Full wwPDB X-ray Structure Validation Report ⓘ

Aug 15, 2021 – 04:07 PM JST

PDB ID	:	7CUJ
Title	:	Crystal structure of fission yeast Ccq1 and Tpz1
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Deposited on	:	2020-08-23
Resolution	:	2.40 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:

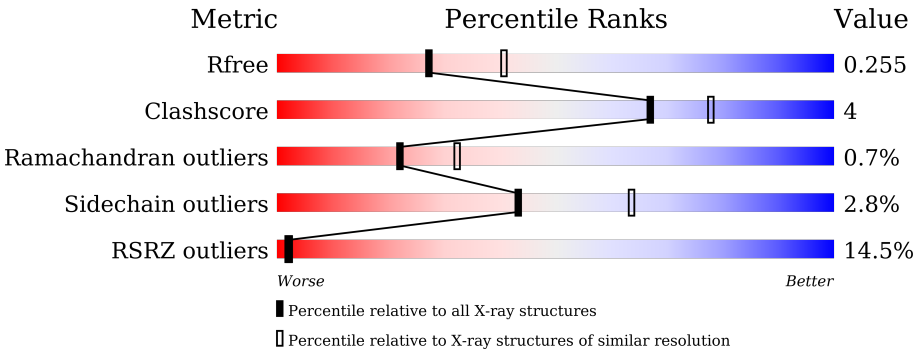
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.23.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.1

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 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	317	11% 74% 7% • 19%
1	B	317	12% 73% 6% • 19%
2	C	45	4% 78% • • 16%
2	D	45	22% 78% • 20%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4806 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 Coiled-coil quantitatively-enriched protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	258	Total	C	N	O	S	0	0	0
			2046	1318	338	380	10			
1	B	256	Total	C	N	O	S	0	0	0
			2031	1310	336	375	10			

- Molecule 2 is a protein called Protection of telomeres protein tpz1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	38	Total	C	N	O	S	0	0	0
			334	217	56	60	1			
2	D	36	Total	C	N	O	S	0	0	0
			315	202	54	58	1			

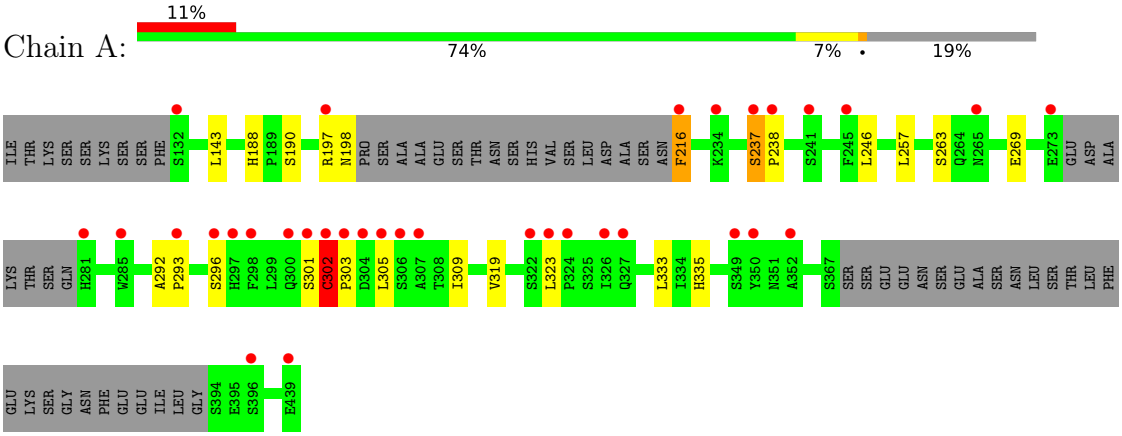
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	37	Total	O	0	0
			37	37		
3	C	9	Total	O	0	0
			9	9		
3	B	28	Total	O	0	0
			28	28		
3	D	6	Total	O	0	0
			6	6		

