



Full wwPDB X-ray Structure Validation Report

Sep 16, 2014 – 06:55 PM EDT

PDB ID : 3RVB
Title : The structure of HCV NS3 helicase (Heli-80) bound with inhibitor ITMN-3479
Authors : Mather, O.; Cheng, R.; Schonfield, D.; Barker, J.
Deposited on : 2011-05-06
Resolution : 2.20 Å(reported)

This is a full wwPDB validation 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/ValidationPDFNotes.html>

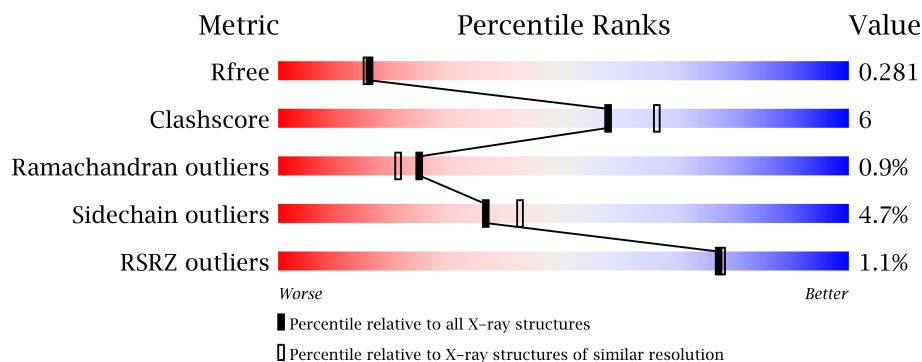
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.16 November 2013
Xtriage (Phenix) : dev-1439
EDS : stable23489
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable23489

1 Overall quality at a glance


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}	66092	2938 (2.20-2.20)
Clashscore	79885	3751 (2.20-2.20)
Ramachandran outliers	78287	3681 (2.20-2.20)
Sidechain outliers	78261	3682 (2.20-2.20)
RSRZ outliers	66119	2939 (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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	493	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	I79	A	1	-	X
3	MG	A	3	-	X
4	CL	A	4	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 3511 atoms, of which 0 are hydrogen and 0 are deuterium.

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 RNA helicase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	443	Total	C	N	O	S	0	1	0
			3344	2115	572	638	19			

There are 37 discrepancies between the modelled and reference sequences:

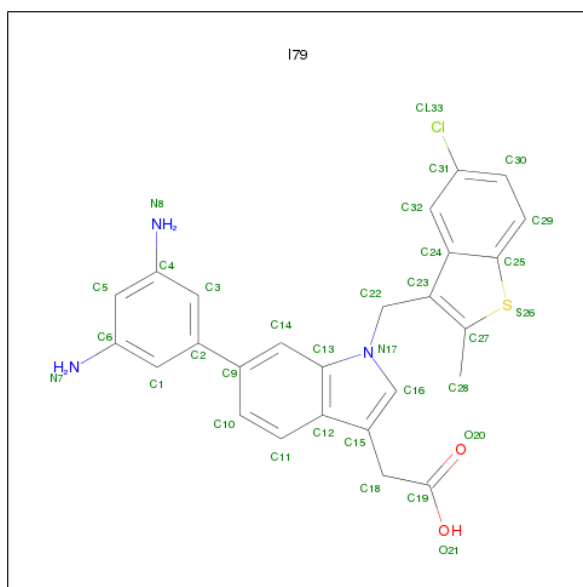
Chain	Residue	Modelled	Actual	Comment	Reference
A	145	MET	-	EXPRESSION TAG	UNP P26663
A	146	GLY	-	EXPRESSION TAG	UNP P26663
A	147	ARG	-	EXPRESSION TAG	UNP P26663
A	148	GLY	-	EXPRESSION TAG	UNP P26663
A	149	SER	-	EXPRESSION TAG	UNP P26663
A	150	HIS	-	EXPRESSION TAG	UNP P26663
A	151	HIS	-	EXPRESSION TAG	UNP P26663
A	152	HIS	-	EXPRESSION TAG	UNP P26663
A	153	HIS	-	EXPRESSION TAG	UNP P26663
A	154	HIS	-	EXPRESSION TAG	UNP P26663
A	155	HIS	-	EXPRESSION TAG	UNP P26663
A	156	GLY	-	EXPRESSION TAG	UNP P26663
A	157	MET	-	EXPRESSION TAG	UNP P26663
A	158	ALA	-	EXPRESSION TAG	UNP P26663
A	159	SER	-	EXPRESSION TAG	UNP P26663
A	196	THR	SER	CONFLICT	UNP P26663
A	240	VAL	ALA	CONFLICT	UNP P26663
A	258	ALA	THR	CONFLICT	UNP P26663
A	263	GLY	ALA	CONFLICT	UNP P26663
A	265	ILE	VAL	CONFLICT	UNP P26663
A	299	SER	THR	CONFLICT	UNP P26663
A	358	VAL	ALA	CONFLICT	UNP P26663
A	383	ALA	GLY	CONFLICT	UNP P26663
A	386	LEU	ILE	CONFLICT	UNP P26663
A	403	SER	ILE	CONFLICT	UNP P26663
A	447	ASP	GLU	CONFLICT	UNP P26663
A	584	SER	CYS	CONFLICT	UNP P26663

