

Full wwPDB X-ray Structure Validation Report (i)

May 13, 2020 – 09:48 pm BST

PDB ID	:	1WBJ
Title	:	wildtype tryptophan synthase complexed with glycerol phosphate
Authors	:	Kulik, V.; Weyand, M.; Schlichting, I.
Deposited on		
Resolution	:	1.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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 following versions of software and data (see references (1)) were used in the production of this report:

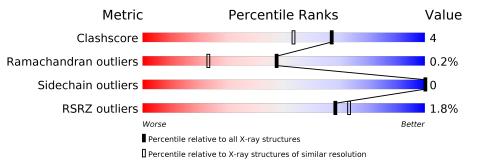
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
$\rm CCP4$:	$7.0.044 (\mathrm{Gargrove})$
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 1.50 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
Clashscore	141614	$3144 \ (1.50 - 1.50)$
Ramachandran outliers	138981	$3066 \ (1.50-1.50)$
Sidechain outliers	138945	3064 (1.50-1.50)
RSRZ outliers	127900	2884 (1.50-1.50)

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 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	А	268	87%	13%	
2	В	396	% 	9%	·

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	\mathbf{Res}	Chirality	Geometry	Clashes	Electron density
3	G3P	А	1268	Х	-	-	-



$1 \mathrm{WBJ}$

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 5569 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.

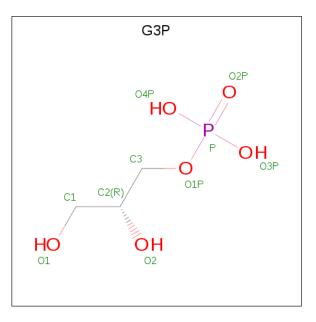
• Molecule 1 is a protein called TRYPTOPHAN SYNTHASE ALPHA CHAIN.

Mol	Chain	Residues		Ate	oms			ZeroOcc	AltConf	Trace
1	А	267	Total 2019	C 1284	$rac{N}{352}$	O 375	S 8	0	2	0

• Molecule 2 is a protein called TRYPTOPHAN SYNTHASE BETA CHAIN.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
2	В	390	Total 2991	C 1882	N 521	O 568	S 20	0	10	0

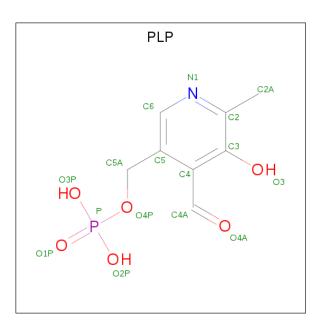
• Molecule 3 is SN-GLYCEROL-3-PHOSPHATE (three-letter code: G3P) (formula: $C_3H_9O_6P$).



Mo	Chair	n Residues	Atoms				ZeroOcc	AltConf
3	А	1	Total 10	С 3	О 6	Р 1	0	0

• Molecule 4 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: $C_8H_{10}NO_6P$).





Mol	Chain	Residues		Ate	oms			ZeroOcc	AltConf
4	В	1	Total	С	Ν	0	Р	0	Ο
4	D	T	15	8	1	5	1	0	0

• Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	В	1	Total Na 1 1	0	0

• Molecule 6 is water.

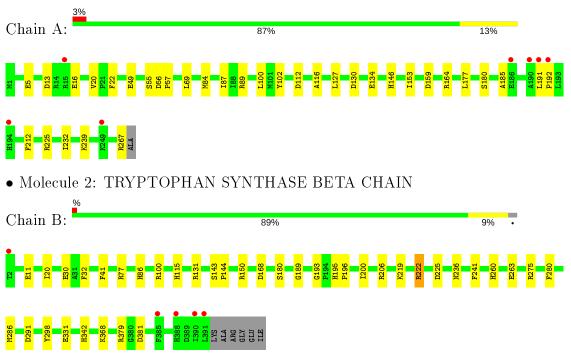
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	А	192	Total O 192 192	2	0
6	В	341	Total O 341 341	0	0



