



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:56 AM UTC

PDB ID : 6LBI / pdb_00006lbi
Title : Crystal Structure of FOXO1-DBD homodimer bound to a palindromic DNA sequence
Authors : Li, J.; Dai, S.Y.; Chen, Y.H.
Deposited on : 2019-11-14
Resolution : 3.07 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

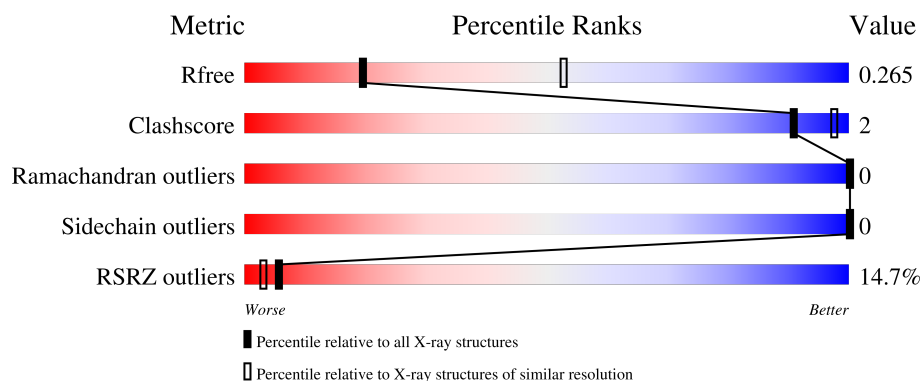
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.07 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	2469 (3.10-3.02)
Clashscore	190562	2569 (3.10-3.02)
Ramachandran outliers	187476	2424 (3.10-3.02)
Sidechain outliers	187428	2423 (3.10-3.02)
RSRZ outliers	180081	2469 (3.10-3.02)

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	20	90% 10%
1	B	20	90% 10%
1	E	20	10% 90% 10%
1	F	20	100%
1	I	20	15% 90% 10%

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Mol	Chain	Length	Quality of chain
1	J	20	
2	C	118	
2	D	118	
2	G	118	
2	H	118	
2	K	118	
2	L	118	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6172 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 DNA chain called IRE0.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	20	Total	C	N	O	P	0	0	0
			407	196	74	118	19			
1	B	20	Total	C	N	O	P	0	0	0
			407	196	74	118	19			
1	E	20	Total	C	N	O	P	0	0	0
			407	196	74	118	19			
1	F	20	Total	C	N	O	P	0	0	0
			407	196	74	118	19			
1	I	20	Total	C	N	O	P	0	0	0
			407	196	74	118	19			
1	J	20	Total	C	N	O	P	0	0	0
			407	196	74	118	19			

- Molecule 2 is a protein called Forkhead box protein O1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	84	Total	C	N	O	S	0	0	0
			644	411	108	123	2			
2	D	81	Total	C	N	O	S	0	0	0
			634	405	110	117	2			
2	G	83	Total	C	N	O	S	0	0	0
			648	412	111	123	2			
2	H	74	Total	C	N	O	S	0	0	0
			587	379	102	104	2			
2	K	80	Total	C	N	O	S	0	0	0
			611	389	105	116	1			
2	L	76	Total	C	N	O	S	0	0	0
			606	390	105	109	2			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	148	GLY	-	expression tag	UNP Q12778

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Chain	Residue	Modelled	Actual	Comment	Reference
C	149	PRO	-	expression tag	UNP Q12778
C	150	SER	-	expression tag	UNP Q12778
D	148	GLY	-	expression tag	UNP Q12778
D	149	PRO	-	expression tag	UNP Q12778
D	150	SER	-	expression tag	UNP Q12778
G	148	GLY	-	expression tag	UNP Q12778
G	149	PRO	-	expression tag	UNP Q12778
G	150	SER	-	expression tag	UNP Q12778
H	148	GLY	-	expression tag	UNP Q12778
H	149	PRO	-	expression tag	UNP Q12778
H	150	SER	-	expression tag	UNP Q12778
K	148	GLY	-	expression tag	UNP Q12778
K	149	PRO	-	expression tag	UNP Q12778
K	150	SER	-	expression tag	UNP Q12778
L	148	GLY	-	expression tag	UNP Q12778
L	149	PRO	-	expression tag	UNP Q12778
L	150	SER	-	expression tag	UNP Q12778

