



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 21, 2021 – 11:03 am BST

PDB ID : 6XTD
Title : Rhs1-CT in complex with cognate immunity protein RhsI1
Authors : Hagan, M.R.; Hunter, B.; Coulthurst, S.
Deposited on : 2020-01-16
Resolution : 1.30 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 following versions of software and data (see [references ⓘ](#)) 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 : 2.22
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) : 2.22

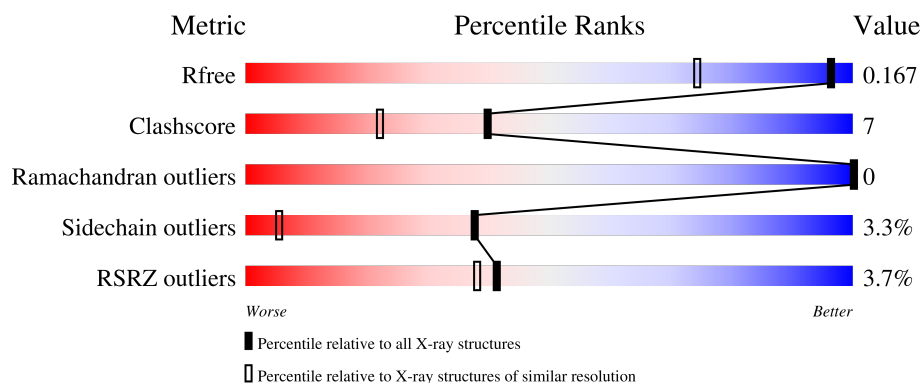
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.30 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}	130704	1058 (1.30-1.30)
Clashscore	141614	1101 (1.30-1.30)
Ramachandran outliers	138981	1058 (1.30-1.30)
Sidechain outliers	138945	1058 (1.30-1.30)
RSRZ outliers	127900	1029 (1.30-1.30)

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	155	<div> <div style="width: 100%; height: 10px; background-color: red; position: relative;"> % </div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> 74% 11% • 15% </div> </div>
2	BBB	163	<div> <div style="width: 100%; height: 10px; background-color: red; position: relative;"> 6% </div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> 87% 12% • </div> </div>

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	BR	AAA	1502	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 2847 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 Putative deoxyribonuclease RhsA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	132	Total	C	N	O	S	0	5	0
			1069	681	191	196	1			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	1319	MET	-	initiating methionine	UNP A0A1C3HFI3
AAA	1320	GLY	-	expression tag	UNP A0A1C3HFI3
AAA	1321	SER	-	expression tag	UNP A0A1C3HFI3
AAA	1322	SER	-	expression tag	UNP A0A1C3HFI3
AAA	1323	HIS	-	expression tag	UNP A0A1C3HFI3
AAA	1324	HIS	-	expression tag	UNP A0A1C3HFI3
AAA	1325	HIS	-	expression tag	UNP A0A1C3HFI3
AAA	1326	HIS	-	expression tag	UNP A0A1C3HFI3
AAA	1327	HIS	-	expression tag	UNP A0A1C3HFI3
AAA	1328	HIS	-	expression tag	UNP A0A1C3HFI3
AAA	1329	SER	-	expression tag	UNP A0A1C3HFI3
AAA	1330	GLN	-	expression tag	UNP A0A1C3HFI3
AAA	1331	ASP	-	expression tag	UNP A0A1C3HFI3
AAA	1332	PRO	-	expression tag	UNP A0A1C3HFI3

- Molecule 2 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	BBB	163	Total	C	N	O	S	0	10	0
			1366	877	226	254	9			

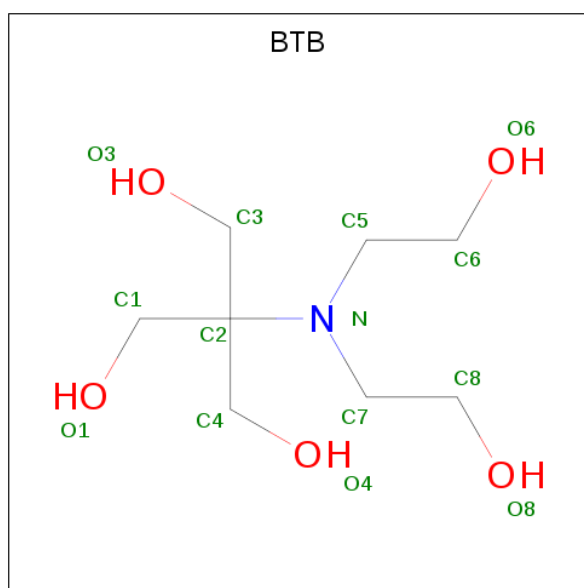
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BBB	1	MET	-	initiating methionine	UNP A0A2G8A4T5

- Molecule 3 is BROMIDE ION (three-letter code: BR) (formula: Br).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	AAA	2	Total	Br	0	0
			2	2		
3	BBB	4	Total	Br	0	0
			4	4		