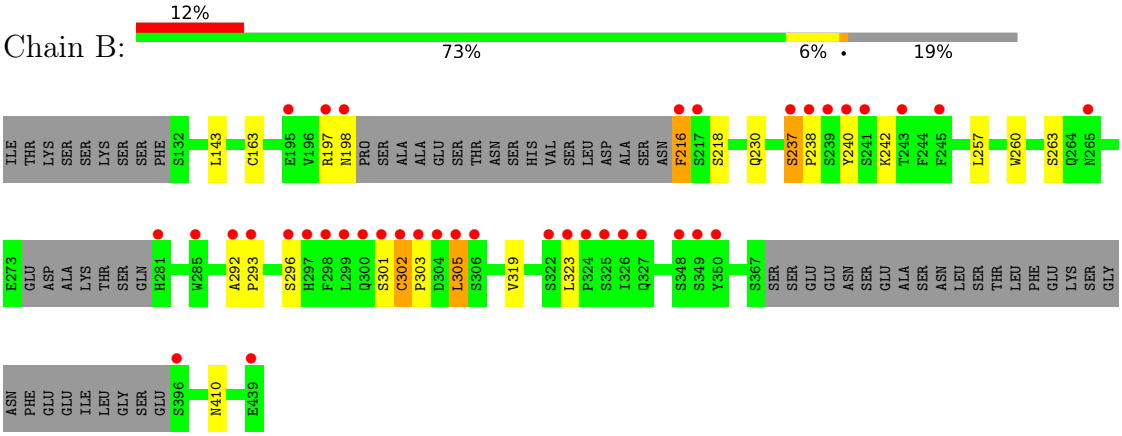
3 Residue-property plots (i)

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.

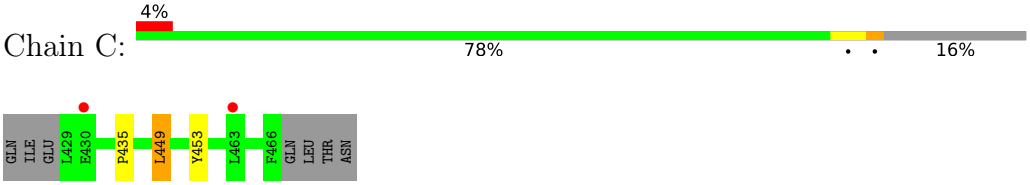
• Molecule 1: Coiled-coil quantitatively-enriched protein 1



• Molecule 1: Coiled-coil quantitatively-enriched protein 1

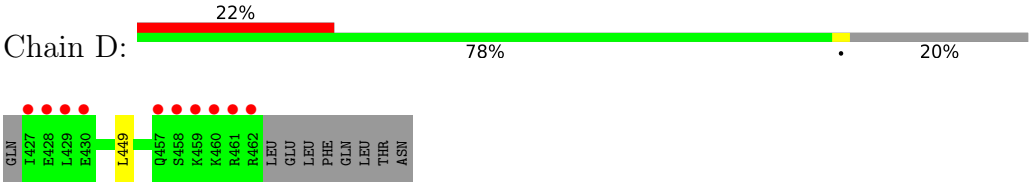


• Molecule 2: Protection of telomeres protein tpz1



• Molecule 2: Protection of telomeres protein tpz1

Chain D:


22%
78%
20%
GLN
I427
E428
L429
E430
L449
Q457
S458
K459
K460
R461
R462
LEU
GLU
LEU
PHE
GLN
LEU
THR
ASN

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	58.30Å 71.75Å 95.18Å 90.00° 103.89° 90.00°	Depositor
Resolution (Å)	38.87 – 2.40 38.84 – 2.39	Depositor EDS
% Data completeness (in resolution range)	83.5 (38.87-2.40) 83.0 (38.84-2.39)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.75 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.197 , 0.255 0.197 , 0.255	Depositor DCC
R_{free} test set	1240 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å^2)	33.9	Xtriage
Anisotropy	0.126	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 52.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	4806	wwPDB-VP
Average B, all atoms (Å^2)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.47% 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

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	0.27	0/2096	0.50	0/2841
1	B	0.27	0/2081	0.50	0/2821
2	C	0.26	0/341	0.47	0/455
2	D	0.26	0/321	0.50	0/428
All	All	0.27	0/4839	0.50	0/6545

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	2046	0	2023	17	0
1	B	2031	0	2012	19	0
2	C	334	0	340	3	0
2	D	315	0	320	0	0
3	A	37	0	0	1	0
3	B	28	0	0	0	0
3	C	9	0	0	0	0
3	D	6	0	0	0	0
All	All	4806	0	4695	37	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.

