



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 14, 2022 – 09:09 am GMT

PDB ID : 6Z6D
Title : Crystal structure of the HK97 bacteriophage large terminase
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Deposited on : 2020-05-28
Resolution : 2.20 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 : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.31.3
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) : 2.31.3

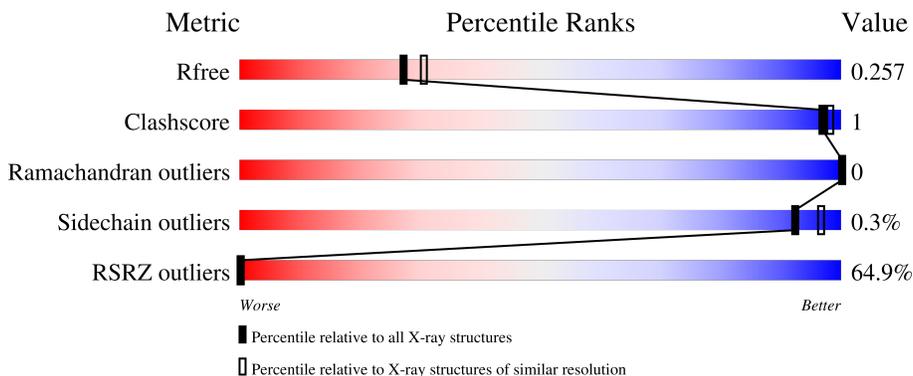
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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	514	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 3633 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 Terminase large subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	479	3522	2242	600	660	20	0	0	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-9	MET	-	initiating methionine	UNP Q9MCT1
A	-8	GLY	-	expression tag	UNP Q9MCT1
A	-7	SER	-	expression tag	UNP Q9MCT1
A	-6	SER	-	expression tag	UNP Q9MCT1
A	-5	HIS	-	expression tag	UNP Q9MCT1
A	-4	HIS	-	expression tag	UNP Q9MCT1
A	-3	HIS	-	expression tag	UNP Q9MCT1
A	-2	HIS	-	expression tag	UNP Q9MCT1
A	-1	HIS	-	expression tag	UNP Q9MCT1
A	0	HIS	-	expression tag	UNP Q9MCT1

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	17	Total	Br	0	1
			18	18		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	93	Total	O	0	0
			93	93		

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	211.79Å 39.15Å 65.45Å 90.00° 103.39° 90.00°	Depositor
Resolution (Å)	103.23 – 2.20 45.53 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.5 (103.23-2.20) 99.6 (45.53-2.20)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.45 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.205 , 0.254 0.211 , 0.257	Depositor DCC
R_{free} test set	1244 reflections (4.64%)	wwPDB-VP
Wilson B-factor (Å ²)	35.1	Xtriage
Anisotropy	0.371	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	0.95	EDS
Total number of atoms	3633	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.94% 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

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	0.40	0/3591	0.61	0/4895

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	A	3522	0	3404	6	0
2	A	18	0	0	1	0
3	A	93	0	0	0	0
All	All	3633	0	3404	6	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 (6) 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:71:HIS:O	2:A:607:BR:BR	2.84	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:194:LEU:HD21	1:A:198:TRP:CZ2	2.52	0.45
1:A:61:THR:HG22	1:A:99:LEU:HD23	1.99	0.44
1:A:78:VAL:HG23	1:A:81:THR:HG21	2.02	0.41
1:A:194:LEU:HD21	1:A:198:TRP:CH2	2.55	0.41
1:A:71:HIS:CG	1:A:149:LEU:HD22	2.57	0.40

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	A	475/514 (92%)	463 (98%)	12 (2%)	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	A	349/424 (82%)	348 (100%)	1 (0%)	92 97

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

Mol	Chain	Res	Type
1	A	162	GLN

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

Mol	Chain	Res	Type
1	A	162	GLN
1	A	266	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 18 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

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	479/514 (93%)	2.64	311 (64%) 0 0	23, 36, 65, 92	0

