wwPDB X-ray Structure Validation Summary Report (i)

Aug 16, 2023 – 12:19 PM EDT

PDB ID	:	2AQ7
Title	:	Structure-activity relationships at the 5-posiiton of thiolactomycin: an intact 5(R)-isoprene unit is required for activity against the condensing enzymes from Mycobacterium tuberculosis and Escherichia coli
Authors	:	Kim, P.; Zhang, Y.M.; Shenoy, G.; Nguyen, Q.A.; Boshoff, H.I.; Manjunatha, U.H.; Goodwin, M.B.; Lonsdale, J.; Price, A.C.; Miller, D.J.
Deposited on	:	2005-08-17
Resolution	:	2.30 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:

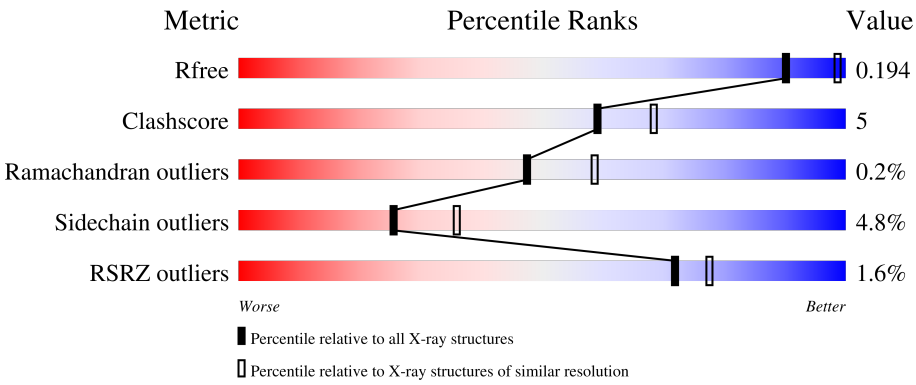
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	406	2%, 88%, 11%
1	B	406	90%, 8%
1	C	406	2%, 90%, 8%
1	D	406	2%, 84%, 13%

2 Entry composition (i)

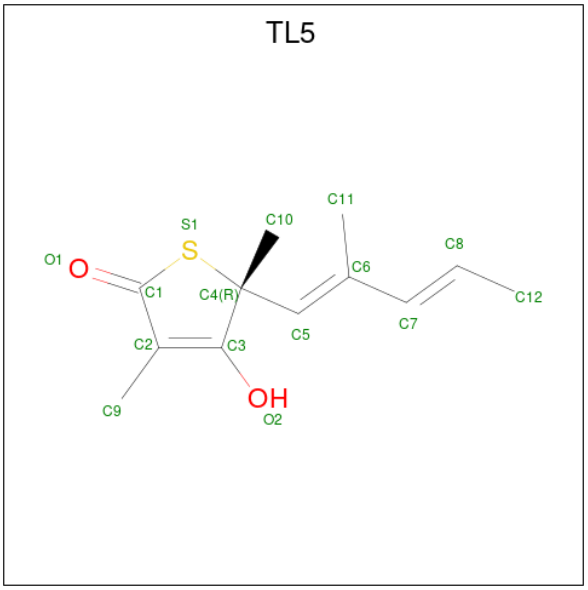
There are 3 unique types of molecules in this entry. The entry contains 12408 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 3-oxoacyl-[acyl-carrier-protein] synthase I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	404	2960	1841	516	581	22	0	0	0
1	B	403	2955	1838	515	580	22	0	0	0
1	C	403	2955	1838	515	580	22	0	0	0
1	D	403	2955	1838	515	580	22	0	0	0

- Molecule 2 is (5R)-4-HYDROXY-3,5-DIMETHYL-5-[(1E,3E)-2-METHYLPENTA-1,3-DIENYL]THIOPHEN-2(5H)-ONE (three-letter code: TL5) (formula: $C_{12}H_{16}O_2S$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	S		
2	A	1	15	12	2	1	0	0
2	B	1	15	12	2	1	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	S		
2	D	1	15	12	2	1	0	0

- Molecule 3 is water.

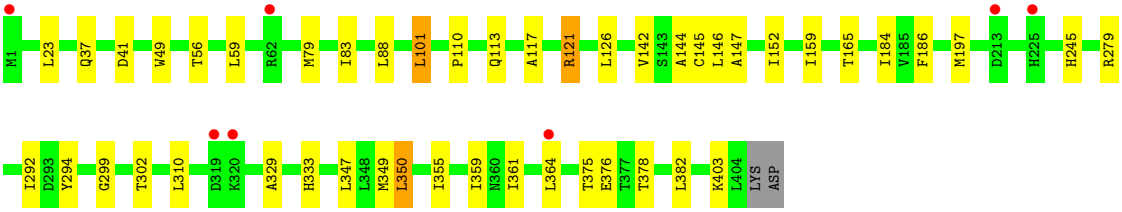
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	123	123	123	0	0
			Total	O		
3	B	143	143	143	0	0
			Total	O		
3	C	126	126	126	0	0
			Total	O		
3	D	146	146	146	0	0

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.

