



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:51 AM UTC

PDB ID : 5OHN / pdb_00005ohn
Title : Crystal structure of USP30 in covalent complex with ubiquitin propargylamide (low resolution)
Authors : Gersch, M.; Komander, D.
Deposited on : 2017-07-17
Resolution : 3.60 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

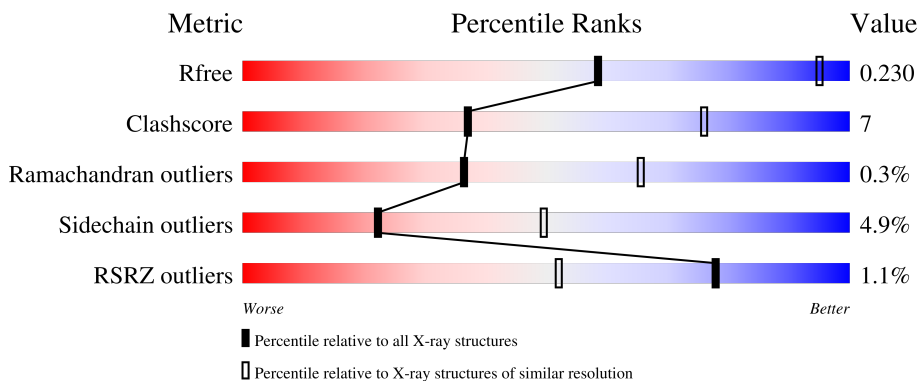
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 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}	180053	1747 (3.70-3.50)
Clashscore	190562	1827 (3.70-3.50)
Ramachandran outliers	187476	1773 (3.70-3.50)
Sidechain outliers	187428	1772 (3.70-3.50)
RSRZ outliers	180081	1745 (3.70-3.50)

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 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 $\leq 5\%$. 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	370	 67% 13% 19%
1	C	370	 65% 14% 20%
2	B	76	 86% 13%
2	D	76	 82% 17%

2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 5789 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 Ubiquitin carboxyl-terminal hydrolase 30, Ubiquitin carboxyl-terminal hydrolase 30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	299	2331	1480	404	430	17	0	0	0
1	C	297	2312	1462	404	429	17	0	0	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	62	GLY	-	expression tag	UNP Q70CQ3
A	63	PRO	-	expression tag	UNP Q70CQ3
A	348	ASP	PHE	engineered mutation	UNP Q70CQ3
A	350	ASP	MET	engineered mutation	UNP Q70CQ3
A	353	GLU	ILE	engineered mutation	UNP Q70CQ3
A	358	SER	-	linker	UNP Q70CQ3
A	359	ASN	-	linker	UNP Q70CQ3
A	360	ALA	-	linker	UNP Q70CQ3
C	62	GLY	-	expression tag	UNP Q70CQ3
C	63	PRO	-	expression tag	UNP Q70CQ3
C	348	ASP	PHE	engineered mutation	UNP Q70CQ3
C	350	ASP	MET	engineered mutation	UNP Q70CQ3
C	353	GLU	ILE	engineered mutation	UNP Q70CQ3
C	358	SER	-	linker	UNP Q70CQ3
C	359	ASN	-	linker	UNP Q70CQ3
C	360	ALA	-	linker	UNP Q70CQ3

- Molecule 2 is a protein called Polyubiquitin-B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	76	572	360	99	112	1	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	D	76	572	360	99	112	1	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	76	AYE	GLY	engineered mutation	UNP P0CG47
D	76	AYE	GLY	engineered mutation	UNP P0CG47

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		
3	C	1	Total	Zn	0	0
			1	1		

