Full wwPDB X-ray Structure Validation Report ⓘ

Nov 15, 2023 – 12:50 AM JST

PDB ID	:	6IPA
Title	:	C-terminal EMAP II-like domain of p43 refined against twinned data
Authors	:	Manickam, Y.; Harlos, K.; Gupta, S.; Sharma, A.
Deposited on	:	2018-11-02
Resolution	:	2.47 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:

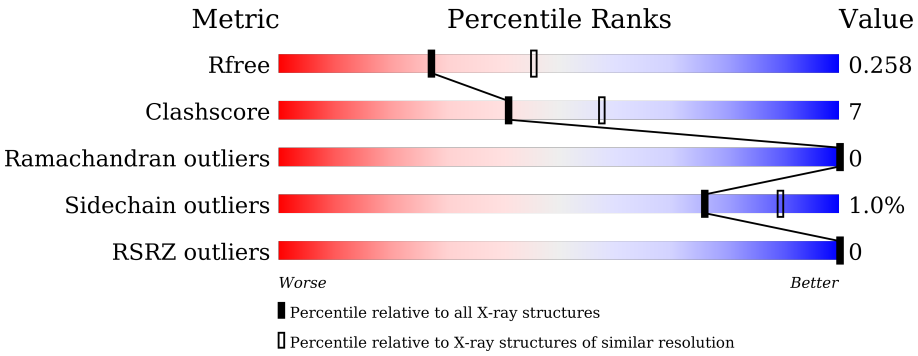
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.47 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}	130704	5857 (2.50-2.46)
Clashscore	141614	6594 (2.50-2.46)
Ramachandran outliers	138981	6469 (2.50-2.46)
Sidechain outliers	138945	6471 (2.50-2.46)
RSRZ outliers	127900	5738 (2.50-2.46)

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 <=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	204	70% 10% 19%
1	B	204	65% 16% 19%
1	C	204	68% 12% 19%
1	D	204	66% 15% 19%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 5342 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 aminoacyl-tRNA synthetase-interacting multifunctional protein p43.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	165	Total	C	N	O	S	0	0	0
			1295	820	221	247	7			
1	B	165	Total	C	N	O	S	0	0	0
			1301	823	224	247	7			
1	C	165	Total	C	N	O	S	0	0	0
			1301	823	224	247	7			
1	D	165	Total	C	N	O	S	0	0	0
			1301	823	224	247	7			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	202	GLY	-	expression tag	UNP A0A1G4HHT8
A	203	ALA	-	expression tag	UNP A0A1G4HHT8
A	204	MET	-	expression tag	UNP A0A1G4HHT8
A	205	ALA	-	expression tag	UNP A0A1G4HHT8
B	202	GLY	-	expression tag	UNP A0A1G4HHT8
B	203	ALA	-	expression tag	UNP A0A1G4HHT8
B	204	MET	-	expression tag	UNP A0A1G4HHT8
B	205	ALA	-	expression tag	UNP A0A1G4HHT8
C	202	GLY	-	expression tag	UNP A0A1G4HHT8
C	203	ALA	-	expression tag	UNP A0A1G4HHT8
C	204	MET	-	expression tag	UNP A0A1G4HHT8
C	205	ALA	-	expression tag	UNP A0A1G4HHT8
D	202	GLY	-	expression tag	UNP A0A1G4HHT8
D	203	ALA	-	expression tag	UNP A0A1G4HHT8
D	204	MET	-	expression tag	UNP A0A1G4HHT8
D	205	ALA	-	expression tag	UNP A0A1G4HHT8

- Molecule 2 is water.

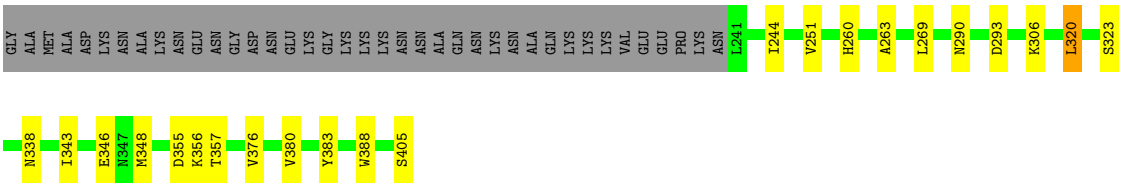
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	45	Total O 45 45	0	0
2	B	18	Total O 18 18	0	0
2	C	41	Total O 41 41	0	0
2	D	40	Total O 40 40	0	0

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.

