.40
1	D	635	ARC	NE CZ NH1	-9.00	124.83	120.30
1		115	ARC	NE-CZ-NH2	9.00	115.81	120.30 120.30
1		635	ARC	NE CZ NH2	-0.90 8 20	116.01	120.30 120.30
1	B	352	ARC	NE-CZ-NH1	$\frac{-0.29}{7.05}$	110.13	120.30 120.30
1	B	583	ARC	NE-CZ-NH1	7.90	124.27	120.30 120.30
1	D	000 014	CIN	NCA CR	-7.09	110.40	120.50
1	D	570	CLU	CR CA C	7.14	06.12	110.00
1	C	592	APC	NE CZ NH2	7.06	90.12	110.40
1	D D	197	CLU	$\frac{\text{NE-CZ-NH2}}{\text{CC-CD-OF2}}$	6.00	123.03	120.30 118.20
1		545	MET	CC SD CE	-0.99 6.01	104.55	110.00
1	A C	040 496		NE CZ NH2	6.75	111.20	100.20
1	D	420 602	ANG	CC CD NE	-0.75	08.95	120.30
1	В	<u>602</u>	ARG	CG-CD-NE	-0.40	98.20	111.80
1	A	579	GLU	CB-CA-C	-0.23	97.94	110.40
1	В	435	MET	CG-SD-CE	6.21	110.14	100.20
1	A	01 171	THR	OGI-CB-CG2	-5.98	96.25	110.00
1	В	171	GLU	CG-CD-OEI	-5.87	106.55	118.30
1	A	683	LEU	CB-CG-CDI	-5.86	101.03	111.00
1	B	583	ARG	CD-NE-CZ	5.83	131.76	123.60
1	A	276	ARG	NE-CZ-NH1	-5.73	117.44	120.30
1	B	673	ARG	NE-CZ-NH1	5.71	123.15	120.30
1	A	579	GLU	N-CA-CB	5.63	120.74	110.60
1	A	602	ARG	CG-CD-NE	-5.58	100.09	111.80
1	С	276	ARG	NE-CZ-NH2	5.57	123.08	120.30
1	D	276	ARG	NE-CZ-NH1	-5.56	117.52	120.30
1	В	51	ASP	CB-CG-OD2	-5.52	113.33	118.30
1	D	214	GLN	CB-CA-C	-5.50	99.40	110.40
1	В	250	ASP	CB-CG-OD2	-5.42	113.42	118.30
1	D	503	GLU	OE1-CD-OE2	5.37	129.75	123.30
1	С	122	ARG	NE-CZ-NH2	-5.37	117.61	120.30
1	A	583	ARG	NE-CZ-NH2	-5.31	$117.6\overline{4}$	120.30
1	В	536	MET	CG-SD-CE	-5.22	91.84	100.20
1	А	140	LEU	CB-CG-CD2	5.21	119.86	111.00
1	С	376	ASP	CB-CG-OD1	-5.21	113.61	118.30
1	D	98	ARG	NE-CZ-NH1	-5.17	117.71	120.30
1	А	422	ARG	CD-NE-CZ	5.15	130.81	123.60
1	D	147	GLU	CB-CA-C	-5.15	100.10	110.40
1	В	187	GLU	CG-CD-OE1	5.13	128.56	118.30
1	D	441	ASP	CB-CA-C	5.12	120.65	110.40
1	С	579	GLU	N-CA-CB	5.08	119.74	110.60
1	С	292	LYS	CD-CE-NZ	5.06	123.34	111.70
1	D	146	LYS	CD-CE-NZ	-5.06	100.06	111.70



Mol	Chain	Res	Type	Atoms	Ζ	$Observed(^{o})$	$Ideal(^{o})$
1	D	593	ASP	CB-CG-OD2	5.04	122.84	118.30
1	D	664	LYS	N-CA-CB	5.03	119.66	110.60
1	А	422	ARG	NE-CZ-NH2	5.01	122.81	120.30

There are no chirality outliers.

