



wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 2WQZ / pdb_00002wqz
Title : Crystal structure of synaptic protein neuroligin-4 in complex with neurexin-beta 1: alternative refinement
Authors : Fabrichny, I.P.; Leone, P.; Sulzenbacher, G.; Comoletti, D.; Miller, M.T.; Taylor, P.; Bourne, Y.; Marchot, P.
Deposited on : 2009-08-28
Resolution : 3.90 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 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

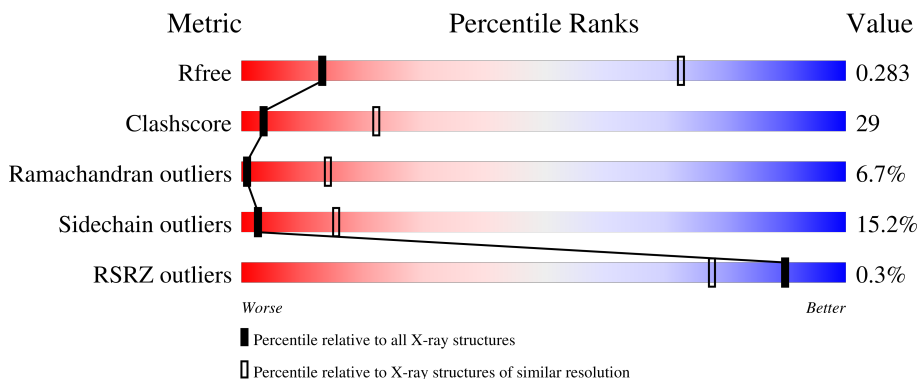
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.90 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}	180053	1270 (4.10-3.70)
Clashscore	190562	1034 (4.08-3.72)
Ramachandran outliers	187476	1251 (4.10-3.70)
Sidechain outliers	187428	1243 (4.10-3.70)
RSRZ outliers	180081	1269 (4.10-3.70)

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	A	588	40% 39% 11% 7%
1	B	588	46% 36% 9% 7%
2	C	179	53% 36% 9% 2%
2	D	179	50% 39% 9% 2%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11360 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 NEUROLIGIN 4, X-LINKED.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	545	Total	C	N	O	S	0	0	0
			4310	2756	712	821	21			
1	B	544	Total	C	N	O	S	0	0	0
			4302	2749	713	819	21			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	561	ARG	LYS	conflict	UNP Q8N0W4
B	561	ARG	LYS	conflict	UNP Q8N0W4

- Molecule 2 is a protein called NEUREXIN-1-BETA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	177	Total	C	N	O	S	0	0	0
			1359	857	243	258	1			
2	D	177	Total	C	N	O	S	0	0	0
			1359	857	243	258	1			

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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		

