



wwPDB X-ray Structure Validation Summary Report

Apr 7, 2014 – 09:17 PM EDT

PDB ID : 2E9T
Title : Foot-and-mouth disease virus RNA-polymerase RNA dependent in complex with a template-primer RNA and 5F-UTP
Authors : Ferrer-Orta, C.; Arias, A.; Perez-Luque, R.; Escarmis, C.; Domingo, E.; Verdaguier, N.
Deposited on : 2007-01-26
Resolution : 2.60 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

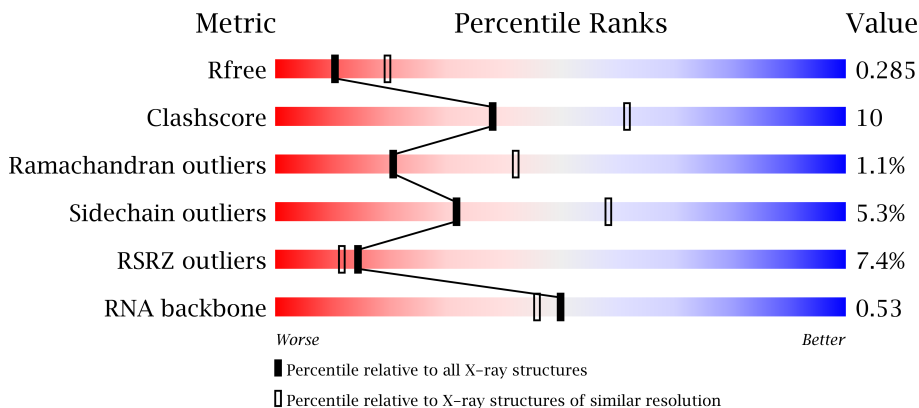
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	FAILED
Xtriage (Phenix)	:	dev-1439
EDS	:	stable22978
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)	:	stable22978

1 Overall quality at a glance

The reported resolution of this entry is 2.60 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}	66092	1718 (2.60-2.60)
Clashscore	79885	2154 (2.60-2.60)
Ramachandran outliers	78287	2113 (2.60-2.60)
Sidechain outliers	78261	2113 (2.60-2.60)
RSRZ outliers	66119	1718 (2.60-2.60)
RNA backbone	1838	1002 (3.12-2.08)

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	B	8	
1	E	8	
2	C	7	
2	F	7	
3	A	476	
3	D	476	

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

Mol	Type	Chain	Res	Geometry	Electron density
4	MG	A	780	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8205 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 RNA chain called 5'-R(P*UP*AP*GP*GP*GP*CP*CP*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	8	Total	C	N	O	P	0	0	0
			171	76	31	56	8			
1	E	8	Total	C	N	O	P	0	0	0
			171	76	31	56	8			

- Molecule 2 is a RNA chain called 5'-R(*GP*GP*GP*CP*CP*CP*(5FU))-3'.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	C	7	Total 147	C 66	F 1	N 26	O 48	P 6	0	0	0
2	F	7	Total 147	C 66	F 1	N 26	O 48	P 6	0	0	0

- Molecule 3 is a protein called RNA-dependent RNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	474	Total	C	N	O	S	0	0	0
			3741	2378	647	695	21			
3	D	474	Total	C	N	O	S	0	0	0
			3741	2378	647	695	21			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	471	ALA	-	CLONING ARTIFACT	UNP Q0QEE1
A	472	ALA	-	CLONING ARTIFACT	UNP Q0QEE1
A	473	LEU	-	CLONING ARTIFACT	UNP Q0QEE1
A	474	GLU	-	CLONING ARTIFACT	UNP Q0QEE1
A	475	HIS	-	CLONING ARTIFACT	UNP Q0QEE1
A	476	HIS	-	CLONING ARTIFACT	UNP Q0QEE1
D	471	ALA	-	CLONING ARTIFACT	UNP Q0QEE1
D	472	ALA	-	CLONING ARTIFACT	UNP Q0QEE1

