



wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 6NS7 / pdb_00006ns7
Title : Crystal structure of murine caspase-11
Authors : Yang, J.; Liu, Z.; Xiao, T.S.
Deposited on : 2019-01-24
Resolution : 2.40 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

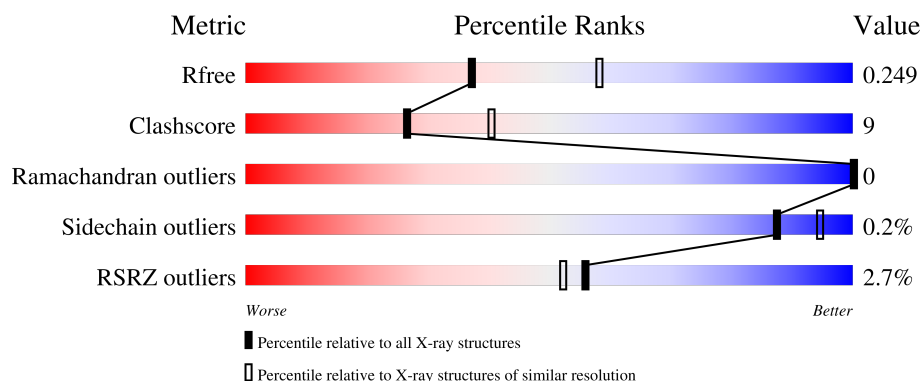
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (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 $\leq 5\%$. 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	284	 2% 69% 15% 14%
1	B	284	 2% 73% 12% 15%
1	C	284	 3% 66% 18% 15%
1	D	284	 3% 67% 18% 15%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7887 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 Caspase-11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	244	Total	C	N	O	S	0	0	0
			1952	1237	336	364	15			
1	B	242	Total	C	N	O	S	0	0	0
			1940	1231	334	360	15			
1	C	242	Total	C	N	O	S	0	0	0
			1940	1231	334	360	15			
1	D	241	Total	C	N	O	S	0	0	0
			1932	1227	332	358	15			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	90	GLY	-	expression tag	UNP P70343
A	91	SER	-	expression tag	UNP P70343
A	254	ALA	CYS	conflict	UNP P70343
B	90	GLY	-	expression tag	UNP P70343
B	91	SER	-	expression tag	UNP P70343
B	254	ALA	CYS	conflict	UNP P70343
C	90	GLY	-	expression tag	UNP P70343
C	91	SER	-	expression tag	UNP P70343
C	254	ALA	CYS	conflict	UNP P70343
D	90	GLY	-	expression tag	UNP P70343
D	91	SER	-	expression tag	UNP P70343
D	254	ALA	CYS	conflict	UNP P70343

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

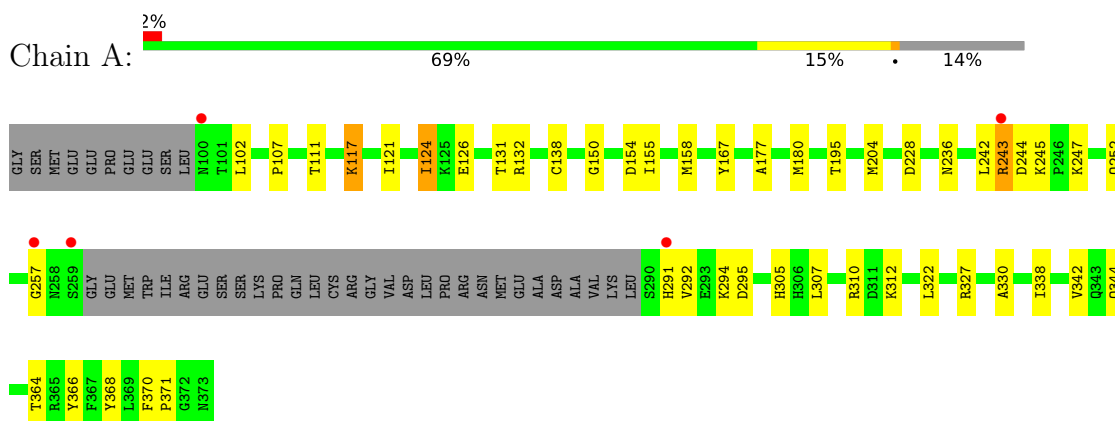
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	32	Total	O	0	0
			32	32		
3	B	39	Total	O	0	0
			39	39		
3	C	18	Total	O	0	0
			18	18		
3	D	14	Total	O	0	0
			14	14		

