



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 11, 2022 – 10:10 am BST

PDB ID : 7O5T
Title : Crystal Structure of a Class D Carbapenemase Complexed with Bromide
Authors : Zhou, Q.; He, Y.; Jin, Y.
Deposited on : 2021-04-09
Resolution : 1.81 Å(reported)

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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.27
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0267
CCP4 : 7.1.010 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.27

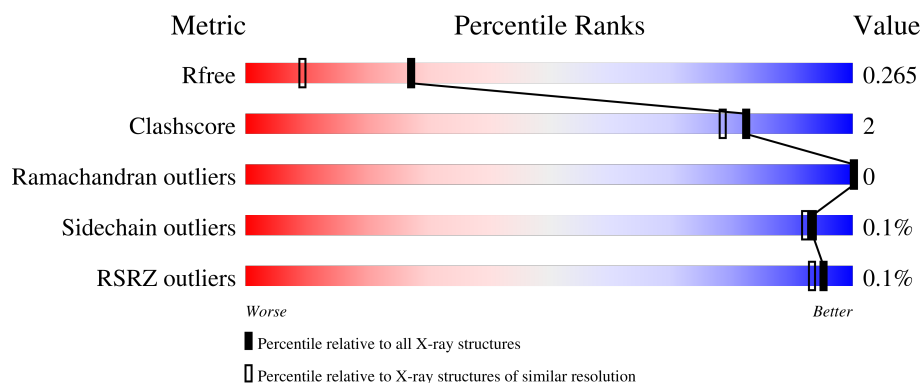
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.81 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	7484 (1.84-1.80)
Clashscore	141614	8401 (1.84-1.80)
Ramachandran outliers	138981	8290 (1.84-1.80)
Sidechain outliers	138945	8290 (1.84-1.80)
RSRZ outliers	127900	7371 (1.84-1.80)

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	260	<div> <div>90%</div> <div>6%</div> </div>
1	BBB	260	<div> <div>89%</div> <div>5%</div> <div>6%</div> </div>
1	CCC	260	<div> <div>88%</div> <div>6%</div> <div>7%</div> </div>
1	DDD	260	<div> <div>88%</div> <div>6%</div> <div>6%</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
2	BR	AAA	302[A]	-	-	X	-
2	BR	AAA	302[B]	-	-	X	-
2	BR	BBB	302[B]	-	-	X	-
2	BR	BBB	304[B]	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 16683 atoms, of which 7905 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 Beta-lactamase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	AAA	244	Total	C	H	N	O	S	48	3	0
			3998	1283	1979	356	373	7			
1	BBB	244	Total	C	H	N	O	S	49	3	0
			3992	1281	1976	355	372	8			
1	CCC	243	Total	C	H	N	O	S	47	2	0
			3985	1279	1976	354	368	8			
1	DDD	245	Total	C	H	N	O	S	47	1	0
			3987	1280	1974	355	370	8			

There are 68 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	6	MET	-	initiating methionine	UNP A0A482LRD5
AAA	7	HIS	-	expression tag	UNP A0A482LRD5
AAA	8	HIS	-	expression tag	UNP A0A482LRD5
AAA	9	HIS	-	expression tag	UNP A0A482LRD5
AAA	10	HIS	-	expression tag	UNP A0A482LRD5
AAA	11	HIS	-	expression tag	UNP A0A482LRD5
AAA	12	HIS	-	expression tag	UNP A0A482LRD5
AAA	13	SER	-	expression tag	UNP A0A482LRD5
AAA	14	ALA	-	expression tag	UNP A0A482LRD5
AAA	15	GLY	-	expression tag	UNP A0A482LRD5
AAA	16	GLU	-	expression tag	UNP A0A482LRD5
AAA	17	ASN	-	expression tag	UNP A0A482LRD5
AAA	18	LEU	-	expression tag	UNP A0A482LRD5
AAA	19	TYR	-	expression tag	UNP A0A482LRD5
AAA	20	PHE	-	expression tag	UNP A0A482LRD5
AAA	21	GLN	-	expression tag	UNP A0A482LRD5
AAA	22	GLY	-	expression tag	UNP A0A482LRD5
BBB	6	MET	-	initiating methionine	UNP A0A482LRD5
BBB	7	HIS	-	expression tag	UNP A0A482LRD5
BBB	8	HIS	-	expression tag	UNP A0A482LRD5
BBB	9	HIS	-	expression tag	UNP A0A482LRD5

