



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 08:58 PM GMT

PDB ID : 1MWU
Title : Structure of methicillin acyl-Penicillin binding protein 2a from methicillin resistant *Staphylococcus aureus* strain 27r at 2.60 Å resolution.
Authors : Lim, D.C.; Strynadka, N.C.J.
Deposited on : 2002-10-01
Resolution : 2.60 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
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

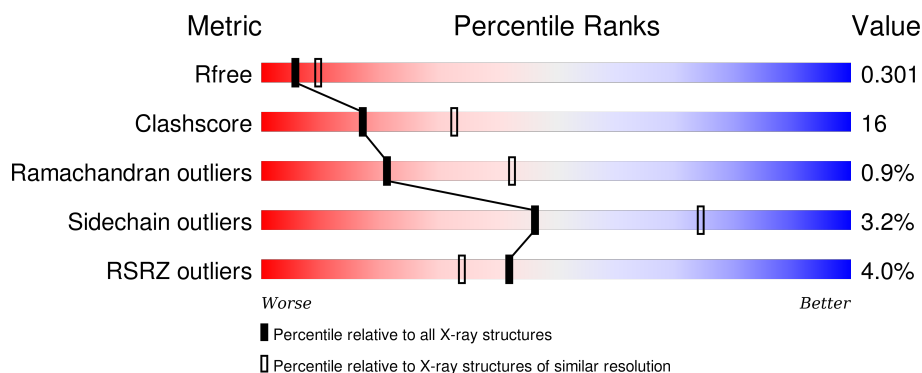
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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}	91344	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	646	<div> <div>2%</div> <div>63%</div> <div>33%</div> <div>• •</div> </div>
1	B	646	<div> <div>5%</div> <div>61%</div> <div>31%</div> <div>• 6%</div> </div>

2 Entry composition [i](#)

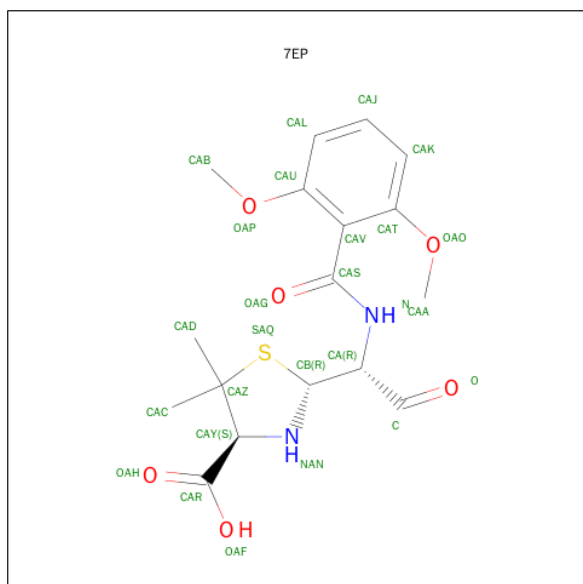
There are 5 unique types of molecules in this entry. The entry contains 10109 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 penicillin-binding protein 2a.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	632	Total	C	N	O	S	0	0	0
			5077	3202	853	1007	15			
1	B	609	Total	C	N	O	S	0	0	0
			4904	3099	822	969	14			

- Molecule 2 is (2R,4S)-2-[(1R)-1-[(2,6-DIMETHOXYPHENYL)CARBONYL]AMINO}-2-OXOETHYL]-5,5-DIMETHYL-1,3-THIAZOLIDINE-4-CARBOXYLIC ACID (three-letter code: 7EP) (formula: C₁₇H₂₂N₂O₆S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			26	17	2	6	1		
2	B	1	Total	C	N	O	S	0	0
			26	17	2	6	1		

- Molecule 3 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	3	Total 3	Cd 3	0	0
3	A	2	Total 2	Cd 2	0	0

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	3	Total 3	Cl 3	0	0
4	A	1	Total 1	Cl 1	0	0

