Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2024 – 12:04 PM EST

PDB ID	:	8TOQ
Title	:	ACE2-peptide 1 complex
Authors	:	Christie, M.; Payne, R.J.
Deposited on	:	2023-08-03
Resolution	:	2.30 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 (i) 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 (i)) were used in the production of this report:

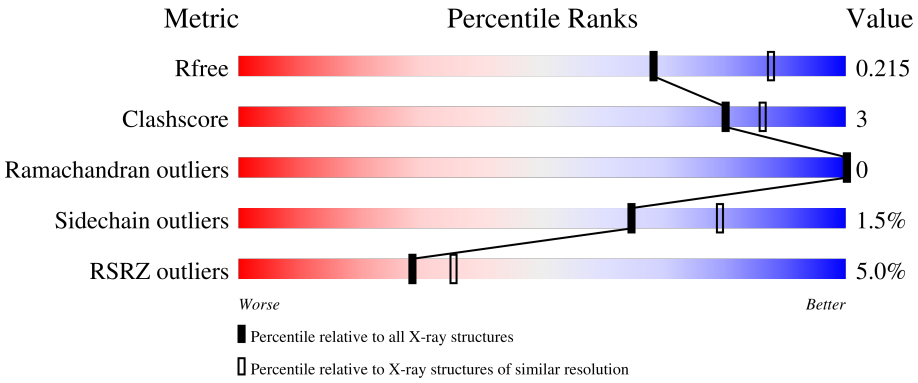
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 <=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	625	4% 87% 8% 5%
2	E	15	13% 73% 13% 13%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 5133 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 Angiotensin-converting enzyme 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	592	4834	3094	799	912	29	0	0	0

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	615	GLY	-	expression tag	UNP Q9BYF1
A	616	SER	-	expression tag	UNP Q9BYF1
A	617	HIS	-	expression tag	UNP Q9BYF1
A	618	HIS	-	expression tag	UNP Q9BYF1
A	619	HIS	-	expression tag	UNP Q9BYF1
A	620	HIS	-	expression tag	UNP Q9BYF1
A	621	HIS	-	expression tag	UNP Q9BYF1
A	622	HIS	-	expression tag	UNP Q9BYF1
A	623	HIS	-	expression tag	UNP Q9BYF1
A	624	HIS	-	expression tag	UNP Q9BYF1
A	625	HIS	-	expression tag	UNP Q9BYF1
A	626	HIS	-	expression tag	UNP Q9BYF1
A	627	SER	-	expression tag	UNP Q9BYF1
A	628	GLY	-	expression tag	UNP Q9BYF1
A	629	LEU	-	expression tag	UNP Q9BYF1
A	630	ASN	-	expression tag	UNP Q9BYF1
A	631	ASP	-	expression tag	UNP Q9BYF1
A	632	ILE	-	expression tag	UNP Q9BYF1
A	633	PHE	-	expression tag	UNP Q9BYF1
A	634	GLU	-	expression tag	UNP Q9BYF1
A	635	ALA	-	expression tag	UNP Q9BYF1
A	636	GLN	-	expression tag	UNP Q9BYF1
A	637	LYS	-	expression tag	UNP Q9BYF1
A	638	ILE	-	expression tag	UNP Q9BYF1
A	639	GLU	-	expression tag	UNP Q9BYF1
A	640	TRP	-	expression tag	UNP Q9BYF1
A	641	HIS	-	expression tag	UNP Q9BYF1

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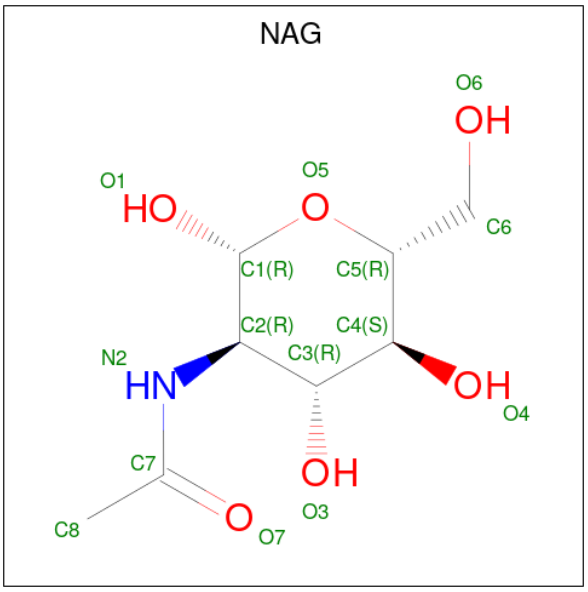
Chain	Residue	Modelled	Actual	Comment	Reference
A	642	GLU	-	expression tag	UNP Q9BYF1