All (15) planarity outliers are listed below:

Mol	Chain	\mathbf{Res}	Type	Group
1	А	115	ARG	Sidechain
1	А	267	ARG	Sidechain
1	А	341	ARG	Sidechain
1	А	602	ARG	Sidechain
1	В	115	ARG	Sidechain
1	В	352	ARG	Sidechain
1	В	602	ARG	Sidechain
1	С	341	ARG	Sidechain
1	С	352	ARG	Sidechain
1	С	602	ARG	Sidechain
1	С	673	ARG	Sidechain
1	D	115	ARG	Sidechain
1	D	352	ARG	Sidechain
1	D	602	ARG	Sidechain
1	D	703	ALA	Peptide

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	5476	0	5259	37	0
1	В	5471	0	5253	29	0
1	С	5476	0	5259	24	0
1	D	5495	0	5273	27	0
2	Е	34	0	27	0	0
2	F	34	0	27	0	0
2	G	34	0	29	0	0
2	Н	34	0	28	0	0
3	A	1	0	0	0	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	В	1	0	0	0	0
3	С	1	0	0	0	0
3	D	1	0	0	0	0
4	А	8	0	12	2	0
4	В	4	0	6	0	0
4	С	8	0	12	0	0
4	D	4	0	6	0	0
5	А	1	0	0	0	0
5	С	2	0	0	0	0
6	А	130	0	0	1	0
6	В	89	0	0	4	0
6	С	121	0	0	3	0
6	D	92	0	0	3	0
All	All	22517	0	21191	113	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 3.

All (113) 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	$distance (\text{\AA})$	overlap (Å)
1:D:674:LYS:HB3	6:D:991:HOH:O	1.46	1.14
1:B:583:ARG:NH1	6:B:901:HOH:O	2.06	0.82
1:B:583:ARG:NE	6:B:901:HOH:O	1.91	0.80
1:C:640:ASP:OD2	1:C:682:LYS:HE2	1.88	0.73
1:B:114:ASP:OD2	1:C:673:ARG:NH1	2.27	0.66
1:B:545:MET:HG3	1:B:553:VAL:HB	1.78	0.66
1:C:380:HIS:CE1	6:C:1004:HOH:O	2.48	0.65
1:A:405:HIS:HE1	1:A:438:TYR:O	1.81	0.63
1:A:142:TYR:OH	1:B:376:ASP:OD2	2.16	0.62
1:C:32:HIS:HB2	6:C:966:HOH:O	1.99	0.62
1:A:67:LYS:O	1:A:68:SER:HB2	2.00	0.61
1:A:545:MET:HG3	1:A:553:VAL:HB	1.82	0.61
1:D:639:ILE:HD12	1:D:683:LEU:HD23	1.81	0.61
1:C:545:MET:HG3	1:C:553:VAL:HB	1.82	0.60
1:D:545:MET:HG3	1:D:553:VAL:HB	1.84	0.60
1:B:405:HIS:HE1	1:B:438:TYR:O	1.86	0.57
1:A:602:ARG:NH1	1:A:602:ARG:CG	2.68	0.56
1:C:398:LYS:NZ	1:C:402:GLU:OE1	2.36	0.56
1:D:405:HIS:HE1	1:D:438:TYR:O	1.87	0.56
1:A:638:ASN:OD1	1:A:684:SER:OG	2.24	0.56



