



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 12:59 PM UTC

PDB ID : 9US3 / pdb_00009us3
Title : Klebsiella pneumoniae maltohexaose-producing alpha-amylase
Authors : Fujimoto, Z.; Kishine, N.; Momma, M.
Deposited on : 2025-05-01
Resolution : 1.90 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

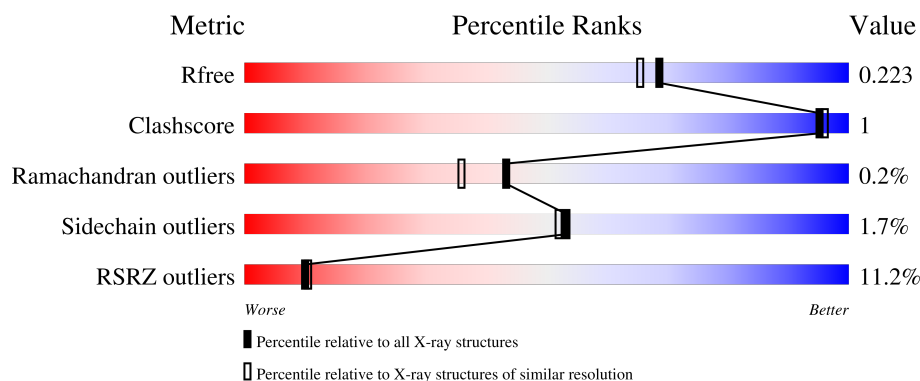
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	A	660	4% 95% ••
1	B	660	18% 93% 5% •

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11227 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 Maltohexaose-producing amylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	649	Total	C	N	O	S	0	3	0
			5173	3281	894	974	24			
1	B	651	Total	C	N	O	S	0	3	0
			5192	3292	902	974	24			

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Ca	0	0
			2	2		
2	B	2	Total	Ca	0	0
			2	2		

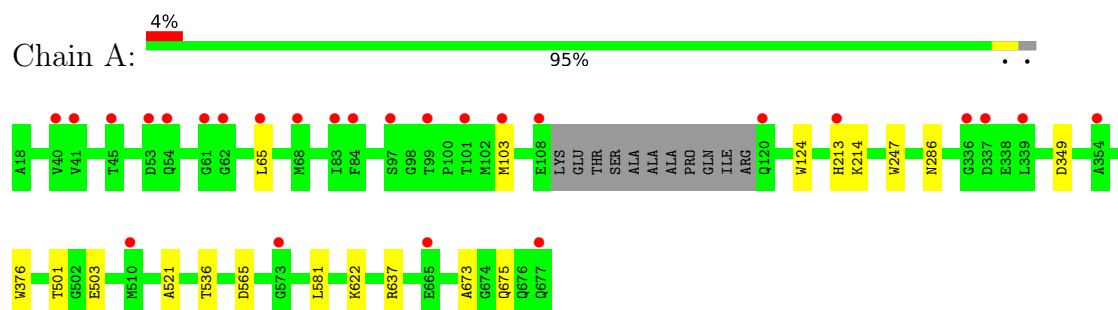
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	552	Total	O	0	0
			552	552		
3	B	306	Total	O	0	0
			306	306		

