



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 29, 2020 – 05:01 PM BST

PDB ID : 6IZY
Title : The RNA-dependent RNA polymerase domain of dengue 2 NS5
Authors : Shimizu, H.; Sekine, S.
Deposited on : 2018-12-20
Resolution : 2.11 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.13
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13

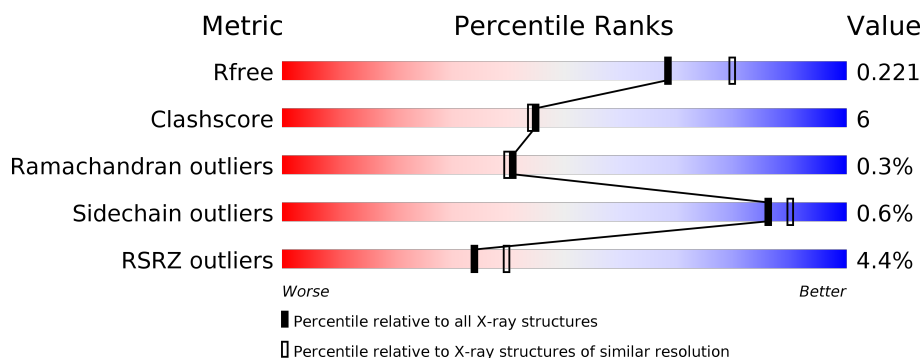
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.11 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}	130704	6241 (2.14-2.10)
Clashscore	141614	6778 (2.14-2.10)
Ramachandran outliers	138981	6705 (2.14-2.10)
Sidechain outliers	138945	6706 (2.14-2.10)
RSRZ outliers	127900	6112 (2.14-2.10)

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 $\leq 5\%$. 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	686	<div> <div>4%</div> <div>75%</div> <div>10%</div> <div>15%</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5003 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 Genome polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	586	Total	C	N	O	S	0	0	0
			4776	3010	852	881	33			

There are 43 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	211	MET	-	initiating methionine	UNP C6L435
A	212	LYS	-	expression tag	UNP C6L435
A	213	ASP	-	expression tag	UNP C6L435
A	214	HIS	-	expression tag	UNP C6L435
A	215	LEU	-	expression tag	UNP C6L435
A	216	ILE	-	expression tag	UNP C6L435
A	217	HIS	-	expression tag	UNP C6L435
A	218	ASN	-	expression tag	UNP C6L435
A	219	HIS	-	expression tag	UNP C6L435
A	220	HIS	-	expression tag	UNP C6L435
A	221	LYS	-	expression tag	UNP C6L435
A	222	HIS	-	expression tag	UNP C6L435
A	223	GLU	-	expression tag	UNP C6L435
A	224	HIS	-	expression tag	UNP C6L435
A	225	ALA	-	expression tag	UNP C6L435
A	226	HIS	-	expression tag	UNP C6L435
A	227	ALA	-	expression tag	UNP C6L435
A	228	GLU	-	expression tag	UNP C6L435
A	229	HIS	-	expression tag	UNP C6L435
A	230	ASP	-	expression tag	UNP C6L435
A	231	TYR	-	expression tag	UNP C6L435
A	232	LYS	-	expression tag	UNP C6L435
A	233	ASP	-	expression tag	UNP C6L435
A	234	ASP	-	expression tag	UNP C6L435
A	235	ASP	-	expression tag	UNP C6L435
A	236	ASP	-	expression tag	UNP C6L435
A	237	LYS	-	expression tag	UNP C6L435