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:382:LYS:HE2	1:A:385:VAL:HA	1.88	0.55
1:D:351:LYS:CE	6:D:915:HOH:O	2.53	0.55
1:C:405:HIS:HE1	1:C:438:TYR:O	1.92	0.53
1:D:639:ILE:HD12	1:D:683:LEU:CD2	2.40	0.52
1:C:544:GLU:OE1	6:C:901:HOH:O	2.19	0.52
1:B:413:MET:HA	6:B:917:HOH:O	2.11	0.51
1:B:356:PHE:CD1	1:B:578:PRO:HB3	2.46	0.51
1:B:66:ASN:OD1	1:B:66:ASN:N	2.44	0.50
1:D:652:ALA:HA	1:D:696:SER:O	2.11	0.49
1:A:602:ARG:NH1	1:A:602:ARG:HG2	2.28	0.49
1:C:638:ASN:OD1	1:C:684:SER:OG	2.27	0.49
1:A:192:LYS:HA	1:A:197:GLN:HE22	1.78	0.48
1:C:207:THR:HA	1:C:208:SER:C	2.34	0.48
1:A:285:TYR:CE2	4:A:802:EDO:H22	2.49	0.48
1:D:290:PRO:O	1:D:291:SER:C	2.52	0.48
1:D:511:GLN:NE2	1:D:518:ASN:HB2	2.29	0.48
1:A:290:PRO:O	1:A:291:SER:C	2.52	0.48
1:B:207:THR:HA	1:B:208:SER:C	2.35	0.47
1:B:583:ARG:CZ	6:B:901:HOH:O	2.33	0.47
1:C:168:ASP:HA	1:C:458:HIS:HB2	1.96	0.47
1:A:207:THR:HA	1:A:208:SER:C	2.34	0.47
1:A:527:PRO:HG2	1:A:612:ILE:HD12	1.97	0.47
1:C:290:PRO:O	1:C:291:SER:C	2.53	0.47
1:C:369:GLY:HA2	1:C:374:TRP:CD1	2.49	0.47
1:A:42:VAL:HA	1:A:56:SER:O	2.14	0.46
1:A:285:TYR:CZ	4:A:802:EDO:H22	2.49	0.46
1:B:52:VAL:HG11	1:B:271:VAL:HG21	1.97	0.46
1:B:511:GLN:NE2	1:B:518:ASN:HB2	2.30	0.46
1:C:42:VAL:HA	1:C:56:SER:O	2.15	0.46
1:A:220:ASN:HB3	1:A:270:ILE:HB	1.97	0.46
1:D:356:PHE:CD1	1:D:578:PRO:HB3	2.51	0.46
1:D:80:THR:HA	1:D:103:GLU:O	2.16	0.46
1:B:80:THR:HA	1:B:103:GLU:O	2.16	0.46
1:A:52:VAL:HG11	1:A:271:VAL:HG21	1.98	0.45
1:A:511:GLN:NE2	1:A:518:ASN:HB2	2.31	0.45
1:B:369:GLY:HA2	1:B:374:TRP:CD1	2.50	0.45
1:C:80:THR:HA	1:C:103:GLU:O	2.16	0.45
1:C:444:LYS:HA	1:C:482:ASN:O	2.17	0.45
1:B:293:ILE:HD12	1:B:497:PRO:HD2	1.98	0.45
1:A:369:GLY:HA2	1:A:374:TRP:CD1	2.52	0.45
1:C:52:VAL:HG11	1:C:271:VAL:HG21	1.99	0.45



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:D:42:VAL:HA	1:D:56:SER:O	2.17	0.44
1:D:207:THR:HA	1:D:208:SER:C	2.37	0.44
1:B:42:VAL:HA	1:B:56:SER:O	2.18	0.44
1:A:80:THR:HA	1:A:103:GLU:O	2.18	0.44
1:B:168:ASP:HA	1:B:458:HIS:HB2	1.99	0.44
1:A:168:ASP:HA	1:A:458:HIS:HB2	1.99	0.44
1:D:91:TRP:HE3	1:D:568:TYR:HH	1.64	0.44
1:D:444:LYS:HA	1:D:482:ASN:O	2.18	0.44
1:A:444:LYS:HA	1:A:482:ASN:O	2.17	0.44
1:A:382:LYS:HD2	1:B:142:TYR:OH	2.18	0.44
1:A:101:TYR:CE2	1:A:122:ARG:HD3	2.53	0.43
1:D:527:PRO:HG2	1:D:612:ILE:HD12	1.99	0.43
1:C:356:PHE:CD1	1:C:578:PRO:HB3	2.53	0.43
1:D:527:PRO:HG2	1:D:612:ILE:CD1	2.48	0.43
1:B:557:ILE:HG13	1:B:668:GLN:HA	2.00	0.43
1:B:444:LYS:HA	1:B:482:ASN:O	2.19	0.43
1:C:511:GLN:NE2	1:C:518:ASN:HB2	2.33	0.43
1:A:356:PHE:CD1	1:A:578:PRO:HB3	2.54	0.43
1:B:432:TYR:O	1:B:435:MET:HB2	2.19	0.43
1:B:290:PRO:O	1:B:291:SER:C	2.58	0.43
1:D:222:HIS:CG	1:D:223:GLU:H	2.37	0.43
1:A:527:PRO:HG2	1:A:612:ILE:CD1	2.48	0.42
1:D:35:LEU:HD11	1:D:75:ILE:HG13	2.01	0.42
1:D:168:ASP:HA	1:D:458:HIS:HB2	2.01	0.42
1:D:228:ASN:HD22	1:D:228:ASN:HA	1.67	0.42
1:C:526:LEU:N	1:C:527:PRO:CD	2.82	0.42
1:A:526:LEU:N	1:A:527:PRO:CD	2.83	0.42
1:A:432:TYR:O	1:A:435:MET:HB2	2.19	0.42
1:D:432:TYR:O	1:D:435:MET:HB2	2.19	0.42
1:B:527:PRO:HG2	1:B:612:ILE:CD1	2.49	0.42
1:D:420:ALA:HB3	6:D:965:HOH:O	2.20	0.42
1:A:346:THR:O	1:A:350:VAL:HG23	2.20	0.42
1:B:222:HIS:CG	1:B:223:GLU:H	2.38	0.42
1:A:304:TYR:OH	1:A:537:ASP:OD1	2.36	0.42
1:D:369:GLY:HA2	1:D:374:TRP:CD1	2.55	0.42
1:D:161:TYR:CD1	1:D:161:TYR:N	2.88	0.41
1:A:63:LYS:HD2	6:A:1020:HOH:O	2.19	0.41
1:A:602:ARG:HG2	1:A:602:ARG:HH11	1.85	0.41
1:D:526:LEU:N	1:D:527:PRO:CD	2.83	0.41
1:A:405:HIS:CE1	1:A:438:TYR:O	2.67	0.41
1:C:163:ILE:HG23	1:C:174:TYR:CD2	2.55	0.41



