wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 04:41 AM GMT

PDB ID	:	2NTF
Title	:	Crystal Structure of a Quorum-Quenching Antibody in Complex with an N-Acyl-L-Homoserine Lactone Analog
Authors	:	Debler, E.W.; Wilson, I.A.
Deposited on	:	2006-11-07
Resolution	:	3.18 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

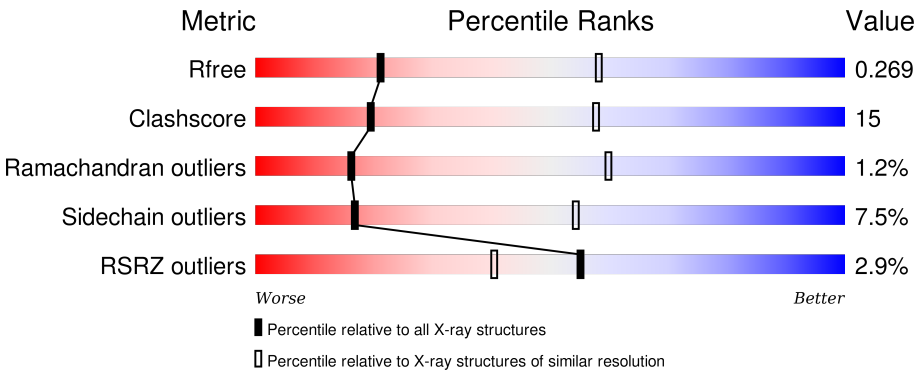
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.18 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	1115 (3.22-3.14)
Clashscore	102246	1125 (3.20-3.16)
Ramachandran outliers	100387	1105 (3.20-3.16)
Sidechain outliers	100360	1104 (3.20-3.16)
RSRZ outliers	91569	1120 (3.22-3.14)

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 <=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	211	% 73% 25% •
1	L	211	71% 27% •
2	B	222	6% 63% 35% ••
2	H	222	4% 62% 35% •

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 6652 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.

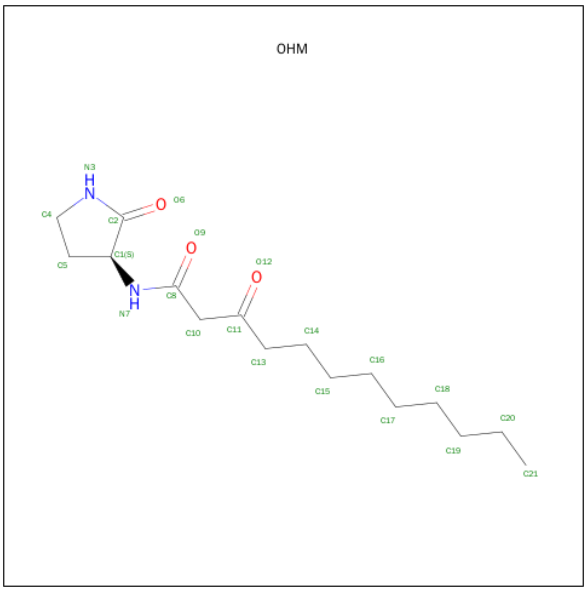
- Molecule 1 is a protein called Murine Antibody Fab RS2-1G9 Lambda Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	L	211	1606	1005	272	323	6	0	0	0
1	A	211	1606	1005	272	323	6	0	0	0

- Molecule 2 is a protein called Murine Antibody Fab RS2-1G9 IGG1 Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	H	222	1699	1084	276	333	6	0	0	0
2	B	222	1699	1084	276	333	6	0	0	0

- Molecule 3 is 3-OXO-N-[(3S)-2-OXOPYRROLIDIN-3-YL]DODECANAMIDE (three-letter code: OHM) (formula: $C_{16}H_{28}N_2O_3$).



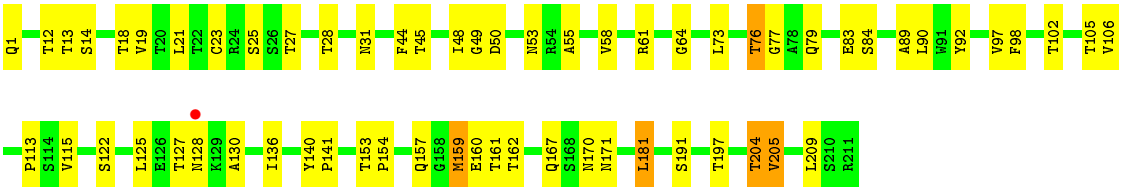
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	H	1	21	16	2	3	0	0
			Total	C	N	O		
3	B	1	21	16	2	3	0	0

3 Residue-property plots (i)

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.

