



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 14, 2017 – 09:54 pm GMT

PDB ID : 2E4O
Title : X-ray Crystal Structure of Aristolochene Synthase from *Aspergillus terreus* and the Evolution of Templates for the Cyclization of Farnesyl Diphosphate
Authors : Shishova, E.Y.; Di Costanzo, L.; Cane, D.E.; Christianson, D.W.
Deposited on : 2006-12-15
Resolution : 2.20 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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : recalc28949

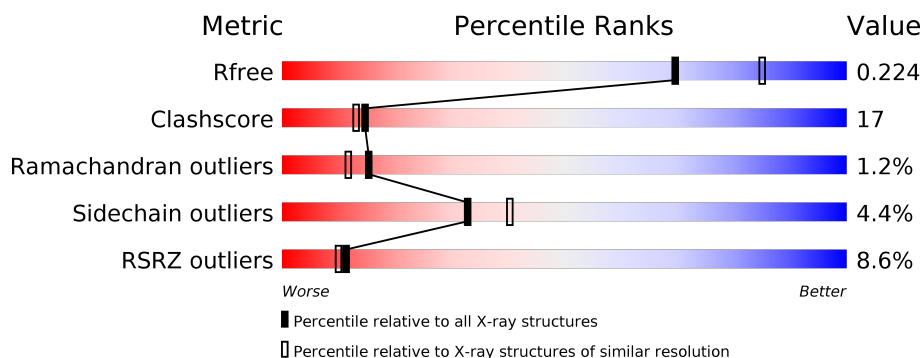
1 Overall quality at a glance

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}	100719	4002 (2.20-2.20)
Clashscore	112137	4730 (2.20-2.20)
Ramachandran outliers	110173	4656 (2.20-2.20)
Sidechain outliers	110143	4657 (2.20-2.20)
RSRZ outliers	101464	4033 (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 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	320	<div> <div>6%</div> <div>68% 24% 8%</div> </div>
1	B	320	<div> <div>6%</div> <div>68% 23% 8%</div> </div>
1	C	320	<div> <div>11%</div> <div>57% 33% 8%</div> </div>
1	D	320	<div> <div>10%</div> <div>59% 29% 8%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	BME	C	502	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9795 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.

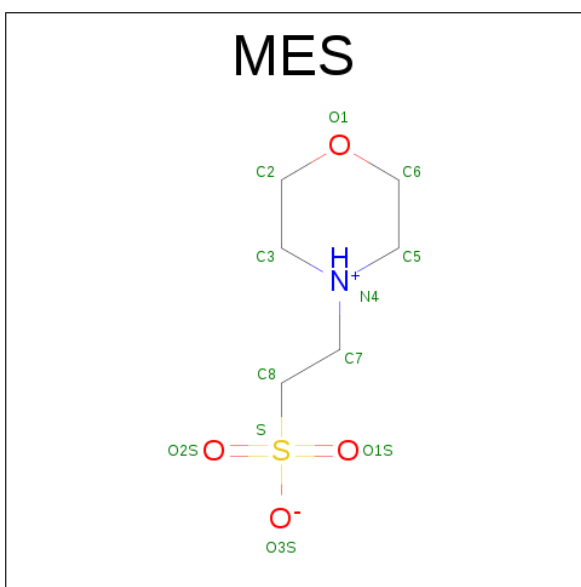
- Molecule 1 is a protein called Aristolochene synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	295	Total	C	N	O	S	0	0	0
			2392	1529	403	445	15			
1	B	295	Total	C	N	O	S	0	0	0
			2393	1531	403	444	15			
1	C	296	Total	C	N	O	S	0	0	0
			2400	1535	404	446	15			
1	D	294	Total	C	N	O	S	0	0	0
			2385	1525	402	443	15			

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

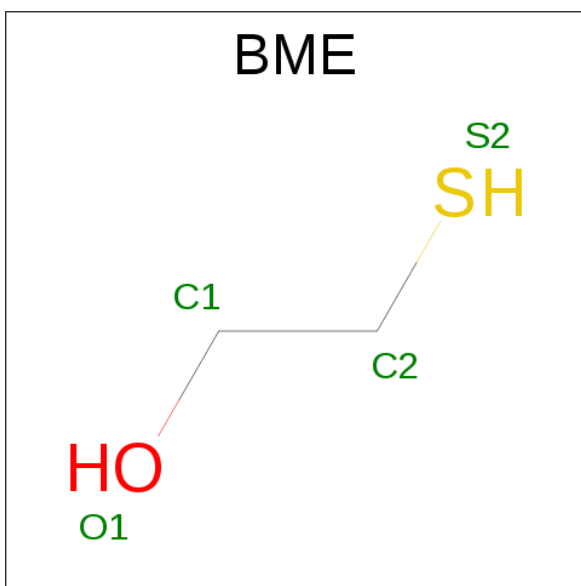
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Cl	0	0
			1	1		
2	C	1	Total	Cl	0	0
			1	1		

- Molecule 3 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C₆H₁₃NO₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	D	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 4 is BETA-MERCAPTOETHANOL (three-letter code: BME) (formula: C₂H₆OS).



