



wwPDB X-ray Structure Validation Summary Report

Mar 1, 2014 – 04:14 AM GMT

PDB ID : 2DVB
Title : Crystal structure of peanut lectin GAL-beta-1,6-GalNAc complex
Authors : Natchiar, S.K.; Srinivas, O.; Mitra, N.; Surolia, A.; Jayaraman, N.; Vijayan, M.
Deposited on : 2006-07-30
Resolution : 2.25 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

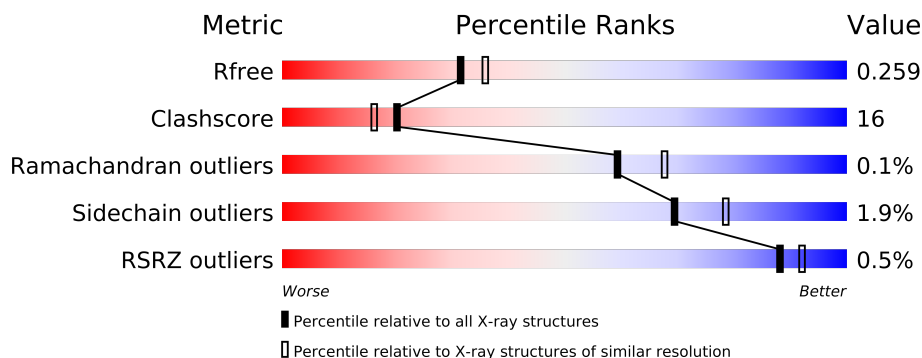
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.25 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}	66092	1108 (2.28-2.24)
Clashscore	79885	1326 (2.28-2.24)
Ramachandran outliers	78287	1291 (2.28-2.24)
Sidechain outliers	78261	1291 (2.28-2.24)
RSRZ outliers	66119	1110 (2.28-2.24)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	236	
1	B	236	
1	C	236	
1	D	236	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
4	CA	B	237	-	X
4	CA	D	237	-	X
6	SO4	C	3240	-	X

2 Entry composition i

There are 7 unique types of molecules in this entry. The entry contains 8047 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

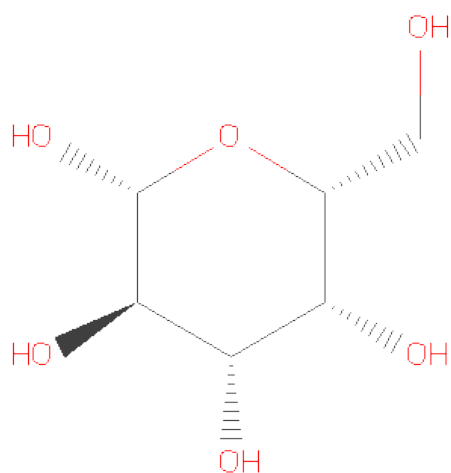
- Molecule 1 is a protein called Galactose-binding lectin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	232	Total	C	N	O	S	9	0	0
			1743	1102	287	352	2			
1	B	232	Total	C	N	O	S	12	0	0
			1743	1102	287	352	2			
1	C	232	Total	C	N	O	S	7	0	0
			1743	1102	287	352	2			
1	D	232	Total	C	N	O	S	11	0	0
			1743	1102	287	352	2			

- Molecule 2 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	2	Total	C	N	O	0	0
			26	14	1	11		

- Molecule 3 is SUGAR (D-GALACTOSE) (three-letter code: GAL) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C O 12 6 6	0	0
3	C	1	Total C O 12 6 6	0	0
3	D	1	Total C O 12 6 6	0	0

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Ca 1 1	0	0
4	A	1	Total Ca 1 1	0	0
4	D	1	Total Ca 1 1	0	0
4	C	1	Total Ca 1 1	0	0

- Molecule 5 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total Mn 1 1	0	0
5	A	1	Total Mn 1 1	0	0
5	D	1	Total Mn 1 1	0	0
5	C	1	Total Mn 1 1	0	0

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		
6	C	1	Total	O	S	0	0
			5	4	1		
6	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	240	Total	O	0	0
			240	240		
7	B	260	Total	O	0	0
			260	260		
7	C	255	Total	O	0	0
			255	255		
7	D	230	Total	O	0	0
			230	230		

