wwPDB X-ray Structure Validation Summary Report (i)

Jul 31, 2023 – 01:31 AM EDT

PDB ID	:	1UBP
Title	:	CRYSTAL STRUCTURE OF UREASE FROM BACILLUS PASTEURII INHIBITED WITH BETA-MERCAPTOETHANOL AT 1.65 ANGSTROMS RESOLUTION
Authors	:	Benini, S.; Rypniewski, W.R.; Wilson, K.S.; Ciurli, S.; Mangani, S.
Deposited on	:	1998-01-21
Resolution	:	1.65 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 (i) 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 (i)) were used in the production of this report:

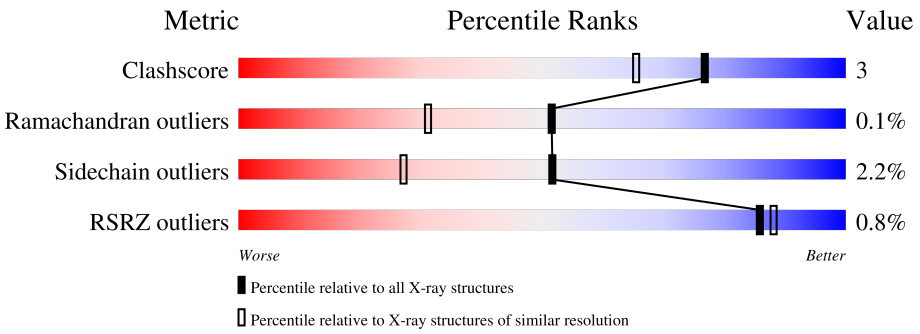
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.34
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.34

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.65 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))
Clashscore	141614	1931 (1.66-1.66)
Ramachandran outliers	138981	1891 (1.66-1.66)
Sidechain outliers	138945	1891 (1.66-1.66)
RSRZ outliers	127900	1791 (1.66-1.66)

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 <=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	100	85% 13% •
2	B	122	% 87% 11% •
3	C	570	% 91% 8% •

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 7077 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 UREASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	100	782	493	133	150	6	7	0	0

- Molecule 2 is a protein called UREASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	122	951	589	171	190	1	21	0	0

- Molecule 3 is a protein called UREASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	570	4323	2714	743	843	23	34	0	0

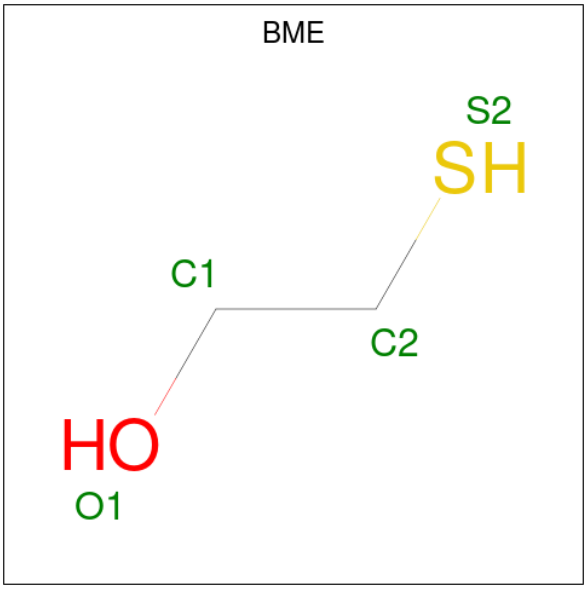
There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	19	GLU	ARG	variant	UNP P41020
C	28	TRP	-	insertion	UNP P41020
C	29	ILE	GLY	variant	UNP P41020
C	36	THR	TYR	variant	UNP P41020
C	37	THR	TYR	variant	UNP P41020
C	38	TYR	LEU	variant	UNP P41020
C	220	KCX	LYS	modified residue	UNP P41020
C	263	LEU	VAL	variant	UNP P41020
C	420	ILE	MET	variant	UNP P41020

- Molecule 4 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ni		
4	C	2	2	2	0	0

- Molecule 5 is BETA-MERCAPTOETHANOL (three-letter code: BME) (formula: C_2H_6OS).



