Full wwPDB X-ray Structure Validation Report (i)

Sep 30, 2019 – 12:00 pm BST

PDB ID	:	6SW8
Title	:	Crystal structure of the NS1 (H7N1) RNA-binding domain
Deposited on	:	2019-09-20
Resolution	:	1.93 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report.

This report is produced by the wwPDB biocuration pipeline after annotation of the structure.

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	:	1.8.0 (224370), CSD as540be (2019)
Xtriage (Phenix)	:	1.13
EDS	:	2.5
Percentile statistics	:	20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac	:	5.8.0158
CCP4	:	7.0 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.5

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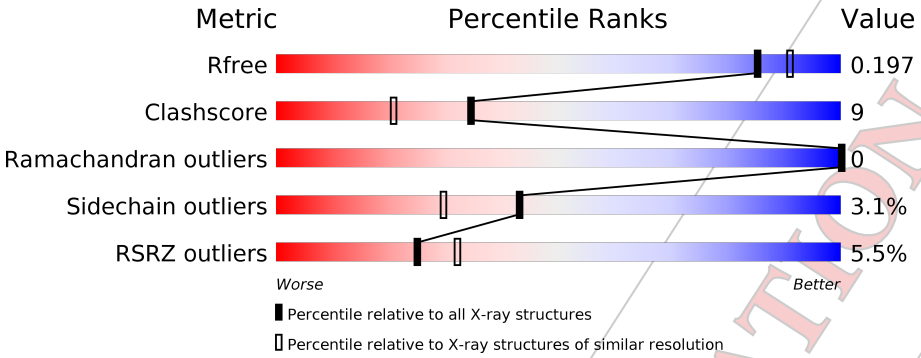
1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.93 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}	111664	3622 (1.96-1.92)
Clashscore	122126	3795 (1.96-1.92)
Ramachandran outliers	120053	3757 (1.96-1.92)
Sidechain outliers	120020	3757 (1.96-1.92)
RSRZ outliers	108989	3554 (1.96-1.92)

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 <=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	77	8% 77% 17% • 5%
1	B	77	3% 74% 21% 5%

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:

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	PEG	A	103	-	-	X	-

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2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 1270 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 Non-structural protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	73	Total	C	N	O	S	0	2	0
			591	367	105	113	6			
1	B	73	Total	C	N	O	S	0	1	0
			587	364	105	113	5			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP Q1PST0
A	-2	SER	-	expression tag	UNP Q1PST0
A	-1	HIS	-	expression tag	UNP Q1PST0
A	0	MET	-	expression tag	UNP Q1PST0
A	1	SER	-	expression tag	UNP Q1PST0
B	-3	GLY	-	expression tag	UNP Q1PST0
B	-2	SER	-	expression tag	UNP Q1PST0
B	-1	HIS	-	expression tag	UNP Q1PST0
B	0	MET	-	expression tag	UNP Q1PST0
B	1	SER	-	expression tag	UNP Q1PST0

- Molecule 2 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).

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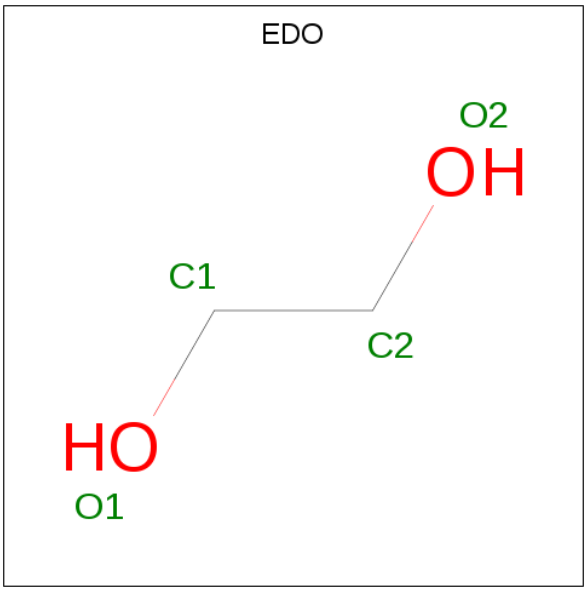
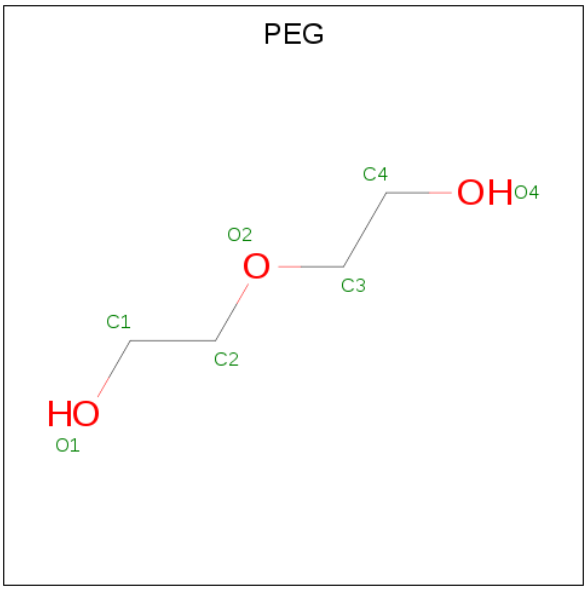