Atom-1	Atom-2	Interatomic	Clash
	1100111 =	distance (A)	overlap (Å)
1:A:453:PRO:HG3	1:B:462:TRP:CE2	2.55	0.41
1:C:346:THR:O	1:C:350:VAL:HG23	2.19	0.41
1:D:192:LYS:HA	1:D:197:GLN:HE22	1.85	0.41
1:B:120:ARG:O	1:B:130:PHE:HA	2.21	0.41
1:B:91:TRP:HE3	1:B:568:TYR:HH	1.69	0.41
1:C:212:LYS:HA	1:C:217:LEU:O	2.21	0.41
1:B:511:GLN:HA	1:B:517:ARG:HB3	2.03	0.41
1:A:161:TYR:CD1	1:A:161:TYR:N	2.89	0.40
1:A:287:LEU:HD23	1:A:287:LEU:HA	1.88	0.40
1:C:432:TYR:O	1:C:435:MET:HB2	2.21	0.40
1:A:654:ILE:N	1:A:654:ILE:HD12	2.36	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	Perce	entiles
1	А	681/685~(99%)	641 (94%)	38~(6%)	2(0%)	41	47
1	В	680/685~(99%)	645~(95%)	33~(5%)	2(0%)	41	47
1	С	681/685~(99%)	645~(95%)	34~(5%)	2(0%)	41	47
1	D	684/685~(100%)	649~(95%)	34~(5%)	1 (0%)	51	62
All	All	2726/2740~(100%)	2580 (95%)	139 (5%)	7 (0%)	41	47

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	С	308	TRP
1	А	308	TRP
1	В	503	GLU
1	А	141	ILE



 $Continued \ from \ previous \ page...$

Mol	Chain	Res	Type
1	В	141	ILE
1	С	141	ILE
1	D	141	ILE

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	582/582~(100%)	576~(99%)	6 (1%)	76 85
1	В	581/582~(100%)	571~(98%)	10 (2%)	60 72
1	С	582/582~(100%)	575~(99%)	7 (1%)	71 82
1	D	583/582~(100%)	576~(99%)	7 (1%)	71 82
All	All	2328/2328~(100%)	2298~(99%)	30 (1%)	69 79

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	72	ASP
1	А	267	ARG
1	А	488	ARG
1	А	545	MET
1	А	579	GLU
1	А	662	ASN
1	В	72	ASP
1	В	114	ASP
1	В	267	ARG
1	В	295	GLU
1	В	488	ARG
1	В	516	ASP
1	В	545	MET
1	В	579	GLU
1	В	637	SER
1	В	682	LYS
1	С	66	ASN
1	С	72	ASP



Mol	Chain	Res	Type
1	С	267	ARG
1	С	488	ARG
1	С	579	GLU
1	С	602	ARG
1	С	637	SER
1	D	72	ASP
1	D	267	ARG
1	D	488	ARG
1	D	545	MET
1	D	579	GLU
1	D	637	SER
1	D	646	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	66	ASN
1	А	197	GLN
1	А	252	HIS
1	В	197	GLN
1	В	252	HIS
1	С	86	ASN
1	С	197	GLN
1	D	64	ASN
1	D	197	GLN
1	D	228	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)

12 monosaccharides are modelled in this entry.