Chain D:  82% 17%



4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	181.83Å 181.83Å 94.96Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	157.47 – 3.60 157.47 – 3.60	Depositor EDS
% Data completeness (in resolution range)	99.3 (157.47-3.60) 99.3 (157.47-3.60)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.33 (at 3.58Å)	Xtriage
Refinement program	PHENIX (1.12rc2_2821: ???)	Depositor
R, R_{free}	0.211 , 0.253 0.200 , 0.230	Depositor DCC
R_{free} test set	972 reflections (4.65%)	wwPDB-VP
Wilson B-factor (Å ²)	147.1	Xtriage
Anisotropy	0.229	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 194.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.20$	Xtriage
Estimated twinning fraction	0.398 for h,-h-k,-l	Xtriage
Reported twinning fraction	0.521 for H, K, L 0.479 for K, H, -L	Depositor
Outliers	0 of 20774 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5789	wwPDB-VP
Average B, all atoms (Å ²)	165.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.15% 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

5.1 Standard geometry

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

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	0.71	0/2388	0.81	1/3245 (0.0%)
1	C	0.69	2/2365 (0.1%)	0.82	3/3210 (0.1%)
2	B	0.59	0/574	0.70	0/778
2	D	0.57	0/574	0.72	0/778
All	All	0.68	2/5901 (0.0%)	0.79	4/8011 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	286	ASN	CG-OD1	5.44	1.33	1.23
1	C	286	ASN	CG-ND2	5.30	1.44	1.33

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	281	ASP	N-CA-C	5.50	119.16	111.74
1	C	262	HIS	CA-C-N	5.46	125.36	119.85
1	C	262	HIS	C-N-CA	5.46	125.36	119.85
1	C	281	ASP	N-CA-C	5.34	118.95	111.74

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	2331	0	2144	32	3
1	C	2312	0	2139	42	3
2	B	572	0	569	6	0
2	D	572	0	569	18	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
All	All	5789	0	5421	80	3

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 7.