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Chain	Residue	Modelled	Actual	Comment	Reference
A	238	GLU	-	expression tag	UNP C6L435
A	239	HIS	-	expression tag	UNP C6L435
A	240	LEU	-	expression tag	UNP C6L435
A	241	TYR	-	expression tag	UNP C6L435
A	242	PHE	-	expression tag	UNP C6L435
A	243	GLN	-	expression tag	UNP C6L435
A	244	GLY	-	See Sequence Details	UNP C6L435
A	245	SER	-	See Sequence Details	UNP C6L435
A	246	SER	-	See Sequence Details	UNP C6L435
A	247	GLY	-	See Sequence Details	UNP C6L435
A	248	SER	-	See Sequence Details	UNP C6L435
A	249	SER	-	See Sequence Details	UNP C6L435
A	250	GLY	-	See Sequence Details	UNP C6L435
A	628	VAL	ILE	See Sequence Details	UNP C6L435
A	749	ARG	LYS	See Sequence Details	UNP C6L435
A	836	ILE	VAL	See Sequence Details	UNP C6L435

- Molecule 2 is COBALT (II) ION (three-letter code: CO) (formula: Co).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	4	Total Co 4 4	0	0

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

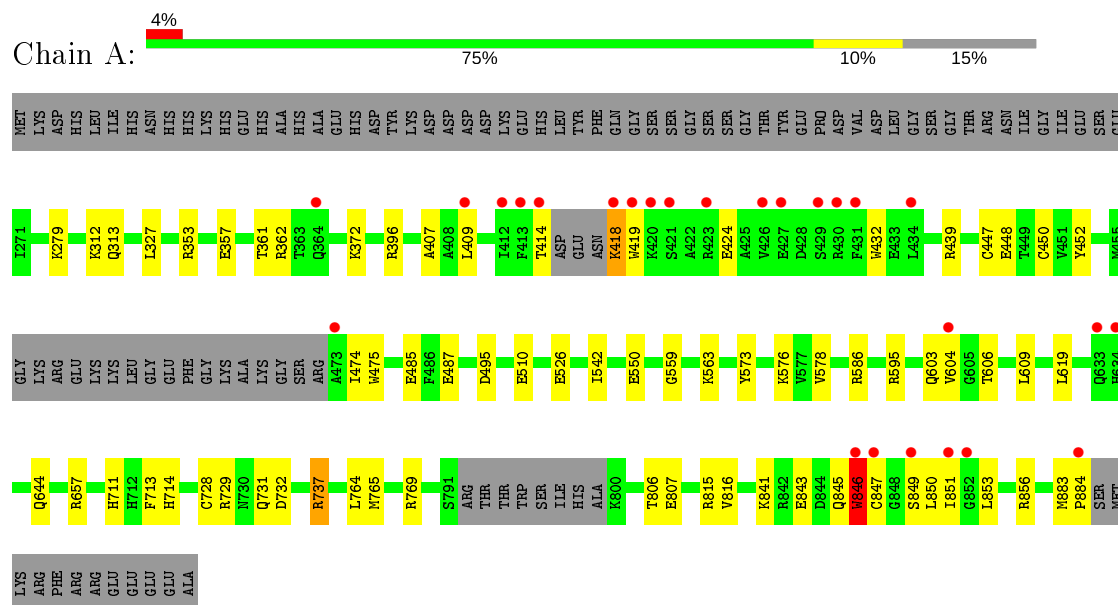
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	222	Total O 222 222	0	0

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: Genome polypeptide



4 Data and refinement statistics

Property	Value	Source
Space group	I 4 3 2	Depositor
Cell constants a, b, c, α , β , γ	237.35Å 237.35Å 237.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.96 – 2.11 41.96 – 2.11	Depositor EDS
% Data completeness (in resolution range)	95.7 (41.96-2.11) 95.7 (41.96-2.11)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.39 (at 2.10Å)	Xtriage
Refinement program	PHENIX 1.12_2829	Depositor
R, R_{free}	0.195 , 0.221 0.195 , 0.221	Depositor DCC
R_{free} test set	1993 reflections (3.20%)	wwPDB-VP
Wilson B-factor (Å ²)	45.6	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 53.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5003	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.03% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.32	1/4888 (0.0%)	0.52	2/6603 (0.0%)

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
1	A	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	846	TRP	CB-CG	-5.02	1.41	1.50

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	737	ARG	NE-CZ-NH1	6.64	123.62	120.30
1	A	846	TRP	CA-CB-CG	-6.43	101.48	113.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	846	TRP	Peptide

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	4776	0	4674	61	0
2	A	4	0	0	0	0
3	A	1	0	0	0	0
4	A	222	0	0	11	0
All	All	5003	0	4674	61	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 6.