All (311) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	369	VAL	9.7
1	A	142	THR	9.0
1	A	467	THR	8.8
1	A	368	PHE	8.0
1	A	144	GLY	7.5
1	A	366	TYR	7.2
1	A	143	HIS	7.1
1	A	11	ILE	6.7
1	A	141	THR	6.3
1	A	139	GLY	6.2
1	A	334	LYS	6.0
1	A	367	SER	5.9
1	A	393	ASP	5.8
1	A	361	GLY	5.7
1	A	319	ASP	5.7
1	A	401	ALA	5.7
1	A	394	GLN	5.6
1	A	348	ASP	5.6
1	A	255	MET	5.5
1	A	363	SER	5.5
1	A	69	LEU	5.4
1	A	483	ALA	5.4
1	A	360	PRO	5.3
1	A	336	LEU	5.3
1	A	399	ALA	5.2
1	A	374	ALA	5.2
1	A	337	GLU	5.2

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Mol	Chain	Res	Type	RSRZ
1	A	478	MET	5.1
1	A	145	LEU	5.0
1	A	428	LEU	5.0
1	A	140	LYS	5.0
1	A	108	PRO	4.9
1	A	335	THR	4.9
1	A	7	VAL	4.8
1	A	320	ASP	4.8
1	A	333	GLN	4.7
1	A	468	GLY	4.6
1	A	273	THR	4.6
1	A	303	LEU	4.6
1	A	466	ALA	4.5
1	A	354	GLY	4.5
1	A	160	GLY	4.5
1	A	378	GLY	4.4
1	A	306	ARG	4.4
1	A	347	TYR	4.4
1	A	377	ILE	4.3
1	A	256	PRO	4.3
1	A	365	ASP	4.3
1	A	237	GLY	4.3
1	A	351	VAL	4.3
1	A	364	VAL	4.3
1	A	166	ILE	4.2
1	A	199	ILE	4.2
1	A	441	VAL	4.1
1	A	67	ILE	4.0
1	A	293	THR	4.0
1	A	422	VAL	4.0
1	A	402	ILE	4.0
1	A	222	ASP	3.9
1	A	342	THR	3.9
1	A	358	THR	3.9
1	A	383	THR	3.9
1	A	395	PHE	3.9
1	A	177	GLU	3.9
1	A	376	ILE	3.9
1	A	349	VAL	3.9
1	A	387	PHE	3.8
1	A	318	ALA	3.8
1	A	432	GLY	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	346	PRO	3.8
1	A	375	GLU	3.8
1	A	271	VAL	3.8
1	A	2	THR	3.7
1	A	63	LEU	3.7
1	A	96	VAL	3.7
1	A	110	LEU	3.7
1	A	398	ASP	3.7
1	A	307	ASN	3.7
1	A	341	LYS	3.7
1	A	442	LEU	3.7
1	A	116	ILE	3.7
1	A	275	SER	3.7
1	A	350	TRP	3.7
1	A	396	ARG	3.7
1	A	73	VAL	3.7
1	A	219	LYS	3.6
1	A	64	ILE	3.6
1	A	207	ASP	3.6
1	A	279	SER	3.6
1	A	23	ILE	3.6
1	A	390	TRP	3.6
1	A	61	THR	3.6
1	A	8	ILE	3.6
1	A	72	LEU	3.6
1	A	381	ASP	3.6
1	A	161	PRO	3.6
1	A	113	ILE	3.5
1	A	248	GLN	3.5
1	A	425	LEU	3.5
1	A	244	ASP	3.5
1	A	397	LYS	3.4
1	A	276	PRO	3.4
1	A	175	ALA	3.4
1	A	16	ILE	3.4
1	A	235	ALA	3.4
1	A	18	PRO	3.3
1	A	26	PRO	3.3
1	A	470	ILE	3.3
1	A	331	THR	3.3
1	A	440	PRO	3.3
1	A	128	CYS	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	304	SER	3.2
1	A	392	ILE	3.2
1	A	339	ARG	3.2
1	A	119	SER	3.2
1	A	254	ARG	3.2
1	A	261	THR	3.2
1	A	54	ILE	3.2
1	A	373	ILE	3.2
1	A	359	THR	3.2
1	A	27	MET	3.2
1	A	184	ILE	3.2
1	A	321	GLY	3.2
1	A	101	VAL	3.2
1	A	477	THR	3.2
1	A	38	LEU	3.2
1	A	249	ALA	3.2
1	A	340	THR	3.1
1	A	43	ASN	3.1
1	A	288	GLU	3.1
1	A	408	LEU	3.1
1	A	343	ASP	3.1
1	A	123	LEU	3.1
1	A	380	PHE	3.1
1	A	99	LEU	3.1
1	A	194	LEU	3.1
1	A	25	GLN	3.1
1	A	24	GLY	3.1
1	A	449	ALA	3.1
1	A	447	VAL	3.1
1	A	400	ASP	3.1
1	A	431	ASN	3.0
1	A	50	ALA	3.0
1	A	308	ASP	3.0
1	A	229	TRP	3.0
1	A	93	ALA	3.0
1	A	252	ALA	3.0
1	A	106	LEU	3.0
1	A	167	ASP	3.0
1	A	291	ILE	3.0
1	A	481	GLY	3.0
1	A	285	LEU	3.0