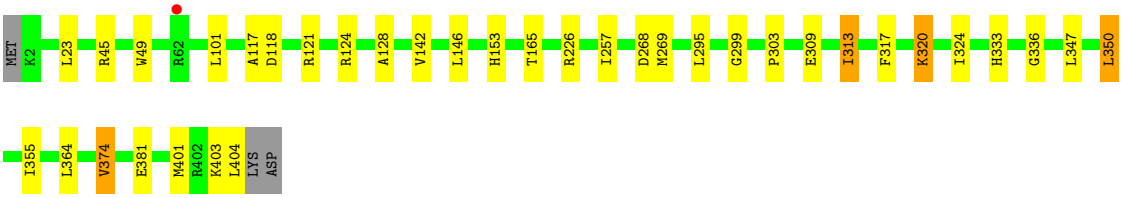
• Molecule 1: 3-oxoacyl-[acyl-carrier-protein] synthase I

Chain A:



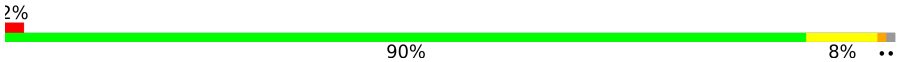
• Molecule 1: 3-oxoacyl-[acyl-carrier-protein] synthase I

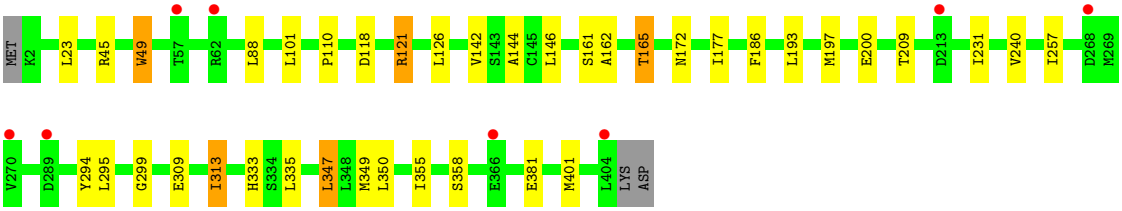
Chain B:



• Molecule 1: 3-oxoacyl-[acyl-carrier-protein] synthase I

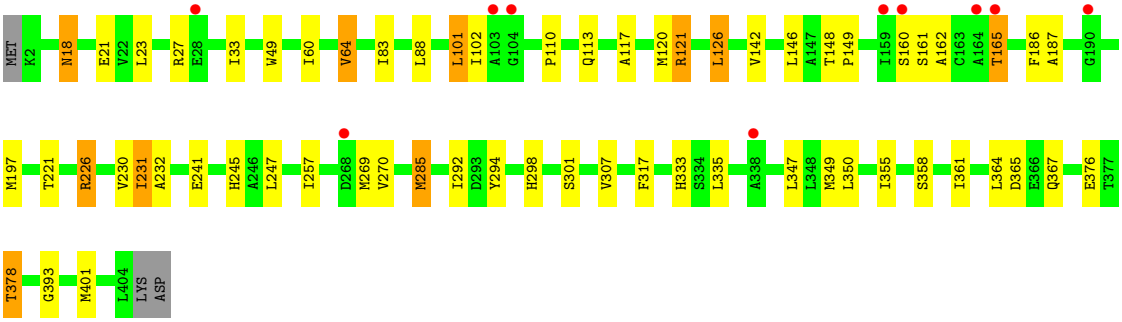
Chain C:





• Molecule 1: 3-oxoacyl-[acyl-carrier-protein] synthase I

Chain D:


MET K2 N18 E21 V22 L23 R27 E28 I33 W49 I60 V64 I83 L88 L101 I102 A103 G104 P110 Q113 A117 M120 R121 L126 V142 L146 A147 T148 P149 I159 S160 S161 A162 C163 A164 T165 F186 A187 G190
M197 T221 R226 V230 I231 A232 E241 H245 A246 L247 I257 D268 M269 V270 M285 I292 D293 Y294 H298 S301 V307 F317 H333 S334 L335 A338 L347 L348 M349 L350 I355 S358 I361 L364 D365 E366 Q367 E376 T377
T378 G393 M401 L404 LYS ASP

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	59.12Å 139.00Å 212.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.78 – 2.30 38.77 – 2.30	Depositor EDS
% Data completeness (in resolution range)	96.2 (38.78-2.30) 96.2 (38.77-2.30)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	7.92 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.182 , 0.228 0.193 , 0.194	Depositor DCC
R_{free} test set	3807 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	18.1	Xtriage
Anisotropy	0.114	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 38.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	12408	wwPDB-VP
Average B, all atoms (Å^2)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.32% 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: TL5