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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	134	134	134	0	0
			Total	O		
6	B	200	200	200	0	0
			Total	O		
6	C	677	677	677	0	0

3 Residue-property plots (i)

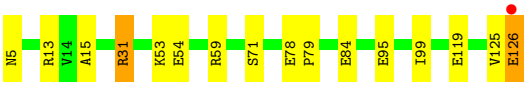
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: UREASE

Chain A:

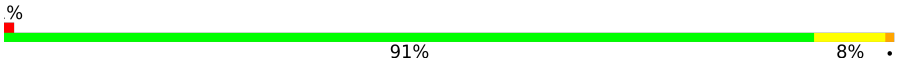
- Molecule 2: UREASE

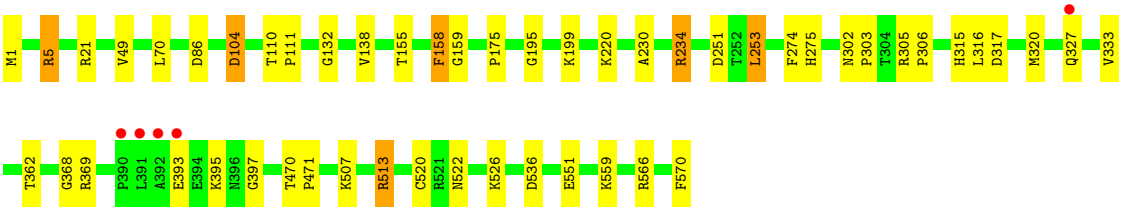
Chain B:



- Molecule 3: UREASE

Chain C:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 63 2 2	Depositor
Cell constants a, b, c, α, β, γ	131.34Å 131.34Å 190.01Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	14.00 – 1.65 13.94 – 1.65	Depositor EDS
% Data completeness (in resolution range)	98.7 (14.00-1.65) 98.7 (13.94-1.65)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	2.49 (at 1.65Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.158 , (Not available) 0.171 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	14.9	Xtriage
Anisotropy	0.144	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 54.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	7077	wwPDB-VP
Average B, all atoms (Å^2)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.24% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: KCX, CXM, NI, BME

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	0.88	1/782 (0.1%)	0.95	3/1053 (0.3%)
2	B	0.72	3/963 (0.3%)	1.04	5/1296 (0.4%)
3	C	0.50	3/4392 (0.1%)	1.03	10/5955 (0.2%)
All	All	0.60	7/6137 (0.1%)	1.02	18/8304 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	C	0	1

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	100	SER	C-OXT	21.39	1.64	1.23
2	B	125	VAL	C-N	-10.94	1.08	1.34
3	C	393	GLU	CA-CB	-6.54	1.39	1.53
3	C	570	PHE	C-OXT	6.48	1.35	1.23
2	B	126	GLU	N-CA	5.89	1.58	1.46

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	5	ARG	NE-CZ-NH2	-11.97	114.32	120.30
2	B	125	VAL	C-N-CA	10.94	149.05	121.70
3	C	393	GLU	CB-CA-C	8.47	127.35	110.40
2	B	13	ARG	NE-CZ-NH2	7.55	124.07	120.30
2	B	31	ARG	NE-CZ-NH2	7.51	124.06	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	104	ASP	Mainchain

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	782	0	801	8	0
2	B	951	0	936	7	0
3	C	4323	0	4289	24	0
4	C	2	0	0	0	0
5	C	8	0	10	0	0
6	A	134	0	0	3	0
6	B	200	0	0	2	1
6	C	677	0	0	8	4
All	All	7077	0	6036	36	4

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 3.

