



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:54 PM UTC

PDB ID : 7ZS6 / pdb_00007zs6
Title : Crystal structure of Apis mellifera RidA
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Deposited on : 2022-05-06
Resolution : 1.31 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
Mogul : 2022.3.0, CSD as543be (2022)
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

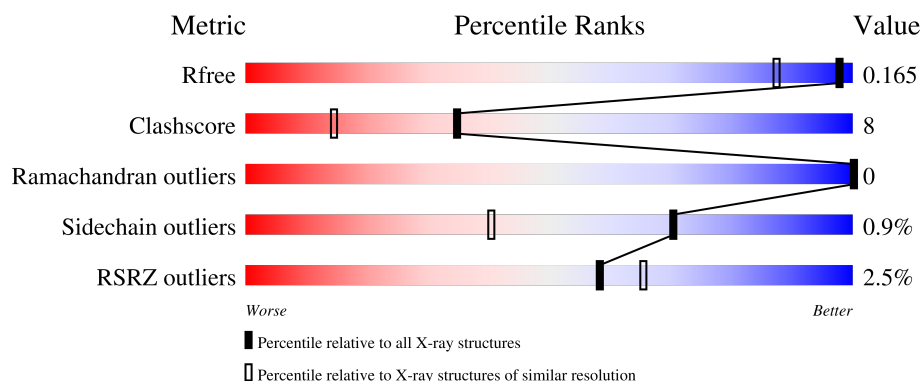
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.31 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	2531 (1.34-1.30)
Clashscore	190562	2585 (1.34-1.30)
Ramachandran outliers	187476	2528 (1.34-1.30)
Sidechain outliers	187428	2528 (1.34-1.30)
RSRZ outliers	180081	2528 (1.34-1.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	AAA	140	4% 79% 15% • 5%
1	BBB	140	% 82% 12% • 5%
1	CCC	140	2% 76% 16% • 5%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 3991 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 Reactive intermediate deaminase A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	133	Total	C	N	O	S	4	27	0
			1176	775	182	214	5			
1	BBB	133	Total	C	N	O	S	0	31	0
			1221	807	190	219	5			
1	CCC	133	Total	C	N	O	S	0	23	0
			1167	772	179	211	5			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	-2	GLY	-	expression tag	UNP A0A7M7GBQ0
AAA	-1	SER	-	expression tag	UNP A0A7M7GBQ0
AAA	0	HIS	-	expression tag	UNP A0A7M7GBQ0
BBB	-2	GLY	-	expression tag	UNP A0A7M7GBQ0
BBB	-1	SER	-	expression tag	UNP A0A7M7GBQ0
BBB	0	HIS	-	expression tag	UNP A0A7M7GBQ0
CCC	-2	GLY	-	expression tag	UNP A0A7M7GBQ0
CCC	-1	SER	-	expression tag	UNP A0A7M7GBQ0
CCC	0	HIS	-	expression tag	UNP A0A7M7GBQ0

- Molecule 2 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	BBB	1	Total	C	O	0	0
			4	2	2		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	BBB	1	Total	Mg	0	0
			1	1		

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	BBB	1	Total	Na	0	0
			1	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	AAA	144	Total	O	0	1
			145	145		
5	BBB	160	Total	O	0	0
			160	160		
5	CCC	116	Total	O	0	0
			116	116		

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: Reactive intermediate deaminase A

Chain AAA: 



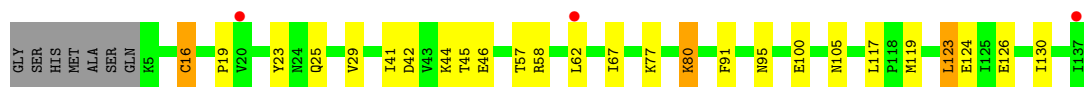
- Molecule 1: Reactive intermediate deaminase A

Chain BBB: 



- Molecule 1: Reactive intermediate deaminase A

Chain CCC: 



4 Data and refinement statistics

Property	Value	Source
Space group	I 41 2 2	Depositor
Cell constants a, b, c, α , β , γ	109.50Å 109.50Å 141.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.30 – 1.31 43.30 – 1.31	Depositor EDS
% Data completeness (in resolution range)	99.4 (43.30-1.31) 99.5 (43.30-1.31)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.42 (at 1.31Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.131 , 0.164 0.130 , 0.165	Depositor DCC
R_{free} test set	5097 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	18.7	Xtriage
Anisotropy	0.121	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 41.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	3991	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.28% 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: NA, EDO, 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	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	AAA	1.07	1/1265 (0.1%)	1.13	0/1714
1	BBB	0.97	0/1315	1.01	2/1776 (0.1%)
1	CCC	1.07	0/1246	1.20	7/1689 (0.4%)
All	All	1.04	1/3826 (0.0%)	1.12	9/5179 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AAA	137	ILE	C-OXT	5.84	1.35	1.23