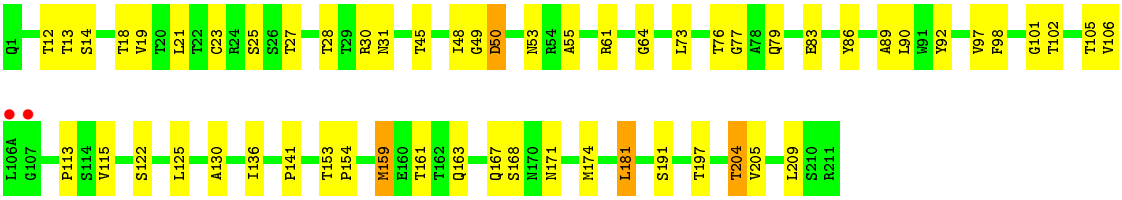
- Molecule 1: Murine Antibody Fab RS2-1G9 Lambda Light Chain

Chain L:



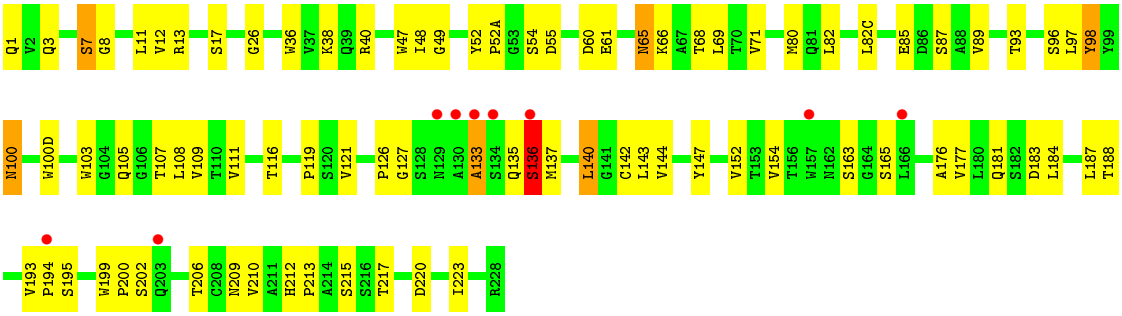
- Molecule 1: Murine Antibody Fab RS2-1G9 Lambda Light Chain

Chain A:



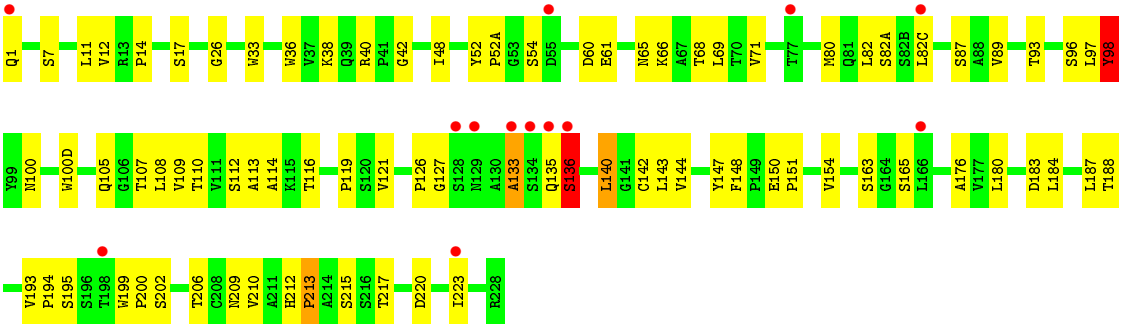
- Molecule 2: Murine Antibody Fab RS2-1G9 IGG1 Heavy Chain

Chain H:



- Molecule 2: Murine Antibody Fab RS2-1G9 IGG1 Heavy Chain

Chain B:


Q1
S7
L11
V12
R13
P14
S17
G26
W33
W36
V37
K38
Q39
R40
P41
G42
I48
Y52
P52A
G53
S54
D55
D60
E61
N65
K66
A67
T68
L69
T70
V71
T77
M80
Q81
L82
S82A
S82B
L82C
S87
A88
V89
T93
S96
L97
Y98
Y99
N100
W100D
Q105
G106
T107
L108
V109
T110
V111
S112
A113
A114
K115
T116
P119
S120
V121
P126
G127
S128
N129
A130
A133
S134
Q135
S136
L140
G141
C142
L143
V144
Y147
F148
P149
E150
P151
V154
S163
G164
S165
L166
A176
V177
L180
D183
L184
L187
T188
V193
P194
S195
S196
T198
W199
P200
S202
T206
C208
N209
V210
A211
H212
P213
A214
S215
S216
T217
D220
I223
R228

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	118.66Å 118.66Å 176.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.02 – 3.18 44.01 – 3.18	Depositor EDS
% Data completeness (in resolution range)	89.1 (44.02-3.18) 89.2 (44.01-3.18)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	2.35 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.3.0017	Depositor
R, R_{free}	0.210 , 0.265 0.210 , 0.269	Depositor DCC
R_{free} test set	992 reflections (5.37%)	DCC
Wilson B-factor (Å^2)	80.6	Xtriage
Anisotropy	0.120	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 82.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.30$	Xtriage
Outliers	0 of 19449 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	6652	wwPDB-VP
Average B, all atoms (Å^2)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.60% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: OHM