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 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: TRYPTOPHAN SYNTHASE ALPHA CHAIN





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants	182.04Å 59.56 Å 67.41 Å	Depositor
a, b, c, α , β , γ	90.00° 94.56° 90.00°	Depositor
Resolution (Å)	20.00 - 1.50	Depositor
Resolution (A)	36.29 - 1.34	EDS
% Data completeness	93.8 (20.00-1.50)	Depositor
(in resolution range)	82.7 (36.29-1.34)	EDS
R _{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.00 (at 1.34 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.0	Depositor
B B.	0.179 , 0.202	Depositor
R, R_{free}	0.182 , (Not available)	DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	8.8	Xtriage
Anisotropy	0.331	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.38 , 46.0	EDS
L-test for twinning ²	$ \langle L \rangle = 0.48, \langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5569	wwPDB-VP
Average B, all atoms $(Å^2)$	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.99% of the height of the origin peak. No significant pseudotranslation is detected.

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.



¹Intensities estimated from amplitudes.

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: G3P, NA, PLP

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 Chair	Chain	Bond lengths		Bond angles		
	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	1.00	1/2069~(0.0%)	1.10	9/2811~(0.3%)	
2	В	1.10	6/3092~(0.2%)	1.16	18/4174~(0.4%)	
All	All	1.06	7/5161~(0.1%)	1.13	27/6985~(0.4%)	

All (7) bond length outliers are listed below:

Mol	Chain	\mathbf{Res}	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	$\operatorname{Ideal}(\operatorname{\AA})$
2	В	263	GLU	CD-OE1	6.66	1.32	1.25
2	В	41	PHE	CD1-CE1	6.21	1.51	1.39
2	В	291	ASP	CB-CG	-6.16	1.38	1.51
2	В	298	TYR	CE1-CZ	6.12	1.46	1.38
1	А	55	SER	CB-OG	-5.80	1.34	1.42
2	В	331	GLU	CD-OE2	5.69	1.31	1.25
2	В	206	ARG	CG-CD	5.09	1.64	1.51

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
2	В	222	ARG	NE-CZ-NH1	11.11	125.86	120.30
2	В	206	ARG	NE-CZ-NH2	10.13	125.37	120.30
2	В	222	ARG	NE-CZ-NH2	-9.84	115.38	120.30
1	А	225	ARG	NE-CZ-NH2	-9.34	115.63	120.30
2	В	77	ARG	NE-CZ-NH2	-9.07	115.77	120.30
2	В	206	ARG	NE-CZ-NH1	-7.75	116.42	120.30
1	А	225	ARG	NE-CZ-NH1	7.60	124.10	120.30
2	В	241	PHE	CB-CG-CD2	-7.21	115.75	120.80
2	В	168	ASP	CB-CG-OD2	7.01	124.61	118.30
2	В	131	ARG	NE-CZ-NH1	6.94	123.77	120.30
1	А	13	ASP	CB-CG-OD2	6.82	124.43	118.30
2	В	368	LYS	CD-CE-NZ	-6.59	96.54	111.70

Continued on next page...



1	W	ΒJ

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	В	275	ARG	NE-CZ-NH2	6.34	123.47	120.30
2	В	286	MET	CA-CB-CG	6.29	124.00	113.30
1	А	164	ARG	NE-CZ-NH2	-5.95	117.33	120.30
2	В	286	MET	CG-SD-CE	-5.80	90.91	100.20
1	А	159	ASP	CB-CG-OD2	5.78	123.51	118.30
2	В	381	ASP	CB-CG-OD2	5.56	123.30	118.30
1	А	56	ASP	CB-CG-OD2	5.40	123.16	118.30
1	А	89	ARG	NE-CZ-NH1	5.35	122.97	120.30
2	В	298	TYR	CA-CB-CG	-5.33	103.28	113.40
1	А	134	GLU	OE1-CD-OE2	-5.29	116.96	123.30
2	В	100	ARG	NE-CZ-NH1	5.26	122.93	120.30
2	В	222	ARG	CG-CD-NE	5.25	122.83	111.80
1	А	130	ASP	CB-CG-OD1	5.24	123.01	118.30
2	В	225	ASP	CB-CG-OD2	5.22	123.00	118.30
2	В	150	ARG	NE-CZ-NH2	-5.05	117.77	120.30

Continued from previous page...