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: IRE0

Chain A: 



- Molecule 1: IRE0

Chain B: 

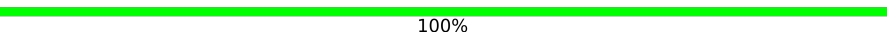


- Molecule 1: IRE0

Chain E: 



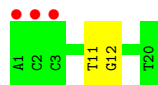
- Molecule 1: IRE0

Chain F: 

There are no outlier residues recorded for this chain.

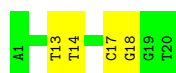
- Molecule 1: IRE0

Chain I: 

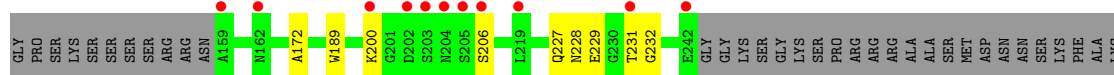


- Molecule 1: IRE0

Chain J: 



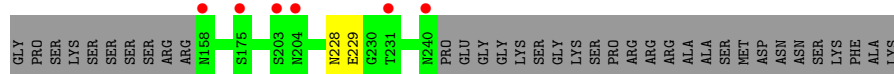
- Molecule 2: Forkhead box protein O1



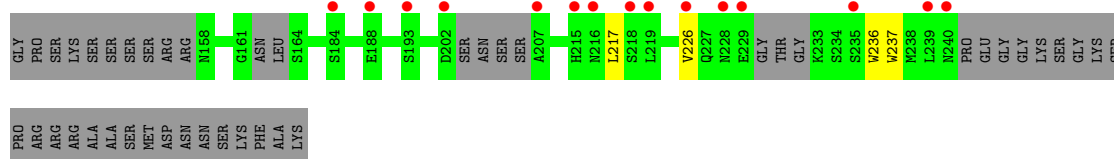
- Molecule 2: Forkhead box protein O1



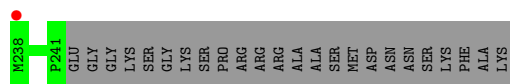
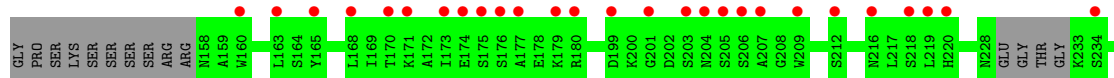
- Molecule 2: Forkhead box protein O1



