



wwPDB X-ray Structure Validation Summary Report ⓘ

Jul 25, 2022 – 04:07 pm BST

PDB ID : 7QPJ
Title : Crystal structure of engineered TCR (756) complexed to HLA-A*02:01 presenting MAGE-A10 9-mer peptide
Authors : Simister, P.C.; Border, E.C.; Vieira, J.F.; Pumphrey, N.J.
Deposited on : 2022-01-04
Resolution : 1.54 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtrriage (Phenix) : 1.13
EDS : 2.29
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0267
CCP4 : 7.1.010 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.29

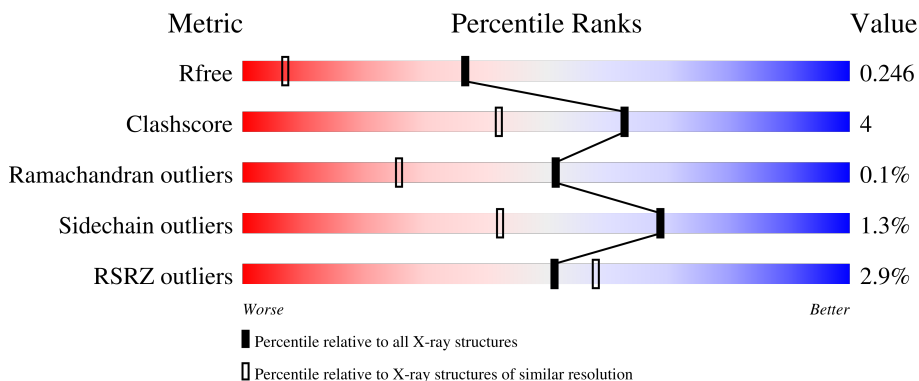
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.54 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	2556 (1.56-1.52)
Clashscore	141614	2634 (1.56-1.52)
Ramachandran outliers	138981	2580 (1.56-1.52)
Sidechain outliers	138945	2577 (1.56-1.52)
RSRZ outliers	127900	2524 (1.56-1.52)

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	C	277	 3% (poor fit), 91% (0-1 outliers), 9% (2-3 outliers)
2	D	100	 91% (0-1 outliers), 8% (2-3 outliers), . (not modelled)
3	E	9	 89% (0-1 outliers), 11% (2-3 outliers)
4	A	206	 3% (poor fit), 89% (0-1 outliers), 8% (2-3 outliers), . (not modelled)
5	B	241	 3% (poor fit), 88% (0-1 outliers), 10% (2-3 outliers), . (not modelled)

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:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	GOL	C	303	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 13302 atoms, of which 6204 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 MHC class I antigen.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	C	276	4370	1414	2115	406	426	9	91	8	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	1	MET	-	initiating methionine	UNP Q861F7

- Molecule 2 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
2	D	100	1575	517	765	136	153	4	37	1	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	1	MET	-	initiating methionine	UNP P61769

- Molecule 3 is a protein called Melanoma-associated antigen 10.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
3	E	9	138	45	66	11	15	1	3	0	0

- Molecule 4 is a protein called T-cell receptor alpha chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
4	A	200	2990	955	1449	261	317	8	57	3	0

- Molecule 5 is a protein called T-cell receptor beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
5	B	238	3645	1189	1777	315	355	9	64	3	0

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
6	C	1	14	3	8	3	2	0
6	C	1	14	3	8	3	2	0
6	C	1	14	3	8	3	2	0
6	C	1	14	3	8	3	2	0

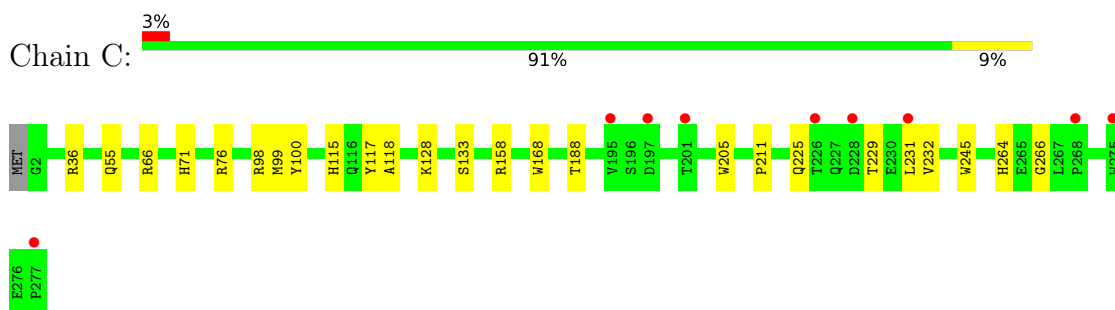
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	C	192	Total	O	0	0
			192	192		
7	D	77	Total	O	0	0
			77	77		
7	E	4	Total	O	0	0
			4	4		
7	A	136	Total	O	0	0
			136	136		
7	B	119	Total	O	0	0
			119	119		