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Chain	Residue	Modelled	Actual	Comment	Reference
A	586	THR	ILE	CONFLICT	UNP P26663
A	605	LEU	VAL	CONFLICT	UNP P26663
A	615	VAL	ILE	CONFLICT	UNP P26663
A	618	PHE	TYR	CONFLICT	UNP P26663
A	632	ALA	SER	CONFLICT	UNP P26663
A	633	ALA	-	INSERTION	UNP P26663
A	634	ALA	-	INSERTION	UNP P26663
A	635	ARG	-	INSERTION	UNP P26663
A	636	GLU	-	INSERTION	UNP P26663
A	637	ALA	-	INSERTION	UNP P26663

- Molecule 2 is {1-[(5-CHLORO-2-METHYL-1-BENZOTHIOPHEN-3-YL)METHYL]-6-(3,5-DIAMINOPHENYL)-1H-INDOL-3-YL}ACETICACID (three-letter code: I79) (formula: C₂₆H₂₂ClN₃O₂S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	Cl	N	O	S	0	0
			33	26	1	3	2	1		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Mg	0	0
			2	2		

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total 1	Cl 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	131	Total 131	O 131	0	0

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 ($\text{RSRZ} > 2$). 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: RNA helicase

Chain A:

4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	92.35Å 92.35Å 104.46Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	34.82 – 2.20 34.60 – 2.20	Depositor EDS
% Data completeness (in resolution range)	96.6 (34.82-2.20) 96.6 (34.60-2.20)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.62 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.224 , 0.287 0.221 , 0.281	Depositor DCC
R_{free} test set	1322 reflections (5.42%)	DCC
Wilson B-factor (Å ²)	42.0	Xtriage
Anisotropy	0.071	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 26.7	EDS
Estimated twinning fraction	0.022 for -h,-k,l	Xtriage
L-test for twinning	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 25723 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3511	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.01% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, I79, CL

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	0.87	2/3427 (0.1%)	0.83	2/4683 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	480	GLU	CG-CD	5.49	1.60	1.51
1	A	608	GLU	CG-CD	5.07	1.59	1.51

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	570	ARG	NE-CZ-NH1	5.19	122.89	120.30
1	A	514	ARG	NE-CZ-NH1	5.12	122.86	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3344	0	3304	42	0
2	A	33	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	2	0	0	0	0
4	A	1	0	0	0	0
5	A	131	0	0	1	0
All	All	3511	0	3304	42	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 6.

All (42) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:333:HIS:HD2	1:A:335:ASN:H	1.28	0.80
1:A:583:LYS:HA	1:A:586:THR:HG23	1.74	0.68
1:A:626:ASP:O	1:A:630:VAL:HG23	1.93	0.68
1:A:374:CYS:HA	1:A:409:VAL:HG12	1.79	0.65
1:A:419:THR:HG23	1:A:420:GLY:H	1.62	0.65
1:A:419:THR:O	1:A:464:ARG:NH2	2.30	0.64
1:A:550:THR:HG21	1:A:558:PRO:HA	1.80	0.64
1:A:533:GLU:O	1:A:537:THR:HG23	1.98	0.63
1:A:415:MET:HA	1:A:464:ARG:NH1	2.15	0.62
1:A:374:CYS:HA	1:A:409:VAL:CG1	2.31	0.60
1:A:346:GLU:OE1	1:A:356:ILE:HG22	2.03	0.58
1:A:429:ASN:HA	1:A:453:GLN:NE2	2.19	0.57
1:A:194:PRO:HG3	1:A:198:GLN:CB	2.36	0.55
1:A:248:ILE:O	1:A:250:PRO:HD3	2.07	0.55
1:A:550:THR:CG2	1:A:558:PRO:HA	2.37	0.55
1:A:429:ASN:HD21	1:A:475:PHE:HB2	1.71	0.54
1:A:333:HIS:CD2	1:A:334:PRO:HD2	2.43	0.53
1:A:436:VAL:HG11	1:A:488:SER:HB3	1.92	0.52
1:A:423:ASP:OD1	1:A:469:ARG:NH2	2.41	0.51
1:A:194:PRO:HG3	1:A:198:GLN:HB3	1.93	0.51
1:A:415:MET:HA	1:A:464:ARG:HH12	1.75	0.51
1:A:393:ARG:HH22	1:A:416:THR:CG2	2.23	0.50
1:A:420:GLY:HA2	1:A:467:ARG:NH1	2.26	0.49
1:A:624:SER:HA	1:A:630:VAL:HG22	1.96	0.47
1:A:371:LYS:HG2	1:A:392:TYR:CG	2.49	0.47
1:A:429:ASN:ND2	1:A:477:THR:H	2.13	0.47
1:A:296:ASP:HA	5:A:12:HOH:O	2.14	0.46
1:A:465:THR:HG21	1:A:472:ILE:O	2.16	0.46
1:A:253:ARG:HH21	1:A:276:ASP:CG	2.19	0.46
1:A:356:ILE:HD12	1:A:386:LEU:HD21	1.99	0.45
1:A:253:ARG:O	1:A:268:SER:HA	2.16	0.45
1:A:433:THR:CG2	1:A:451:VAL:HG21	2.48	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:456:VAL:HG23	1:A:483:SER:HB3	1.99	0.43
1:A:393:ARG:HH22	1:A:416:THR:HG22	1.83	0.43
1:A:356:ILE:HG23	1:A:357:GLU:OE2	2.20	0.41
1:A:333:HIS:CD2	1:A:335:ASN:H	2.19	0.41
1:A:420:GLY:O	1:A:421:ASP:HB2	2.20	0.41
1:A:415:MET:SD	1:A:460:GLN:HB3	2.60	0.41
1:A:458:ARG:NH2	1:A:477:THR:O	2.54	0.41
1:A:333:HIS:HD2	1:A:335:ASN:N	2.07	0.41
1:A:589:LYS:HB3	1:A:590:PRO:HD3	2.02	0.40
1:A:436:VAL:CG1	1:A:488:SER:HB3	2.51	0.40