All (80) 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:159:GLU:O	2:D:74:ARG:CD	1.80	1.26
1:C:159:GLU:O	2:D:74:ARG:HD3	1.11	1.26
1:C:262:HIS:CB	1:C:263:PRO:HD2	1.69	1.21
1:C:262:HIS:CB	1:C:263:PRO:CD	2.22	1.17
1:C:262:HIS:HB3	1:C:263:PRO:CD	1.73	1.17
1:C:262:HIS:HB2	1:C:263:PRO:HD2	1.20	1.14
1:A:262:HIS:CB	1:A:263:PRO:CD	2.26	1.13
1:A:262:HIS:HB2	1:A:263:PRO:HD2	1.32	1.09
1:A:262:HIS:HB2	1:A:263:PRO:CD	1.84	1.07
1:A:262:HIS:HB3	1:A:263:PRO:HD3	1.30	1.06
1:C:257:ALA:O	1:C:261:GLY:N	1.91	1.02
1:C:262:HIS:HB3	1:C:263:PRO:HD3	1.39	1.00
1:A:482:ARG:NH1	1:C:483:LYS:O	1.96	0.98
1:A:262:HIS:CB	1:A:263:PRO:HD3	1.93	0.95
1:C:159:GLU:O	2:D:74:ARG:CG	2.26	0.83
1:C:159:GLU:C	2:D:74:ARG:HG2	2.07	0.79
2:D:23:ILE:HD11	2:D:51:GLU:C	2.15	0.72
2:B:23:ILE:HD11	2:B:51:GLU:C	2.17	0.69
1:C:159:GLU:O	2:D:74:ARG:HG2	1.92	0.68
1:C:240:GLN:OE1	1:C:240:GLN:N	2.27	0.67
1:C:160:GLN:CA	2:D:74:ARG:HG2	2.24	0.67
1:A:240:GLN:N	1:A:240:GLN:OE1	2.28	0.66
1:C:160:GLN:HA	2:D:74:ARG:HG2	1.80	0.63
1:C:159:GLU:C	2:D:74:ARG:CD	2.71	0.62
1:A:287:CYS:O	1:A:289:LYS:N	2.32	0.62
1:C:160:GLN:N	2:D:74:ARG:HG2	2.16	0.61
1:C:287:CYS:O	1:C:289:LYS:N	2.34	0.60
1:C:286:ASN:O	1:C:288:THR:HG23	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:159:GLU:C	2:D:74:ARG:CG	2.74	0.58
1:C:443:VAL:HB	1:C:454:VAL:HG12	1.86	0.58
1:C:257:ALA:C	1:C:261:GLY:N	2.62	0.57
1:A:443:VAL:HB	1:A:454:VAL:HG12	1.87	0.56
1:A:262:HIS:HB3	1:A:263:PRO:CD	2.01	0.55
1:A:145:ASP:O	1:A:149:MET:HG3	2.06	0.55
1:A:286:ASN:O	1:A:288:THR:HG23	2.07	0.55
1:C:433:THR:O	1:C:501:ARG:NH2	2.38	0.55
1:A:433:THR:O	1:A:501:ARG:NH2	2.39	0.54
1:C:145:ASP:O	1:C:149:MET:HG3	2.07	0.53
1:A:152:TRP:CE3	1:A:154:ILE:HD13	2.45	0.52
1:C:453:PHE:CE2	2:D:75:GLY:HA3	2.45	0.52
1:C:328:LEU:HG	2:D:73:LEU:HD13	1.91	0.52
1:A:148:ARG:NH1	1:A:155:SER:HA	2.24	0.51
1:C:152:TRP:CE3	1:C:154:ILE:HD13	2.45	0.51
1:A:243:VAL:HG11	1:A:356:TYR:OH	2.10	0.50
1:A:229:THR:HG21	1:A:356:TYR:CD2	2.47	0.50
1:C:243:VAL:HG11	1:C:356:TYR:OH	2.11	0.49
1:C:229:THR:HG21	1:C:356:TYR:CD2	2.48	0.49
1:C:148:ARG:NH1	1:C:155:SER:HA	2.30	0.47
1:A:164:GLU:HG3	2:B:49:GLN:OE1	2.15	0.47
2:D:22:THR:HA	2:D:55:THR:HA	1.97	0.46
1:A:284:CYS:HB3	1:A:287:CYS:HB2	1.99	0.45
2:B:22:THR:HA	2:B:55:THR:HA	1.97	0.45
1:C:77:CYS:HB3	2:D:76:AYE:H3A	1.93	0.45
1:A:151:ARG:NH1	1:A:175:ASP:OD2	2.47	0.44
1:A:231:ASN:HD21	1:A:356:TYR:HE1	1.65	0.44
1:A:72:ASN:HA	1:A:76:THR:HG22	2.00	0.44
1:C:239:HIS:CB	1:C:286:ASN:ND2	2.81	0.44
1:C:142:CYS:O	1:C:146:VAL:HG13	2.18	0.43
1:C:231:ASN:HD21	1:C:356:TYR:HE1	1.65	0.43
1:A:116:LEU:HD21	1:A:147:LEU:HD21	2.01	0.43
2:D:1:MET:HE1	2:D:61:ILE:O	2.19	0.43
1:A:148:ARG:NE	1:A:154:ILE:O	2.52	0.43
2:D:26:VAL:HG21	2:D:56:LEU:HD11	2.01	0.43
2:B:26:VAL:HG21	2:B:56:LEU:HD11	2.01	0.42
1:C:151:ARG:NH1	1:C:175:ASP:OD2	2.47	0.42
1:A:142:CYS:O	1:A:146:VAL:HG13	2.19	0.42
1:A:482:ARG:HD3	1:C:482:ARG:HD2	2.01	0.42
1:C:72:ASN:HA	1:C:76:THR:HG22	2.01	0.42
1:C:116:LEU:HD21	1:C:147:LEU:HD21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1:MET:HE1	2:B:61:ILE:O	2.19	0.42
1:A:178:ASP:O	1:A:179:ARG:CB	2.68	0.42
1:C:284:CYS:HB3	1:C:287:CYS:HB2	2.01	0.41
1:A:77:CYS:HB3	2:B:76:AYE:H3A	2.01	0.41
1:A:306:THR:OG1	1:A:307:THR:N	2.54	0.41
1:C:164:GLU:HG3	2:D:49:GLN:OE1	2.20	0.41
1:A:224:PHE:CE1	1:A:320:CYS:HB3	2.56	0.41
1:A:152:TRP:CE2	1:A:154:ILE:HG21	2.56	0.41
1:C:152:TRP:CE2	1:C:154:ILE:HG21	2.57	0.40
1:C:306:THR:OG1	1:C:307:THR:N	2.55	0.40
1:A:442:VAL:HB	1:A:496:LEU:HB2	2.03	0.40