The worst 5 of 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)
1:A:100:SER:OXT	1:A:100:SER:C	1.64	1.33
3:C:251:ASP:OD1	6:C:1153:HOH:O	2.08	0.71
3:C:507:LYS:HD3	6:C:1172:HOH:O	1.92	0.70
2:B:54:GLU:HG3	6:B:289:HOH:O	1.93	0.66
1:A:3:LEU:HD23	6:A:196:HOH:O	1.99	0.63

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:1369:HOH:O	6:C:1369:HOH:O[10_665]	1.84	0.36

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:1371:HOH:O	6:C:1371:HOH:O[12_565]	2.12	0.08
6:B:205:HOH:O	6:C:1174:HOH:O[2_665]	2.15	0.05
6:C:1107:HOH:O	6:C:1324:HOH:O[2_665]	2.16	0.04

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	98/100 (98%)	98 (100%)	0	0	100 100
2	B	120/122 (98%)	115 (96%)	4 (3%)	1 (1%)	19 5
3	C	567/570 (100%)	543 (96%)	24 (4%)	0	100 100
All	All	785/792 (99%)	756 (96%)	28 (4%)	1 (0%)	51 31

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	99	ILE

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	84/84 (100%)	82 (98%)	2 (2%)	49 23
2	B	101/101 (100%)	98 (97%)	3 (3%)	41 15
3	C	460/460 (100%)	451 (98%)	9 (2%)	55 32

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	645/645 (100%)	631 (98%)	14 (2%)	52 27

5 of 14 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	253	LEU
3	C	317	ASP
3	C	551	GLU
3	C	526	LYS
3	C	536	ASP

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)

2 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	$\#\|Z\| > 2$
3	KCX	C	220	4,3	9,11,12	2.36	2 (22%)	5,12,14	1.55	1 (20%)
1	CXM	A	1	1	8,10,11	1.42	1 (12%)	7,11,13	2.77	2 (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
3	KCX	C	220	4,3	-	0/9/10/12	-
1	CXM	A	1	1	-	2/9/10/12	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	220	KCX	CX-NZ	6.57	1.46	1.35
1	A	1	CXM	CN-N	-3.51	1.28	1.35
3	C	220	KCX	OQ1-CX	2.27	1.25	1.21

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1	CXM	ON1-CN-N	6.59	135.66	124.85
3	C	220	KCX	CD-CE-NZ	-2.40	105.34	112.21
1	A	1	CXM	CA-N-CN	-2.01	118.76	122.44

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1	CXM	CB-CA-N-CN
1	A	1	CXM	C-CA-N-CN

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 4 ligands modelled in this entry, 2 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	$\#\|Z\| > 2$
5	BME	C	600	4	3,3,3	0.32	0	1,2,2	0.65	0
5	BME	C	601	3	3,3,3	0.53	0	1,2,2	1.31	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
5	BME	C	600	4	-	0/1/1/1	-
5	BME	C	601	3	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	601	BME	O1-C1-C2-S2

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)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	125:VAL	C	126:GLU	N	1.08

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	99/100 (99%)	-0.56	0	100	100	10, 13, 20, 29	2 (2%)
2	B	122/122 (100%)	-0.38	1 (0%)	86	88	12, 16, 25, 42	8 (6%)
3	C	568/570 (99%)	-0.56	5 (0%)	84	86	9, 13, 24, 49	12 (2%)
All	All	789/792 (99%)	-0.53	6 (0%)	86	88	9, 14, 24, 49	22 (2%)

The worst 5 of 6 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	392	ALA	4.1
3	C	390	PRO	3.4
3	C	391	LEU	3.2
3	C	327	GLN	3.1
3	C	393	GLU	2.5

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	CXM	A	1	11/12	0.97	0.06	11,12,18,20	0
3	KCX	C	220	12/13	0.98	0.05	9,11,12,15	0

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
5	BME	C	601	4/4	0.96	0.15	23,26,26,30	0
5	BME	C	600	4/4	0.97	0.10	14,16,18,21	0
4	NI	C	701	1/1	0.99	0.03	14,14,14,14	0
4	NI	C	702	1/1	0.99	0.03	12,12,12,12	0

6.5 Other polymers (i)

There are no such residues in this entry.