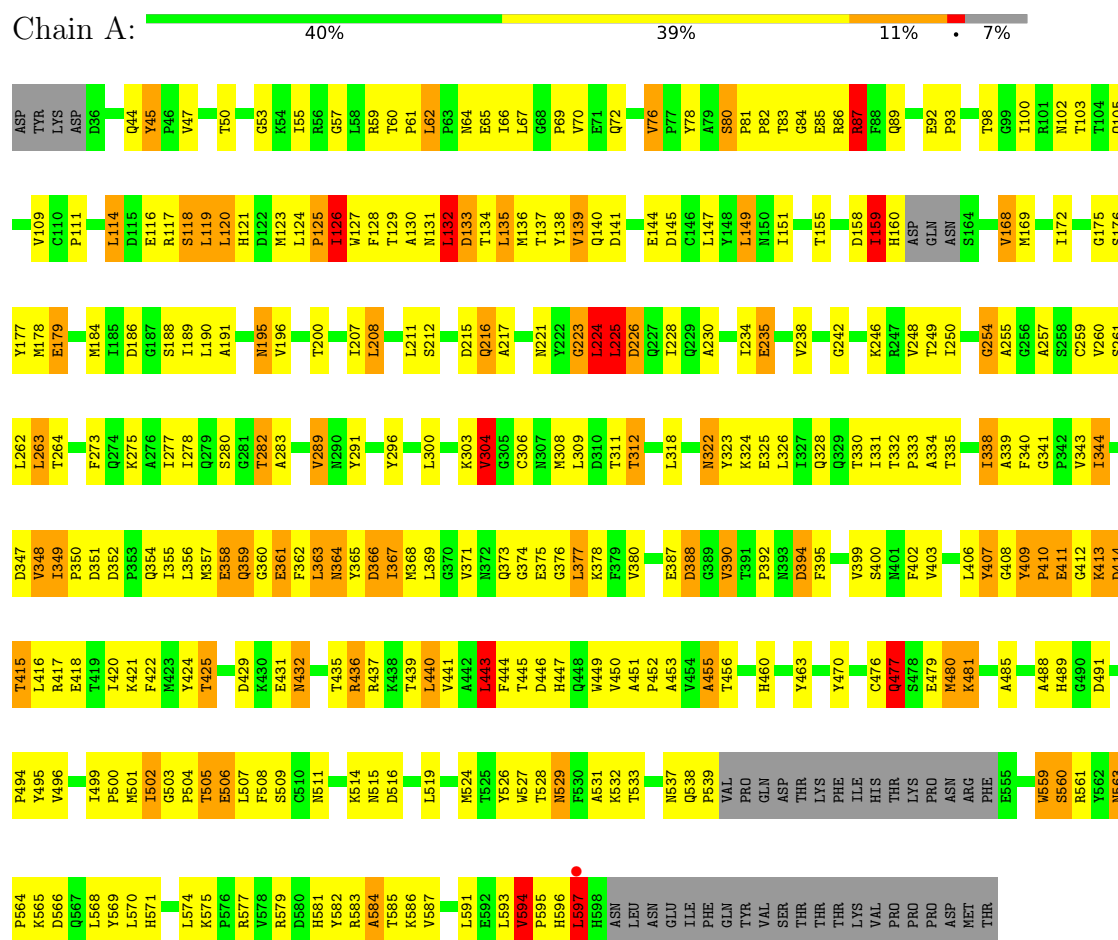
- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

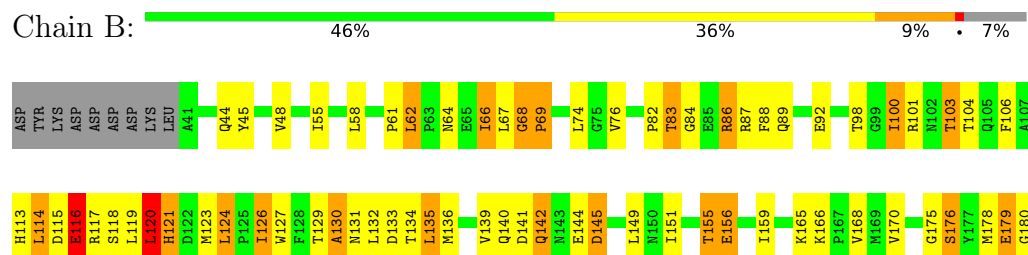
3 Residue-property plots

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: NEUROLIGIN 4, X-LINKED



• Molecule 1: NEUROLIGIN 4, X-LINKED





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	158.52Å 198.67Å 85.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.90 30.00 – 3.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (30.00-3.90) 99.2 (30.00-3.90)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.43 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.205 , 0.276 0.212 , 0.283	Depositor DCC
R_{free} test set	2178 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	92.0	Xtriage
Anisotropy	0.258	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 115.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	11360	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.35% 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: NAG, CA

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	0.70	1/4429 (0.0%)	0.95	8/6040 (0.1%)
1	B	0.68	0/4422	0.94	13/6033 (0.2%)
2	C	0.61	0/1384	0.82	0/1874
2	D	0.90	2/1384 (0.1%)	0.99	6/1874 (0.3%)
All	All	0.71	3/11619 (0.0%)	0.94	27/15821 (0.2%)

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
1	A	0	5
1	B	0	3
All	All	0	8

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	176	VAL	CA-CB	6.27	1.60	1.53
2	D	245	ILE	CA-CB	5.55	1.59	1.53
1	A	347	ASP	CA-C	5.47	1.55	1.52

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	503	GLY	CA-C-N	10.20	132.59	119.84
1	A	503	GLY	C-N-CA	10.20	132.59	119.84
1	A	563	ASN	CA-C-N	8.06	129.92	119.84
1	A	563	ASN	C-N-CA	8.06	129.92	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	236	ILE	N-CA-C	7.76	118.98	108.11

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	360	GLY	Peptide
1	A	410	PRO	Peptide
1	A	411	GLU	Peptide
1	A	537	ASN	Peptide
1	A	597	LEU	Peptide

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	4310	0	4133	283	0
1	B	4302	0	4122	225	0
2	C	1359	0	1346	73	0
2	D	1359	0	1346	90	0
3	A	28	0	26	8	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
All	All	11360	0	10973	651	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 29.