All (3) 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)
1:A:356:TYR:OH	1:C:356:TYR:OH[5_555]	1.67	0.53
1:A:148:ARG:NH1	1:C:145:ASP:OD2[4_654]	2.16	0.04
1:A:148:ARG:NH2	1:C:145:ASP:CG[4_654]	2.19	0.01

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	287/370 (78%)	268 (93%)	18 (6%)	1 (0%)	36	65
1	C	285/370 (77%)	267 (94%)	17 (6%)	1 (0%)	30	61
2	B	73/76 (96%)	72 (99%)	1 (1%)	0	100	100
2	D	73/76 (96%)	72 (99%)	1 (1%)	0	100	100
All	All	718/892 (80%)	679 (95%)	37 (5%)	2 (0%)	36	65

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	262	HIS
1	C	262	HIS

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	247/343 (72%)	235 (95%)	12 (5%)	22	49
1	C	247/343 (72%)	233 (94%)	14 (6%)	18	46
2	B	61/68 (90%)	59 (97%)	2 (3%)	33	58
2	D	61/68 (90%)	59 (97%)	2 (3%)	33	58
All	All	616/822 (75%)	586 (95%)	30 (5%)	22	49

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	76	THR
1	A	144	LEU
1	A	146	VAL
1	A	170	THR
1	A	220	SER
1	A	232	MET
1	A	233	VAL
1	A	234	CYS
1	A	335	THR
1	A	438	LEU
1	A	448	MET
1	A	454	VAL
2	B	55	THR
2	B	70	VAL
1	C	76	THR
1	C	144	LEU
1	C	146	VAL
1	C	170	THR
1	C	220	SER
1	C	232	MET

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Mol	Chain	Res	Type
1	C	233	VAL
1	C	234	CYS
1	C	264	LEU
1	C	278	SER
1	C	335	THR
1	C	438	LEU
1	C	448	MET
1	C	454	VAL
2	D	55	THR
2	D	70	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	222	HIS
1	A	342	HIS
1	A	487	GLN
2	B	25	ASN
1	C	342	HIS
1	C	487	GLN
2	D	25	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

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

There are no such residues in this entry.

5.8 Polymer linkage issues

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	299/370 (80%)	-0.67	4 (1%) 75 48	101, 157, 225, 277	0
1	C	297/370 (80%)	-0.69	3 (1%) 79 54	112, 157, 226, 267	0
2	B	75/76 (98%)	-0.84	1 (1%) 75 48	127, 165, 209, 221	0
2	D	75/76 (98%)	-0.88	0 100 100	122, 159, 199, 233	0
All	All	746/892 (83%)	-0.72	8 (1%) 78 52	101, 158, 222, 277	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	103	TYR	4.9
1	A	218	TRP	3.8
1	A	462	SER	3.1
1	C	132	VAL	2.6
2	B	19	PRO	2.6
1	A	220	SER	2.4
1	A	156	SER	2.2
1	C	462	SER	2.1

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 oligosaccharides 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
3	ZN	A	800	1/1	1.00	0.01	107,107,107,107	0
3	ZN	C	800	1/1	1.00	0.03	116,116,116,116	0

6.5 Other polymers [i](#)

There are no such residues in this entry.