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

Mol	Type	Chain	Bos	Link	Bo	ond leng	ths	B	ond ang	les
WIOI	Type	Ullalli	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2
2	BGC	Е	1	2	12,12,12	0.98	1 (8%)	$17,\!17,\!17$	3.14	8 (47%)
2	GLC	Е	2	3,2	11,11,12	0.47	0	$15,\!15,\!17$	2.05	6 (40%)
2	GLC	Е	3	3,2	11,11,12	0.55	0	$15,\!15,\!17$	1.73	4 (26%)
2	BGC	F	1	2	12,12,12	0.84	0	17,17,17	1.71	5 (29%)
2	GLC	F	2	3,2	11,11,12	0.60	0	15,15,17	1.60	2 (13%)
2	GLC	F	3	3,2	11,11,12	0.31	0	15,15,17	2.08	3 (20%)
2	BGC	G	1	2	12,12,12	1.11	1 (8%)	17,17,17	1.56	6 (35%)
2	GLC	G	2	3,2	11,11,12	0.87	0	$15,\!15,\!17$	1.57	2 (13%)
2	GLC	G	3	3,2	11,11,12	0.87	0	$15,\!15,\!17$	2.43	8 (53%)
2	BGC	Н	1	2	12,12,12	0.96	0	17,17,17	1.96	4 (23%)
2	GLC	Н	2	3,2	11,11,12	0.52	0	15,15,17	2.39	5 (33%)
2	GLC	Н	3	3,2	11,11,12	0.70	0	15,15,17	2.10	3 (20%)

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	BGC	Е	1	2	-	2/2/22/22	0/1/1/1
2	GLC	Е	2	3,2	-	2/2/19/22	0/1/1/1
2	GLC	Е	3	3,2	-	0/2/19/22	0/1/1/1
2	BGC	F	1	2	-	0/2/22/22	0/1/1/1
2	GLC	F	2	3,2	-	2/2/19/22	0/1/1/1
2	GLC	F	3	3,2	-	0/2/19/22	0/1/1/1
2	BGC	G	1	2	-	2/2/22/22	0/1/1/1
2	GLC	G	2	3,2	-	1/2/19/22	0/1/1/1
2	GLC	G	3	3,2	-	0/2/19/22	0/1/1/1
2	BGC	Н	1	2	-	2/2/22/22	0/1/1/1
2	GLC	Н	2	3,2	-	1/2/19/22	0/1/1/1
2	GLC	Н	3	3,2	-	0/2/19/22	0/1/1/1



Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	$\operatorname{Ideal}(\operatorname{\AA})$
2	Е	1	BGC	01-C1	-2.42	1.31	1.39
2	G	1	BGC	O4-C4	2.10	1.47	1.43

All (2) bond length outliers are listed below:

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	Н	2	GLC	C1-O5-C5	7.11	121.83	112.19
2	Е	1	BGC	O5-C1-C2	6.89	122.58	110.28
2	F	3	GLC	C1-O5-C5	5.66	119.86	112.19
2	Н	3	GLC	C2-C3-C4	-5.59	101.22	110.89
2	Е	1	BGC	01-C1-C2	-4.94	95.13	109.03
2	G	3	GLC	C2-C3-C4	-4.74	102.69	110.89
2	Е	1	BGC	C1-C2-C3	-4.62	100.73	110.31
2	Е	3	GLC	C2-C3-C4	-4.41	103.27	110.89
2	F	2	GLC	C1-O5-C5	4.36	118.10	112.19
2	G	2	GLC	C3-C4-C5	4.27	117.86	110.24
2	Е	1	BGC	O2-C2-C1	4.26	119.05	109.16
2	Е	1	BGC	O3-C3-C2	-4.26	100.50	110.35
2	Н	3	GLC	O3-C3-C2	4.25	118.13	109.99
2	Н	1	BGC	O4-C4-C3	-4.00	101.11	110.35
2	G	3	GLC	O4-C4-C3	3.80	119.13	110.35
2	Е	2	GLC	O5-C5-C6	-3.61	101.54	107.20
2	Е	2	GLC	C1-O5-C5	3.57	117.03	112.19
2	Н	2	GLC	C2-C3-C4	3.46	116.88	110.89
2	G	3	GLC	O3-C3-C2	-3.40	103.49	109.99
2	Е	2	GLC	C2-C3-C4	-3.36	105.08	110.89
2	Н	1	BGC	O5-C1-C2	3.23	116.06	110.28
2	F	1	BGC	C3-C4-C5	3.13	115.83	110.24
2	F	3	GLC	O2-C2-C3	3.12	116.38	110.14
2	Н	1	BGC	O3-C3-C4	3.05	117.40	110.35
2	Е	1	BGC	O4-C4-C3	-2.95	103.54	110.35
2	G	3	GLC	O2-C2-C1	2.92	115.12	109.15
2	F	1	BGC	O2-C2-C1	2.91	115.91	109.16
2	G	1	BGC	O4-C4-C5	2.84	116.34	109.30
2	Н	2	GLC	O2-C2-C1	2.83	114.93	109.15
2	F	1	BGC	O3-C3-C2	-2.82	103.83	110.35
2	G	1	BGC	O2-C2-C1	2.82	115.69	109.16
2	E	1	BGC	C4-C3-C2	2.73	115.59	110.82
2	Н	1	BGC	C6-C5-C4	2.65	119.20	113.00
2	F	2	GLC	O5-C5-C6	-2.62	103.10	107.20
2	F	3	GLC	O5-C5-C6	-2.60	103.13	107.20
2	Е	2	GLC	C3-C4-C5	2.59	114.87	110.24