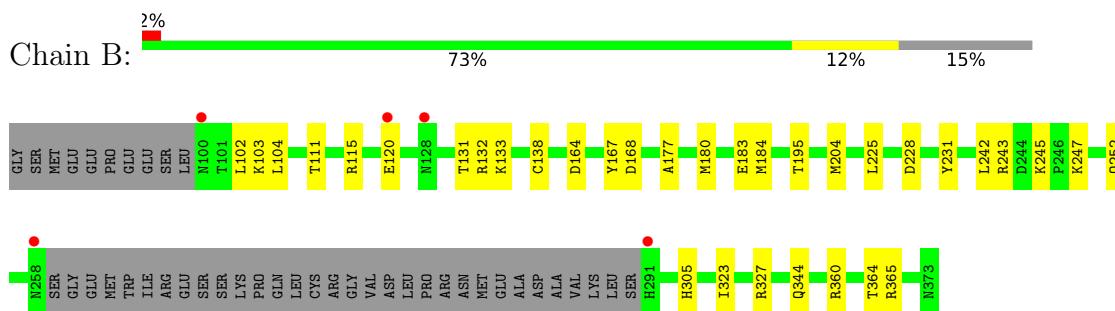
3 Residue-property plots [i](#)

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.

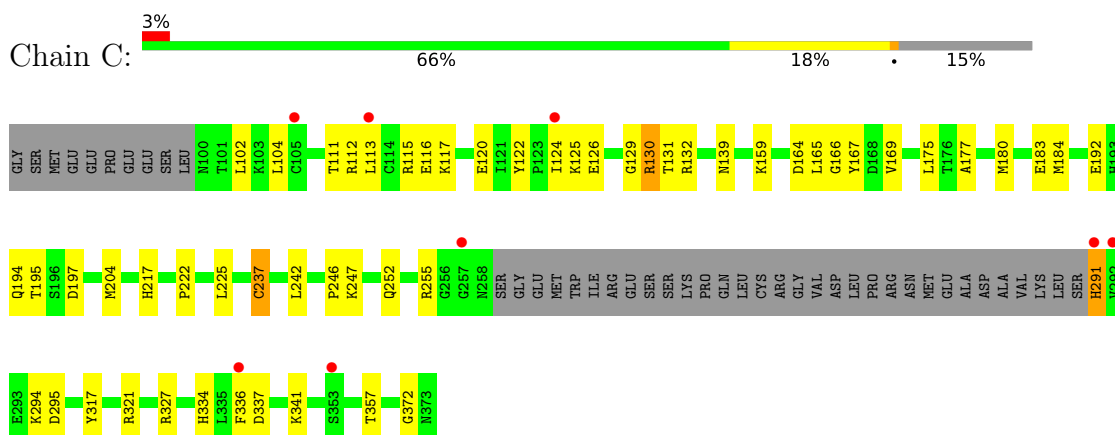
• Molecule 1: Caspase-11



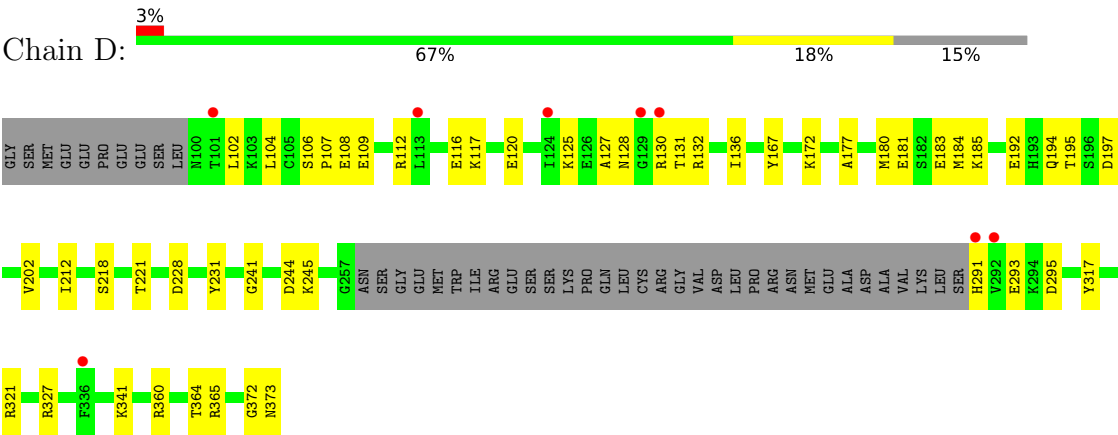
• Molecule 1: Caspase-11



• Molecule 1: Caspase-11



● Molecule 1: Caspase-11



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	120.71Å 121.09Å 78.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.93 – 2.40 47.93 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.9 (47.93-2.40) 99.8 (47.93-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.14 (at 2.39Å)	Xtriage
Refinement program	PHENIX (1.12_2829: ???)	Depositor
R, R_{free}	0.194 , 0.242 0.202 , 0.249	Depositor DCC
R_{free} test set	1993 reflections (4.36%)	wwPDB-VP
Wilson B-factor (Å ²)	52.0	Xtriage
Anisotropy	0.413	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 64.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.014 for k,h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7887	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 32.51 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 9.2864e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.46	0/1995	0.77	7/2686 (0.3%)
1	B	0.40	0/1983	0.69	0/2670
1	C	0.47	1/1983 (0.1%)	0.73	0/2670
1	D	0.47	0/1975	0.77	1/2659 (0.0%)
All	All	0.45	1/7936 (0.0%)	0.74	8/10685 (0.1%)

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	C	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	237	CYS	CA-CB	5.05	1.61	1.53

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	158	MET	CA-CB-CG	-7.13	99.84	114.10
1	A	126	GLU	CB-CA-C	6.82	122.09	109.54
1	A	126	GLU	CA-CB-CG	6.56	127.22	114.10
1	A	126	GLU	CB-CG-CD	6.41	123.50	112.60
1	A	117	LYS	CD-CE-NZ	-6.14	92.26	111.90

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	126	GLU	Peptide
1	C	291	HIS	Peptide

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	A	1952	0	1920	40	0
1	B	1940	0	1910	29	0
1	C	1940	0	1910	41	0
1	D	1932	0	1904	43	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
3	A	32	0	0	0	0
3	B	39	0	0	2	0
3	C	18	0	0	2	0
3	D	14	0	0	1	0
All	All	7887	0	7644	144	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 9.