- Molecule 2 is a protein called Peptide 1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	13	Total	C	N	O	0	0	0
			109	75	18	16			

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

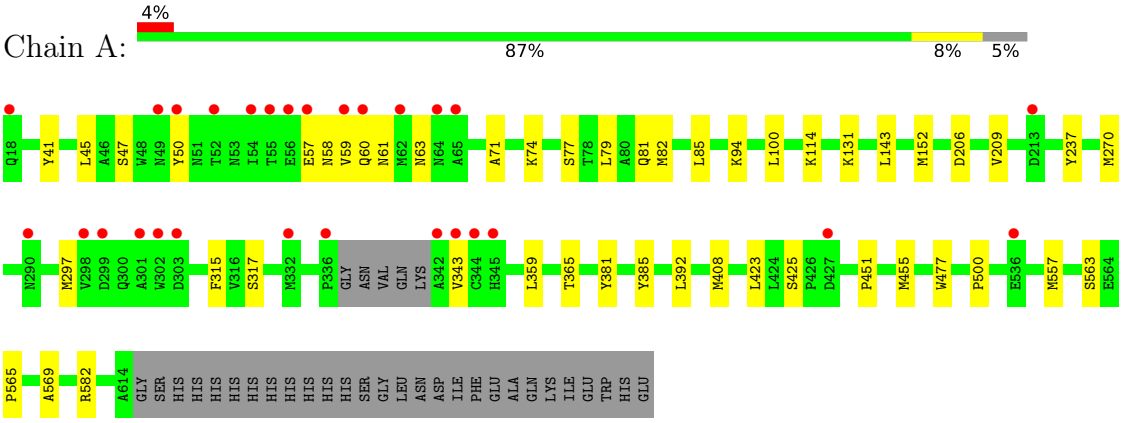
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	143	Total O 143 143	0	0
6	E	3	Total O 3 3	0	0

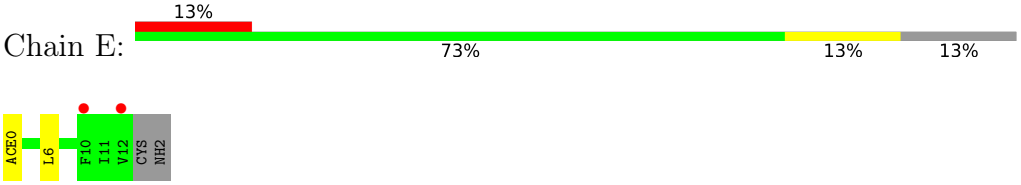
3 Residue-property plots (i)

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: Angiotensin-converting enzyme 2



• Molecule 2: Peptide 1



4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α, β, γ	180.28Å 180.28Å 71.65Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	45.55 – 2.30 45.55 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.8 (45.55-2.30) 99.8 (45.55-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.07 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.182 , 0.215 0.181 , 0.215	Depositor DCC
R_{free} test set	2022 reflections (5.26%)	wwPDB-VP
Wilson B-factor (Å^2)	39.2	Xtriage
Anisotropy	0.397	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 33.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.015 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	5133	wwPDB-VP
Average B, all atoms (Å^2)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.08% 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.

5 Model quality

5.1 Standard geometry

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

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	0.28	0/4970	0.47	0/6752
2	E	0.28	0/110	0.59	0/149
All	All	0.28	0/5080	0.47	0/6901

There are no bond length outliers.

There are no bond angle outliers.

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	4834	0	4604	26	0
2	E	109	0	115	2	0
3	A	42	0	39	0	0
4	A	1	0	0	0	0
5	A	1	0	0	0	0
6	A	143	0	0	0	0
6	E	3	0	0	1	0
All	All	5133	0	4758	26	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 3.