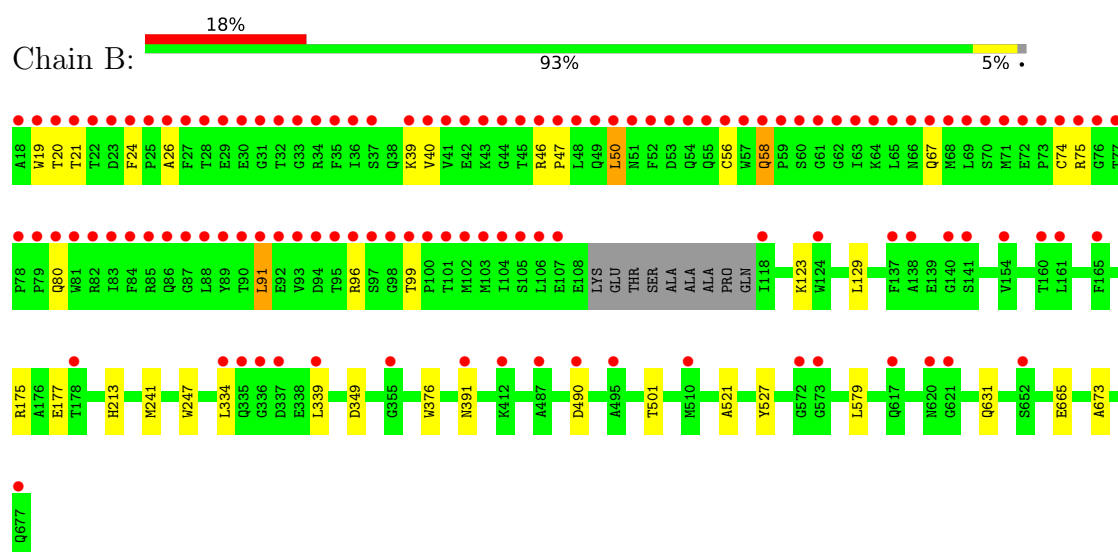
3 Residue-property plots

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: Maltohexaose-producing amylase



- Molecule 1: Maltohexaose-producing amylase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	74.73Å 107.84Å 82.36Å 90.00° 97.35° 90.00°	Depositor
Resolution (Å)	30.68 – 1.90 30.68 – 1.90	Depositor EDS
% Data completeness (in resolution range)	96.8 (30.68-1.90) 96.8 (30.68-1.90)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.64 (at 1.89Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.188 , 0.217 0.196 , 0.223	Depositor DCC
R_{free} test set	4923 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å ²)	19.9	Xtriage
Anisotropy	0.013	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 36.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	11227	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.91% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA

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	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.97	0/5333	1.29	0/7232
1	B	0.99	0/5355	1.33	0/7260
All	All	0.98	0/10688	1.31	0/14492

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

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	A	5173	0	4903	9	0
1	B	5192	0	4928	16	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	552	0	0	1	0
3	B	306	0	0	0	0
All	All	11227	0	9831	25	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 1.

All (25) 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:B:19:TRP:HE3	1:B:50:LEU:HD11	1.55	0.69
1:B:501:THR:HA	1:B:521:ALA:O	2.05	0.57
1:B:19:TRP:CE3	1:B:50:LEU:HD11	2.40	0.54
1:B:20:THR:HG22	1:B:26:ALA:HA	1.90	0.53
1:B:527:TYR:OH	1:B:579:LEU:O	2.19	0.51
1:A:501:THR:HA	1:A:521:ALA:O	2.10	0.51
1:B:213:HIS:HE1	1:B:349:ASP:OD1	1.96	0.49
1:B:241:MET:HA	1:B:631:GLN:HA	1.96	0.47
1:B:247:TRP:CD1	1:B:247:TRP:C	2.93	0.47
1:B:129:LEU:HD11	1:B:673:ALA:HB2	1.97	0.47
1:B:56:CYS:SG	1:B:58:GLN:OE1	2.73	0.46
1:B:24:PHE:CE2	1:B:91:LEU:HD21	2.50	0.46
1:B:213:HIS:CE1	1:B:349:ASP:OD1	2.68	0.46
1:B:21:THR:HB	1:B:50:LEU:HB2	1.97	0.46
1:B:490:ASP:OD1	1:B:490:ASP:N	2.49	0.46
1:A:213:HIS:CE1	1:A:349:ASP:OD1	2.70	0.45
1:B:47:PRO:HA	1:B:80:GLN:HA	1.99	0.44
1:B:175:ARG:NH2	1:B:665:GLU:O	2.50	0.44
1:A:124:TRP:CG	1:A:673:ALA:HB1	2.53	0.43
1:A:247:TRP:C	1:A:247:TRP:CD1	2.96	0.43
1:A:581:LEU:O	1:A:637:ARG:HD2	2.18	0.43
1:A:536:THR:O	1:A:675:GLN:NE2	2.53	0.42
1:A:214:LYS:NZ	3:A:801:HOH:O	2.32	0.42
1:A:103:MET:SD	1:A:622:LYS:HA	2.60	0.41
1:A:503:GLU:OE1	1:A:565[B]:ASP:OD2	2.39	0.41