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	0.37	0/3008	0.58	0/4065
1	B	0.38	0/3003	0.60	0/4058
1	C	0.38	0/3003	0.59	1/4058 (0.0%)
1	D	0.40	0/3003	0.60	1/4058 (0.0%)
All	All	0.38	0/12017	0.59	2/16239 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	226	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	C	121	ARG	NE-CZ-NH2	-5.04	117.78	120.30

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	A	2960	0	2915	28	0
1	B	2955	0	2910	21	0
1	C	2955	0	2910	19	0
1	D	2955	0	2910	43	0
2	A	15	0	15	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	15	0	15	1	0
2	D	15	0	15	6	0
3	A	123	0	0	1	0
3	B	143	0	0	1	0
3	C	126	0	0	0	0
3	D	146	0	0	3	0
All	All	12408	0	11690	110	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 5.

The worst 5 of 110 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:D:285:MET:SD	1:D:292:ILE:HD11	2.13	0.89
1:D:221:THR:O	1:D:361:ILE:HD11	1.76	0.86
1:B:309:GLU:O	1:B:313:ILE:HD13	1.84	0.78
1:A:101:LEU:HB2	1:A:152:ILE:HD13	1.65	0.77
1:C:349:MET:HE3	1:C:355:ILE:HA	1.67	0.75

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	402/406 (99%)	384 (96%)	17 (4%)	1 (0%)	47	58
1	B	401/406 (99%)	388 (97%)	12 (3%)	1 (0%)	47	58
1	C	401/406 (99%)	388 (97%)	12 (3%)	1 (0%)	47	58
1	D	401/406 (99%)	386 (96%)	14 (4%)	1 (0%)	47	58
All	All	1605/1624 (99%)	1546 (96%)	55 (3%)	4 (0%)	47	58

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	299	GLY
1	C	299	GLY
1	B	299	GLY
1	D	301	SER

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	306/309 (99%)	292 (95%)	14 (5%)	27	38
1	B	306/309 (99%)	294 (96%)	12 (4%)	32	46
1	C	306/309 (99%)	292 (95%)	14 (5%)	27	38
1	D	306/309 (99%)	287 (94%)	19 (6%)	18	25
All	All	1224/1236 (99%)	1165 (95%)	59 (5%)	25	36

5 of 59 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	88	LEU
1	D	350	LEU
1	C	333	HIS
1	D	347	LEU
1	D	231	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	37	GLN
1	D	341	GLN
1	D	372	ASN
1	D	245	HIS
1	B	372	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)

3 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	$\#\|Z\| > 2$
2	TL5	A	600	-	8,15,15	0.51	0	10,22,22	1.87	4 (40%)
2	TL5	D	603	-	8,15,15	0.45	0	10,22,22	1.85	5 (50%)
2	TL5	B	601	-	8,15,15	0.48	0	10,22,22	1.90	4 (40%)

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	TL5	A	600	-	-	0/5/27/27	0/1/1/1
2	TL5	D	603	-	-	0/5/27/27	0/1/1/1
2	TL5	B	601	-	-	0/5/27/27	0/1/1/1

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	601	TL5	C12-C8-C7	-3.16	119.11	125.34
2	A	600	TL5	C12-C8-C7	-3.01	119.40	125.34
2	D	603	TL5	C12-C8-C7	-3.00	119.43	125.34
2	A	600	TL5	C9-C2-C3	-2.90	123.77	131.27
2	A	600	TL5	O1-C1-C2	-2.85	123.21	128.35

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	600	TL5	2	0
2	D	603	TL5	6	0
2	B	601	TL5	1	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	404/406 (99%)	-0.10	7 (1%)	70	76	12, 20, 35, 46	0
1	B	403/406 (99%)	-0.20	1 (0%)	95	96	9, 17, 26, 32	0
1	C	403/406 (99%)	-0.07	8 (1%)	65	71	12, 20, 29, 39	0
1	D	403/406 (99%)	-0.13	10 (2%)	57	64	9, 17, 25, 33	0
All	All	1613/1624 (99%)	-0.12	26 (1%)	72	77	9, 18, 29, 46	0

The worst 5 of 26 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	319	ASP	4.0
1	C	270	VAL	3.5
1	C	213	ASP	3.3
1	C	62	ARG	2.9
1	B	62	ARG	2.8

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	TL5	D	603	15/15	0.80	0.31	26,26,26,26	15
2	TL5	A	600	15/15	0.83	0.28	26,26,26,26	15
2	TL5	B	601	15/15	0.84	0.23	26,26,26,26	15

6.5 Other polymers (i)

There are no such residues in this entry.