- Molecule 2: Forkhead box protein O1

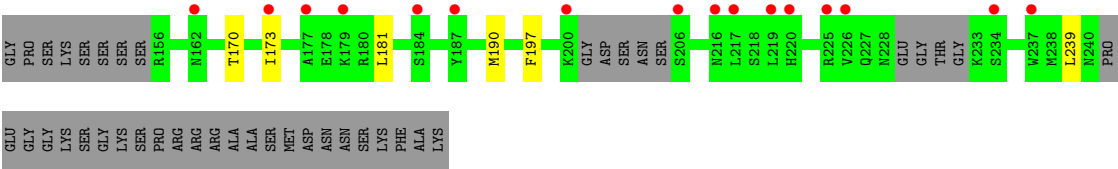


- Molecule 2: Forkhead box protein O1



- Molecule 2: Forkhead box protein O1





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	67.73Å 89.09Å 194.17Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.79 – 3.07 46.79 – 3.07	Depositor EDS
% Data completeness (in resolution range)	76.1 (46.79-3.07) 76.4 (46.79-3.07)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	12.45 (at 3.06Å)	Xtriage
Refinement program	PHENIX 1.11.1 _2575	Depositor
R, R_{free}	0.227 , 0.264 0.230 , 0.265	Depositor DCC
R_{free} test set	873 reflections (3.81%)	wwPDB-VP
Wilson B-factor (Å ²)	26.6	Xtriage
Anisotropy	0.512	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 60.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	6172	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.00% 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	0.20	0/456	0.38	0/702
1	B	0.19	0/456	0.38	0/702
1	E	0.19	0/456	0.38	0/702
1	F	0.20	0/456	0.38	0/702
1	I	0.19	0/456	0.39	0/702
1	J	0.19	0/456	0.38	0/702
2	C	0.07	0/662	0.22	0/902
2	D	0.08	0/651	0.23	0/883
2	G	0.07	0/665	0.19	0/902
2	H	0.07	0/601	0.23	0/811
2	K	0.09	0/628	0.22	0/858
2	L	0.10	0/621	0.24	0/841
All	All	0.14	0/6564	0.30	0/9409

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	A	407	0	228	1	0
1	B	407	0	228	1	0
1	E	407	0	228	1	0
1	F	407	0	228	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	I	407	0	228	1	0
1	J	407	0	228	2	0
2	C	644	0	586	5	0
2	D	634	0	591	2	0
2	G	648	0	602	1	0
2	H	587	0	550	2	0
2	K	611	0	541	0	0
2	L	606	0	567	4	0
All	All	6172	0	4805	19	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 2.

All (19) 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:200:LYS:O	2:C:206:SER:OG	2.22	0.58
2:L:170:THR:HG23	2:L:239:LEU:HD21	1.88	0.56
2:L:190:MET:HB3	2:L:197:PHE:CD2	2.41	0.55
2:C:231:THR:HG23	2:C:232:GLY:H	1.72	0.54
1:I:11:DT:H2''	1:I:12:DG:H5''	1.89	0.53
2:C:228:ASN:OD1	2:C:229:GLU:N	2.39	0.53
1:J:17:DC:H2''	1:J:18:DG:C8	2.45	0.52
2:H:217:LEU:HB3	2:H:237:TRP:CZ3	2.49	0.48
2:L:190:MET:HB3	2:L:197:PHE:HD2	1.76	0.47
2:H:226:VAL:HB	2:H:236:TRP:HB2	1.95	0.47
1:E:11:DT:H2''	1:E:12:DG:H5''	1.96	0.47
1:A:11:DT:H2''	1:A:12:DG:H5''	2.01	0.43
2:D:196:TYR:O	2:D:200:LYS:NZ	2.36	0.43
2:C:227:GLN:HB2	2:D:227:GLN:HB2	2.00	0.42
1:J:13:DT:H2''	1:J:14:DT:H5''	2.00	0.42
2:G:228:ASN:OD1	2:G:229:GLU:N	2.52	0.42
1:B:17:DC:H2''	1:B:18:DG:C8	2.56	0.41
2:L:173:ILE:HD13	2:L:181:LEU:HD12	2.02	0.41
2:C:172:ALA:HB2	2:C:189:TRP:CE3	2.56	0.41

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	
2	C	82/118 (70%)	77 (94%)	5 (6%)	0	100	100
2	D	77/118 (65%)	74 (96%)	3 (4%)	0	100	100
2	G	81/118 (69%)	76 (94%)	5 (6%)	0	100	100
2	H	66/118 (56%)	61 (92%)	5 (8%)	0	100	100
2	K	76/118 (64%)	72 (95%)	4 (5%)	0	100	100
2	L	70/118 (59%)	68 (97%)	2 (3%)	0	100	100
All	All	452/708 (64%)	428 (95%)	24 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	
2	C	65/101 (64%)	65 (100%)	0	100	100
2	D	65/101 (64%)	65 (100%)	0	100	100
2	G	67/101 (66%)	67 (100%)	0	100	100
2	H	59/101 (58%)	59 (100%)	0	100	100
2	K	61/101 (60%)	61 (100%)	0	100	100
2	L	62/101 (61%)	62 (100%)	0	100	100
All	All	379/606 (62%)	379 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	D	162	ASN
2	L	158	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	20/20 (100%)	0.50	0	100 100	16, 24, 47, 53	0
1	B	20/20 (100%)	0.32	0	100 100	11, 24, 53, 54	0
1	E	20/20 (100%)	1.10	2 (10%)	12 6	30, 49, 59, 61	0
1	F	20/20 (100%)	0.81	0	100 100	31, 38, 62, 63	0
1	I	20/20 (100%)	0.93	3 (15%)	5 3	36, 44, 62, 67	0
1	J	20/20 (100%)	0.70	0	100 100	30, 42, 55, 55	0
2	C	84/118 (71%)	0.82	11 (13%)	7 4	12, 33, 74, 82	0
2	D	81/118 (68%)	0.88	7 (8%)	16 9	15, 32, 69, 78	0
2	G	83/118 (70%)	0.90	6 (7%)	21 11	16, 34, 67, 74	0
2	H	74/118 (62%)	1.46	15 (20%)	3 1	31, 52, 68, 82	0
2	K	80/118 (67%)	1.81	28 (35%)	1 0	26, 65, 81, 95	0
2	L	76/118 (64%)	1.28	16 (21%)	2 1	26, 54, 70, 80	0
All	All	598/828 (72%)	1.09	88 (14%)	6 3	11, 45, 74, 95	0