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	A	648/660 (98%)	634 (98%)	13 (2%)	1 (0%)	43	36
1	B	650/660 (98%)	621 (96%)	28 (4%)	1 (0%)	43	36
All	All	1298/1320 (98%)	1255 (97%)	41 (3%)	2 (0%)	43	36

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	376	TRP
1	B	376	TRP

5.3.2 Protein sidechains ⓘ

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	A	535/540 (99%)	533 (100%)	2 (0%)	84	87
1	B	537/540 (99%)	521 (97%)	16 (3%)	36	30
All	All	1072/1080 (99%)	1054 (98%)	18 (2%)	53	52

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	65	LEU
1	A	286	ASN
1	B	39	LYS
1	B	40	VAL
1	B	46	ARG
1	B	50	LEU
1	B	58	GLN
1	B	67	GLN
1	B	74	CYS
1	B	75	ARG
1	B	91	LEU
1	B	96	ARG
1	B	99	THR
1	B	123	LYS

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Mol	Chain	Res	Type
1	B	177	GLU
1	B	334	LEU
1	B	339	LEU
1	B	391	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	GLN
1	A	49	GLN
1	A	55	GLN
1	A	86	GLN
1	A	120	GLN
1	A	208	ASN
1	A	362	ASN
1	A	391	ASN
1	A	511	GLN
1	B	38	GLN
1	B	67	GLN
1	B	120	GLN
1	B	150	ASN
1	B	162	GLN
1	B	213	HIS
1	B	362	ASN
1	B	511	GLN
1	B	675	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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, 95th 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	A	649/660 (98%)	0.08	26 (4%)	42 45	9, 17, 38, 56	3 (0%)
1	B	651/660 (98%)	0.94	119 (18%)	3 3	15, 27, 95, 109	3 (0%)
All	All	1300/1320 (98%)	0.51	145 (11%)	10 10	9, 21, 86, 109	6 (0%)

All (145) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	41	VAL	8.2
1	B	48	LEU	7.4
1	B	19	TRP	6.2
1	B	81	TRP	6.2
1	B	103	MET	6.1
1	B	104	ILE	5.8
1	B	74	CYS	5.7
1	B	57	TRP	5.6
1	B	93	VAL	5.4
1	B	63	ILE	5.3
1	B	50	LEU	5.1
1	B	36	ILE	5.1
1	B	73	PRO	5.0
1	B	106	LEU	4.9
1	B	65	LEU	4.9
1	B	78	PRO	4.9
1	B	79	PRO	4.9
1	B	88	LEU	4.8
1	B	68	MET	4.8
1	B	18	ALA	4.8
1	B	26	ALA	4.7
1	B	27	PHE	4.7
1	B	52	PHE	4.6
1	B	83	ILE	4.6