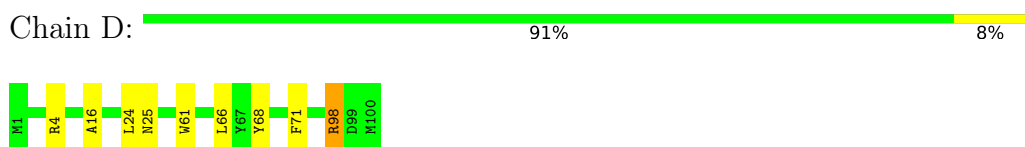
3 Residue-property plots [i](#)

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.

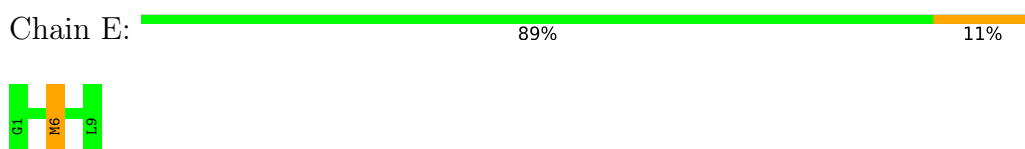
- Molecule 1: MHC class I antigen



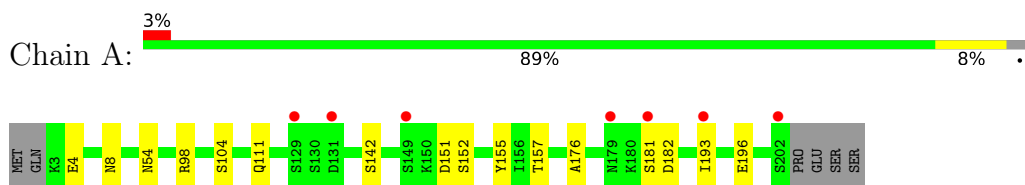
- Molecule 2: Beta-2-microglobulin



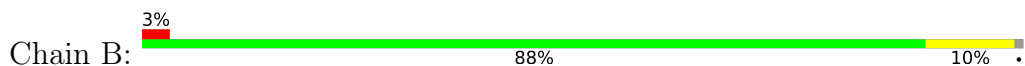
- Molecule 3: Melanoma-associated antigen 10

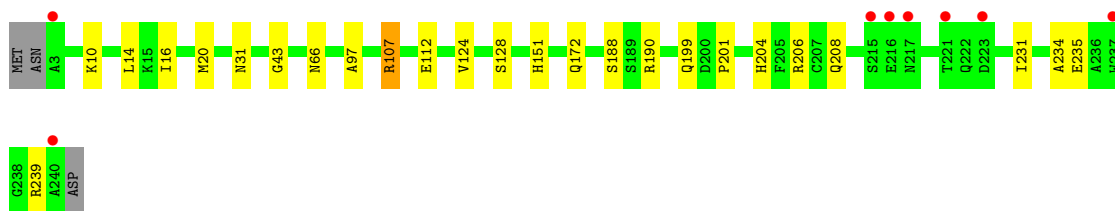


- Molecule 4: T-cell receptor alpha chain



- Molecule 5: T-cell receptor beta chain





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	54.20Å 77.45Å 116.68Å 90.00° 102.70° 90.00°	Depositor
Resolution (Å)	64.11 – 1.54 64.03 – 1.54	Depositor EDS
% Data completeness (in resolution range)	96.7 (64.11-1.54) 89.1 (64.03-1.54)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.13 (at 1.54Å)	Xtrriage
Refinement program	REFMAC 5.8.0267, REFMAC 5.8.0267	Depositor
R, R_{free}	0.202 , 0.236 0.212 , 0.246	Depositor DCC
R_{free} test set	6100 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	18.4	Xtrriage
Anisotropy	0.423	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	(Not available) , (Not available)	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	0.037 for h,-k,-h-l	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	13302	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.71% 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: GOL

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	C	0.78	0/2350	0.91	3/3195 (0.1%)
2	D	0.67	0/836	0.85	0/1137
3	E	1.19	0/73	1.13	1/95 (1.1%)
4	A	0.77	0/1578	0.91	0/2141
5	B	0.70	0/1929	0.85	0/2633
All	All	0.75	0/6766	0.89	4/9201 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	158	ARG	NE-CZ-NH1	8.26	124.43	120.30
1	C	158	ARG	NE-CZ-NH2	-6.01	117.30	120.30
1	C	117	TYR	CB-CG-CD1	-5.88	117.47	121.00
3	E	6	MET	CG-SD-CE	5.76	109.42	100.20