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	CCC	16[A]	CYS	CB-CA-C	6.82	119.14	108.63
1	CCC	16[B]	CYS	CB-CA-C	6.82	119.14	108.63
1	CCC	105	ASN	OD1-CG-ND2	6.66	129.25	122.60
1	CCC	80	LYS	CG-CD-CE	5.75	124.53	111.30
1	CCC	44	LYS	CA-C-O	-5.50	114.67	120.55
1	CCC	42	ASP	CA-CB-CG	5.28	117.88	112.60
1	CCC	105	ASN	N-CA-C	-5.15	104.28	111.39
1	BBB	16[A]	CYS	CB-CA-C	-5.11	103.02	109.31
1	BBB	16[B]	CYS	CB-CA-C	-5.11	103.02	109.31

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	AAA	1176	0	1296	24	0
1	BBB	1221	0	1348	21	0
1	CCC	1167	0	1268	22	0
2	BBB	4	0	6	2	0
3	BBB	1	0	0	0	0
4	BBB	1	0	0	0	0
5	AAA	145	0	0	2	0
5	BBB	160	0	0	5	0
5	CCC	116	0	0	3	0
All	All	3991	0	3918	56	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.

All (56) 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:CCC:58[A]:ARG:NH2	1:CCC:100[A]:GLU:OE2	1.90	1.04
1:BBB:74[A]:ASN:OD1	1:BBB:76[A]:ASN:OD1	1.82	0.96
1:AAA:22:PRO:HD2	1:CCC:95[B]:ASN:OD1	1.66	0.96
1:AAA:22:PRO:CD	1:CCC:95[B]:ASN:OD1	2.17	0.93
1:AAA:16[B]:CYS:SG	1:AAA:67[B]:ILE:HG13	2.12	0.90
1:CCC:41:ILE:HD11	1:CCC:119[B]:MET:HE1	1.60	0.83
1:BBB:79[B]:ILE:HD12	1:CCC:29[B]:VAL:HG21	1.64	0.80
1:BBB:16[B]:CYS:SG	1:BBB:67[B]:ILE:HG13	2.23	0.78
1:BBB:16[B]:CYS:SG	1:BBB:66:HIS:HB2	2.23	0.78
1:BBB:116[B]:LYS:HD3	5:BBB:735:HOH:O	1.87	0.75
1:BBB:137:ILE:OXT	5:BBB:601:HOH:O	2.04	0.73
1:AAA:80[B]:LYS:HZ1	1:BBB:126[B]:GLU:CD	1.98	0.71
1:BBB:49[B]:VAL:HG22	2:BBB:501:EDO:O2	1.92	0.70
1:AAA:79[B]:ILE:HD12	1:BBB:29[B]:VAL:HG21	1.78	0.64
1:AAA:80[B]:LYS:HB3	1:AAA:128[B]:ILE:HG22	1.79	0.63
1:AAA:51:GLY:O	5:AAA:202:HOH:O	2.15	0.63
1:CCC:58[A]:ARG:HH22	1:CCC:100[A]:GLU:CD	2.02	0.62
1:CCC:45:THR:HG21	5:CCC:202:HOH:O	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CCC:117[A]:LEU:HD23	1:CCC:124[A]:GLU:HB2	1.86	0.58
1:CCC:16[A]:CYS:SG	1:CCC:67[A]:ILE:HD11	2.46	0.55
1:AAA:5:LYS:HE3	1:AAA:7:ILE:HD11	1.88	0.55
1:AAA:16[B]:CYS:HB2	1:AAA:25[B]:GLN:NE2	2.23	0.54
1:AAA:80[B]:LYS:HB3	1:AAA:128[B]:ILE:CG2	2.37	0.54
1:AAA:22:PRO:CG	1:CCC:95[B]:ASN:OD1	2.56	0.54
1:CCC:41:ILE:CD1	1:CCC:119[B]:MET:HE1	2.33	0.53
1:AAA:95[B]:ASN:OD1	1:AAA:109:ARG:NH1	2.41	0.53
1:AAA:41:ILE:HD11	1:AAA:119[A]:MET:SD	2.49	0.53
1:AAA:6:THR:HG21	1:CCC:130[B]:ILE:HG21	1.92	0.52
1:AAA:29[A]:VAL:HG11	1:CCC:130[A]:ILE:HD11	1.92	0.52
1:BBB:123[B]:LEU:C	1:BBB:123[B]:LEU:HD22	2.36	0.51
1:AAA:16[B]:CYS:SG	1:AAA:66:HIS:HB2	2.52	0.50
1:BBB:18[A]:LYS:HE3	5:BBB:612:HOH:O	2.12	0.49
1:AAA:22:PRO:HD3	1:CCC:95[B]:ASN:HD21	1.77	0.48
1:CCC:62[B]:LEU:HD12	5:CCC:268:HOH:O	2.14	0.47
1:BBB:69[B]:LYS:NZ	5:BBB:602:HOH:O	2.33	0.47
1:CCC:25:GLN:OE1	1:CCC:67[B]:ILE:HD12	2.15	0.47
1:CCC:19:PRO:HB3	1:CCC:23[B]:TYR:CE2	2.50	0.47
1:BBB:79[A]:ILE:HD11	1:BBB:130[A]:ILE:HG12	1.98	0.46
1:BBB:116[B]:LYS:HE3	1:BBB:116[B]:LYS:HB2	1.73	0.46
1:AAA:95[B]:ASN:ND2	5:AAA:204:HOH:O	2.49	0.45
1:BBB:46[A]:GLU:HG2	5:BBB:715:HOH:O	2.17	0.44
1:CCC:45:THR:O	1:CCC:46[B]:GLU:HG2	2.18	0.44
1:CCC:57:THR:HA	1:CCC:123[B]:LEU:HD11	1.98	0.43
1:AAA:12[B]:SER:HA	1:AAA:25[B]:GLN:OE1	2.17	0.43
1:BBB:49[B]:VAL:CG2	2:BBB:501:EDO:O2	2.64	0.43
1:AAA:137:ILE:HG13	1:BBB:9[B]:LYS:HG3	2.00	0.43
1:AAA:17:PRO:HG2	1:AAA:41:ILE:HB	2.01	0.42
1:AAA:22:PRO:CD	1:CCC:95[B]:ASN:CG	2.92	0.42
1:AAA:61:LEU:HD23	1:AAA:61:LEU:HA	1.93	0.42
1:CCC:126[A]:GLU:HA	5:CCC:255:HOH:O	2.19	0.42
1:BBB:79[A]:ILE:CG1	1:BBB:130[A]:ILE:HG12	2.50	0.42
1:BBB:74[A]:ASN:CG	1:BBB:76[A]:ASN:OD1	2.61	0.41
1:CCC:77:LYS:O	1:CCC:130[B]:ILE:HG13	2.21	0.41
1:BBB:70[B]:GLU:OE2	1:BBB:70[B]:GLU:HA	2.21	0.40