All (88) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	K	219	LEU	7.3
2	K	203	SER	5.0
2	K	205	SER	4.5
2	H	219	LEU	4.5
2	D	232	GLY	4.4
2	K	204	ASN	4.4
2	L	216	ASN	4.4
2	H	218	SER	4.2
2	K	220	HIS	4.0
2	G	158	ASN	4.0
2	L	200	LYS	3.9

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Mol	Chain	Res	Type	RSRZ
2	C	242	GLU	3.8
2	L	162	ASN	3.8
2	H	216	ASN	3.8
2	H	207	ALA	3.6
2	L	237	TRP	3.6
2	K	199	ASP	3.4
2	C	159	ALA	3.4
2	C	200	LYS	3.4
2	G	204	ASN	3.3
2	H	240	ASN	3.3
2	D	160	TRP	3.2
2	L	225	ARG	3.2
2	K	176	SER	3.2
2	L	184	SER	3.1
1	I	1	DA	3.1
2	H	228	ASN	3.1
2	D	177	ALA	3.1
2	H	229	GLU	3.1
2	G	175	SER	3.0
2	L	173	ILE	3.0
2	D	231	THR	2.9
2	D	211	ASN	2.9
2	G	203	SER	2.8
2	G	231	THR	2.8
2	C	206	SER	2.8
2	K	238	MET	2.8
2	C	203	SER	2.8
2	H	202	ASP	2.8
2	L	219	LEU	2.8
2	K	179	LYS	2.7
2	K	174	GLU	2.7
2	D	162	ASN	2.7
2	G	240	ASN	2.7
2	C	219	LEU	2.7
2	C	204	ASN	2.7
2	K	160	TRP	2.7
2	K	218	SER	2.7
2	D	161	GLY	2.6
2	K	177	ALA	2.6
2	H	215	HIS	2.6
2	K	165	TYR	2.5
2	K	175	SER	2.5

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Mol	Chain	Res	Type	RSRZ
2	H	193	SER	2.5
2	C	231	THR	2.5
2	H	235	SER	2.4
2	K	170	THR	2.4
2	K	180	ARG	2.4
1	E	10	DA	2.4
2	L	177	ALA	2.4
2	H	188	GLU	2.4
2	K	216	ASN	2.4
2	K	171	LYS	2.4
2	C	162	ASN	2.3
2	L	234	SER	2.3
2	K	201	GLY	2.3
2	C	205	SER	2.3
2	L	187	TYR	2.3
2	L	179	LYS	2.3
2	L	220	HIS	2.2
2	H	184	SER	2.2
2	L	217	LEU	2.2
2	K	212	SER	2.2
2	C	202	ASP	2.1
2	L	226	VAL	2.1
2	K	207	ALA	2.1
2	K	173	ILE	2.1
2	K	206	SER	2.1
2	H	239	LEU	2.1
2	L	206	SER	2.0
2	K	163	LEU	2.0
2	K	209	TRP	2.0
2	K	168	LEU	2.0
2	K	234	SER	2.0
1	E	1	DA	2.0
1	I	2	DC	2.0
1	I	3	DC	2.0
2	H	226	VAL	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 [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.