All (37) 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:B:198:ASN:C	1:B:216:PHE:N	2.28	0.88
1:B:296:SER:HB2	1:B:323:LEU:HD22	1.58	0.86
1:A:197:ARG:NH1	2:C:453:TYR:OH	2.22	0.72
1:A:292:ALA:N	1:A:293:PRO:HD2	2.06	0.71
1:B:237:SER:HB3	1:B:238:PRO:HD2	1.77	0.67
1:A:237:SER:HB3	1:A:238:PRO:HD2	1.76	0.66
1:B:302:CYS:N	1:B:303:PRO:CD	2.62	0.63
1:A:302:CYS:N	1:A:303:PRO:CD	2.63	0.62
1:B:292:ALA:N	1:B:293:PRO:HD2	2.14	0.62
1:A:237:SER:HB3	1:A:238:PRO:CD	2.32	0.58
1:A:296:SER:HB2	1:A:323:LEU:HD13	1.86	0.56
1:A:302:CYS:N	1:A:303:PRO:HD2	2.21	0.56
1:B:237:SER:HB3	1:B:238:PRO:CD	2.38	0.52
1:B:197:ARG:HD3	1:B:218:SER:CB	2.39	0.52
1:A:198:ASN:C	1:A:216:PHE:N	2.63	0.52
1:B:296:SER:CB	1:B:323:LEU:HD22	2.38	0.50
1:A:296:SER:HB2	1:A:323:LEU:HD22	1.95	0.48
1:B:301:SER:C	1:B:303:PRO:HD2	2.34	0.48
1:B:302:CYS:N	1:B:303:PRO:HD2	2.28	0.47
1:A:301:SER:C	1:A:303:PRO:HD2	2.35	0.47
1:A:292:ALA:N	1:A:293:PRO:CD	2.78	0.47
1:B:292:ALA:HB2	1:B:319:VAL:HG22	1.96	0.46
1:A:188:HIS:HD2	1:A:190:SER:H	1.63	0.46
1:A:237:SER:CB	1:A:238:PRO:CD	2.94	0.44
1:B:230:GLN:HB2	1:B:260:TRP:CH2	2.53	0.43
1:B:296:SER:HB2	1:B:323:LEU:CD2	2.39	0.43
1:B:240:TYR:CE2	1:B:242:LYS:HB3	2.54	0.43
1:A:335:HIS:HE1	3:A:502:HOH:O	2.00	0.43
1:B:197:ARG:HD3	1:B:218:SER:HB2	1.99	0.42
2:C:435:PRO:HG3	1:B:163:CYS:HB2	2.01	0.42
1:A:237:SER:CB	1:A:238:PRO:HD2	2.49	0.42
1:B:296:SER:HB2	1:B:323:LEU:HD13	2.01	0.42
1:A:246:LEU:HA	1:A:309:ILE:O	2.20	0.42
1:A:319:VAL:HG13	1:A:323:LEU:HD12	2.02	0.41
2:C:449:LEU:HD12	2:C:449:LEU:HA	1.90	0.41
1:B:260:TRP:O	1:B:263:SER:HB3	2.21	0.41
1:B:302:CYS:O	1:B:305:LEU:N	2.50	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	250/317 (79%)	236 (94%)	12 (5%)	2 (1%)	19 29
1	B	248/317 (78%)	229 (92%)	17 (7%)	2 (1%)	19 29
2	C	36/45 (80%)	36 (100%)	0	0	100 100
2	D	34/45 (76%)	34 (100%)	0	0	100 100
All	All	568/724 (78%)	535 (94%)	29 (5%)	4 (1%)	22 32

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	237	SER
1	B	237	SER
1	A	302	CYS
1	B	302	CYS

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	233/285 (82%)	225 (97%)	8 (3%)	37 56
1	B	231/285 (81%)	226 (98%)	5 (2%)	52 71
2	C	37/44 (84%)	36 (97%)	1 (3%)	44 65
2	D	35/44 (80%)	34 (97%)	1 (3%)	42 62
All	All	536/658 (82%)	521 (97%)	15 (3%)	43 63