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Chain	Residue	Modelled	Actual	Comment	Reference
BBB	10	HIS	-	expression tag	UNP A0A482LRD5
BBB	11	HIS	-	expression tag	UNP A0A482LRD5
BBB	12	HIS	-	expression tag	UNP A0A482LRD5
BBB	13	SER	-	expression tag	UNP A0A482LRD5
BBB	14	ALA	-	expression tag	UNP A0A482LRD5
BBB	15	GLY	-	expression tag	UNP A0A482LRD5
BBB	16	GLU	-	expression tag	UNP A0A482LRD5
BBB	17	ASN	-	expression tag	UNP A0A482LRD5
BBB	18	LEU	-	expression tag	UNP A0A482LRD5
BBB	19	TYR	-	expression tag	UNP A0A482LRD5
BBB	20	PHE	-	expression tag	UNP A0A482LRD5
BBB	21	GLN	-	expression tag	UNP A0A482LRD5
BBB	22	GLY	-	expression tag	UNP A0A482LRD5
CCC	6	MET	-	initiating methionine	UNP A0A482LRD5
CCC	7	HIS	-	expression tag	UNP A0A482LRD5
CCC	8	HIS	-	expression tag	UNP A0A482LRD5
CCC	9	HIS	-	expression tag	UNP A0A482LRD5
CCC	10	HIS	-	expression tag	UNP A0A482LRD5
CCC	11	HIS	-	expression tag	UNP A0A482LRD5
CCC	12	HIS	-	expression tag	UNP A0A482LRD5
CCC	13	SER	-	expression tag	UNP A0A482LRD5
CCC	14	ALA	-	expression tag	UNP A0A482LRD5
CCC	15	GLY	-	expression tag	UNP A0A482LRD5
CCC	16	GLU	-	expression tag	UNP A0A482LRD5
CCC	17	ASN	-	expression tag	UNP A0A482LRD5
CCC	18	LEU	-	expression tag	UNP A0A482LRD5
CCC	19	TYR	-	expression tag	UNP A0A482LRD5
CCC	20	PHE	-	expression tag	UNP A0A482LRD5
CCC	21	GLN	-	expression tag	UNP A0A482LRD5
CCC	22	GLY	-	expression tag	UNP A0A482LRD5
DDD	6	MET	-	initiating methionine	UNP A0A482LRD5
DDD	7	HIS	-	expression tag	UNP A0A482LRD5
DDD	8	HIS	-	expression tag	UNP A0A482LRD5
DDD	9	HIS	-	expression tag	UNP A0A482LRD5
DDD	10	HIS	-	expression tag	UNP A0A482LRD5
DDD	11	HIS	-	expression tag	UNP A0A482LRD5
DDD	12	HIS	-	expression tag	UNP A0A482LRD5
DDD	13	SER	-	expression tag	UNP A0A482LRD5
DDD	14	ALA	-	expression tag	UNP A0A482LRD5
DDD	15	GLY	-	expression tag	UNP A0A482LRD5
DDD	16	GLU	-	expression tag	UNP A0A482LRD5
DDD	17	ASN	-	expression tag	UNP A0A482LRD5

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Chain	Residue	Modelled	Actual	Comment	Reference
DDD	18	LEU	-	expression tag	UNP A0A482LRD5
DDD	19	TYR	-	expression tag	UNP A0A482LRD5
DDD	20	PHE	-	expression tag	UNP A0A482LRD5
DDD	21	GLN	-	expression tag	UNP A0A482LRD5
DDD	22	GLY	-	expression tag	UNP A0A482LRD5

- Molecule 2 is BROMIDE ION (three-letter code: BR) (formula: Br).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	AAA	4	Total Br 5 5	0	1
2	BBB	4	Total Br 6 6	0	2
2	CCC	1	Total Br 1 1	0	0
2	DDD	1	Total Br 1 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	AAA	193	Total O 193 193	0	0
3	BBB	198	Total O 198 198	0	0
3	CCC	168	Total O 168 168	0	0
3	DDD	148	Total O 149 149	0	1

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: Beta-lactamase

Chain AAA:  90% 6%



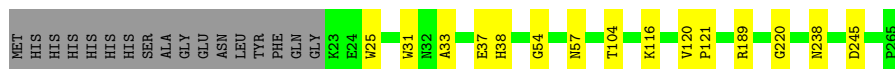
- Molecule 1: Beta-lactamase

Chain BBB:  89% 5% 6%



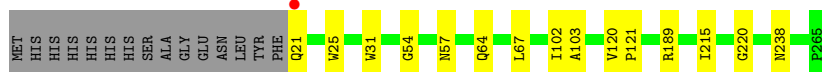
- Molecule 1: Beta-lactamase

Chain CCC:  88% 6% 7%



- Molecule 1: Beta-lactamase

Chain DDD:  88% 6% 6%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	82.57Å 107.26Å 124.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	81.30 – 1.81 81.30 – 1.81	Depositor EDS
% Data completeness (in resolution range)	99.8 (81.30-1.81) 99.8 (81.30-1.81)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.70 (at 1.81Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.187 , 0.261 0.194 , 0.265	Depositor DCC
R_{free} test set	5093 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	20.7	Xtriage
Anisotropy	1.022	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	(Not available) , (Not available)	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	16683	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 39.33 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.2245e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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, KCX

