



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 22, 2020 – 03:58 AM BST

PDB ID : 6PHC
Title : Pfs25 in complex with the human transmission blocking antibody 2544
Authors : McLeod, B.R.; Julien, J.P.
Deposited on : 2019-06-25
Resolution : 2.90 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 following versions of software and data (see [references ⓘ](#)) 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 : 2.13.1
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) : 2.13.1

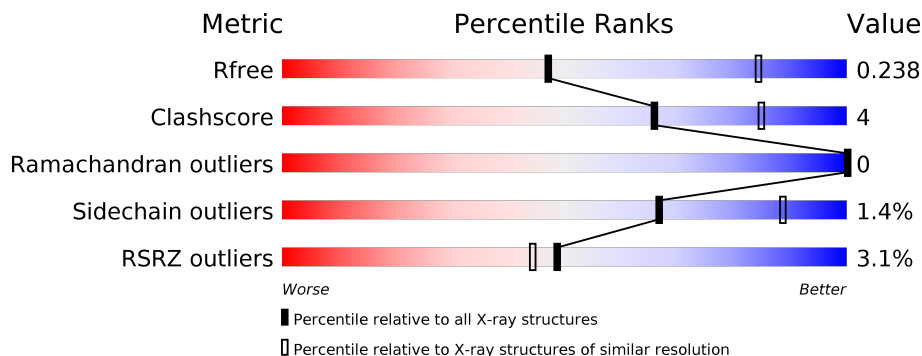
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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	E	184	
1	I	184	
2	A	228	
2	C	228	
3	B	217	
3	D	217	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 9000 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 25 kDa ookinete surface antigen.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	I	158	1124	680	191	229	24	0	0	0
1	E	155	1106	668	186	229	23	0	0	0

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	-2	GLU	-	expression tag	UNP P13829
I	-1	THR	-	expression tag	UNP P13829
I	0	GLY	-	expression tag	UNP P13829
I	91	GLN	ASN	conflict	UNP P13829
I	144	GLN	ASN	conflict	UNP P13829
I	164B	GLN	ASN	conflict	UNP P13829
I	172	GLY	-	expression tag	UNP P13829
I	173	THR	-	expression tag	UNP P13829
I	174	LYS	-	expression tag	UNP P13829
I	175	HIS	-	expression tag	UNP P13829
I	176	HIS	-	expression tag	UNP P13829
I	177	HIS	-	expression tag	UNP P13829
I	178	HIS	-	expression tag	UNP P13829
I	179	HIS	-	expression tag	UNP P13829
I	180	HIS	-	expression tag	UNP P13829
E	-2	GLU	-	expression tag	UNP P13829
E	-1	THR	-	expression tag	UNP P13829
E	0	GLY	-	expression tag	UNP P13829
E	91	GLN	ASN	conflict	UNP P13829
E	144	GLN	ASN	conflict	UNP P13829
E	166	GLN	ASN	conflict	UNP P13829
E	173	GLY	-	expression tag	UNP P13829
E	174	THR	-	expression tag	UNP P13829
E	175	LYS	-	expression tag	UNP P13829
E	176	HIS	-	expression tag	UNP P13829

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Chain	Residue	Modelled	Actual	Comment	Reference
E	177	HIS	-	expression tag	UNP P13829
E	178	HIS	-	expression tag	UNP P13829
E	179	HIS	-	expression tag	UNP P13829
E	180	HIS	-	expression tag	UNP P13829
E	181	HIS	-	expression tag	UNP P13829

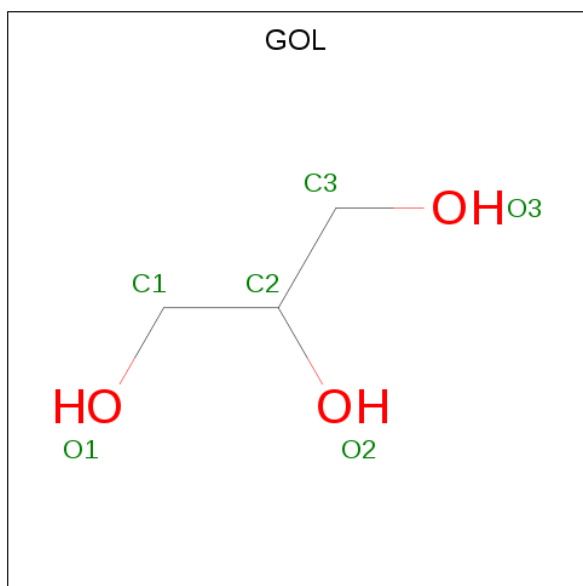
- Molecule 2 is a protein called 2544 Antibody Fab, Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	A	228	Total	C	N	O	S	0	0	0
			1716	1085	281	342	8			
2	C	228	Total	C	N	O	S	0	0	0
			1716	1084	281	343	8			

- Molecule 3 is a protein called 2544 Antibody Fab, Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	B	217	Total	C	N	O	S	0	0	0
			1670	1046	281	336	7			
3	D	217	Total	C	N	O	S	0	0	0
			1644	1028	273	336	7			

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).