All (61) 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:409:LEU:HD21	1:A:474:ILE:HD11	1.43	0.98
1:A:845:GLN:HA	1:A:849:SER:HB3	1.45	0.97
1:A:847:CYS:SG	4:A:1190:HOH:O	2.23	0.94
1:A:806:THR:O	4:A:1001:HOH:O	1.85	0.94
1:A:884:PRO:O	4:A:1002:HOH:O	1.90	0.90
1:A:845:GLN:HB3	1:A:846:TRP:HE3	1.36	0.88
1:A:845:GLN:HB3	1:A:846:TRP:CE3	2.12	0.85
1:A:732:ASP:OD1	4:A:1003:HOH:O	1.95	0.84
1:A:510:GLU:O	4:A:1004:HOH:O	1.99	0.80
1:A:728:CYS:SG	4:A:1190:HOH:O	2.45	0.74
1:A:414:THR:HA	1:A:418:LYS:HG3	1.70	0.74
1:A:526:GLU:O	1:A:657:ARG:NH2	2.19	0.71
1:A:731:GLN:N	1:A:847:CYS:O	2.21	0.69
1:A:769:ARG:NH1	1:A:847:CYS:HB2	2.08	0.68
1:A:495:ASP:OD2	4:A:1006:HOH:O	2.11	0.68
1:A:644:GLN:OE1	4:A:1005:HOH:O	2.11	0.67
1:A:414:THR:HA	1:A:418:LYS:CG	2.27	0.62
1:A:312:LYS:HE3	1:A:313:GLN:O	2.01	0.60
1:A:807:GLU:OE2	1:A:815:ARG:NH2	2.34	0.59
1:A:419:TRP:HD1	1:A:424:GLU:HG2	1.70	0.56
1:A:485:GLU:HG2	1:A:604:VAL:HB	1.87	0.56
1:A:362:ARG:HA	1:A:595:ARG:HH22	1.72	0.54
1:A:439:ARG:NH1	1:A:487:GLU:OE2	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:603:GLN:HG3	4:A:1023:HOH:O	2.08	0.53
1:A:714:HIS:ND1	1:A:843:GLU:OE1	2.44	0.51
1:A:731:GLN:NE2	1:A:849:SER:HA	2.26	0.51
1:A:559:GLY:O	1:A:563:LYS:HE2	2.12	0.50
1:A:845:GLN:O	1:A:849:SER:N	2.45	0.48
1:A:396:ARG:HG2	1:A:432:TRP:CZ3	2.49	0.48
1:A:769:ARG:HH12	1:A:847:CYS:HB2	1.79	0.48
1:A:452:TYR:HB2	1:A:578:VAL:HG22	1.95	0.47
1:A:576:LYS:HG2	1:A:595:ARG:O	2.14	0.47
1:A:644:GLN:NE2	4:A:1018:HOH:O	2.46	0.47
1:A:485:GLU:OE2	1:A:573:TYR:OH	2.18	0.47
1:A:418:LYS:HD2	1:A:419:TRP:O	2.15	0.47
1:A:372:LYS:NZ	4:A:1014:HOH:O	2.46	0.47
1:A:845:GLN:HG3	1:A:851:ILE:CG1	2.45	0.46
1:A:353:ARG:O	1:A:357:GLU:HG3	2.16	0.46
1:A:475:TRP:HZ3	1:A:576:LYS:HD3	1.81	0.46
1:A:279:LYS:HE3	1:A:448:GLU:HB2	1.97	0.46
1:A:586:ARG:NH1	1:A:586:ARG:HB3	2.31	0.46
1:A:764:LEU:HG	1:A:765:MET:HE3	1.97	0.46
1:A:550:GLU:HB3	1:A:609:LEU:HD22	2.00	0.43
1:A:713:PHE:C	1:A:714:HIS:HD2	2.22	0.43
1:A:841:LYS:HG3	1:A:851:ILE:HD12	1.99	0.43
1:A:419:TRP:CD1	1:A:424:GLU:HG2	2.52	0.43
1:A:475:TRP:CZ3	1:A:576:LYS:HD3	2.55	0.42
1:A:452:TYR:OH	1:A:603:GLN:OE1	2.24	0.42
1:A:850:LEU:HD22	1:A:853:LEU:HD22	2.02	0.42
1:A:603:GLN:O	1:A:606:THR:HG22	2.20	0.42
1:A:845:GLN:HG3	1:A:851:ILE:HG12	2.02	0.42
1:A:418:LYS:HD2	1:A:419:TRP:N	2.35	0.41
1:A:851:ILE:HA	1:A:856:ARG:HD2	2.03	0.41
1:A:711:HIS:CD2	1:A:729:ARG:HB2	2.56	0.41
1:A:714:HIS:CE1	1:A:843:GLU:OE1	2.73	0.41
1:A:327:LEU:HA	1:A:327:LEU:HD23	1.83	0.41
1:A:764:LEU:HD21	1:A:816:VAL:HG21	2.03	0.41
1:A:619:LEU:HD23	1:A:619:LEU:HA	1.92	0.41
1:A:361:THR:O	1:A:595:ARG:NH2	2.54	0.40
1:A:542:ILE:HD13	1:A:542:ILE:HA	1.98	0.40
1:A:447:CYS:SG	1:A:450:CYS:HB2	2.61	0.40