- Molecule 4 is 2-[BIS-(2-HYDROXY-ETHYL)-AMINO]-2-HYDROXYMETHYL-PROPAN E-1,3-DIOL (three-letter code: BTB) (formula: C₈H₁₉NO₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	AAA	1	Total	C	N	O	0	0
			14	8	1	5		

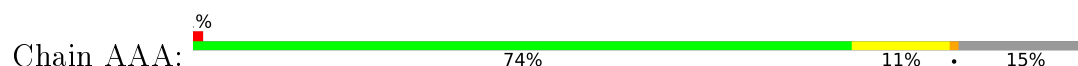
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	AAA	187	Total	O	0	0
			187	187		
5	BBB	205	Total	O	0	0
			205	205		

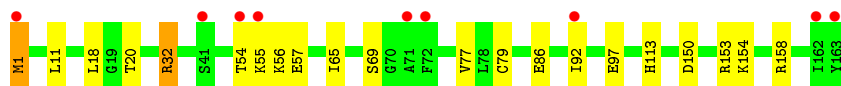
3 Residue-property plots [i](#)

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: Putative deoxyribonuclease RhsA



- Molecule 2: Uncharacterized protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	39.66Å 44.11Å 46.81Å 101.20° 96.13° 114.15°	Depositor
Resolution (Å)	35.42 – 1.30 35.39 – 1.30	Depositor EDS
% Data completeness (in resolution range)	96.0 (35.42-1.30) 96.1 (35.39-1.30)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.16 (at 1.30Å)	Xtriage
Refinement program	REFMAC 5.8.0257	Depositor
R, R_{free}	0.121 , 0.165 0.122 , 0.167	Depositor DCC
R_{free} test set	3327 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	14.3	Xtriage
Anisotropy	0.148	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 47.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	2847	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.73% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.94	1/1107 (0.1%)	1.01	3/1486 (0.2%)
2	BBB	0.96	1/1425 (0.1%)	1.12	5/1925 (0.3%)
All	All	0.95	2/2532 (0.1%)	1.07	8/3411 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	BBB	97	GLU	CD-OE1	5.49	1.31	1.25
1	AAA	1463	GLU	CD-OE2	5.21	1.31	1.25

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	BBB	158	ARG	NE-CZ-NH1	12.08	126.34	120.30
2	BBB	32	ARG	NE-CZ-NH1	-9.36	115.62	120.30
2	BBB	153	ARG	NE-CZ-NH2	-7.65	116.48	120.30
2	BBB	158	ARG	NE-CZ-NH2	-7.49	116.55	120.30
1	AAA	1425	ARG	NE-CZ-NH2	-5.80	117.40	120.30
1	AAA	1458	TYR	CB-CG-CD2	-5.78	117.53	121.00
2	BBB	158	ARG	CD-NE-CZ	5.21	130.90	123.60
1	AAA	1343	ASP	CB-CG-OD1	-5.04	113.76	118.30

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	AAA	1069	0	1053	13	0
2	BBB	1366	0	1373	23	0
3	AAA	2	0	0	2	0
3	BBB	4	0	0	2	0
4	AAA	14	0	19	1	0
5	AAA	187	0	0	3	0
5	BBB	205	0	0	10	0
All	All	2847	0	2445	36	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 7.