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	0.73	0/1646	0.77	0/2250
1	L	0.75	0/1646	0.79	0/2250
2	B	0.67	1/1749 (0.1%)	0.74	1/2395 (0.0%)
2	H	0.70	0/1749	0.75	1/2395 (0.0%)
All	All	0.71	1/6790 (0.0%)	0.76	2/9290 (0.0%)

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
2	B	0	2
2	H	0	2
All	All	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	98	TYR	CD2-CE2	5.35	1.47	1.39

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	127	GLY	N-CA-C	-5.87	98.43	113.10
2	H	127	GLY	N-CA-C	-5.58	99.15	113.10

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	126	PRO	Peptide
2	B	54	SER	Peptide
2	H	126	PRO	Peptide
2	H	54	SER	Peptide

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	1606	0	1543	48	0
1	L	1606	0	1543	54	0
2	B	1699	0	1646	58	0
2	H	1699	0	1646	54	1
3	B	21	0	28	2	0
3	H	21	0	28	0	0
All	All	6652	0	6434	196	1

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 15.

The worst 5 of 196 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:H:48:ILE:HG21	2:H:80:MET:HE1	1.44	0.99
1:L:154:PRO:HG2	1:A:27:THR:HG21	1.47	0.96
2:B:48:ILE:HG21	2:B:80:MET:HE1	1.51	0.88
2:B:143:LEU:HA	2:B:188:THR:HG22	1.55	0.88
2:H:52(A):PRO:HA	2:H:71:VAL:HG11	1.56	0.84

All (1) 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)
2:H:3:GLN:OE1	2:H:13:ARG:NH2[7_555]	2.12	0.08

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	209/211 (99%)	190 (91%)	18 (9%)	1 (0%)	34	77
1	L	209/211 (99%)	190 (91%)	19 (9%)	0	100	100
2	B	220/222 (99%)	192 (87%)	24 (11%)	4 (2%)	11	50
2	H	220/222 (99%)	196 (89%)	19 (9%)	5 (2%)	8	43
All	All	858/866 (99%)	768 (90%)	80 (9%)	10 (1%)	16	60

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	136	SER
2	B	136	SER
2	B	133	ALA
2	H	133	ALA
2	H	55	ASP

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	180/180 (100%)	168 (93%)	12 (7%)	20	59
1	L	180/180 (100%)	166 (92%)	14 (8%)	16	52
2	B	192/192 (100%)	177 (92%)	15 (8%)	16	52
2	H	192/192 (100%)	177 (92%)	15 (8%)	16	52
All	All	744/744 (100%)	688 (92%)	56 (8%)	17	54

5 of 56 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	140	LEU
1	A	30	ARG
2	B	136	SER
2	H	142	CYS
2	H	202	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	53	ASN
2	H	100	ASN
1	A	53	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 carbohydrates in this entry.

5.6 Ligand geometry (i)

2 ligands 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	OHM	B	1002	-	20,21,21	0.97	0	20,25,25	1.47	3 (15%)
3	OHM	H	1001	-	20,21,21	0.93	0	20,25,25	1.11	2 (10%)

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	OHM	B	1002	-	-	0/17/27/27	0/1/1/1
3	OHM	H	1001	-	-	0/17/27/27	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	H	1001	OHM	C2-C1-N7	-3.16	106.33	111.46
3	B	1002	OHM	C4-C5-C1	-3.02	99.39	104.45
3	B	1002	OHM	C4-N3-C2	-2.27	108.46	113.60
3	H	1001	OHM	C4-N3-C2	-2.02	109.02	113.60
3	B	1002	OHM	C10-C8-N7	3.47	120.72	115.93

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1002	OHM	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	211/211 (100%)	0.06	2 (0%)	85	78	53, 71, 93, 105	0
1	L	211/211 (100%)	0.05	1 (0%)	91	87	53, 71, 93, 105	0
2	B	222/222 (100%)	0.31	13 (5%)	26	14	48, 77, 93, 98	0
2	H	222/222 (100%)	0.24	9 (4%)	41	26	48, 77, 93, 98	0
All	All	866/866 (100%)	0.17	25 (2%)	55	40	48, 77, 93, 105	0

The worst 5 of 25 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	129	ASN	4.5
2	B	1	GLN	3.6
2	B	128	SER	3.5
2	H	166	LEU	3.5
2	B	129	ASN	3.2

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 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(Å^2)	Q<0.9
3	OHM	H	1001	21/21	0.95	0.21	-0.14	49,52,68,69	0
3	OHM	B	1002	21/21	0.96	0.20	-0.57	54,58,71,73	0

6.5 Other polymers (i)

There are no such residues in this entry.