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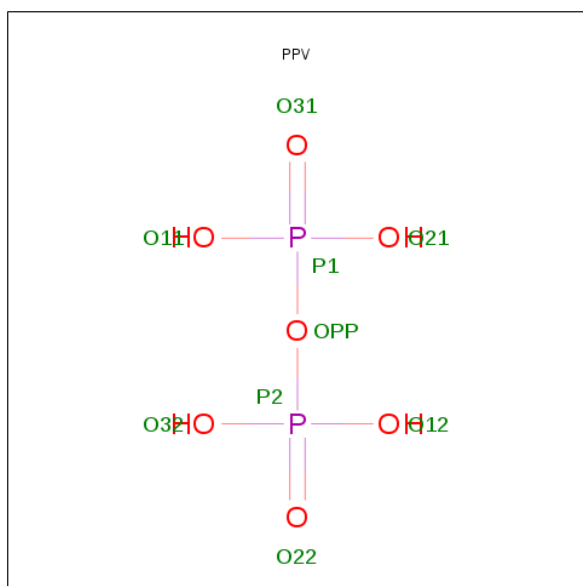
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Chain	Residue	Modelled	Actual	Comment	Reference
D	473	LEU	-	CLONING ARTIFACT	UNP Q0QEE1
D	474	GLU	-	CLONING ARTIFACT	UNP Q0QEE1
D	475	HIS	-	CLONING ARTIFACT	UNP Q0QEE1
D	476	HIS	-	CLONING ARTIFACT	UNP Q0QEE1

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	2	Total Mg 2 2	0	0
4	D	2	Total Mg 2 2	0	0

- Molecule 5 is PYROPHOSPHATE (three-letter code: PPV) (formula: $\text{H}_4\text{O}_7\text{P}_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total O P 9 7 2	0	0
5	D	1	Total O P 9 7 2	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	35	Total O 35 35	0	0

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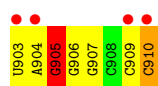
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	2	Total 2	O 2	0	0
6	C	1	Total 1	O 1	0	0
6	D	24	Total 24	O 24	0	0
6	E	2	Total 2	O 2	0	0
6	F	1	Total 1	O 1	0	0

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 ($RSRZ > 2$). 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: 5'-R(P*UP*AP*GP*GP*GP*CP*CP*C)-3'

Chain B: 



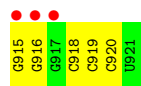
- Molecule 1: 5'-R(P*UP*AP*GP*GP*GP*CP*CP*C)-3'

Chain E: 



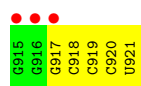
- Molecule 2: 5'-R(*GP*GP*GP*CP*CP*CP*(5FU))-3'

Chain C: 



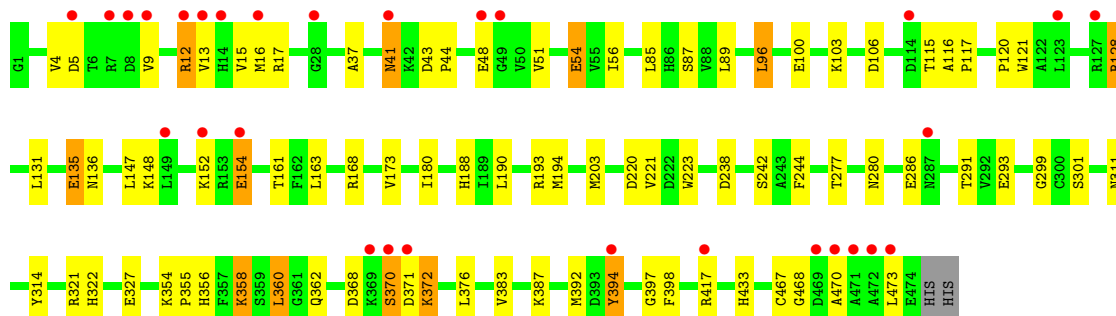
- Molecule 2: 5'-R(*GP*GP*GP*CP*CP*CP*(5FU))-3'