All (36) 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)
2:BBB:69[B]:SER:OG	2:BBB:79[B]:CYS:SG	1.97	1.16
2:BBB:77[A]:VAL:HG13	5:BBB:317:HOH:O	1.52	1.09
2:BBB:54:THR:HG22	5:BBB:422:HOH:O	1.53	1.07
3:BBB:204:BR:BR	5:BBB:440:HOH:O	2.37	0.95
2:BBB:55:LYS:HG3	5:BBB:356:HOH:O	1.66	0.95
2:BBB:54:THR:HG21	5:BBB:454:HOH:O	1.70	0.90
2:BBB:150[B]:ASP:OD1	3:BBB:201:BR:BR	2.51	0.84
1:AAA:1375:ILE:HD12	1:AAA:1465:ILE:HD11	1.60	0.83
1:AAA:1342:ASN:HA	5:AAA:1699:HOH:O	1.80	0.81
1:AAA:1413:GLU:HG3	2:BBB:65[B]:ILE:CD1	2.19	0.73
1:AAA:1459:LYS:HD3	5:BBB:307:HOH:O	1.90	0.70
2:BBB:150[B]:ASP:OD2	2:BBB:154:LYS:NZ	2.23	0.70
2:BBB:77[A]:VAL:CG1	5:BBB:317:HOH:O	2.24	0.68
1:AAA:1413:GLU:HG3	2:BBB:65[B]:ILE:HD11	1.78	0.64
1:AAA:1342:ASN:N	1:AAA:1457:ASN:ND2	2.46	0.64
2:BBB:11:LEU:HD23	2:BBB:18:LEU:HD12	1.84	0.58
2:BBB:54:THR:HG21	2:BBB:57:GLU:HB2	1.85	0.57
1:AAA:1375:ILE:HD12	1:AAA:1465:ILE:CD1	2.32	0.56
2:BBB:150[B]:ASP:OD1	2:BBB:154:LYS:NZ	2.40	0.55
2:BBB:54:THR:CG2	5:BBB:454:HOH:O	2.40	0.53
2:BBB:150[B]:ASP:CG	2:BBB:154:LYS:NZ	2.61	0.53
4:AAA:1503:BTB:H82	4:AAA:1503:BTB:H61	1.94	0.50
2:BBB:54:THR:CG2	2:BBB:57:GLU:HB3	2.42	0.50
2:BBB:54:THR:HG21	2:BBB:57:GLU:CB	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:BBB:54:THR:CG2	5:BBB:422:HOH:O	2.33	0.49
1:AAA:1436:LYS:HE3	5:AAA:1628:HOH:O	2.13	0.49
1:AAA:1441[B]:ASP:HA	3:AAA:1502:BR:BR	2.70	0.46
5:AAA:1616:HOH:O	2:BBB:92:ILE:HD12	2.15	0.45
2:BBB:54:THR:CG2	2:BBB:57:GLU:CB	2.96	0.44
2:BBB:20:THR:O	2:BBB:77[A]:VAL:CG2	2.66	0.44
1:AAA:1402[B]:LYS:HB3	1:AAA:1402[B]:LYS:HE3	1.44	0.43
1:AAA:1342:ASN:N	1:AAA:1457:ASN:HD21	2.17	0.42
1:AAA:1369:MET:CG	1:AAA:1429:GLU:HG2	2.49	0.42
1:AAA:1441[A]:ASP:HA	3:AAA:1502:BR:BR	2.74	0.42
2:BBB:32:ARG:NH2	2:BBB:32:ARG:HG3	2.35	0.41
2:BBB:1:MET:N	5:BBB:314:HOH:O	2.52	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	AAA	135/155 (87%)	132 (98%)	3 (2%)	0	100	100
2	BBB	171/163 (105%)	168 (98%)	3 (2%)	0	100	100
All	All	306/318 (96%)	300 (98%)	6 (2%)	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	108/122 (88%)	103 (95%)	5 (5%)	27	2
2	BBB	149/139 (107%)	145 (97%)	4 (3%)	44	9
All	All	257/261 (98%)	248 (96%)	9 (4%)	38	5

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

Mol	Chain	Res	Type
1	AAA	1342	ASN
1	AAA	1362[A]	ARG
1	AAA	1362[B]	ARG
1	AAA	1420	LYS
1	AAA	1467	LYS
2	BBB	1	MET
2	BBB	56	LYS
2	BBB	86	GLU
2	BBB	113	HIS

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

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 7 ligands modelled in this entry, 6 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
4	BTB	AAA	1503	-	13,13,13	1.36	1 (7%)	7,16,16	0.52	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	BTB	AAA	1503	-	-	3/21/21/21	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	AAA	1503	BTB	C5-N	4.47	1.54	1.48

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	AAA	1503	BTB	C4-C2-C3-O3
4	AAA	1503	BTB	N-C2-C3-O3
4	AAA	1503	BTB	C1-C2-C3-O3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	AAA	1503	BTB	1	0

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 [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	132/155 (85%)	-0.02	2 (1%) 73 75	11, 16, 34, 63	0
2	BBB	163/163 (100%)	0.17	9 (5%) 25 22	10, 19, 37, 68	0
All	All	295/318 (92%)	0.08	11 (3%) 41 38	10, 17, 36, 68	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	BBB	162	ILE	7.0
2	BBB	54	THR	4.6
2	BBB	163	TYR	4.1
2	BBB	72	PHE	3.9
2	BBB	55	LYS	3.9
1	AAA	1342	ASN	3.8
2	BBB	41	SER	3.3
2	BBB	71	ALA	2.5
2	BBB	1	MET	2.4
1	AAA	1343	ASP	2.2
2	BBB	92	ILE	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 monosaccharides 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(\AA^2)	Q<0.9
3	BR	BBB	202	1/1	0.83	0.16	43,43,43,43	1
4	BTB	AAA	1503	14/14	0.95	0.08	14,17,23,28	0
3	BR	BBB	203	1/1	0.98	0.11	34,34,34,34	1
3	BR	BBB	201	1/1	0.99	0.15	29,29,29,29	1
3	BR	BBB	204	1/1	0.99	0.14	41,41,41,41	1
3	BR	AAA	1502	1/1	0.99	0.07	44,44,44,44	1
3	BR	AAA	1501	1/1	1.00	0.09	24,24,24,24	1

6.5 Other polymers [i](#)

There are no such residues in this entry.