



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 06:31 PM GMT

PDB ID : 1B70
Title : PHENYLALANYL TRNA SYNTHETASE COMPLEXED WITH PHENYLALANINE
Authors : Reshetnikova, L.; Moor, N.; Lavrik, O.; Vassilyev, D.G.
Deposited on : 1999-01-26
Resolution : 2.70 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

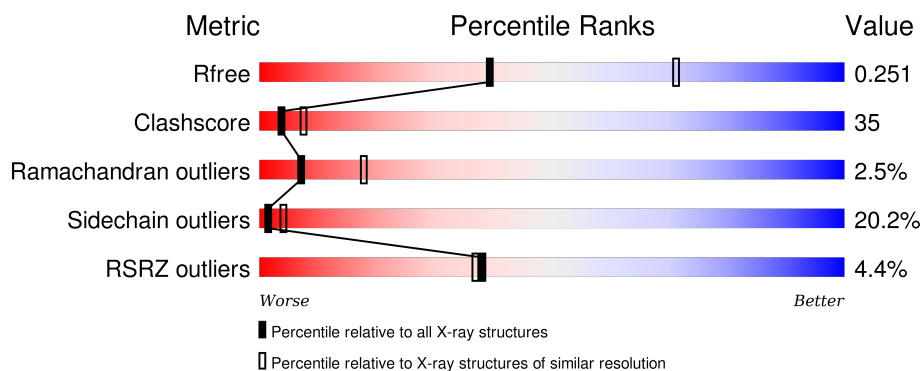
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

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	350	<div> <div>2%</div> <div>34%</div> <div>33%</div> <div>8%</div> <div>24%</div> </div>
2	B	785	<div> <div>5%</div> <div>44%</div> <div>42%</div> <div>12%</div> <div>..</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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	PHE	A	352	-	-	-	X

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 8313 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 PHENYLALANYL-TRNA SYNTHETASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	265	Total	C	N	O	S	0	0	0
			2112	1382	359	364	7			

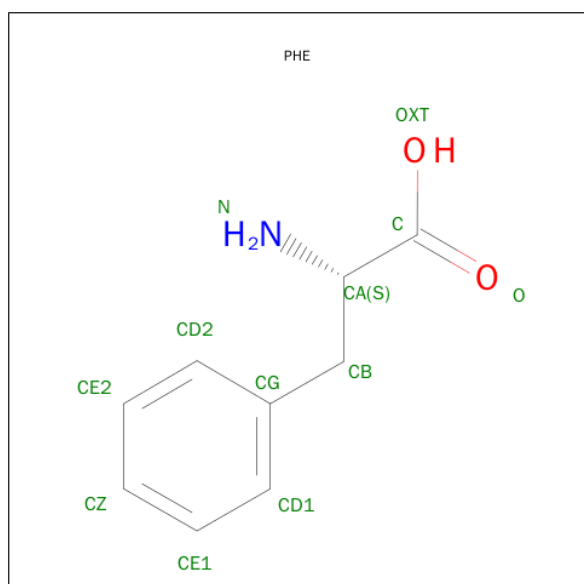
- Molecule 2 is a protein called PHENYLALANYL-TRNA SYNTHETASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	775	Total	C	N	O	S	0	0	0
			6054	3879	1078	1087	10			

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		

- Molecule 4 is PHENYLALANINE (three-letter code: PHE) (formula: C₉H₁₁NO₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			12	9	1	2		

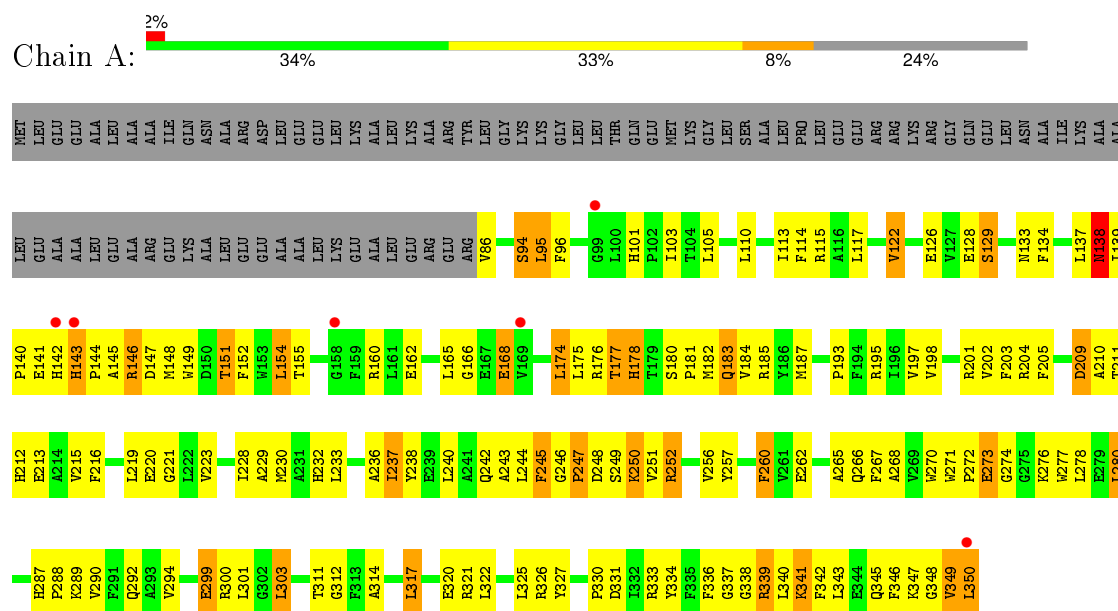
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	28	Total	O	0	0
			28	28		
5	B	106	Total	O	0	0
			106	106		