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	F	1	BGC	C4-C3-C2	2.57	115.31	110.82
2	G	3	GLC	O4-C4-C5	-2.55	102.96	109.30
2	Е	1	BGC	O2-C2-C3	2.54	116.22	110.35
2	Е	2	GLC	O2-C2-C3	2.51	115.17	110.14
2	G	3	GLC	O3-C3-C4	2.43	115.97	110.35
2	G	2	GLC	O2-C2-C1	2.40	114.06	109.15
2	G	3	GLC	C1-O5-C5	2.28	115.28	112.19
2	G	1	BGC	C6-C5-C4	2.22	118.19	113.00
2	F	1	BGC	O5-C1-C2	2.18	114.17	110.28
2	Е	3	GLC	O5-C5-C6	-2.18	103.79	107.20
2	G	1	BGC	O4-C4-C3	-2.17	105.34	110.35
2	Е	2	GLC	O3-C3-C2	2.14	114.09	109.99
2	G	3	GLC	O5-C5-C6	-2.14	103.85	107.20
2	Ε	3	GLC	O2-C2-C3	-2.09	105.95	110.14
2	G	1	BGC	O5-C1-C2	2.08	114.00	110.28
2	Н	2	GLC	O3-C3-C2	-2.06	106.05	109.99
2	Н	2	GLC	C1-C2-C3	-2.05	107.14	109.67
2	Н	3	GLC	O <u>5-C5-C6</u>	-2.04	104.01	107.20
2	Е	3	GLC	C6-C5-C4	-2.04	108.23	113.00
2	G	1	BGC	O3-C3-C4	2.01	114.99	110.35

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	\mathbf{Res}	Type	Atoms
2	Е	2	GLC	O5-C5-C6-O6
2	Е	1	BGC	C4-C5-C6-O6
2	F	2	GLC	O5-C5-C6-O6
2	Е	1	BGC	O5-C5-C6-O6
2	Е	2	GLC	C4-C5-C6-O6
2	Н	2	GLC	O5-C5-C6-O6
2	G	2	GLC	O5-C5-C6-O6
2	F	2	GLC	C4-C5-C6-O6
2	Н	1	BGC	C4-C5-C6-O6
2	G	1	BGC	C4-C5-C6-O6
2	G	1	BGC	O5-C5-C6-O6
2	Н	1	BGC	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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 13 ligands modelled in this entry, 7 are monoatomic - leaving 6 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	Turne	Chain	Dec	Tiple	B	ond leng	gths	E	Bond ang	gles
MOI	туре	Unain	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
4	EDO	А	803	-	3,3,3	0.81	0	$2,\!2,\!2$	0.97	0
4	EDO	C	802	-	3,3,3	1.32	1 (33%)	$2,\!2,\!2$	0.81	0
4	EDO	D	802	-	3,3,3	1.92	1 (33%)	2,2,2	1.06	0
4	EDO	А	802	-	3,3,3	0.73	0	2,2,2	1.19	0
4	EDO	C	803	-	3,3,3	1.76	1 (33%)	$2,\!2,\!2$	0.72	0
4	EDO	В	802	-	3,3,3	0.37	0	2,2,2	0.76	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	EDO	А	803	-	-	1/1/1/1	-
4	EDO	С	802	-	-	0/1/1/1	-
4	EDO	D	802	-	-	1/1/1/1	-
4	EDO	А	802	-	-	1/1/1/1	-
4	EDO	С	803	-	-	0/1/1/1	-
4	EDO	В	802	-	-	0/1/1/1	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	$\mathrm{Ideal}(\mathrm{\AA})$
4	D	802	EDO	01-C1	2.72	1.56	1.42
4	С	803	EDO	O1-C1	2.10	1.52	1.42
4	С	802	EDO	O1-C1	2.01	1.52	1.42

