



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 6DHV / pdb_00006dhv
Title : Structure of Arabidopsis Fatty Acid Amide Hydrolase
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Deposited on : 2018-05-21
Resolution : 2.10 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 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
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

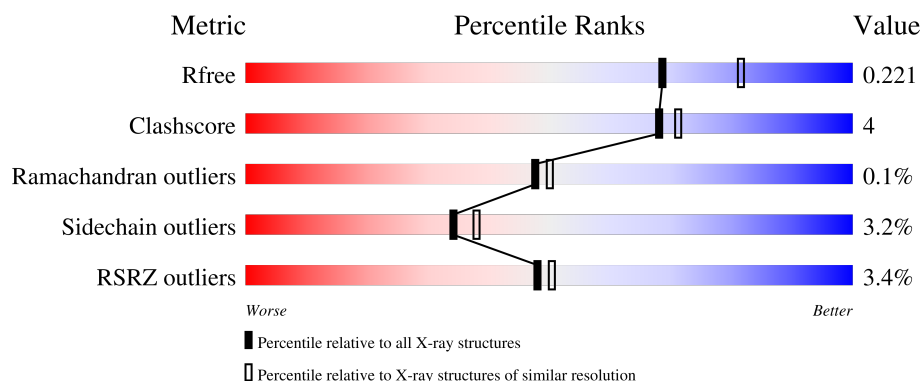
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	636	
1	B	636	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9537 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 Fatty acid amide hydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	594	Total	C	N	O	S	0	0	0
			4549	2887	768	871	23			
1	B	597	Total	C	N	O	S	0	0	0
			4570	2900	772	874	24			

There are 58 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	608	LYS	-	expression tag	UNP Q7XJJ7
A	609	GLY	-	expression tag	UNP Q7XJJ7
A	610	GLU	-	expression tag	UNP Q7XJJ7
A	611	PHE	-	expression tag	UNP Q7XJJ7
A	612	GLU	-	expression tag	UNP Q7XJJ7
A	613	ALA	-	expression tag	UNP Q7XJJ7
A	614	TYR	-	expression tag	UNP Q7XJJ7
A	615	VAL	-	expression tag	UNP Q7XJJ7
A	616	GLU	-	expression tag	UNP Q7XJJ7
A	617	GLN	-	expression tag	UNP Q7XJJ7
A	618	LYS	-	expression tag	UNP Q7XJJ7
A	619	LEU	-	expression tag	UNP Q7XJJ7
A	620	ILE	-	expression tag	UNP Q7XJJ7
A	621	SER	-	expression tag	UNP Q7XJJ7
A	622	GLU	-	expression tag	UNP Q7XJJ7
A	623	GLU	-	expression tag	UNP Q7XJJ7
A	624	ASP	-	expression tag	UNP Q7XJJ7
A	625	LEU	-	expression tag	UNP Q7XJJ7
A	626	ASN	-	expression tag	UNP Q7XJJ7
A	627	SER	-	expression tag	UNP Q7XJJ7
A	628	ALA	-	expression tag	UNP Q7XJJ7
A	629	VAL	-	expression tag	UNP Q7XJJ7
A	630	ASP	-	expression tag	UNP Q7XJJ7
A	631	HIS	-	expression tag	UNP Q7XJJ7
A	632	HIS	-	expression tag	UNP Q7XJJ7

