

wwPDB X-ray Structure Validation Summary Report (i)

Jun 17, 2024 – 12:15 PM EDT

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This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org A user guide is available at https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

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

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

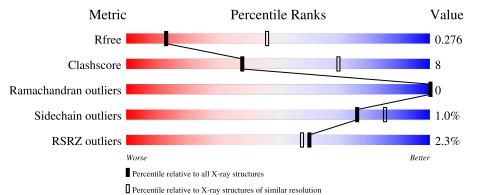
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.25 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	$\begin{array}{c} \textbf{Whole archive} \\ (\#\textbf{Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R_{free}	130704	1191 (3.30-3.22)
Clashscore	141614	1251 (3.30-3.22)
Ramachandran outliers	138981	1229 (3.30-3.22)
Sidechain outliers	138945	1228 (3.30-3.22)
RSRZ outliers	127900	1154 (3.30-3.22)

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						
			2%						
1	A	328	78%	21% •					
	D	1 - 0	.% ■						
2	В	173	84%	16%					
	тт	224	4%						
3	Н	226	81%	19%					
	т	014	2%						
4	L	214	80%	20%					
	0	9							
5	C	2	100%						



The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	NAG	С	2	-	-	-	Х



$8 \mathrm{TXM}$

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 7300 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 Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	А	326	Total 2544	C 1610	N 438	0 485	S 11	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	7	ALA	-	expression tag	UNP C3W5S1
А	8	ASP	-	expression tag	UNP C3W5S1
A	9	PRO	-	expression tag	UNP C3W5S1
А	10	GLY	-	expression tag	UNP C3W5S1

• Molecule 2 is a protein called Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	В	173	Total 1392	C 874	N 236	0 276	S 6	0	0	0

• Molecule 3 is a protein called GC_w13_B, Fab heavy chain.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
3	Н	226	Total 1664	C 1052	N 279	0 324	S 9	0	0	0

• Molecule 4 is a protein called GC_w13_B, Fab light chain.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
4	L	214	Total 1642	C 1023	N 279	O 335	${ m S}{ m 5}$	0	0	0

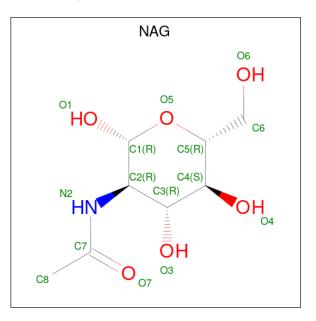
• Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-a cetamido-2-deoxy-beta-D-glucopyranose.





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
5	С	2	Total C N O 28 16 2 10	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	Atoms	ZeroOcc	AltConf
6	А	1	Total C N O 14 8 1 5	0	0
6	L	1	Total C N O 14 8 1 5	0	0

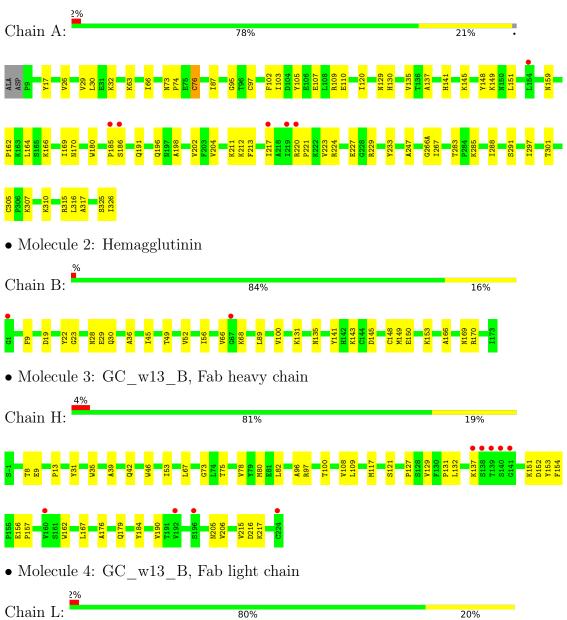
• Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	А	2	Total Mg 2 2	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: Hemagglutinin



DI 52 DI 155 DI 155 1155 125 1155 125 1155 125 1155 12 N159 88 8160 88 9161 121 9167 121 9167 121 9169 88 8183 88 9183 122 9183 123 1202 124 1203 124 1204 123 1205 124 1205 124 1206 124 1207 124 1208 936 1209 936 123 149 129 129 129 179 129 179 120 110 110 1110 1110 1110 1110 1110 1110 1110 1110

• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:

100%

NAG1 NAG2



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants a, b, c, α , β , γ	$\frac{167.53 \text{\AA}}{90.00^{\circ}} \frac{167.53 \text{\AA}}{90.00^{\circ}} \frac{167.53 \text{\AA}}{90.00^{\circ}}$	Depositor
Resolution (Å)	$\begin{array}{rrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrr$	Depositor EDS
% Data completeness	$100.0\ (44.77-3.25)$	Depositor
(in resolution range)	$100.0 \ (48.36 - 3.05)$	EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.14 (at 3.07 \text{\AA})$	Xtriage
Refinement program	PHENIX (1.19.2_4158: ???)	Depositor
R, R_{free}	$\begin{array}{rrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrr$	Depositor DCC
R_{free} test set	1509 reflections (5.02%)	wwPDB-VP
Wilson B-factor $(Å^2)$	92.4	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.29, 47.3	EDS
L-test for $twinning^2$	$< L > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.027 for l,-k,h	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	7300	wwPDB-VP
Average B, all atoms $(Å^2)$	99.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 1.92% 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: NAG, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with |Z| > 5 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond	lengths	Bond angles		
	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.24	0/2609	0.47	0/3546	
2	В	0.24	0/1420	0.41	0/1913	
3	Н	0.25	0/1701	0.47	0/2314	
4	L	0.24	0/1676	0.48	0/2276	
All	All	0.24	0/7406	0.46	0/10049	

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	2544	0	2497	49	0
2	В	1392	0	1318	18	0
3	Н	1664	0	1667	30	0
4	L	1642	0	1588	25	0
5	С	28	0	25	0	0
6	А	14	0	13	0	0
6	L	14	0	13	0	0
7	А	2	0	0	0	0
All	All	7300	0	7121	109	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 8.

The worst 5 of 109 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:HIS:HE1	1:A:164:LEU:HB3	1.40	0.87
4:L:4:GLN:H	4:L:27:ASN:HB2	1.43	0.82
3:H:100:THR:HG23	3:H:108:VAL:HG21	1.67	0.77
4:L:148:GLN:HB2	4:L:196:GLU:HB3	1.68	0.75
1:A:325:SER:O	1:A:326:ILE:HG23	1.86	0.74

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	А	324/328~(99%)	306~(94%)	18~(6%)	0	100 100
2	В	171/173~(99%)	169 (99%)	2(1%)	0	100 100
3	Н	224/226~(99%)	219~(98%)	5(2%)	0	100 100
4	L	212/214~(99%)	206 (97%)	6 (3%)	0	100 100
All	All	931/941~(99%)	900~(97%)	31 (3%)	0	100 100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.



Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	А	286/287~(100%)	283~(99%)	3~(1%)	76 85
2	В	148/148~(100%)	146~(99%)	2(1%)	67 81
3	Н	187/187~(100%)	186 (100%)	1 (0%)	88 93
4	L	187/187~(100%)	185~(99%)	2(1%)	73 84
All	All	808/809~(100%)	800~(99%)	8 (1%)	76 85

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	L	64	SER
4	L	2	ASP
2	В	148	CYS
2	В	22	TYR
3	Н	9	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	129	ASN
4	L	167	GLN

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)

2 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



Mol	Type	Chain	Res	Link	Bo	ond leng	ths	В	ond ang	les
	туре	Chain	nes	LIIIK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
5	NAG	С	1	5,1	14,14,15	0.38	0	$17,\!19,\!21$	0.46	0
5	NAG	С	2	5	14,14,15	0.26	0	17,19,21	0.54	0

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).

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.

Mo	bl	Type	Chain	Res	Link	Chirals	Torsions	Rings
5		NAG	С	1	5,1	-	0/6/23/26	0/1/1/1
5		NAG	С	2	5	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	С	2	NAG	C4-C5-C6-O6
5	С	2	NAG	O5-C5-C6-O6
5	С	2	NAG	C3-C2-N2-C7