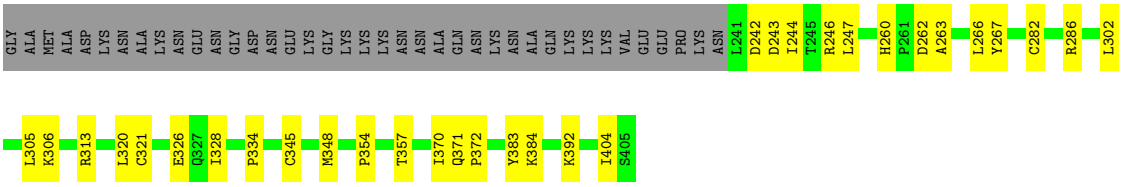
• Molecule 1: aminoacyl-tRNA synthetase-interacting multifunctional protein p43

Chain A:



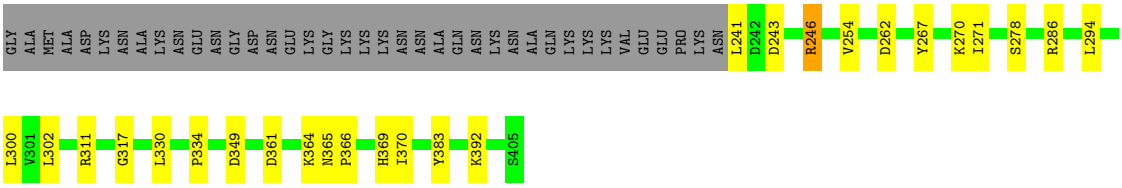
• Molecule 1: aminoacyl-tRNA synthetase-interacting multifunctional protein p43

Chain B:



• Molecule 1: aminoacyl-tRNA synthetase-interacting multifunctional protein p43

Chain C:



• Molecule 1: aminoacyl-tRNA synthetase-interacting multifunctional protein p43

Chain D:


K297
Y298
V299
L300
L305
K306
G317
M318
C321
P334
I343
I344
C345
E346
F360
H369
H373
Y383
K384
K387
K392
S405

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	37.17Å 146.90Å 146.93Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.73 – 2.47 36.73 – 2.47	Depositor EDS
% Data completeness (in resolution range)	99.7 (36.73-2.47) 99.7 (36.73-2.47)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.95 (at 2.48Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.202 , 0.261 0.203 , 0.258	Depositor DCC
R_{free} test set	1995 reflections (6.69%)	wwPDB-VP
Wilson B-factor (Å^2)	44.9	Xtriage
Anisotropy	0.271	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 21.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.366 for -h,l,k	Xtriage
Reported twinning fraction	0.646 for H, K, L 0.354 for -H, L, K	Depositor
Outliers	1 of 29839 reflections (0.003%)	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	5342	wwPDB-VP
Average B, all atoms (Å^2)	50.0	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 27.95 % 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 2.0096e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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

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	0.75	0/1317	0.85	1/1775 (0.1%)
1	B	0.83	0/1323	0.89	1/1782 (0.1%)
1	C	0.87	0/1323	0.94	4/1782 (0.2%)
1	D	0.82	1/1323 (0.1%)	0.92	1/1782 (0.1%)
All	All	0.82	1/5286 (0.0%)	0.90	7/7121 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	383	TYR	CE1-CZ	-5.32	1.31	1.38

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	243	ASP	CB-CG-OD1	6.99	124.59	118.30
1	C	246	ARG	NE-CZ-NH1	6.17	123.39	120.30
1	C	349	ASP	CB-CG-OD1	5.82	123.54	118.30
1	D	243	ASP	CB-CG-OD1	5.73	123.46	118.30
1	C	349	ASP	CB-CG-OD2	-5.19	113.63	118.30
1	C	383	TYR	N-CA-C	-5.12	97.16	111.00
1	A	320	LEU	CA-CB-CG	5.06	126.93	115.30

There are no chirality outliers.