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Chain	Residue	Modelled	Actual	Comment	Reference
A	633	HIS	-	expression tag	UNP Q7XJJ7
A	634	HIS	-	expression tag	UNP Q7XJJ7
A	635	HIS	-	expression tag	UNP Q7XJJ7
A	636	HIS	-	expression tag	UNP Q7XJJ7
B	608	LYS	-	expression tag	UNP Q7XJJ7
B	609	GLY	-	expression tag	UNP Q7XJJ7
B	610	GLU	-	expression tag	UNP Q7XJJ7
B	611	PHE	-	expression tag	UNP Q7XJJ7
B	612	GLU	-	expression tag	UNP Q7XJJ7
B	613	ALA	-	expression tag	UNP Q7XJJ7
B	614	TYR	-	expression tag	UNP Q7XJJ7
B	615	VAL	-	expression tag	UNP Q7XJJ7
B	616	GLU	-	expression tag	UNP Q7XJJ7
B	617	GLN	-	expression tag	UNP Q7XJJ7
B	618	LYS	-	expression tag	UNP Q7XJJ7
B	619	LEU	-	expression tag	UNP Q7XJJ7
B	620	ILE	-	expression tag	UNP Q7XJJ7
B	621	SER	-	expression tag	UNP Q7XJJ7
B	622	GLU	-	expression tag	UNP Q7XJJ7
B	623	GLU	-	expression tag	UNP Q7XJJ7
B	624	ASP	-	expression tag	UNP Q7XJJ7
B	625	LEU	-	expression tag	UNP Q7XJJ7
B	626	ASN	-	expression tag	UNP Q7XJJ7
B	627	SER	-	expression tag	UNP Q7XJJ7
B	628	ALA	-	expression tag	UNP Q7XJJ7
B	629	VAL	-	expression tag	UNP Q7XJJ7
B	630	ASP	-	expression tag	UNP Q7XJJ7
B	631	HIS	-	expression tag	UNP Q7XJJ7
B	632	HIS	-	expression tag	UNP Q7XJJ7
B	633	HIS	-	expression tag	UNP Q7XJJ7
B	634	HIS	-	expression tag	UNP Q7XJJ7
B	635	HIS	-	expression tag	UNP Q7XJJ7
B	636	HIS	-	expression tag	UNP Q7XJJ7

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	207	Total O 207 207	0	0
2	B	211	Total O 211 211	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	72.08Å 79.66Å 132.59Å 90.00° 104.44° 90.00°	Depositor
Resolution (Å)	33.00 – 2.10 33.00 – 2.10	Depositor EDS
% Data completeness (in resolution range)	98.5 (33.00-2.10) 98.4 (33.00-2.10)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.76 (at 2.10Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.192 , 0.220 0.193 , 0.221	Depositor DCC
R_{free} test set	4315 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	44.8	Xtriage
Anisotropy	0.077	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 51.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.021 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	9537	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.48% 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](#)

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	0.38	0/4645	0.44	1/6307 (0.0%)
1	B	0.52	1/4666 (0.0%)	0.50	5/6333 (0.1%)
All	All	0.46	1/9311 (0.0%)	0.47	6/12640 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	308	ILE	C-O	-6.73	1.18	1.24

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	543	LEU	N-CA-C	7.14	119.15	111.36
1	B	542	VAL	N-CA-C	6.23	120.88	113.22
1	A	25	MET	N-CA-C	-5.59	101.57	109.96
1	B	306	VAL	N-CA-C	-5.37	107.55	111.90
1	B	357	ILE	N-CA-C	5.16	119.67	112.50
1	B	358	LEU	N-CA-C	5.07	117.07	110.43