The worst 5 of 144 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:D:125:LYS:O	1:D:130:ARG:NH1	2.06	0.89
1:D:131:THR:OG1	1:D:195:THR:HG23	1.72	0.89
1:D:228:ASP:OD1	1:D:360:ARG:NH2	2.13	0.82
1:C:130:ARG:NH1	3:C:501:HOH:O	2.11	0.82
1:B:102:LEU:HD12	1:B:327:ARG:HA	1.65	0.78

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	240/284 (84%)	230 (96%)	10 (4%)	0	100	100
1	B	238/284 (84%)	230 (97%)	8 (3%)	0	100	100
1	C	238/284 (84%)	228 (96%)	10 (4%)	0	100	100
1	D	237/284 (84%)	227 (96%)	10 (4%)	0	100	100
All	All	953/1136 (84%)	915 (96%)	38 (4%)	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	217/252 (86%)	217 (100%)	0	100	100
1	B	215/252 (85%)	215 (100%)	0	100	100
1	C	215/252 (85%)	214 (100%)	1 (0%)	81	91
1	D	214/252 (85%)	213 (100%)	1 (0%)	81	91
All	All	861/1008 (85%)	859 (100%)	2 (0%)	87	94

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	130	ARG
1	D	212	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	152	ASN
1	C	329	HIS
1	D	373	ASN
1	D	152	ASN
1	D	329	HIS

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](#)

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	$\# Z > 2$
2	SO4	D	401	-	4,4,4	0.31	0	6,6,6	0.29	0
2	SO4	C	401	-	4,4,4	0.26	0	6,6,6	0.27	0
2	SO4	B	401	-	4,4,4	0.31	0	6,6,6	0.24	0
2	SO4	A	401	-	4,4,4	0.34	0	6,6,6	0.42	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 [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	244/284 (85%)	-0.10	5 (2%) 65 60	37, 59, 92, 120	0
1	B	242/284 (85%)	-0.21	5 (2%) 63 59	35, 58, 91, 117	0
1	C	242/284 (85%)	0.13	8 (3%) 49 45	43, 70, 121, 157	0
1	D	241/284 (84%)	0.26	8 (3%) 49 45	42, 79, 136, 163	0
All	All	969/1136 (85%)	0.02	26 (2%) 56 52	35, 65, 112, 163	0

The worst 5 of 26 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	113	LEU	4.7
1	C	291	HIS	3.4
1	D	291	HIS	3.3
1	C	113	LEU	3.0
1	A	257	GLY	3.0

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
2	SO4	A	401	5/5	0.96	0.08	56,58,66,67	0
2	SO4	C	401	5/5	0.96	0.07	56,57,60,66	0
2	SO4	B	401	5/5	0.97	0.07	47,52,65,68	0
2	SO4	D	401	5/5	0.97	0.06	48,63,66,68	0

6.5 Other polymers [i](#)

There are no such residues in this entry.