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Mol	Chain	Res	Type	RSRZ
1	B	84	PHE	4.5
1	B	76	GLY	4.4
1	A	510	MET	4.4
1	B	59	PRO	4.4
1	B	24	PHE	4.3
1	B	64	LYS	4.2
1	B	77	THR	4.2
1	B	102	MET	4.2
1	B	101	THR	4.2
1	B	35	PHE	4.1
1	B	510	MET	4.1
1	B	47	PRO	4.1
1	B	62	GLY	4.1
1	B	91	LEU	4.1
1	B	69	LEU	4.1
1	B	95	THR	4.0
1	A	354	ALA	4.0
1	B	34[A]	ARG	4.0
1	B	40	VAL	4.0
1	B	45	THR	4.0
1	B	90	THR	4.0
1	B	89	TYR	4.0
1	B	100	PRO	4.0
1	B	54	GLN	3.9
1	B	339	LEU	3.8
1	B	22	THR	3.8
1	B	21	THR	3.8
1	A	62	GLY	3.7
1	B	98	GLY	3.7
1	B	20	THR	3.7
1	B	51	ASN	3.7
1	B	99	THR	3.7
1	B	28	THR	3.6
1	B	53	ASP	3.6
1	B	573	GLY	3.6
1	B	97	SER	3.5
1	B	82	ARG	3.5
1	B	80	GLN	3.5
1	B	335	GLN	3.4
1	B	87	GLY	3.4
1	B	140	GLY	3.4
1	B	55	GLN	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	105	SER	3.4
1	B	56	CYS	3.4
1	B	46	ARG	3.3
1	B	49	GLN	3.3
1	A	84	PHE	3.3
1	B	71	MET	3.2
1	B	44	GLY	3.2
1	B	92	GLU	3.2
1	B	334	LEU	3.1
1	B	75	ARG	3.0
1	B	25	PRO	3.0
1	B	138	ALA	3.0
1	A	53	ASP	3.0
1	B	72	GLU	3.0
1	B	621	GLY	3.0
1	B	677	GLN	2.9
1	A	83	ILE	2.9
1	A	97	SER	2.9
1	B	31	GLY	2.9
1	A	336	GLY	2.9
1	B	67	GLN	2.8
1	B	37	SER	2.8
1	B	495	ALA	2.8
1	A	45	THR	2.8
1	B	70	SER	2.8
1	B	336	GLY	2.8
1	A	99	THR	2.8
1	B	85	ARG	2.7
1	B	32	THR	2.7
1	B	337	ASP	2.6
1	A	677	GLN	2.6
1	B	572	GLY	2.6
1	B	29	GLU	2.6
1	A	54	GLN	2.6
1	B	58	GLN	2.5
1	B	118	ILE	2.5
1	B	96	ARG	2.5
1	B	86	GLN	2.5
1	B	490	ASP	2.5
1	A	68	MET	2.5
1	A	65	LEU	2.5
1	B	61	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	30	GLU	2.5
1	A	337	ASP	2.5
1	B	94	ASP	2.5
1	A	120	GLN	2.4
1	B	66	ASN	2.4
1	B	391	ASN	2.4
1	B	412	LYS	2.4
1	B	107	GLU	2.3
1	B	161	LEU	2.3
1	B	160	THR	2.3
1	B	355	GLY	2.3
1	B	620	ASN	2.3
1	B	165	PHE	2.3
1	B	652	SER	2.3
1	A	41	VAL	2.3
1	A	665	GLU	2.2
1	B	154	VAL	2.2
1	B	39	LYS	2.2
1	B	487	ALA	2.2
1	B	43	LYS	2.2
1	A	108	GLU	2.2
1	B	60	SER	2.2
1	B	137	PHE	2.2
1	B	42	GLU	2.2
1	B	617	GLN	2.1
1	B	141	SER	2.1
1	A	339	LEU	2.1
1	B	23	ASP	2.1
1	A	61	GLY	2.1
1	A	573	GLY	2.1
1	A	103	MET	2.1
1	A	101	THR	2.1
1	A	213	HIS	2.1
1	A	40	VAL	2.1
1	B	124	TRP	2.1
1	B	178	THR	2.0
1	B	33	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

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, 95th 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($\text{\AA}^2$)	Q<0.9
2	CA	A	702	1/1	0.98	0.02	13,13,13,13	0
2	CA	B	702	1/1	0.99	0.03	17,17,17,17	0
2	CA	B	701	1/1	1.00	0.03	16,16,16,16	0
2	CA	A	701	1/1	1.00	0.01	12,12,12,12	0

6.5 Other polymers [i](#)

There are no such residues in this entry.