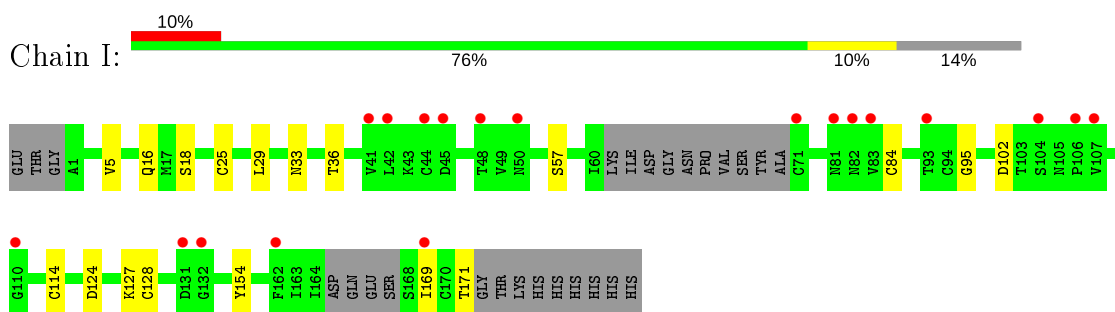


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	I	1	Total 6	C 3	O 3	0	0
4	I	1	Total 6	C 3	O 3	0	0
4	C	1	Total 6	C 3	O 3	0	0
4	C	1	Total 6	C 3	O 3	0	0

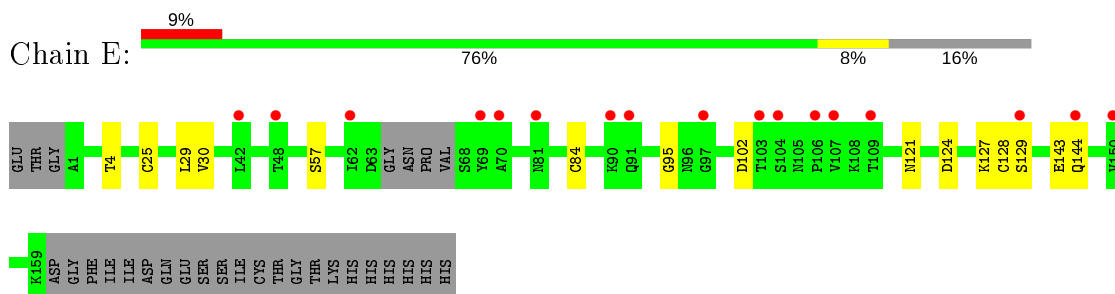
3 Residue-property plots [i](#)

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.

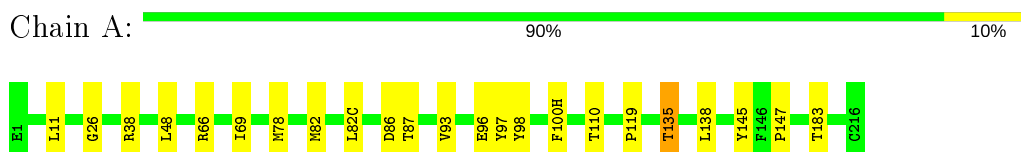
- Molecule 1: 25 kDa ookinete surface antigen



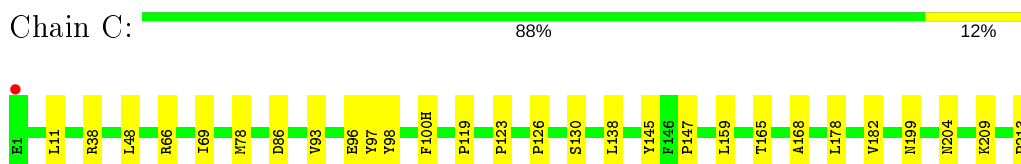
- Molecule 1: 25 kDa ookinete surface antigen