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	А	802	EDO	O1-C1-C2-O2
4	А	803	EDO	O1-C1-C2-O2
4	D	802	EDO	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	А	802	EDO	2	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	< RSRZ >	#RSRZ>2			$OWAB(Å^2)$	Q<0.9
1	А	682/685~(99%)	-0.25	1 (0%)	95	98	22, 31, 48, 72	0
1	В	682/685~(99%)	-0.09	7 (1%)	82	88	23, 35, 53, 84	0
1	С	682/685~(99%)	-0.18	4 (0%)	89	93	21, 32, 49, 71	0
1	D	685/685~(100%)	-0.22	1 (0%)	95	98	23, 34, 52, 75	0
All	All	2731/2740 (99%)	-0.18	13 (0%)	91	95	21, 33, 51, 84	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	В	701	ALA	6.4
1	В	683	LEU	5.0
1	С	701	ALA	3.5
1	А	701	ALA	2.9
1	В	361	GLY	2.5
1	С	602	ARG	2.4
1	В	37	ALA	2.4
1	В	682	LYS	2.4
1	D	682	LYS	2.4
1	В	20	SER	2.3
1	В	639	ILE	2.3
1	С	66	ASN	2.1
1	С	188	LYS	2.1

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	${f B} ext{-factors}({ m \AA}^2)$	Q < 0.9
2	BGC	G	1	12/12	0.85	0.16	41,52,59,60	0
2	BGC	Н	1	12/12	0.88	0.17	32,43,49,55	0
2	BGC	Е	1	12/12	0.89	0.14	29,39,43,43	0
2	BGC	F	1	12/12	0.93	0.15	$35,\!46,\!50,\!53$	0
2	GLC	G	3	11/12	0.95	0.17	24,28,33,36	0
2	GLC	G	2	11/12	0.95	0.12	30,38,43,44	0
2	GLC	Е	3	11/12	0.96	0.12	24,26,28,29	0
2	GLC	F	2	11/12	0.96	0.12	23,28,30,32	0
2	GLC	Н	2	11/12	0.96	0.12	$27,\!29,\!31,\!33$	0
2	GLC	F	3	11/12	0.97	0.15	25,31,33,34	0
2	GLC	Е	2	11/12	0.97	0.10	22,26,30,33	0
2	GLC	Н	3	11/12	0.97	0.13	23,30,33,34	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	$B-factors(Å^2)$	Q<0.9
4	EDO	С	803	4/4	0.62	0.37	$41,\!43,\!53,\!54$	0
4	EDO	А	803	4/4	0.81	0.20	45,47,49,54	0
4	EDO	D	802	4/4	0.87	0.18	27,30,31,35	0
4	EDO	С	802	4/4	0.88	0.21	$27,\!27,\!27,\!31$	0
3	CA	А	801	1/1	0.93	0.05	37,37,37,37	0
4	EDO	В	802	4/4	0.94	0.13	32,36,38,41	0
5	MG	С	804	1/1	0.94	0.06	30,30,30,30	0
3	CA	В	801	1/1	0.95	0.05	46,46,46,46	0
4	EDO	А	802	4/4	0.95	0.20	$28,\!29,\!29,\!30$	0
5	MG	С	805	1/1	0.95	0.05	44,44,44,44	0
5	MG	А	804	1/1	0.97	0.03	$27,\!27,\!27,\!27$	0
3	CA	C	801	1/1	0.98	0.15	45,45,45,45	0
3	CA	D	801	1/1	0.99	0.06	39,39,39,39	0

6.5 Other polymers (i)

There are no such residues in this entry.