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0

- Molecule 3 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 7 4 3	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 7 4 3	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	39	Total O 39 39	0	0
4	B	27	Total O 27 27	0	0

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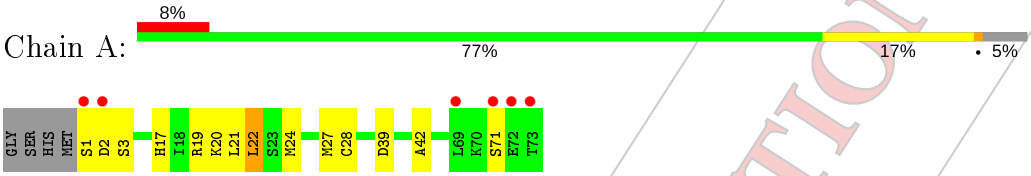
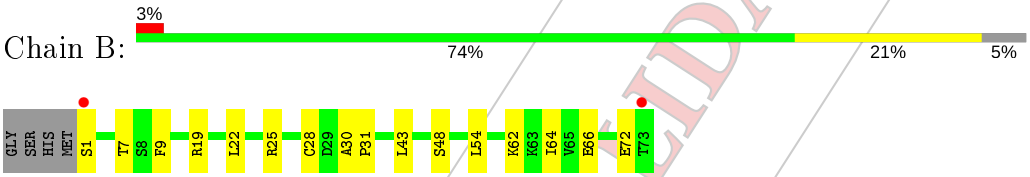
3 Residue-property plots (i)

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 geometryand 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: Non-structural protein 1



- Molecule 1: Non-structural protein 1



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4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	83.83Å 83.83Å 68.53Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.83 – 1.93 49.83 – 1.93	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.83-1.93) 100.0 (49.83-1.93)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.63 (at 1.94Å)	Xtriage
Refinement program	PHENIX 1.12_2829	Depositor
R, R_{free}	0.175 , 0.193 0.178 , 0.197	Depositor DCC
R_{free} test set	977 reflections (4.62%)	wwPDB-VP
Wilson B-factor (Å^2)	43.3	Xtriage
Anisotropy	0.044	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 57.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	0.032 for -h,-k,l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	1270	wwPDB-VP
Average B, all atoms (Å^2)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.98% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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5 Model quality

5.1 Standard geometry

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

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	0.93	1/603 (0.2%)	0.93	1/806 (0.1%)
1	B	0.82	0/596	0.86	1/797 (0.1%)
All	All	0.88	1/1199 (0.1%)	0.89	2/1603 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	28	CYS	CB-SG	5.42	1.91	1.82

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	19	ARG	NE-CZ-NH1	-6.91	116.85	120.30
1	B	19	ARG	NE-CZ-NH1	-6.06	117.27	120.30

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	591	0	606	11	0
1	B	587	0	599	9	0
2	A	8	0	12	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	4	0	6	1	0
3	A	14	0	20	6	0
4	A	39	0	0	2	0
4	B	27	0	0	1	0
All	All	1270	0	1243	22	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 9.