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	A	4549	0	4573	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	4570	0	4601	37	0
2	A	207	0	0	0	0
2	B	211	0	0	2	0
All	All	9537	0	9174	65	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 (65) 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:A:9:ARG:O	1:A:13:VAL:HG23	1.87	0.75
1:B:438:ARG:NH1	2:B:701:HOH:O	2.23	0.68
1:B:144:THR:HG23	1:B:147:GLN:H	1.59	0.68
1:A:603:ILE:HG22	1:A:604:LEU:N	2.10	0.67
1:B:23:GLU:OE2	1:B:23:GLU:HA	1.96	0.66
1:A:603:ILE:O	1:A:604:LEU:HB2	1.96	0.66
1:A:144:THR:HG23	1:A:147:GLN:H	1.63	0.64
1:A:406:ASP:OD2	1:A:561:LYS:HD2	2.00	0.61
1:B:29:HIS:NE2	1:B:529:GLU:OE1	2.32	0.60
1:A:417:LEU:HB3	1:A:590:LEU:HD13	1.85	0.58
1:B:324:ARG:HD3	2:B:846:HOH:O	2.03	0.58
1:A:171:ARG:HB2	1:A:248:LYS:HB2	1.86	0.57
1:B:140:SER:HB2	1:B:142:LEU:HD12	1.86	0.57
1:A:6:VAL:HG23	1:A:68:THR:HG23	1.86	0.56
1:B:92:VAL:HG22	1:B:373:PRO:HG2	1.86	0.56
1:A:603:ILE:CG2	1:A:604:LEU:N	2.73	0.51
1:A:148:VAL:HG13	1:A:603:ILE:HG21	1.92	0.51
1:A:144:THR:HG22	1:A:147:GLN:HB2	1.93	0.50
1:B:563:GLY:O	1:B:595:LYS:NZ	2.41	0.50
1:B:14:ASP:OD2	1:B:16:SER:OG	2.23	0.50
1:A:603:ILE:HG22	1:A:604:LEU:H	1.74	0.50
1:A:603:ILE:N	1:A:603:ILE:HD12	2.26	0.50
1:A:5:GLN:HE21	1:A:7:MET:HE1	1.79	0.48
1:A:495:MET:HE3	1:A:499:LEU:HD21	1.96	0.48
1:B:9:ARG:O	1:B:493:ARG:NH2	2.45	0.48
1:B:23:GLU:HG3	1:B:540:ARG:HH21	1.78	0.48
1:B:90:VAL:HG11	1:B:108:CYS:SG	2.54	0.47
1:B:539:MET:HE2	1:B:543:LEU:HD21	1.97	0.47
1:B:110:PRO:HD3	1:B:378:LEU:O	2.15	0.46
1:A:603:ILE:CG2	1:A:604:LEU:H	2.28	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:HIS:CE1	1:A:257:GLY:HA3	2.50	0.46
1:B:9:ARG:CA	1:B:493:ARG:HH12	2.29	0.46
1:B:23:GLU:OE1	1:B:536:THR:HG23	2.15	0.45
1:B:131:ILE:HG23	1:B:200:ILE:HG12	1.97	0.45
1:A:113:ASP:O	1:A:115:SER:N	2.44	0.45
1:B:14:ASP:O	1:B:17:THR:HG22	2.15	0.45
1:A:146:LEU:HG	1:A:150:LYS:HE2	1.98	0.45
1:B:381:HIS:HA	1:B:382:ASN:HA	1.68	0.45
1:A:281:SER:H	1:A:305:SER:HB3	1.80	0.45
1:B:23:GLU:CG	1:B:540:ARG:HH21	2.30	0.44
1:B:90:VAL:HG13	1:B:375:PHE:HB2	2.00	0.44
1:B:137:ALA:HB1	1:B:143:THR:HG22	2.00	0.44
1:B:203:THR:CG2	1:B:249:ALA:HB2	2.48	0.44
1:B:358:LEU:C	1:B:358:LEU:HD12	2.43	0.44
1:B:201:PHE:O	1:B:294:CYS:HB2	2.17	0.44
1:A:137:ALA:HB1	1:A:143:THR:HG22	2.00	0.43
1:A:369:LYS:HE2	1:A:369:LYS:HB2	1.67	0.43
1:A:491:ARG:HG3	1:A:547:LEU:HG	2.01	0.43
1:B:281:SER:H	1:B:305:SER:HB3	1.83	0.43
1:B:148:VAL:HG13	1:B:603:ILE:HG21	2.00	0.42
1:B:382:ASN:HA	1:B:383:GLY:HA3	1.74	0.42
1:A:397:LYS:HZ2	1:A:397:LYS:H	1.66	0.42
1:A:8:LYS:HD2	1:A:68:THR:CG2	2.50	0.42
1:B:27:ALA:HA	1:B:28:PRO:HD3	1.84	0.42
1:B:153:ILE:HD13	1:B:174:ALA:HB1	2.02	0.42
1:B:491:ARG:HG3	1:B:547:LEU:HG	2.01	0.42
1:A:417:LEU:HD12	1:A:417:LEU:HA	1.92	0.41
1:B:258:THR:O	1:B:280:GLY:N	2.52	0.41
1:A:176:GLU:O	1:A:180:GLN:HG3	2.19	0.41
1:B:39:VAL:HG21	1:B:467:TYR:HB3	2.02	0.41
1:B:173:ASP:O	1:B:177:VAL:HG23	2.21	0.41
1:A:293:LEU:HD23	1:A:293:LEU:HA	1.92	0.40
1:B:23:GLU:OE1	1:B:536:THR:CG2	2.69	0.40
1:B:1:MET:C	1:B:3:LYS:H	2.28	0.40
1:B:8:LYS:HD2	1:B:68:THR:HG21	2.02	0.40