The worst 5 of 651 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:119:LEU:O	1:B:120:LEU:HD22	1.53	1.08
1:A:189:ILE:HD11	1:A:502:ILE:HD12	1.28	1.08
1:A:139:VAL:HG13	1:A:140:GLN:H	1.24	0.98
1:A:149:LEU:CD1	1:A:151:ILE:HD11	1.96	0.95
2:D:141:LEU:HD11	2:D:148:ILE:HG23	1.47	0.94

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	539/588 (92%)	388 (72%)	105 (20%)	46 (8%)	0	10
1	B	540/588 (92%)	419 (78%)	81 (15%)	40 (7%)	1	12
2	C	173/179 (97%)	142 (82%)	28 (16%)	3 (2%)	7	35
2	D	173/179 (97%)	125 (72%)	41 (24%)	7 (4%)	2	21
All	All	1425/1534 (93%)	1074 (75%)	255 (18%)	96 (7%)	1	14

5 of 96 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	84	GLY
1	A	87	ARG
1	A	118	SER
1	A	121	HIS
1	A	126	ILE

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	467/510 (92%)	390 (84%)	77 (16%)	2	13
1	B	466/510 (91%)	396 (85%)	70 (15%)	3	16
2	C	143/143 (100%)	120 (84%)	23 (16%)	2	14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	143/143 (100%)	128 (90%)	15 (10%)	6	25
All	All	1219/1306 (93%)	1034 (85%)	185 (15%)	3	16

5 of 185 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	304	VAL
1	B	578	VAL
1	B	332	THR
1	B	425	THR
2	C	108	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 39 such sidechains are listed below:

Mol	Chain	Res	Type
2	C	238	ASN
2	D	103	ASN
2	C	252	GLN
2	C	275	ASN
2	D	165	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	1599	-	14,14,15	0.40	0	17,19,21	1.09	0
3	NAG	A	1600	-	14,14,15	0.34	0	17,19,21	1.09	1 (5%)

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	1599	-	-	3/6/23/26	0/1/1/1
3	NAG	A	1600	-	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1600	NAG	C1-C2-N2	-2.86	105.93	110.43

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1599	NAG	C8-C7-N2-C2
3	A	1599	NAG	O7-C7-N2-C2
3	A	1600	NAG	C8-C7-N2-C2
3	A	1600	NAG	O7-C7-N2-C2
3	A	1599	NAG	O5-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1599	NAG	5	0
3	A	1600	NAG	3	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	D	1
2	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	200:ALA	C	231:GLY	N	2.80
1	C	200:ALA	C	231:GLY	N	2.75

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	A	545/588 (92%)	-0.59	1 (0%) 91 81	50, 72, 77, 86	0
1	B	544/588 (92%)	-0.45	0 100 100	63, 73, 78, 84	0
2	C	177/179 (98%)	-0.72	0 100 100	59, 72, 80, 83	0
2	D	177/179 (98%)	-0.25	3 (1%) 69 48	61, 76, 84, 86	0
All	All	1443/1534 (94%)	-0.52	4 (0%) 90 78	50, 73, 80, 86	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	176	VAL	3.3
2	D	89	PHE	3.0
1	A	597	LEU	2.4
2	D	94	GLY	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 oligosaccharides 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($\text{\AA}^2$)	Q<0.9
3	NAG	A	1599	14/15	0.84	0.06	221,222,224,225	0
3	NAG	A	1600	14/15	0.88	0.07	191,192,193,193	0
4	CA	C	1289	1/1	0.98	0.04	109,109,109,109	0
4	CA	D	1289	1/1	0.99	0.04	134,134,134,134	0

6.5 Other polymers [i](#)

There are no such residues in this entry.