All (26) 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:59:VAL:O	1:A:63:ASN:ND2	2.28	0.65
1:A:477:TRP:CE3	1:A:500:PRO:HG3	2.39	0.57
1:A:58:ASN:HA	1:A:61:ASN:HB3	1.87	0.57
1:A:77:SER:O	1:A:81:GLN:HG2	2.09	0.52
1:A:47:SER:OG	2:E:0:ACE:O	2.26	0.52
1:A:343:VAL:O	1:A:359:LEU:HD21	2.11	0.50
1:A:297:MET:HE1	1:A:365:THR:C	2.32	0.50
1:A:152:MET:HG3	1:A:270:MET:HA	1.94	0.49
1:A:50:TYR:HE2	1:A:59:VAL:HG22	1.78	0.49
1:A:79:LEU:O	1:A:82:MET:HG3	2.13	0.49
1:A:392:LEU:HD13	1:A:563:SER:HA	1.95	0.48
1:A:85:LEU:HD22	1:A:94:LYS:HG2	1.96	0.48
1:A:209:VAL:HG11	1:A:565:PRO:HB3	1.95	0.48
1:A:131:LYS:HB3	1:A:143:LEU:HD23	1.97	0.46
1:A:41:TYR:O	1:A:45:LEU:HB2	2.16	0.46
1:A:315:PHE:CZ	1:A:408:MET:HG3	2.50	0.46
1:A:100:LEU:HD23	2:E:6:LEU:HD21	1.98	0.44
1:A:315:PHE:HZ	1:A:408:MET:HG3	1.82	0.44
1:A:50:TYR:CE2	1:A:59:VAL:HG22	2.53	0.44
1:A:71:ALA:HA	1:A:74:LYS:HD2	1.99	0.44
1:A:557:MET:HG2	1:A:569:ALA:HB1	2.00	0.44
1:A:60:GLN:HA	1:A:63:ASN:HB2	2.01	0.43
1:A:423:LEU:HD23	1:A:423:LEU:HA	1.90	0.42
1:A:206:ASP:HB2	6:E:101:HOH:O	2.19	0.42
1:A:297:MET:HE2	1:A:297:MET:HB2	1.81	0.42
1:A:237:TYR:CE1	1:A:451:PRO:HG2	2.55	0.41

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	588/625 (94%)	578 (98%)	10 (2%)	0	100	100
2	E	11/15 (73%)	11 (100%)	0	0	100	100
All	All	599/640 (94%)	589 (98%)	10 (2%)	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	523/552 (95%)	515 (98%)	8 (2%)	65	79
2	E	12/13 (92%)	12 (100%)	0	100	100
All	All	535/565 (95%)	527 (98%)	8 (2%)	65	79

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	57	GLU
1	A	114	LYS
1	A	317	SER
1	A	381	TYR
1	A	385	TYR
1	A	425	SER
1	A	455	MET
1	A	582	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	63	ASN
1	A	89	GLN
1	A	586	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 5 ligands modelled in this entry, 2 are monoatomic - leaving 3 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	$\#\|Z\| > 2$
3	NAG	A	702	1	14,14,15	0.33	0	17,19,21	0.49	0
3	NAG	A	703	1	14,14,15	0.27	0	17,19,21	0.47	0
3	NAG	A	701	1	14,14,15	0.32	0	17,19,21	0.46	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
3	NAG	A	702	1	-	0/6/23/26	0/1/1/1
3	NAG	A	703	1	-	0/6/23/26	0/1/1/1
3	NAG	A	701	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	701	NAG	C1-C2-N2-C7
3	A	701	NAG	C3-C2-N2-C7

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, 95^{th} 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	592/625 (94%)	-0.08	28 (4%) 31 38	27, 45, 80, 124	0
2	E	12/15 (80%)	0.73	2 (16%) 1 2	45, 61, 83, 87	0
All	All	604/640 (94%)	-0.06	30 (4%) 28 35	27, 45, 80, 124	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	56	GLU	4.5
1	A	343	VAL	4.5
1	A	427	ASP	4.3
1	A	336	PRO	3.8
2	E	12	VAL	3.7
1	A	55	THR	3.4
1	A	64	ASN	3.2
1	A	299	ASP	3.2
1	A	332	MET	3.2
1	A	301	ALA	3.1
1	A	52	THR	3.0
1	A	49	ASN	3.0
1	A	342	ALA	2.9
1	A	54	ILE	2.9
1	A	59	VAL	2.7
1	A	60	GLN	2.7
1	A	18	GLN	2.6
1	A	290	ASN	2.5
1	A	62	MET	2.4
1	A	536	GLU	2.4
1	A	57	GLU	2.3
1	A	213	ASP	2.2
1	A	302	TRP	2.2
2	E	10	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	50	TYR	2.1
1	A	303	ASP	2.0
1	A	65	ALA	2.0
1	A	298	VAL	2.0
1	A	345	HIS	2.0
1	A	344	CYS	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, 95^{th} 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
3	NAG	A	702	14/15	0.81	0.27	75,83,86,92	0
3	NAG	A	701	14/15	0.85	0.23	66,76,86,88	0
3	NAG	A	703	14/15	0.87	0.21	61,73,83,85	0
4	ZN	A	704	1/1	0.91	0.09	59,59,59,59	0
5	CL	A	705	1/1	0.99	0.19	34,34,34,34	0

6.5 Other polymers (i)

There are no such residues in this entry.