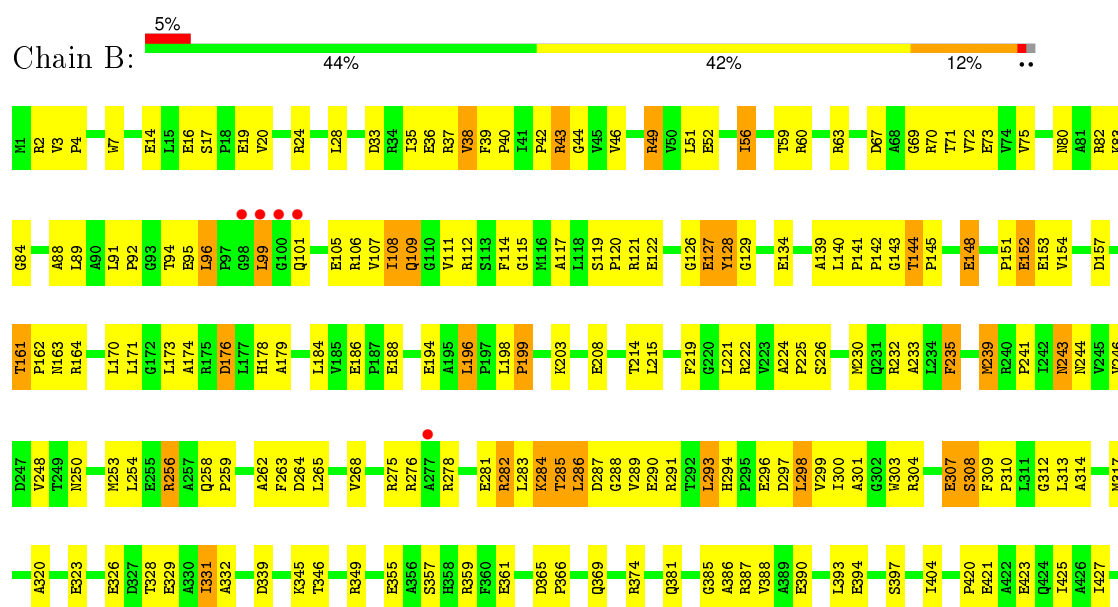
3 Residue-property plots

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: PHENYLALANYL-TRNA SYNTHETASE



• Molecule 2: PHENYLALANYL-TRNA SYNTHETASE



LEU	G719	H656	T583	N516	R430
ARG	F720	P657	H584	D517	
GLY	Y721	B658	L585	P518	V435
LEU	L722	A660	A586	E519	E438
ASP	E723	Q661	G587	D520	
THR	S724	B662	L588		
PRO	L725	L663	L589	R523	T441
	A726	L664	F590	F524	Y442
	L727	B665	G591	R525	R443
	F728	L666	E592	L526	
	D729	P667	G593	D527	P446
	L730	P667	V594	P528	P447
	Y731	P667	G595	S448	S448
	Q732	V668	L596	H449	H449
	G733	H669	P597	R450	R450
	F734	L670	W598	L451	L451
	F735	B671	A599	L532	L532
	L736	B672	X600	L533	D452
	F737	L673	B601	L534	L453
	E738	B674	R602	N535	R454
	G739	L675	L603	P536	
	H740	P676	S604	L537	
	K741		G605	K541	D458
	S742	K680	L608	A542	Y460
	L743	P681	L609	E461	E461
	A744	L682	R610	E462	E462
	F745	A683	L613	R465	
	H746	F684	E614	L466	
	L747	Q685		Y469	
	R748	S688	F617	G551	
	F749	R689		F479	
	R750		L622	L552	
	H751	A692	A623	V553	
	P752	A693	F624	R554	A482
	R753	F694	Q629	V555	
	R754	B695	A630	L556	N485
	T755	P696	F633	K557	R486
	L756	L697	H634	G487	G487
	R757	A698	P635	V488	
	D758	V699	G637	A490	
	E759	V700	S639	P491	
	E760	V701	V642	K494	
	V761	P702	L643		
	E762	A703	V644	R497	
	E763	P704	B645	L498	
	A764	T705	G646	R499	
	V765	P706	E647	E500	
	S766	Y707	B648	R499	
	R767	G708	V649	E500	
	V768	E709	G650	V501	
	A769	V710	F651		
	E770	E711	L652	L505	
	A771	A712	L653		
	L772	L713	G653	E509	
	R773	V714		G574	
	A774	R715		V575	
	R775	E716		V576	
	GLY	A717		E579	T512
	PHE			R580	Y513
	GLY			E581	S514
				E582	F515