- Molecule 2: 2544 Antibody Fab, Heavy Chain



- Molecule 2: 2544 Antibody Fab, Heavy Chain



- Molecule 3: 2544 Antibody Fab, Light Chain

Chain B:  87% 12%



• Molecule 3: 2544 Antibody Fab, Light Chain

Chain D:  90% 8%



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	141.22Å 141.22Å 164.37Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.57 – 2.90 39.57 – 2.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (39.57-2.90) 100.0 (39.57-2.90)	Depositor EDS
R_{merge}	0.24	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.72 (at 2.90Å)	Xtrriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.200 , 0.238 0.200 , 0.238	Depositor DCC
R_{free} test set	2125 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	67.5	Xtrriage
Anisotropy	0.214	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 44.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.000 for -h,-k,l	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	9000	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.90% 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	E	0.25	0/1114	0.48	0/1508
1	I	0.25	0/1131	0.48	0/1525
2	A	0.26	0/1759	0.47	0/2395
2	C	0.26	0/1759	0.48	0/2396
3	B	0.25	0/1707	0.46	0/2320
3	D	0.24	0/1681	0.46	0/2293
All	All	0.25	0/9151	0.47	0/12437

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 [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	E	1106	0	1011	8	0
1	I	1124	0	1030	10	0
2	A	1716	0	1654	13	0
2	C	1716	0	1649	15	0
3	B	1670	0	1616	13	0
3	D	1644	0	1550	15	0
4	C	12	0	16	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	I	12	0	16	0	0
All	All	9000	0	8542	70	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 70 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)
2:C:126:PRO:HG3	2:C:138:LEU:HB3	1.67	0.75
3:D:188:HIS:O	3:D:210:ARG:NH1	2.20	0.74
3:D:180:LEU:HD13	3:D:185:TYR:HB2	1.77	0.67
3:B:61:ARG:NH1	3:B:82:ASP:OD2	2.29	0.64
2:A:26:GLY:H	4:C:302:GOL:H32	1.62	0.63

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	E	151/184 (82%)	139 (92%)	12 (8%)	0	100	100
1	I	152/184 (83%)	138 (91%)	14 (9%)	0	100	100
2	A	226/228 (99%)	224 (99%)	2 (1%)	0	100	100
2	C	226/228 (99%)	224 (99%)	2 (1%)	0	100	100
3	B	215/217 (99%)	210 (98%)	5 (2%)	0	100	100
3	D	215/217 (99%)	210 (98%)	5 (2%)	0	100	100
All	All	1185/1258 (94%)	1145 (97%)	40 (3%)	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	E	126/167 (75%)	125 (99%)	1 (1%)	81	94
1	I	127/167 (76%)	127 (100%)	0	100	100
2	A	193/194 (100%)	191 (99%)	2 (1%)	76	92
2	C	193/194 (100%)	191 (99%)	2 (1%)	76	92
3	B	191/192 (100%)	186 (97%)	5 (3%)	46	77
3	D	185/192 (96%)	181 (98%)	4 (2%)	52	81
All	All	1015/1106 (92%)	1001 (99%)	14 (1%)	67	89

5 of 14 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	B	180	LEU
1	E	30	VAL
3	D	121	ASP
3	B	136	ASN
3	D	60	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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

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
4	GOL	I	202	-	5,5,5	0.91	0	5,5,5	0.98	0
4	GOL	C	301	-	5,5,5	0.93	0	5,5,5	0.94	0
4	GOL	C	302	-	5,5,5	0.91	0	5,5,5	0.97	0
4	GOL	I	201	-	5,5,5	0.95	0	5,5,5	0.91	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
4	GOL	I	202	-	-	0/4/4/4	-
4	GOL	C	301	-	-	2/4/4/4	-
4	GOL	C	302	-	-	2/4/4/4	-
4	GOL	I	201	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	302	GOL	O1-C1-C2-O2
4	C	301	GOL	O1-C1-C2-C3
4	C	302	GOL	O1-C1-C2-C3
4	I	201	GOL	C1-C2-C3-O3
4	C	301	GOL	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	302	GOL	1	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	E	155/184 (84%)	0.56	17 (10%) 5 4	50, 91, 123, 166	0
1	I	158/184 (85%)	0.70	19 (12%) 4 3	48, 99, 137, 185	0
2	A	228/228 (100%)	-0.11	0 100 100	34, 46, 66, 97	0
2	C	228/228 (100%)	-0.13	1 (0%) 92 93	39, 52, 101, 138	0
3	B	217/217 (100%)	-0.04	0 100 100	36, 55, 87, 112	0
3	D	217/217 (100%)	0.02	0 100 100	42, 68, 108, 147	0
All	All	1203/1258 (95%)	0.11	37 (3%) 49 44	34, 61, 119, 185	0

The worst 5 of 37 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	69	TYR	4.1
1	E	48	THR	3.9
1	I	162	PHE	3.8
1	I	104	SER	3.7
1	E	70	ALA	3.4

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
4	GOL	C	302	6/6	0.67	0.37	61,83,83,84	0
4	GOL	I	201	6/6	0.75	0.16	69,74,78,82	0
4	GOL	I	202	6/6	0.79	0.30	94,100,101,102	0
4	GOL	C	301	6/6	0.79	0.32	62,73,77,78	0

6.5 Other polymers [i](#)

There are no such residues in this entry.