There are no symmetry-related clashes.

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	578/686 (84%)	558 (96%)	18 (3%)	2 (0%)	41	40

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	407	ALA
1	A	883	MET

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	512/597 (86%)	509 (99%)	3 (1%)	86	90

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	418	LYS
1	A	737	ARG
1	A	846	TRP

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

Mol	Chain	Res	Type
1	A	351	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 5 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 [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 ⓘ

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	586/686 (85%)	0.12	26 (4%) 34 40	32, 51, 91, 129	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	846	TRP	9.1
1	A	419	TRP	5.1
1	A	413	PHE	5.0
1	A	409	LEU	4.6
1	A	849	SER	4.3
1	A	851	ILE	4.3
1	A	420	LYS	4.1
1	A	430	ARG	3.7
1	A	421	SER	3.5
1	A	426	VAL	3.5
1	A	414	THR	3.4
1	A	604	VAL	3.4
1	A	852	GLY	3.4
1	A	429	SER	3.3
1	A	427	GLU	2.9
1	A	847	CYS	2.9
1	A	884	PRO	2.8
1	A	431	PHE	2.7
1	A	418	LYS	2.4
1	A	634	HIS	2.4
1	A	412	ILE	2.3
1	A	423	ARG	2.3
1	A	434	LEU	2.3
1	A	364	GLN	2.1
1	A	473	ALA	2.0
1	A	633	GLN	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 monosaccharides 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(\AA^2)	Q<0.9
2	CO	A	901	1/1	0.58	0.13	129,129,129,129	0
2	CO	A	904	1/1	0.80	0.15	158,158,158,158	0
2	CO	A	902	1/1	0.95	0.14	91,91,91,91	0
2	CO	A	903	1/1	0.95	0.14	129,129,129,129	0
3	ZN	A	905	1/1	0.99	0.12	53,53,53,53	0

6.5 Other polymers [i](#)

There are no such residues in this entry.