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	А	2019	0	2029	24	0
2	В	2991	0	2965	21	0
3	А	10	0	6	0	0
4	В	15	0	6	0	0
5	В	1	0	0	0	0
6	А	192	0	0	1	0
6	В	341	0	0	6	1
All	All	5569	0	5006	39	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 4.

All (39) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.



Atom-1	Atom-2	Interatomic	Clash
Atom-1	At0111-2	distance (Å)	overlap (Å)
1:A:84:MET:O	1:A:87:ILE:HG22	1.59	1.02
2:B:219[A]:LYS:HE2	6:B:2083:HOH:O	1.75	0.86
2:B:222:ARG:NH2	6:B:2217:HOH:O	2.10	0.85
1:A:100[B]:LEU:HD23	1:A:127:LEU:HD23	1.65	0.78
1:A:180:SER:HA	2:B:20:ILE:CD1	2.15	0.76
1:A:84:MET:O	1:A:87:ILE:CG2	2.43	0.62
1:A:180:SER:CB	2:B:20:ILE:HD11	2.30	0.61
1:A:112:ASP:OD1	1:A:146[A]:HIS:HE1	1.84	0.60
2:B:342[B]:HIS:HD2	6:B:2304:HOH:O	1.85	0.59
1:A:180:SER:HA	2:B:20:ILE:HD11	1.86	0.58
2:B:143:SER:OG	2:B:144:PRO:HD3	2.03	0.57
1:A:69:LEU:HD22	6:A:2060:HOH:O	2.06	0.55
1:A:180:SER:HB2	2:B:20:ILE:HD11	1.88	0.55
2:B:260:HIS:HD2	6:B:2148:HOH:O	1.92	0.53
1:A:180:SER:HA	2:B:20:ILE:HD12	1.88	0.53
2:B:379:ARG:NH1	6:B:2332:HOH:O	2.42	0.53
1:A:153:ILE:HG23	1:A:177:LEU:HG	1.93	0.51
1:A:191:LEU:HD12	1:A:192:PRO:HD2	1.93	0.51
1:A:84:MET:C	1:A:87:ILE:HG22	2.28	0.49
1:A:185:ALA:HB3	1:A:239:LYS:NZ	2.27	0.49
1:A:180:SER:CA	2:B:20:ILE:HD11	2.45	0.47
1:A:116:ALA:HB2	1:A:146[B]:HIS:CE1	2.51	0.46
1:A:22:PHE:HA	1:A:49:GLU:O	2.15	0.45
2:B:115:HIS:CE1	2:B:189:GLY:HA2	2.52	0.45
1:A:100[B]:LEU:CD2	1:A:127:LEU:HD23	2.43	0.45
2:B:30:GLU:HG2	6:B:2052:HOH:O	2.15	0.45
1:A:192:PRO:HG2	1:A:192:PRO:O	2.17	0.44
2:B:86:HIS:CE1	2:B:236:ASN:HB3	2.53	0.44
1:A:16:GLU:HG2	1:A:267:ARG:HG2	2.00	0.43
1:A:5:GLU:CD	1:A:5:GLU:H	2.21	0.43
2:B:195:HIS:ND1	2:B:196:PRO:HA	2.35	0.42
2:B:193:GLY:HA2	2:B:280:PHE:O	2.20	0.42
2:B:32:PHE:CD1	2:B:200:ILE:HG12	2.56	0.41
1:A:20:VAL:O	1:A:232:ILE:HA	2.20	0.41
2:B:195:HIS:CG	2:B:196:PRO:HA	2.55	0.41
1:A:57:PRO:HA	1:A:102:TYR:CZ	2.57	0.40