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	AAA	158/140 (113%)	153 (97%)	5 (3%)	0	100	100
1	BBB	163/140 (116%)	159 (98%)	4 (2%)	0	100	100
1	CCC	154/140 (110%)	150 (97%)	4 (3%)	0	100	100
All	All	475/420 (113%)	462 (97%)	13 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	AAA	141/119 (118%)	141 (100%)	0	100	100
1	BBB	146/119 (123%)	146 (100%)	0	100	100
1	CCC	136/119 (114%)	131 (96%)	5 (4%)	30	3
All	All	423/357 (118%)	418 (99%)	5 (1%)	70	28

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	CCC	80	LYS
1	CCC	91[A]	PHE
1	CCC	91[B]	PHE
1	CCC	123[A]	LEU
1	CCC	123[B]	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 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).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	EDO	BBB	501	-	3,3,3	1.60	1 (33%)	2,2,2	0.18	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	BBB	501	-	-	1/1/1/1	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	BBB	501	EDO	O2-C2	2.42	1.54	1.42

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	BBB	501	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
2	BBB	501	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, 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	AAA	133/140 (95%)	-0.01	5 (3%)	44 52	8, 19, 38, 67	27 (20%)
1	BBB	133/140 (95%)	-0.19	2 (1%)	72 78	8, 17, 36, 66	32 (24%)
1	CCC	133/140 (95%)	0.16	3 (2%)	61 68	9, 21, 50, 73	23 (17%)
All	All	399/420 (95%)	-0.01	10 (2%)	58 65	8, 19, 43, 73	82 (20%)

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	20[A]	VAL	6.1
1	CCC	20	VAL	4.2
1	AAA	21	GLY	3.5
1	AAA	7	ILE	3.3
1	CCC	137	ILE	3.2
1	BBB	137	ILE	3.0
1	AAA	137	ILE	2.8
1	CCC	62[A]	LEU	2.7
1	AAA	19	PRO	2.6
1	BBB	20[A]	VAL	2.2

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](#)

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(Å ²)	Q<0.9
2	EDO	BBB	501	4/4	0.83	0.16	31,34,56,63	0
4	NA	BBB	503	1/1	0.89	0.28	46,46,46,46	0
3	MG	BBB	502	1/1	1.00	0.01	13,13,13,13	1

6.5 Other polymers [i](#)

There are no such residues in this entry.