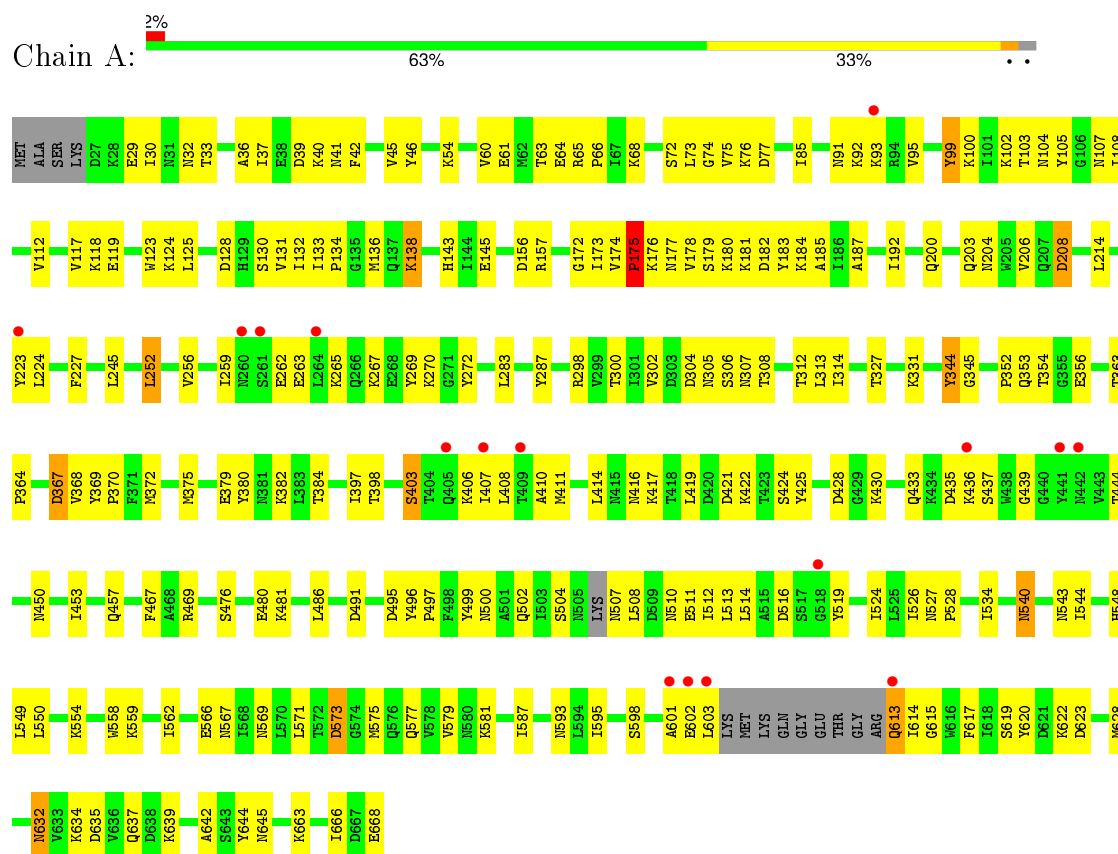
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	42	Total 42	O 42	0	0
5	B	25	Total 25	O 25	0	0

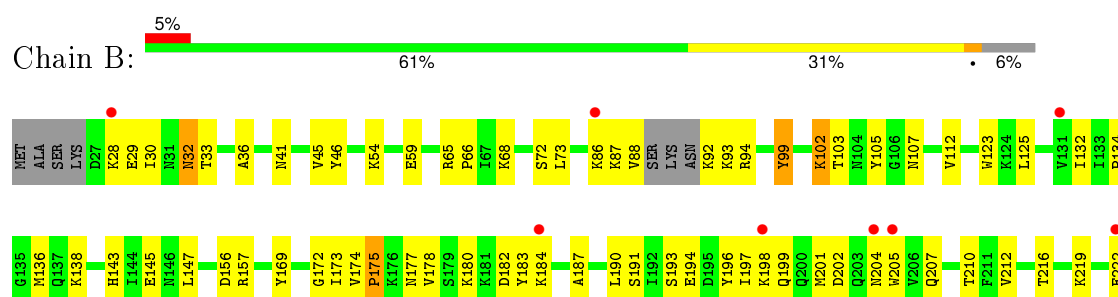
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: penicillin-binding protein 2a



- Molecule 1: penicillin-binding protein 2a



S619	S620	D623	N624	P625	N626	N627	N628	N632	N633	LYS	ASP	VAL	GLN	ASP	LYS	GLY	MET	N642	S643	N644	N645	N646	N647	N648	N651	E658	N659	G660	N661	K662	K663	G664	D665	I666	D667	E668														
S536	A537	N540	I544	L549	L550	K551	D552	T553	I562	I563	S564	K565	E566	N567	I568	N569	L570	L571	T572	D573	Q576	V579	K584	E585	D586	I587	Y588	R589	S590	Y591	K597	S598	GLY	THR	ALA	GLU	LEU	LYS	MET	LYS	GLN	GLY	GLU	THR	GLY	ARG	GLN	I614	F617	I618
G439	GLY	TYR	N442	V443	T444	R445	Y446	E447	V448	V449	N452	I453	D454	L455	I459	S462	D463	N464	I465	F466	F467	A468	R469	V470	A471	S476	G482	D491	N500	A501	Q502	I503	SER	ASN	LYS	ASN	ASN	LEU	D509	N510	E511	I512	I513	L514	G518	Q521	G431	E523	I534	Y535
Q353	L224	S225	D226	K230	F231	K247	H251	L252	V256	I259	E262	E263	L264	K265	Q266	K267	E268	Y272	K273	D274	I278	Y287	R298	V299	T300	I301	V302	N305	I309	T312	L313	I314	Q325	L326	T327	I328	D329	A330	K331	M340	G345	P352								