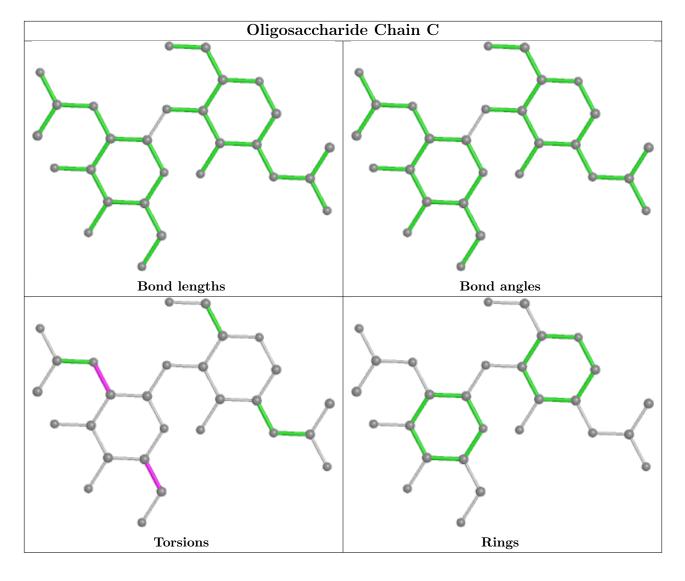
There are no ring outliers.

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 4 ligands modelled in this entry, 2 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	Mol Type Chai	Chain	Res	Link	Bo	ond leng	ths	Bond angles		
		Unam	nes	LIIIK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2
6	NAG	L	301	4	14,14,15	0.21	0	17,19,21	0.38	0
6	NAG	А	401	1	14,14,15	0.23	0	17,19,21	0.44	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.

N	Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
	6	NAG	L	301	4	-	2/6/23/26	0/1/1/1
	6	NAG	А	401	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	А	401	NAG	O5-C5-C6-O6
6	А	401	NAG	C4-C5-C6-O6
6	L	301	NAG	C8-C7-N2-C2
6	L	301	NAG	O7-C7-N2-C2

There are no ring outliers.

No monomer is involved in short contacts.

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	$\mathbf{OWAB}(\mathbf{\AA}^2)$	Q<0.9
1	А	326/328~(99%)	0.16	6 (1%) 68 65	53, 100, 157, 181	0
2	В	173/173~(100%)	0.23	2 (1%) 79 77	55, 86, 127, 139	0
3	Н	226/226~(100%)	0.12	9 (3%) 38 35	59, 95, 142, 160	0
4	L	214/214~(100%)	0.04	5 (2%) 60 58	68, 105, 137, 146	0
All	All	939/941~(99%)	0.14	22 (2%) 60 58	53, 95, 146, 181	0

The worst 5 of 22 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	А	219	ILE	5.0
1	А	185	PRO	4.8
3	Н	138	SER	4.7
4	L	46	ASN	4.0
2	В	1	GLY	3.6

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

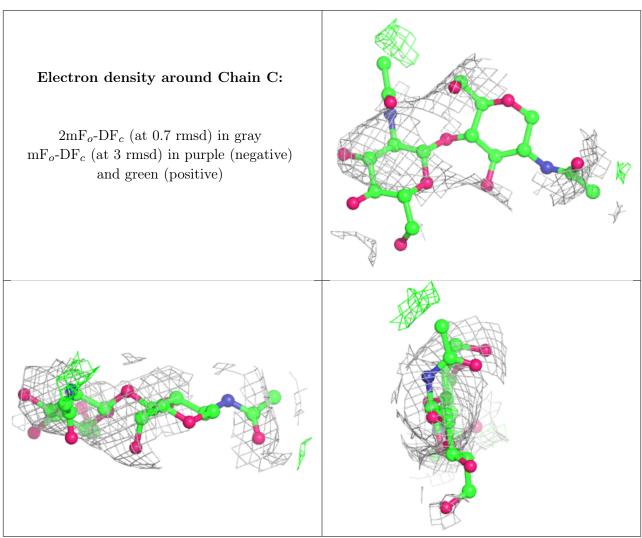
There are no non-standard protein/DNA/RNA residues in this entry.

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	\mathbf{RSR}	B-factors(Å ²)	Q < 0.9
5	NAG	С	2	14/15	0.72	0.52	138,146,151,152	0
5	NAG	С	1	14/15	0.86	0.16	94,111,130,132	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
6	NAG	L	301	14/15	0.69	0.23	96,101,106,106	0
6	NAG	А	401	14/15	0.78	0.28	70,83,97,97	0
7	MG	А	402	1/1	0.93	0.16	87,87,87,87	0
7	MG	А	403	1/1	0.93	0.35	66,66,66,66	0



6.5 Other polymers (i)

There are no such residues in this entry.