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	0.76	0/2055	0.81	0/2776
1	BBB	0.79	0/2052	0.84	1/2772 (0.0%)
1	CCC	0.77	0/2045	0.82	0/2762
1	DDD	0.75	0/2049	0.81	0/2768
All	All	0.77	0/8201	0.82	1/11078 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	BBB	159	ASP	CB-CG-OD2	-5.43	113.41	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	2019	1979	1967	6	0
1	BBB	2016	1976	1964	10	0
1	CCC	2009	1976	1965	10	0
1	DDD	2013	1974	1964	11	0
2	AAA	5	0	0	4	0
2	BBB	6	0	0	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	CCC	1	0	0	0	0
2	DDD	1	0	0	0	0
3	AAA	193	0	0	2	0
3	BBB	198	0	0	1	0
3	CCC	168	0	0	3	0
3	DDD	149	0	0	4	0
All	All	8778	7905	7860	39	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 2.

The worst 5 of 39 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:AAA:302[A]:BR:BR	3:AAA:563:HOH:O	2.39	0.94
2:BBB:302[B]:BR:BR	3:BBB:587:HOH:O	2.46	0.88
1:BBB:137:LYS:HE2	2:BBB:304[B]:BR:BR	2.30	0.86
1:BBB:137:LYS:CE	2:BBB:304[B]:BR:BR	2.96	0.68
1:BBB:137:LYS:HE3	2:BBB:304[A]:BR:BR	2.53	0.63

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	AAA	244/260 (94%)	237 (97%)	7 (3%)	0	100	100
1	BBB	244/260 (94%)	237 (97%)	7 (3%)	0	100	100
1	CCC	242/260 (93%)	237 (98%)	5 (2%)	0	100	100
1	DDD	243/260 (94%)	238 (98%)	5 (2%)	0	100	100
All	All	973/1040 (94%)	949 (98%)	24 (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	214/225 (95%)	214 (100%)	0	100	100
1	BBB	214/225 (95%)	214 (100%)	0	100	100
1	CCC	213/225 (95%)	212 (100%)	1 (0%)	88	87
1	DDD	213/225 (95%)	213 (100%)	0	100	100
All	All	854/900 (95%)	853 (100%)	1 (0%)	93	92

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	CCC	245	ASP

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 ⓘ

4 non-standard protein/DNA/RNA residues 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	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	KCX	AAA	73	1	7,11,12	0.52	0	4,12,14	0.70	0
1	KCX	CCC	73	1	7,11,12	0.52	0	4,12,14	0.67	0
1	KCX	BBB	73	1	7,11,12	0.49	0	4,12,14	0.66	0
1	KCX	DDD	73	1	7,11,12	0.48	0	4,12,14	0.71	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
1	KCX	AAA	73	1	-	0/7/10/12	-
1	KCX	CCC	73	1	-	0/7/10/12	-
1	KCX	BBB	73	1	-	0/7/10/12	-
1	KCX	DDD	73	1	-	0/7/10/12	-

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.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 13 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 [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	243/260 (93%)	-0.47	0 100 100	19, 27, 38, 60	12 (4%)
1	BBB	243/260 (93%)	-0.52	0 100 100	17, 25, 39, 69	11 (4%)
1	CCC	242/260 (93%)	-0.45	0 100 100	18, 28, 43, 64	13 (5%)
1	DDD	244/260 (93%)	-0.42	1 (0%) 92 91	19, 30, 46, 67	18 (7%)
All	All	972/1040 (93%)	-0.47	1 (0%) 95 93	17, 27, 42, 69	54 (5%)

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	DDD	21	GLN	2.2

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	KCX	DDD	73	12/13	0.96	0.09	24,31,34,43	1
1	KCX	BBB	73	12/13	0.97	0.10	18,23,24,25	1
1	KCX	CCC	73	12/13	0.97	0.09	20,27,29,31	1
1	KCX	AAA	73	12/13	0.97	0.07	21,25,28,28	1

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands

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	BR	AAA	303	1/1	0.98	0.04	46,46,46,46	1
2	BR	AAA	302[B]	1/1	0.99	0.07	41,41,41,41	1
2	BR	AAA	302[A]	1/1	0.99	0.07	22,22,22,22	1
2	BR	AAA	304	1/1	0.99	0.02	39,39,39,39	1
2	BR	BBB	302[A]	1/1	0.99	0.12	34,34,34,34	1
2	BR	BBB	302[B]	1/1	0.99	0.12	36,36,36,36	1
2	BR	BBB	303	1/1	0.99	0.02	42,42,42,42	1
2	BR	BBB	304[A]	1/1	0.99	0.07	43,43,43,43	1
2	BR	BBB	304[B]	1/1	0.99	0.07	47,47,47,47	1
2	BR	DDD	301	1/1	0.99	0.03	44,44,44,44	1
2	BR	AAA	301	1/1	1.00	0.02	33,33,33,33	0
2	BR	CCC	301	1/1	1.00	0.02	40,40,40,40	1
2	BR	BBB	301	1/1	1.00	0.01	29,29,29,29	0

6.5 Other polymers

There are no such residues in this entry.