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)
6:B:2076:HOH:O	6:B:2081:HOH:O[2_655]	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	Perce	\mathbf{ntiles}
1	А	267/268~(100%)	262~(98%)	4 (2%)	1 (0%)	34	13
2	В	398/396~(100%)	390~(98%)	8 (2%)	0	100	100
All	All	665/664~(100%)	652 (98%)	12 (2%)	1 (0%)	47	23

All (1) Ramachandran outliers are listed below:

Mol	Chain	\mathbf{Res}	Type
1	А	212	PHE

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	Percentile	es
1	А	209/208~(100%)	209~(100%)	0	100 100)
2	В	316/310~(102%)	316 (100%)	0	100 100)
All	All	525/518~(101%)	525~(100%)	0	100 100)

There are no protein residues with a non-rotameric sidechain to report.

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	В	260	HIS



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 3 ligands modelled in this entry, 1 is 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).

Mal	Mol Type	Chain I	Chain	Chain	Res	Link	Bo	ond leng	\mathbf{ths}	В	ond ang	les
	туре	Cham	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2		
4	PLP	В	1392	2	15, 15, 16	1.27	1(6%)	$20,\!22,\!23$	1.60	2(10%)		
3	G3P	А	1268	-	9, 9, 9	1.07	1 (11%)	$11,\!12,\!12$	1.36	<mark>3 (27%)</mark>		

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	PLP	В	1392	2	-	0/6/6/8	0/1/1/1
3	G3P	А	1268	-	1/1/2/2	1/8/8/8	_

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(A)	Ideal(Å)
4	В	1392	PLP	C6-N1	2.74	1.40	1.34

Continued on next page...



Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	А	1268	G3P	O1-C1	-2.52	1.31	1.42

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
4	В	1392	PLP	O4P-C5A-C5	5.60	120.02	109.35
4	В	1392	PLP	C4A-C4-C5	-2.62	118.24	120.94
3	А	1268	G3P	O3P-P-O1P	-2.48	100.13	106.73
3	А	1268	G3P	O2-C2-C1	-2.26	99.18	109.12
3	А	1268	G3P	O1-C1-C2	2.10	120.25	110.20

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	А	1268	G3P	C2

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	А	1268	G3P	C2-C3-O1P-P

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, 95^{th} 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	А	267/268~(99%)	-0.56	7 (2%) 56 61	10, 15, 31, 42	0
2	В	390/396~(98%)	-0.63	5 (1%) 77 81	7, 12, 22, 38	0
All	All	657/664~(98%)	-0.60	12 (1%) 68 73	7, 14, 27, 42	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	А	191	LEU	3.7
2	В	390	ILE	3.0
1	А	186	GLU	2.9
2	В	2	THR	2.8
2	В	391	LEU	2.5
1	А	15	ARG	2.4
1	А	190	ALA	2.4
1	А	192	PRO	2.3
1	А	194	HIS	2.3
2	В	388	HIS	2.2
1	А	249	LYS	2.2
2	В	385	PHE	2.0

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. The B-factors column lists the minimum, median, 95^{th} 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	\mathbf{RSR}	$\mathbf{B} extsf{-factors}(\mathrm{\AA}^2)$	Q<0.9
3	G3P	A	1268	10/10	0.98	0.05	15, 16, 19, 19	0
4	PLP	В	1392	15/16	0.99	0.07	6, 8, 11, 14	0
5	NA	В	1393	1/1	1.00	0.04	10, 10, 10, 10	0

6.5 Other polymers (i)

There are no such residues in this entry.