1	A	78	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	126	LEU	3.0
1	A	362	ALA	3.0
1	A	457	GLY	3.0
1	A	238	THR	3.0
1	A	45	ALA	2.9
1	A	42	ASP	2.9
1	A	443	THR	2.9
1	A	95	ILE	2.9
1	A	100	ALA	2.9
1	A	221	ALA	2.9
1	A	420	PRO	2.9
1	A	471	ASP	2.9
1	A	36	PHE	2.9
1	A	114	VAL	2.9
1	A	357	ARG	2.9
1	A	278	ILE	2.8
1	A	316	GLY	2.8
1	A	88	LEU	2.8
1	A	332	PRO	2.8
1	A	224	SER	2.8
1	A	282	VAL	2.8
1	A	305	ALA	2.8
1	A	212	CYS	2.8
1	A	197	ILE	2.8
1	A	183	VAL	2.8
1	A	482	ALA	2.8
1	A	198	TRP	2.8
1	A	480	VAL	2.8
1	A	68	LEU	2.8
1	A	186	THR	2.8
1	A	310	THR	2.8
1	A	32	PHE	2.7
1	A	352	ARG	2.8
1	A	423	ASP	2.7
1	A	195	LEU	2.7
1	A	309	LEU	2.7
1	A	105	ASN	2.7
1	A	44	PRO	2.7
1	A	205	SER	2.7
1	A	223	ILE	2.7
1	A	427	SER	2.7
1	A	40	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	170	THR	2.7
1	A	463	LYS	2.7
1	A	66	GLY	2.7
1	A	382	LEU	2.7
1	A	430	LEU	2.7
1	A	294	PRO	2.7
1	A	9	ALA	2.7
1	A	155	THR	2.7
1	A	267	LEU	2.7
1	A	286	CYS	2.6
1	A	146	SER	2.6
1	A	196	SER	2.6
1	A	344	ARG	2.6
1	A	474	VAL	2.6
1	A	103	MET	2.6
1	A	178	ASN	2.6
1	A	465	LYS	2.6
1	A	124	ILE	2.6
1	A	47	THR	2.6
1	A	434	VAL	2.6
1	A	208	PRO	2.6
1	A	65	ALA	2.6
1	A	312	LEU	2.6
1	A	94	ALA	2.6
1	A	75	PRO	2.6
1	A	245	MET	2.5
1	A	200	ASP	2.5
1	A	17	VAL	2.5
1	A	429	MET	2.5
1	A	152	LEU	2.5
1	A	370	VAL	2.5
1	A	52	LEU	2.5
1	A	281	SER	2.5
1	A	329	PHE	2.5
1	A	384	SER	2.5
1	A	338	GLU	2.5
1	A	151	ILE	2.4
1	A	241	SER	2.4
1	A	461	LEU	2.4
1	A	181	LEU	2.4
1	A	176	HIS	2.4
1	A	353	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	372	ASP	2.4
1	A	168	ALA	2.4
1	A	439	HIS	2.4
1	A	182	ILE	2.4
1	A	330	TRP	2.4
1	A	356	LEU	2.4
1	A	234	PRO	2.4
1	A	456	ALA	2.4
1	A	148	ILE	2.3
1	A	132	TYR	2.3
1	A	284	GLU	2.3
1	A	323	TRP	2.3
1	A	258	PHE	2.3
1	A	415	PHE	2.3
1	A	437	GLY	2.3
1	A	218	PRO	2.3
1	A	149	LEU	2.3
1	A	246	ALA	2.3
1	A	473	MET	2.3
1	A	388	ASP	2.3
1	A	169	ILE	2.3
1	A	127	PRO	2.3
1	A	211	VAL	2.3
1	A	74	GLY	2.3
1	A	300	GLY	2.3
1	A	80	ASN	2.3
1	A	135	LEU	2.3
1	A	475	ALA	2.3
1	A	355	LEU	2.3
1	A	424	THR	2.3
1	A	84	VAL	2.3
1	A	192	ALA	2.3
1	A	452	VAL	2.2
1	A	162	GLN	2.2
1	A	37	ILE	2.2
1	A	236	LEU	2.2
1	A	379	ASP	2.2
1	A	445	CYS	2.2
1	A	134	ALA	2.2
1	A	29	LEU	2.2
1	A	476	MET	2.2
1	A	159	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	272	SER	2.2
1	A	417	ASP	2.2
1	A	460	LYS	2.2
1	A	257	SER	2.2
1	A	410	GLU	2.2
1	A	414	GLY	2.2
1	A	188	ALA	2.1
1	A	202	ALA	2.1
1	A	421	ALA	2.1
1	A	130	VAL	2.1
1	A	409	VAL	2.1
1	A	455	ALA	2.1
1	A	15	CYS	2.1
1	A	419	GLY	2.1
1	A	472	GLY	2.1
1	A	10	PHE	2.1
1	A	79	GLN	2.1
1	A	406	LEU	2.1
1	A	226	ARG	2.1
1	A	451	VAL	2.1
1	A	97	PHE	2.1
1	A	165	PHE	2.1
1	A	277	PHE	2.1
1	A	163	ASP	2.1
1	A	313	VAL	2.1
1	A	403	GLY	2.1
1	A	418	MET	2.0
1	A	250	GLU	2.0
1	A	405	SER	2.0
1	A	391	ARG	2.0
1	A	173	GLN	2.0
1	A	446	ALA	2.0