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

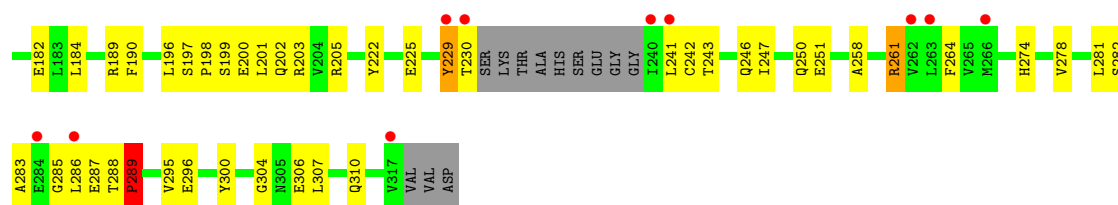
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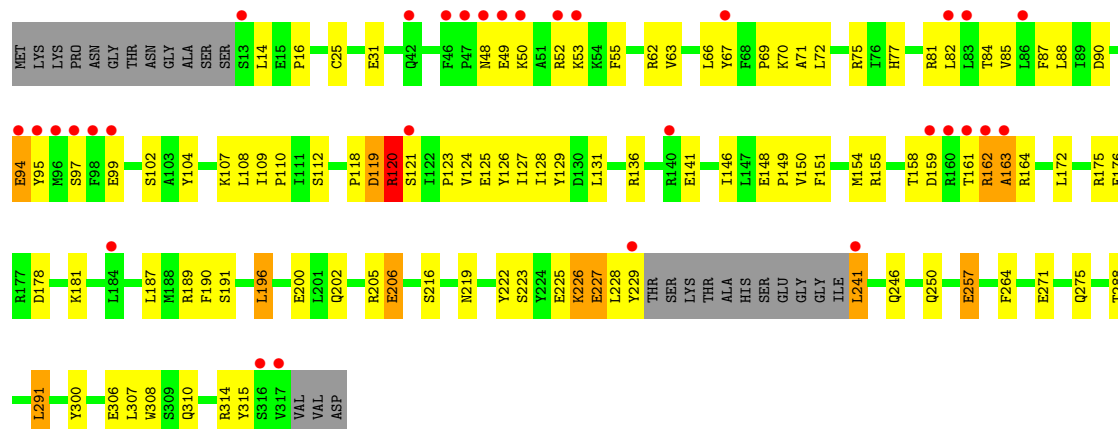
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	S	0	0
			4	2	1	1		
4	C	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	75	Total	O	0	0
			75	75		
5	B	44	Total	O	0	0
			44	44		
5	C	35	Total	O	0	0
			35	35		
5	D	37	Total	O	0	0
			37	37		



• Molecule 1: Aristolochene synthase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	61.19Å 147.24Å 83.74Å 90.00° 97.91° 90.00°	Depositor
Resolution (Å)	50.00 – 2.20 26.49 – 2.18	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.20) 95.8 (26.49-2.18)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.41 (at 2.17Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.222 , 0.272 0.226 , 0.224	Depositor DCC
R_{free} test set	3631 reflections (5.03%)	DCC
Wilson B-factor (Å ²)	36.2	Xtriage
Anisotropy	0.150	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 49.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9795	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.43% 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: CL, MES, 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	0.41	0/2445	0.59	0/3309
1	B	0.42	0/2446	0.57	0/3310
1	C	0.39	0/2453	0.63	2/3320 (0.1%)
1	D	0.38	0/2438	0.57	0/3299
All	All	0.40	0/9782	0.59	2/13238 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	165	PRO	CA-N-CD	-9.59	98.07	111.50
1	C	289	PRO	CA-N-CD	-9.57	98.10	111.50

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	2392	0	2364	65	0
1	B	2393	0	2369	57	0
1	C	2400	0	2375	118	0
1	D	2385	0	2358	97	0
2	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	1	0	0	0	0
3	D	12	0	13	0	0
4	A	8	0	11	4	0
4	C	8	0	11	4	0
4	D	4	0	6	3	0
5	A	75	0	0	3	0
5	B	44	0	0	2	0
5	C	35	0	0	2	0
5	D	37	0	0	1	0
All	All	9795	0	9507	327	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 17.