4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	174.00Å 174.00Å 140.40Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.70 47.29 – 2.70	Depositor EDS
% Data completeness (in resolution range)	89.4 (50.00-2.70) 88.8 (47.29-2.70)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3001.55 (at 2.69Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.224 , 0.256 0.223 , 0.251	Depositor DCC
R_{free} test set	3018 reflections (5.04%)	DCC
Wilson B-factor (Å ²)	51.3	Xtriage
Anisotropy	0.418	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 81.7	EDS
Estimated twinning fraction	0.045 for -h,-k,l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Outliers	0 of 59935 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8313	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.76% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG

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	0.53	0/2180	0.71	0/2957
2	B	0.50	0/6205	0.73	3/8436 (0.0%)
All	All	0.50	0/8385	0.73	3/11393 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	115	GLY	N-CA-C	-5.72	98.80	113.10
2	B	69	GLY	N-CA-C	-5.39	99.64	113.10
2	B	38	VAL	N-CA-C	5.37	125.50	111.00

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	2112	0	2062	143	0
2	B	6054	0	6109	455	0
3	A	1	0	0	0	0
4	A	12	0	8	0	0
5	A	28	0	0	0	0
5	B	106	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	8313	0	8179	576	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 35.

The worst 5 of 576 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:165:LEU:HD12	1:A:301:LEU:HD13	1.35	1.08
2:B:285:THR:HG21	2:B:291:ARG:HE	1.25	0.99
2:B:614:GLU:HG2	2:B:624:PHE:HE1	1.24	0.97
2:B:75:VAL:HG11	2:B:108:ILE:HG21	1.45	0.97
2:B:707:TYR:HE1	2:B:711:GLU:HB2	1.30	0.93

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	263/350 (75%)	243 (92%)	13 (5%)	7 (3%)	6	16
2	B	773/785 (98%)	684 (88%)	70 (9%)	19 (2%)	7	18
All	All	1036/1135 (91%)	927 (90%)	83 (8%)	26 (2%)	7	18

5 of 26 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	138	ASN
2	B	488	VAL
2	B	664	GLU
1	A	94	SER

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Mol	Chain	Res	Type
1	A	338	GLY

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	213/277 (77%)	173 (81%)	40 (19%)	2	5
2	B	623/630 (99%)	494 (79%)	129 (21%)	1	4
All	All	836/907 (92%)	667 (80%)	169 (20%)	1	4

5 of 169 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	256	ARG
2	B	397	SER
2	B	730	LEU
2	B	283	LEU
2	B	308	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	287	HIS
2	B	101	GLN
2	B	243	ASN
1	A	232	HIS
2	B	258	GLN

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 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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	PHE	A	352	-	9,12,12	0.71	0	9,15,15	0.50	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	PHE	A	352	-	-	0/4/8/8	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

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](#)

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	265/350 (75%)	0.03	6 (2%) 64 64	30, 62, 101, 121	0
2	B	775/785 (98%)	0.15	40 (5%) 31 30	28, 66, 115, 130	0
All	All	1040/1135 (91%)	0.12	46 (4%) 38 37	28, 65, 114, 130	0

The worst 5 of 46 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	99	LEU	5.6
2	B	768	VAL	4.5
2	B	718	ALA	4.4
2	B	769	ALA	4.2
2	B	696	ASP	4.1

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	PHE	A	352	12/12	0.95	0.22	3.51	58,64,87,87	0
3	MG	A	351	1/1	0.94	0.18	1.26	36,36,36,36	0

6.5 Other polymers [i](#)

There are no such residues in this entry.