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	80.67Å 103.21Å 186.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.68 – 2.60 24.68 – 2.60	Depositor EDS
% Data completeness (in resolution range)	97.9 (24.68-2.60) 98.0 (24.68-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.85 (at 2.60Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.242 , 0.303 0.240 , 0.301	Depositor DCC
R_{free} test set	2383 reflections (5.00%)	DCC
Wilson B-factor (Å ²)	55.8	Xtriage
Anisotropy	0.616	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 49.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Outliers	0 of 47643 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10109	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.66% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: CL, 7EP, CD

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	0.29	0/5161	0.55	0/6941
1	B	0.29	0/4984	0.55	0/6700
All	All	0.29	0/10145	0.55	0/13641

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	5077	0	5062	167	0
1	B	4904	0	4892	161	0
2	A	26	0	20	1	0
2	B	26	0	20	2	0
3	A	2	0	0	0	0
3	B	3	0	0	0	0
4	A	1	0	0	0	0
4	B	3	0	0	1	0
5	A	42	0	0	1	0
5	B	25	0	0	0	0
All	All	10109	0	9994	325	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 16.

The worst 5 of 325 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:138:LYS:H	1:B:138:LYS:HD2	1.25	0.99
1:A:138:LYS:H	1:A:138:LYS:HD2	1.32	0.94
1:B:455:LEU:HD23	1:B:570:LEU:HD22	1.50	0.93
1:B:579:VAL:HG13	1:B:587:ILE:HG23	1.53	0.88
1:B:392:LEU:HD11	1:B:397:ILE:HD13	1.60	0.83

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	626/646 (97%)	580 (93%)	43 (7%)	3 (0%)	34	60
1	B	597/646 (92%)	537 (90%)	52 (9%)	8 (1%)	15	30
All	All	1223/1292 (95%)	1117 (91%)	95 (8%)	11 (1%)	21	42

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	176	LYS
1	B	432	TRP
1	B	620	TYR
1	A	175	PRO
1	B	305	ASN

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	565/576 (98%)	544 (96%)	21 (4%)	41	69
1	B	546/576 (95%)	531 (97%)	15 (3%)	52	79
All	All	1111/1152 (96%)	1075 (97%)	36 (3%)	46	74

5 of 36 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	554	LYS
1	A	663	LYS
1	B	659	ASN
1	A	613	GLN
1	B	32	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 36 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	32	ASN
1	B	177	ASN
1	B	626	ASN
1	B	44	GLN
1	B	200	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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 9 are monoatomic - leaving 2 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	7EP	A	701	1	20,27,27	1.97	7 (35%)	25,39,39	1.67	6 (24%)
2	7EP	B	701	1	20,27,27	2.29	7 (35%)	25,39,39	1.66	7 (28%)

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	7EP	A	701	1	-	0/12/37/37	0/2/2/2
2	7EP	B	701	1	-	0/12/37/37	0/2/2/2

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701	7EP	CAK-CAT	2.00	1.43	1.39
2	A	701	7EP	CAV-CAU	2.07	1.44	1.40
2	A	701	7EP	CAV-CAT	2.18	1.44	1.40
2	A	701	7EP	CAL-CAU	2.26	1.44	1.39
2	B	701	7EP	CAK-CAT	2.27	1.44	1.39

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	701	7EP	CAL-CAU-CAV	-2.58	115.73	120.43
2	B	701	7EP	CAL-CAU-CAV	-2.44	115.98	120.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	701	7EP	CAK-CAT-CAV	-2.22	116.38	120.43
2	A	701	7EP	CAK-CAT-CAV	-2.16	116.49	120.43
2	A	701	7EP	CB-CA-N	2.02	114.29	109.57

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	701	7EP	1	0
2	B	701	7EP	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	A	632/646 (97%)	0.01	16 (2%) 61 54	25, 56, 93, 122	0
1	B	609/646 (94%)	0.21	34 (5%) 28 21	32, 65, 101, 126	0
All	All	1241/1292 (96%)	0.10	50 (4%) 42 34	25, 60, 99, 126	0

The worst 5 of 50 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	267	LYS	5.9
1	B	436	LYS	4.6
1	B	204	ASN	4.3
1	A	602	GLU	3.9
1	A	603	LEU	3.7

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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
2	7EP	B	701	26/26	0.72	0.36	1.15	59,73,83,86	26
4	CL	B	706	1/1	0.99	0.14	0.29	40,40,40,40	0
2	7EP	A	701	26/26	0.87	0.21	-0.08	52,56,69,73	0
3	CD	B	703	1/1	1.00	0.13	-0.47	46,46,46,46	0
3	CD	A	702	1/1	0.99	0.13	-0.79	42,42,42,42	0
3	CD	A	703	1/1	0.99	0.10	-0.98	54,54,54,54	0
4	CL	B	707	1/1	0.99	0.10	-1.03	47,47,47,47	0
3	CD	B	702	1/1	1.00	0.13	-1.11	46,46,46,46	0
4	CL	A	704	1/1	0.98	0.12	-1.78	40,40,40,40	0
4	CL	B	705	1/1	1.00	0.09	-4.35	38,38,38,38	0
3	CD	B	704	1/1	0.93	0.12	-	80,80,80,80	1

6.5 Other polymers [i](#)

There are no such residues in this entry.