The worst 5 of 327 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:C:242:CYS:SG	4:C:502:BME:S2	2.46	1.13
1:A:96:MET:HE2	1:A:100:GLU:HG2	1.02	1.02
1:A:96:MET:CE	1:A:100:GLU:HG2	1.93	0.99
1:A:96:MET:HE2	1:A:100:GLU:CG	1.97	0.93
1:C:118:PRO:HG2	1:C:120:ARG:NH1	1.82	0.93

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	291/320 (91%)	281 (97%)	10 (3%)	0	100	100
1	B	291/320 (91%)	286 (98%)	3 (1%)	2 (1%)	25	24

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	292/320 (91%)	273 (94%)	13 (4%)	6 (2%)	8	5
1	D	290/320 (91%)	274 (94%)	10 (3%)	6 (2%)	8	5
All	All	1164/1280 (91%)	1114 (96%)	36 (3%)	14 (1%)	15	12

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	120	ARG
1	C	120	ARG
1	C	163	ALA
1	D	162	ARG
1	D	163	ALA

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	260/279 (93%)	252 (97%)	8 (3%)	45	57
1	B	260/279 (93%)	248 (95%)	12 (5%)	31	39
1	C	261/279 (94%)	248 (95%)	13 (5%)	28	34
1	D	259/279 (93%)	246 (95%)	13 (5%)	28	34
All	All	1040/1116 (93%)	994 (96%)	46 (4%)	33	40

5 of 46 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	15	GLU
1	C	165	PRO
1	D	257	GLU
1	C	66	LEU
1	C	145	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	219	ASN
1	B	305	ASN
1	D	22	GLN
1	A	305	ASN
1	C	305	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](#)

Of 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 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	$\# Z > 2$
4	BME	A	501	-	3,3,3	0.57	0	2,2,2	0.55	0
4	BME	A	503	-	3,3,3	0.39	0	2,2,2	0.88	0
4	BME	C	502	-	3,3,3	0.39	0	2,2,2	0.68	0
4	BME	C	504	-	3,3,3	0.31	0	2,2,2	0.95	0
3	MES	D	4246	-	12,12,12	1.32	1 (8%)	14,16,16	1.49	3 (21%)
4	BME	D	500	-	3,3,3	0.54	0	2,2,2	0.58	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
4	BME	A	501	-	-	0/1/1/1	0/0/0/0
4	BME	A	503	-	-	0/1/1/1	0/0/0/0
4	BME	C	502	-	-	0/1/1/1	0/0/0/0
4	BME	C	504	-	-	0/1/1/1	0/0/0/0
3	MES	D	4246	-	-	0/6/14/14	0/1/1/1
4	BME	D	500	-	-	0/1/1/1	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	4246	MES	C8-S	3.37	1.82	1.77

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	4246	MES	O2S-S-C8	2.10	108.60	106.79
3	D	4246	MES	O3S-S-C8	2.92	109.64	106.06
3	D	4246	MES	O1S-S-C8	3.50	109.79	106.79

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	501	BME	1	0
4	A	503	BME	3	0
4	C	502	BME	4	0
4	D	500	BME	3	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	295/320 (92%)	0.21	18 (6%) 22 21	22, 39, 64, 89	0
1	B	295/320 (92%)	0.25	18 (6%) 22 21	24, 40, 65, 78	0
1	C	296/320 (92%)	0.55	34 (11%) 5 5	22, 49, 76, 89	0
1	D	294/320 (91%)	0.51	31 (10%) 7 6	23, 44, 82, 96	0
All	All	1180/1280 (92%)	0.38	101 (8%) 11 10	22, 43, 74, 96	0

The worst 5 of 101 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	240	ILE	6.7
1	D	13	SER	5.5
1	D	159	ASP	5.3
1	D	161	THR	5.0
1	D	160	ARG	5.0

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 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
4	BME	C	502	4/4	0.73	0.20	1.70	58,66,69,80	0
4	BME	C	504	4/4	0.90	0.21	1.53	59,60,63,71	0
4	BME	A	503	4/4	0.84	0.21	1.38	69,70,70,73	0
4	BME	D	500	4/4	0.89	0.17	0.45	47,49,51,63	0
3	MES	D	4246	12/12	0.94	0.19	0.03	57,64,68,69	0
4	BME	A	501	4/4	0.85	0.15	-	65,65,68,72	0
2	CL	B	506	1/1	0.96	0.14	-	60,60,60,60	0
2	CL	C	507	1/1	0.96	0.24	-	56,56,56,56	0

6.5 Other polymers [i](#)

There are no such residues in this entry.