Chain F: 



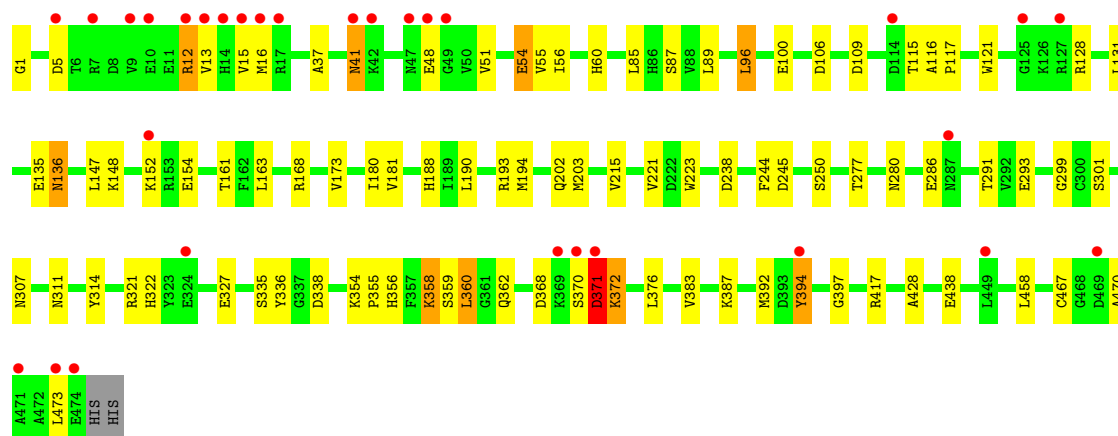
- Molecule 3: RNA-dependent RNA polymerase

Chain A: 



● Molecule 3: RNA-dependent RNA polymerase

Chain D: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	95.60Å 95.60Å 201.16Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.60 29.88 – 2.60	Depositor EDS
% Data completeness (in resolution range)	100.0 (20.00-2.60) 100.0 (29.88-2.60)	Depositor EDS
R_{merge}	0.90	Depositor
R_{sym}	0.74	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.19 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.233 , 0.289 0.233 , 0.285	Depositor DCC
R_{free} test set	1694 reflections (5.32%)	DCC
Wilson B-factor (Å ²)	45.2	Xtriage
Anisotropy	0.080	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 43.6	EDS
Estimated twinning fraction	0.028 for -h,-k,l	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	1 of 33529 reflections (0.003%)	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8205	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 81.22 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 3.7341e-07. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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, 5FU, PPV

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	B	1.01	0/190	1.71	4/294 (1.4%)
1	E	1.06	0/190	1.72	3/294 (1.0%)
2	C	0.84	0/140	1.37	0/217
2	F	0.87	0/140	1.50	0/217
3	A	0.64	0/3830	0.69	0/5186
3	D	0.65	0/3830	0.70	0/5186
All	All	0.67	0/8320	0.82	7/11394 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	D	0	1

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	910	C	C1'-O4'-C4'	-6.98	104.31	109.90
1	E	909	C	O4'-C1'-N1	6.64	113.51	108.20
1	B	909	C	O4'-C1'-N1	6.59	113.48	108.20
1	E	908	C	O4'-C1'-N1	6.33	113.27	108.20
1	B	910	C	O4'-C1'-N1	6.12	113.09	108.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	D	371	ASP	Peptide

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	B	171	0	88	14	0
1	E	171	0	88	11	0
2	C	147	0	77	6	0
2	F	147	0	77	6	0
3	A	3741	0	3669	72	0
3	D	3741	0	3669	68	0
4	A	2	0	0	0	0
4	D	2	0	0	0	0
5	A	9	0	0	0	0
5	D	9	0	0	0	0
6	A	35	0	0	7	0
6	B	2	0	0	0	0
6	C	1	0	0	0	0
6	D	24	0	0	1	0
6	E	2	0	0	0	0
6	F	1	0	0	0	0
All	All	8205	0	7668	156	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 10.