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(Å ²)	Q<0.9
2	BR	A	615	1/1	0.36	0.36	92,92,92,92	0
2	BR	A	612	1/1	0.61	0.29	99,99,99,99	0
2	BR	A	610	1/1	0.63	0.26	35,35,35,35	1
2	BR	A	613	1/1	0.75	0.24	91,91,91,91	0
2	BR	A	614	1/1	0.81	0.25	77,77,77,77	0
2	BR	A	616	1/1	0.81	0.38	94,94,94,94	0
2	BR	A	617	1/1	0.83	0.17	85,85,85,85	0
2	BR	A	605[B]	1/1	0.87	0.10	41,41,41,41	1
2	BR	A	605[A]	1/1	0.87	0.10	41,41,41,41	1
2	BR	A	602	1/1	0.88	0.30	40,40,40,40	1
2	BR	A	607	1/1	0.90	0.24	19,19,19,19	1
2	BR	A	611	1/1	0.90	0.15	30,30,30,30	1
2	BR	A	608	1/1	0.91	0.25	29,29,29,29	1
2	BR	A	604	1/1	0.93	0.32	37,37,37,37	1
2	BR	A	603	1/1	0.95	0.14	30,30,30,30	1
2	BR	A	609	1/1	0.95	0.12	31,31,31,31	1
2	BR	A	606	1/1	0.96	0.18	32,32,32,32	1
2	BR	A	601	1/1	0.97	0.08	44,44,44,44	0

6.5 Other polymers [i](#)

There are no such residues in this entry.