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	143	LEU
1	A	216	PHE
1	A	257	LEU
1	A	263	SER
1	A	269	GLU
1	A	302	CYS
1	A	305	LEU
1	A	333	LEU
2	C	449	LEU
1	B	143	LEU
1	B	216	PHE
1	B	257	LEU
1	B	305	LEU
1	B	410	ASN
2	D	449	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	188	HIS
1	A	335	HIS
2	C	457	GLN
1	B	183	HIS
1	B	188	HIS
1	B	230	GLN
1	B	264	GLN
1	B	410	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

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

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, 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	258/317 (81%)	0.72	34 (13%)	3	3	14, 50, 100, 124	0
1	B	256/317 (80%)	0.83	39 (15%)	2	1	16, 47, 111, 131	0
2	C	38/45 (84%)	0.27	2 (5%)	26	25	26, 46, 69, 76	0
2	D	36/45 (80%)	1.30	10 (27%)	0	0	29, 56, 119, 146	0
All	All	588/724 (81%)	0.78	85 (14%)	2	2	14, 49, 107, 146	0

All (85) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	297	HIS	10.9
1	B	350	TYR	8.2
2	D	461	ARG	7.9
1	B	297	HIS	7.5
1	A	324	PRO	7.1
1	B	300	GLN	6.1
1	B	324	PRO	5.8
1	B	302	CYS	5.8
1	B	293	PRO	5.8
1	B	304	ASP	5.8
1	B	298	PHE	5.7
1	B	299	LEU	5.7
1	A	304	ASP	5.5
1	A	302	CYS	5.5
1	A	326	ILE	5.5
1	A	327	GLN	5.3
1	B	296	SER	5.2
1	B	305	LEU	5.0
1	B	217	SER	4.9
2	D	462	ARG	4.8
2	D	427	ILE	4.8

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Mol	Chain	Res	Type	RSRZ
1	A	350	TYR	4.7
1	A	245	PHE	4.5
1	B	245	PHE	4.4
1	B	439	GLU	4.2
1	A	298	PHE	4.2
2	D	460	LYS	4.2
1	B	281	HIS	4.1
1	A	237	SER	4.0
1	B	197	ARG	3.9
1	B	285	TRP	3.9
1	A	305	LEU	3.7
1	B	195	GLU	3.7
1	B	265	ASN	3.7
1	A	216	PHE	3.6
1	A	273	GLU	3.6
1	B	216	PHE	3.6
1	B	325	SER	3.6
1	A	352	ALA	3.6
1	B	241	SER	3.5
1	A	303	PRO	3.5
1	A	296	SER	3.5
1	A	285	TRP	3.5
1	A	306	SER	3.4
1	A	322	SER	3.3
1	A	238	PRO	3.3
1	B	198	ASN	3.2
1	B	301	SER	3.2
1	A	300	GLN	3.2
2	D	459	LYS	3.2
1	B	303	PRO	3.0
1	A	301	SER	3.0
1	B	327	GLN	3.0
1	A	439	GLU	3.0
1	B	349	SER	2.9
1	A	197	ARG	2.9
1	B	348	SER	2.8
1	A	349	SER	2.8
2	C	430	GLU	2.8
1	B	237	SER	2.7
1	B	326	ILE	2.7
1	B	322	SER	2.7
1	A	281	HIS	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	265	ASN	2.6
1	B	243	THR	2.6
1	B	240	TYR	2.6
2	D	458	SER	2.6
1	B	323	LEU	2.6
1	B	292	ALA	2.5
2	D	457	GLN	2.5
1	B	396	SER	2.5
1	A	293	PRO	2.5
2	D	429	LEU	2.5
1	A	307	ALA	2.4
1	A	234	LYS	2.4
1	A	132	SER	2.4
1	B	306	SER	2.4
1	B	239	SER	2.2
2	D	428	GLU	2.2
1	A	323	LEU	2.1
2	C	463	LEU	2.1
1	A	241	SER	2.1
1	A	396	SER	2.0
2	D	430	GLU	2.0
1	B	238	PRO	2.0

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 monosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.