All (22) 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:39:ASP:HB3	3:A:103:PEG:H21	1.62	0.79
3:A:103:PEG:O1	3:A:103:PEG:H31	1.97	0.63
1:A:1:SER:OG	1:A:2:ASP:N	2.32	0.59
1:A:71:SER:OG	1:B:25:ARG:NH2	2.35	0.59
1:A:24[A]:MET:HE3	4:A:229:HOH:O	2.05	0.56
3:A:104:PEG:O1	3:A:104:PEG:H32	2.06	0.55
1:A:39:ASP:CB	3:A:103:PEG:H21	2.33	0.55
2:A:102:EDO:H22	1:B:72:GLU:HB3	1.88	0.55
1:B:54[B]:LEU:HD23	2:B:101:EDO:H21	1.91	0.52
1:A:22[A]:LEU:HD22	1:A:27:MET:HB2	1.95	0.49
1:A:42:ALA:HB3	3:A:103:PEG:H12	1.93	0.49
1:A:2:ASP:OD1	1:A:3:SER:N	2.46	0.48
3:A:104:PEG:H42	4:A:235:HOH:O	2.15	0.46
1:B:22:LEU:HD23	1:B:28:CYS:HB3	1.98	0.46
1:B:62:LYS:NZ	1:B:66:GLU:OE2	2.48	0.45
1:A:20:LYS:O	1:A:24[A]:MET:HG3	2.16	0.45
1:B:7:THR:HG23	1:B:64:ILE:HD13	1.99	0.45
1:A:17:HIS:NE2	2:A:102:EDO:H21	2.33	0.44
1:A:21:LEU:HD23	1:A:24[A]:MET:CE	2.48	0.44
1:B:30:ALA:HB3	1:B:31:PRO:HD3	2.02	0.42
1:B:9:PHE:HZ	1:B:54[B]:LEU:HD11	1.86	0.40
1:B:54[A]:LEU:HG	4:B:223:HOH:O	2.20	0.40

There are no symmetry-related clashes.

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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	73/77 (95%)	72 (99%)	1 (1%)	0	100	100
1	B	72/77 (94%)	72 (100%)	0	0	100	100
All	All	145/154 (94%)	144 (99%)	1 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	67/69 (97%)	65 (97%)	2 (3%)	44	31
1	B	66/69 (96%)	63 (96%)	3 (4%)	30	15
All	All	133/138 (96%)	128 (96%)	5 (4%)	43	21

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22[A]	LEU
1	A	22[B]	LEU
1	B	1	SER
1	B	43	LEU
1	B	48	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

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Mol	Chain	Res	Type
1	A	10	GLN
1	B	4	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)

5 ligands are modelled in this entry.

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	EDO	A	101	-	3,3,3	0.47	0	2,2,2	0.62	0
2	EDO	A	102	-	3,3,3	0.49	0	2,2,2	0.11	0
3	PEG	A	103	-	6,6,6	0.63	0	5,5,5	1.36	1 (20%)
3	PEG	A	104	-	6,6,6	0.40	0	5,5,5	0.68	0
2	EDO	B	101	-	3,3,3	0.61	0	2,2,2	0.09	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.

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	A	101	-	-	0/1/1/1	-
2	EDO	A	102	-	-	0/1/1/1	-
3	PEG	A	103	-	-	2/4/4/4	-
3	PEG	A	104	-	-	2/4/4/4	-
2	EDO	B	101	-	-	1/1/1/1	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	103	PEG	C3-O2-C2	-2.92	100.62	113.30

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	104	PEG	C1-C2-O2-C3
3	A	103	PEG	O2-C3-C4-O4
3	A	103	PEG	O1-C1-C2-O2
2	B	101	EDO	O1-C1-C2-O2
3	A	104	PEG	C4-C3-O2-C2

There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	102	EDO	2	0
3	A	103	PEG	4	0
3	A	104	PEG	2	0
2	B	101	EDO	1	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.

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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	73/77 (94%)	0.52	6 (8%)	11 17	33, 42, 102, 167	0
1	B	73/77 (94%)	0.37	2 (2%)	54 62	33, 53, 86, 114	0
All	All	146/154 (94%)	0.45	8 (5%)	25 32	33, 47, 97, 167	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	73	THR	11.3
1	A	72	GLU	5.2
1	A	71	SER	4.9
1	B	73	THR	3.5
1	B	1	SER	3.1
1	A	2	ASP	2.4
1	A	1	SER	2.3
1	A	69	LEU	2.3

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. The B-factors column lists the minimum,

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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
2	EDO	A	102	4/4	0.76	0.28	93,93,93,94	0
3	PEG	A	104	7/7	0.79	0.17	73,77,79,79	0
2	EDO	B	101	4/4	0.80	0.15	78,78,78,80	0
2	EDO	A	101	4/4	0.86	0.09	85,86,86,86	0
3	PEG	A	103	7/7	0.90	0.19	42,57,58,60	0

6.5 Other polymers (i)

There are no such residues in this entry.

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