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	C	2255	2115	2083	25	0
2	D	810	765	744	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	72	66	65	1	0
4	A	1541	1449	1435	12	0
5	B	1868	1777	1755	15	0
6	C	24	32	32	6	0
7	A	136	0	0	6	0
7	B	119	0	0	3	0
7	C	192	0	0	4	0
7	D	77	0	0	1	0
7	E	4	0	0	0	0
All	All	7098	6204	6114	54	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 4.

The worst 5 of 54 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:98:ARG:HE	1:C:115:HIS:HE1	1.21	0.87
2:D:4:ARG:NH1	7:D:201:HOH:O	2.10	0.84
1:C:66:ARG:HH22	6:C:303:GOL:H2	1.43	0.83
4:A:196:GLU:OE1	7:A:301:HOH:O	1.97	0.82
1:C:231:LEU:O	1:C:231:LEU:HD12	1.88	0.72

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	C	282/277 (102%)	278 (99%)	4 (1%)	0	100	100
2	D	99/100 (99%)	98 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	E	7/9 (78%)	7 (100%)	0	0	100	100
4	A	201/206 (98%)	195 (97%)	6 (3%)	0	100	100
5	B	239/241 (99%)	230 (96%)	8 (3%)	1 (0%)	34	13
All	All	828/833 (99%)	808 (98%)	19 (2%)	1 (0%)	51	26

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	B	97	ALA

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	C	230/233 (99%)	230 (100%)	0	100	100
2	D	87/95 (92%)	85 (98%)	2 (2%)	50	20
3	E	7/7 (100%)	7 (100%)	0	100	100
4	A	172/182 (94%)	170 (99%)	2 (1%)	71	47
5	B	197/207 (95%)	190 (96%)	7 (4%)	35	8
All	All	693/724 (96%)	682 (98%)	11 (2%)	69	33

5 of 11 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	B	107[A]	ARG
5	B	107[B]	ARG
5	B	190	ARG
5	B	128	SER
5	B	10	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
4	A	111	GLN
4	A	191	ASN
5	B	217	ASN
5	B	31	ASN
5	B	172	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](#)

4 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	$\# Z > 2$
6	GOL	C	301	-	5,5,5	0.19	0	5,5,5	0.55	0
6	GOL	C	302	-	5,5,5	0.11	0	5,5,5	0.31	0
6	GOL	C	304	-	5,5,5	0.10	0	5,5,5	0.45	0
6	GOL	C	303	-	5,5,5	0.17	0	5,5,5	0.60	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.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	GOL	C	301	-	-	4/4/4/4	-
6	GOL	C	302	-	-	2/4/4/4	-
6	GOL	C	304	-	-	2/4/4/4	-
6	GOL	C	303	-	-	1/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	301	GOL	O1-C1-C2-C3
6	C	301	GOL	C1-C2-C3-O3
6	C	301	GOL	O2-C2-C3-O3
6	C	302	GOL	C1-C2-C3-O3
6	C	303	GOL	C1-C2-C3-O3

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	301	GOL	2	0
6	C	303	GOL	4	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.

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	C	276/277 (99%)	0.03	9 (3%) 46 53	10, 22, 52, 73	1 (0%)
2	D	100/100 (100%)	-0.17	0 100 100	12, 27, 42, 52	0
3	E	9/9 (100%)	-0.14	0 100 100	12, 13, 15, 16	0
4	A	200/206 (97%)	0.17	7 (3%) 44 50	12, 25, 62, 102	0
5	B	238/241 (98%)	0.04	8 (3%) 45 51	13, 27, 54, 86	0
All	All	823/833 (98%)	0.04	24 (2%) 51 58	10, 24, 53, 102	1 (0%)

The worst 5 of 24 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	A	129	SER	11.2
4	A	131	ASP	6.4
1	C	195	VAL	5.3
1	C	226	THR	4.3
5	B	223	ASP	4.0

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(Å ²)	Q<0.9
6	GOL	C	302	6/6	0.84	0.11	35,42,48,48	2
6	GOL	C	301	6/6	0.85	0.10	32,39,42,43	2
6	GOL	C	303	6/6	0.87	0.14	31,38,51,51	2
6	GOL	C	304	6/6	0.91	0.11	31,33,34,35	2

6.5 Other polymers [i](#)

There are no such residues in this entry.