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	125.74Å 124.33Å 75.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.98 – 2.25 19.98 – 2.25	Depositor EDS
% Data completeness (in resolution range)	98.1 (19.98-2.25) 98.0 (19.98-2.25)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.91 (at 2.26Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.214 , 0.266 0.209 , 0.259	Depositor DCC
R_{free} test set	2826 reflections (5.34%)	DCC
Wilson B-factor (Å ²)	32.2	Xtriage
Anisotropy	0.527	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 51.2	EDS
Estimated twinning fraction	0.014 for k,h,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 55791 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8047	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.63% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GAL, CA, MN, NGA, SO4

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	0.36	0/1779	0.68	0/2426
1	B	0.36	0/1779	0.69	0/2426
1	C	0.36	0/1779	0.67	0/2426
1	D	0.36	0/1779	0.67	0/2426
All	All	0.36	0/7116	0.68	0/9704

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
2	A	1	0

There are no bond length outliers.

There are no bond angle outliers.

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	240	NGA	C1

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the

chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1743	0	1699	54	0
1	B	1743	0	1699	54	0
1	C	1743	0	1699	65	0
1	D	1743	0	1699	68	0
2	A	26	0	23	0	0
3	B	12	0	12	1	0
3	C	12	0	12	0	0
3	D	12	0	12	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
6	A	5	0	0	0	0
6	B	5	0	0	1	0
6	C	5	0	0	1	0
6	D	5	0	0	0	0
7	A	240	0	0	7	0
7	B	260	0	0	6	0
7	C	255	0	0	13	0
7	D	230	0	0	10	0
All	All	8047	0	6855	218	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 16.

The worst 5 of 218 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:182:ASN:ND2	1:D:184:ASP:H	1.71	0.89
1:C:93:ASP:HB3	7:C:3343:HOH:O	1.80	0.80
1:B:25:THR:HB	7:B:2417:HOH:O	1.84	0.78
1:B:77:LYS:HG2	1:B:78:ASP:OD2	1.84	0.77
1:D:41:ASN:HD22	1:D:211:SER:HA	1.51	0.75

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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	230/236 (98%)	223 (97%)	7 (3%)	0	100	100
1	B	230/236 (98%)	221 (96%)	9 (4%)	0	100	100
1	C	230/236 (98%)	219 (95%)	11 (5%)	0	100	100
1	D	230/236 (98%)	223 (97%)	6 (3%)	1 (0%)	43	46
All	All	920/944 (98%)	886 (96%)	33 (4%)	1 (0%)	59	68

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	180	ASN

5.3.2 Protein sidechains ⓘ

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	197/201 (98%)	194 (98%)	3 (2%)	76	85
1	B	197/201 (98%)	192 (98%)	5 (2%)	60	70
1	C	197/201 (98%)	194 (98%)	3 (2%)	76	85
1	D	197/201 (98%)	193 (98%)	4 (2%)	68	77
All	All	788/804 (98%)	773 (98%)	15 (2%)	69	78

5 of 15 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	80	ASP
1	B	182	ASN
1	D	46	VAL

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Mol	Chain	Res	Type
1	B	78	ASP
1	D	15	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 29 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	216	GLN
1	C	41	ASN
1	D	95	GLN
1	C	15	ASN
1	C	61	ASN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

2 carbohydrates 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	$\# Z > 2$
2	GAL	A	239	2	12,12,12	2.38	4 (33%)	17,17,17	2.72	4 (23%)
2	NGA	A	240	2	13,14,15	3.44	5 (38%)	18,20,21	1.98	3 (16%)

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
2	GAL	A	239	2	-	0/2/22/22	0/1/1/1
2	NGA	A	240	2	1/1/6/7	0/4/24/26	0/1/1/1

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	240	NGA	C4-C5	7.01	1.61	1.52
2	A	240	NGA	O5-C5	6.97	1.55	1.44
2	A	240	NGA	O5-C1	5.03	1.53	1.43
2	A	239	GAL	O5-C1	4.56	1.52	1.43
2	A	239	GAL	C4-C3	4.48	1.64	1.52

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	239	GAL	O6-C6-C5	6.97	135.33	111.36
2	A	239	GAL	C6-C5-C4	6.92	129.73	113.00
2	A	240	NGA	C1-C2-N2	-5.26	104.74	110.85
2	A	240	NGA	C1-O5-C5	3.81	118.40	112.04
2	A	240	NGA	C3-C2-N2	2.60	116.07	110.56

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	240	NGA	C1

There are no torsion outliers.