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	440/493 (89%)	423 (96%)	13 (3%)	4 (1%)	25	21

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	421	ASP
1	A	580	GLN
1	A	422	PHE
1	A	256	VAL

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	365/401 (91%)	348 (95%)	17 (5%)	36	42

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	280	SER
1	A	301	LEU
1	A	386	LEU
1	A	392	TYR
1	A	393	ARG
1	A	399	VAL
1	A	416	THR
1	A	448	THR
1	A	457	SER
1	A	477	THR
1	A	511	VAL
1	A	539	LEU
1	A	583	LYS
1	A	598	LEU
1	A	600	TYR
1	A	611	LEU
1	A	630	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	221	GLN
1	A	246	HIS
1	A	309	GLN
1	A	333	HIS
1	A	429	ASN
1	A	453	GLN
1	A	552	GLN
1	A	572	GLN
1	A	607	ASN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 3 are 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$
2	I79	A	1	-	37,37,37	2.98	9 (24%)	55,55,55	2.20	10 (18%)

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	I79	A	1	-	-	0/12/12/12	0/5/5/5

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1	I79	C27-C23	12.73	1.51	1.36
2	A	1	I79	C23-C24	7.05	1.51	1.41
2	A	1	I79	C13-N17	-5.10	1.33	1.39
2	A	1	I79	C25-S26	-4.41	1.69	1.74
2	A	1	I79	C31-CL33	3.91	1.83	1.74
2	A	1	I79	C16-C15	2.74	1.39	1.37
2	A	1	I79	C28-C27	2.48	1.52	1.50
2	A	1	I79	C15-C12	2.07	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1	I79	C29-C30	2.07	1.41	1.36

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1	I79	C27-S26-C25	10.62	96.21	91.39
2	A	1	I79	C24-C25-S26	5.34	114.19	111.69
2	A	1	I79	C29-C25-C24	-5.05	120.65	123.28
2	A	1	I79	C28-C27-C23	3.88	134.90	128.93
2	A	1	I79	C32-C24-C23	-3.27	128.80	134.30
2	A	1	I79	C16-C15-C12	-3.18	103.08	107.31
2	A	1	I79	C18-C15-C12	2.30	131.32	126.56
2	A	1	I79	C22-C23-C24	-2.20	123.57	126.50
2	A	1	I79	C28-C27-S26	-2.12	117.49	119.95
2	A	1	I79	C30-C31-C32	-2.04	118.92	121.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	443/493 (89%)	-0.19	5 (1%) 77 78	26, 39, 64, 76	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	605	LEU	3.6
1	A	186	ASP	3.2
1	A	343	ASN	2.9
1	A	188	SER	2.4
1	A	417	GLY	2.1

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	I79	A	1	33/33	0.20	6.23	52,66,72,74	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	MG	A	3	1/1	0.16	3.95	22,22,22,22	0
4	CL	A	4	1/1	0.21	2.89	55,55,55,55	0
3	MG	A	2	1/1	0.13	1.84	34,34,34,34	1

6.5 Other polymers ⓘ

There are no such residues in this entry.