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	590/636 (93%)	575 (98%)	15 (2%)	0	100	100
1	B	593/636 (93%)	571 (96%)	21 (4%)	1 (0%)	43	44
All	All	1183/1272 (93%)	1146 (97%)	36 (3%)	1 (0%)	48	50

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	2	GLY

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	503/540 (93%)	487 (97%)	16 (3%)	34	38
1	B	505/540 (94%)	489 (97%)	16 (3%)	34	38
All	All	1008/1080 (93%)	976 (97%)	32 (3%)	34	38

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	GLN
1	A	7	MET
1	A	8	LYS
1	A	33	LEU
1	A	37	LEU

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Mol	Chain	Res	Type
1	A	46	LEU
1	A	49	SER
1	A	127	ARG
1	A	182	GLU
1	A	305	SER
1	A	369	LYS
1	A	381	HIS
1	A	397	LYS
1	A	412	GLU
1	A	417	LEU
1	A	580	VAL
1	B	1	MET
1	B	4	TYR
1	B	5	GLN
1	B	9	ARG
1	B	33	LEU
1	B	90	VAL
1	B	92	VAL
1	B	116	ARG
1	B	127	ARG
1	B	142	LEU
1	B	151	ARG
1	B	178	ILE
1	B	381	HIS
1	B	384	SER
1	B	412	GLU
1	B	453	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	ASN
1	A	192	ASN
1	A	213	HIS
1	B	213	HIS
1	B	421	ASN
1	B	533	GLN
1	B	605	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](#)

There are no ligands in this entry.

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

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	594/636 (93%)	0.19	16 (2%) 56 59	32, 54, 87, 116	0
1	B	597/636 (93%)	0.24	24 (4%) 42 44	33, 57, 94, 128	0
All	All	1191/1272 (93%)	0.21	40 (3%) 48 50	32, 56, 91, 128	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	7	MET	5.5
1	A	7	MET	4.6
1	B	3	LYS	4.4
1	B	4	TYR	4.3
1	B	2	GLY	4.2
1	B	1	MET	4.0
1	B	603	ILE	3.9
1	B	9	ARG	3.6
1	B	6	VAL	3.6
1	B	384	SER	3.3
1	A	93	GLY	3.3
1	A	381	HIS	3.2
1	B	24	THR	3.1
1	B	25	MET	3.1
1	A	9	ARG	3.0
1	A	24	THR	3.0
1	A	116	ARG	3.0
1	B	22	ALA	2.9
1	A	4	TYR	2.9
1	A	384	SER	2.8
1	A	45	PRO	2.7
1	B	5	GLN	2.6
1	B	385	ASN	2.5
1	B	383	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	6	VAL	2.4
1	A	22	ALA	2.3
1	A	413	ASP	2.3
1	B	47	ILE	2.3
1	B	10	ALA	2.3
1	B	381	HIS	2.3
1	B	531	ASN	2.3
1	B	594	THR	2.2
1	A	379	LEU	2.2
1	B	522	PRO	2.1
1	A	46	LEU	2.1
1	A	25	MET	2.1
1	B	27	ALA	2.1
1	A	8	LYS	2.1
1	B	532	ILE	2.1
1	B	8	LYS	2.1

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.