There are no ring outliers.

5.6 Ligand geometry

Of 15 ligands modelled in this entry, 8 are monoatomic - leaving 7 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
6	SO4	A	1240	-	4,4,4	0.27	0	6,6,6	0.08	0
3	GAL	B	1239	-	12,12,12	2.33	4 (33%)	17,17,17	2.85	5 (29%)
6	SO4	B	2240	-	4,4,4	0.23	0	6,6,6	0.06	0
3	GAL	C	2239	-	12,12,12	2.56	4 (33%)	17,17,17	2.83	4 (23%)
6	SO4	C	3240	-	4,4,4	0.24	0	6,6,6	0.14	0
3	GAL	D	3239	-	12,12,12	2.27	4 (33%)	17,17,17	2.84	5 (29%)
6	SO4	D	4240	-	4,4,4	0.25	0	6,6,6	0.08	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	SO4	A	1240	-	-	0/0/0/0	0/0/0/0
3	GAL	B	1239	-	-	0/2/22/22	0/1/1/1
6	SO4	B	2240	-	-	0/0/0/0	0/0/0/0
3	GAL	C	2239	-	-	0/2/22/22	0/1/1/1
6	SO4	C	3240	-	-	0/0/0/0	0/0/0/0
3	GAL	D	3239	-	-	0/2/22/22	0/1/1/1
6	SO4	D	4240	-	-	0/0/0/0	0/0/0/0

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	2239	GAL	O5-C1	5.12	1.53	1.43
3	C	2239	GAL	O5-C5	4.81	1.56	1.44
3	B	1239	GAL	C4-C3	4.66	1.64	1.52
3	C	2239	GAL	C4-C3	4.36	1.64	1.52
3	D	3239	GAL	C4-C3	4.26	1.63	1.52

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1239	GAL	C6-C5-C4	7.58	131.31	113.00
3	C	2239	GAL	C6-C5-C4	7.20	130.40	113.00
3	D	3239	GAL	C6-C5-C4	7.18	130.36	113.00
3	D	3239	GAL	O6-C6-C5	7.01	135.47	111.36
3	C	2239	GAL	O6-C6-C5	6.94	135.23	111.36

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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, 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	232/236 (98%)	-0.36	1 (0%) 90 93	23, 31, 43, 63	2 (0%)
1	B	231/236 (97%)	-0.46	0 100 100	19, 29, 39, 50	1 (0%)
1	C	231/236 (97%)	-0.28	1 (0%) 90 93	21, 31, 46, 59	0
1	D	231/236 (97%)	-0.37	3 (1%) 74 80	21, 31, 45, 62	1 (0%)
All	All	925/944 (97%)	-0.37	5 (0%) 88 92	19, 31, 43, 63	4 (0%)

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	14	GLY	4.1
1	A	232	THR	3.1
1	D	13	GLU	2.6
1	C	16	PRO	2.3
1	D	1	ALA	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 ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	GAL	A	239	12/12	0.15	1.81	33,36,41,49	0
2	NGA	A	240	14/15	0.33	-	57,67,70,70	0

6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(\AA^2)	Q<0.9
6	SO4	C	3240	5/5	0.12	2.36	36,36,37,40	0
4	CA	D	237	1/1	0.18	2.24	32,32,32,32	0
4	CA	B	237	1/1	0.14	2.05	31,31,31,31	0
6	SO4	D	4240	5/5	0.19	1.22	51,51,53,53	0
6	SO4	A	1240	5/5	0.21	1.21	100,100,101,101	0
3	GAL	D	3239	12/12	0.14	0.97	34,42,43,48	0
3	GAL	C	2239	12/12	0.13	0.96	38,42,47,52	0
4	CA	A	237	1/1	0.14	0.86	36,36,36,36	0
3	GAL	B	1239	12/12	0.10	-0.11	31,34,35,38	0
6	SO4	B	2240	5/5	0.08	-1.25	45,45,46,50	0
4	CA	C	237	1/1	0.10	-1.31	36,36,36,36	0
5	MN	B	238	1/1	0.05	-2.06	47,47,47,47	0
5	MN	D	238	1/1	0.03	-3.67	44,44,44,44	0
5	MN	A	238	1/1	0.04	-4.00	57,57,57,57	0
5	MN	C	238	1/1	0.02	-4.72	42,42,42,42	0

6.5 Other polymers ⓘ

There are no such residues in this entry.