The worst 5 of 156 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:D:467:CYS:SG	3:D:470:ALA:HB3	1.64	1.37
3:A:467:CYS:SG	3:A:470:ALA:HB3	1.74	1.26
3:A:85:LEU:HD11	3:A:203:MET:CE	1.72	1.19
3:D:85:LEU:HD11	3:D:203:MET:CE	1.83	1.08
3:D:85:LEU:HD11	3:D:203:MET:HE1	1.01	1.01

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	
3	A	472/476 (99%)	449 (95%)	17 (4%)	6 (1%)	18	35
3	D	472/476 (99%)	446 (94%)	22 (5%)	4 (1%)	27	53
All	All	944/952 (99%)	895 (95%)	39 (4%)	10 (1%)	21	42

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	371	ASP
3	D	371	ASP
3	A	106	ASP
3	A	468	GLY
3	D	106	ASP

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	
3	A	397/399 (100%)	375 (94%)	22 (6%)	30	56
3	D	397/399 (100%)	377 (95%)	20 (5%)	34	61
All	All	794/798 (100%)	752 (95%)	42 (5%)	32	58

5 of 42 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	376	LEU
3	D	41	ASN
3	D	376	LEU
3	A	394	TYR

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Mol	Chain	Res	Type
3	A	473	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
3	A	362	GLN
3	D	60	HIS
3	D	307	ASN
3	A	311	ASN
3	A	356	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	B	7/8 (87%)	1 (14%)	0
1	E	7/8 (87%)	1 (14%)	0
2	C	6/7 (85%)	1 (16%)	0
2	F	6/7 (85%)	1 (16%)	0
All	All	26/30 (86%)	4 (15%)	0

All (4) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	B	905	G
2	C	916	G
1	E	905	G
2	F	917	G

There are no RNA pucker outliers to report.

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

Mogul failed to run properly - this section will therefore be empty.

5.5 Carbohydrates ⓘ

Mogul failed to run properly - this section will therefore be empty.

5.6 Ligand geometry ⓘ

Mogul failed to run properly - this section will therefore be empty.

5.7 Other polymers ⓘ

Mogul failed to run properly - this section will therefore be empty.

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	B	8/8 (100%)	2.08	4 (50%) 0 0	46, 55, 70, 88	8 (100%)
1	E	8/8 (100%)	2.22	4 (50%) 0 0	51, 53, 67, 91	8 (100%)
2	C	7/7 (100%)	1.84	3 (42%) 1 0	34, 44, 73, 78	7 (100%)
2	F	7/7 (100%)	1.86	3 (42%) 1 0	38, 45, 68, 68	7 (100%)
3	A	474/476 (99%)	0.38	29 (6%) 21 17	34, 39, 44, 47	0
3	D	474/476 (99%)	0.37	30 (6%) 19 16	34, 39, 44, 47	0
All	All	978/982 (99%)	0.43	73 (7%) 14 11	34, 39, 46, 91	30 (3%)

The worst 5 of 73 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	371	ASP	6.8
3	A	371	ASP	6.4
3	A	370	SER	6.0
2	C	915	G	5.1
3	D	14	HIS	4.9

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

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	5FU	F	921	21/22	0.24	0.06	20,48,52,53	21
2	5FU	C	921	21/22	0.19	-0.45	20,42,44,46	21

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
4	MG	A	780	1/1	0.29	3.46	41,41,41,41	0
5	PPV	A	930	9/9	0.24	1.48	80,81,84,84	9
5	PPV	D	1930	9/9	0.22	0.57	78,79,79,80	9
4	MG	D	1780	1/1	0.23	0.50	38,38,38,38	0
4	MG	A	781	1/1	0.23	-	57,57,57,57	0
4	MG	D	1781	1/1	0.35	-	66,66,66,66	0

6.5 Other polymers ⓘ

There are no such residues in this entry.