There are no planarity outliers.

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	1295	0	1313	18	0
1	B	1301	0	1324	20	0
1	C	1301	0	1324	15	0
1	D	1301	0	1324	22	0
2	A	45	0	0	0	0
2	B	18	0	0	0	0
2	C	41	0	0	0	0
2	D	40	0	0	0	0
All	All	5342	0	5285	74	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 7.

All (74) 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:265:THR:HG23	1:D:266:LEU:HG	1.48	0.93
1:D:373:HIS:HB3	1:D:384:LYS:HG2	1.65	0.79
1:B:267:TYR:CE2	1:B:286:ARG:HA	2.18	0.78
1:A:306:LYS:HG2	1:A:357:THR:CG2	2.19	0.73
1:D:306:LYS:HD3	1:D:360:PHE:CE2	2.27	0.69
1:A:251:VAL:CG2	1:A:338:ASN:O	2.43	0.66
1:D:346:GLU:OE2	1:D:387:LYS:HB2	1.99	0.62
1:D:346:GLU:OE2	1:D:387:LYS:CB	2.51	0.59
1:A:244:ILE:HG23	1:A:348:MET:HE2	1.86	0.58
1:D:346:GLU:OE2	1:D:387:LYS:N	2.33	0.57
1:C:270:LYS:HD2	1:C:278:SER:OG	2.05	0.57
1:C:294:LEU:HD23	1:C:330:LEU:HD11	1.87	0.56
1:C:246:ARG:HH11	1:C:366:PRO:HG3	1.70	0.56
1:D:257:VAL:HG21	1:D:291:SER:CB	2.37	0.55
1:C:241:LEU:HD23	1:C:369:HIS:NE2	2.22	0.55
1:D:267:TYR:CE2	1:D:286:ARG:HA	2.42	0.55
1:D:334:PRO:HG2	1:D:392:LYS:HB2	1.89	0.54
1:B:242:ASP:OD2	1:B:384:LYS:NZ	2.37	0.54
1:B:302:LEU:HD23	1:B:305:LEU:HD11	1.91	0.52
1:B:371:GLN:HB3	1:B:372:PRO:HD3	1.92	0.52
1:D:257:VAL:HG12	1:D:269:LEU:CD2	2.40	0.52
1:C:267:TYR:CE2	1:C:286:ARG:HA	2.44	0.52
1:A:251:VAL:HG21	1:A:338:ASN:O	2.09	0.52
1:B:306:LYS:HG2	1:B:357:THR:CG2	2.41	0.51
1:A:306:LYS:HG2	1:A:357:THR:HG21	1.95	0.49
1:C:361:ASP:HB3	1:C:364:LYS:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:244:ILE:HD13	1:B:383:TYR:CD1	2.48	0.48
1:B:345:CYS:H	1:B:348:MET:HE3	1.79	0.48
1:D:257:VAL:HG21	1:D:291:SER:HB2	1.95	0.48
1:A:320:LEU:HD13	1:A:388:TRP:HH2	1.77	0.48
1:A:244:ILE:HG23	1:A:348:MET:CE	2.43	0.48
1:B:244:ILE:HG23	1:B:348:MET:CE	2.44	0.48
1:A:320:LEU:HD13	1:A:388:TRP:CH2	2.49	0.47
1:C:262:ASP:O	1:C:311:ARG:HD2	2.13	0.47
1:B:321:CYS:O	1:B:404:ILE:HA	2.15	0.47
1:C:361:ASP:OD2	1:C:364:LYS:HG3	2.15	0.47
1:D:257:VAL:O	1:D:257:VAL:HG23	2.13	0.47
1:A:306:LYS:CG	1:A:357:THR:CG2	2.92	0.46
1:D:241:LEU:HD21	1:D:369:HIS:CE1	2.50	0.46
1:B:244:ILE:HD12	1:B:247:LEU:HD12	1.98	0.46
1:C:302:LEU:O	1:C:317:GLY:HA2	2.16	0.46
1:A:376:VAL:HA	1:A:380:VAL:O	2.16	0.45
1:A:355:ASP:O	1:A:356:LYS:C	2.55	0.45
1:B:334:PRO:HG2	1:B:392:LYS:HB2	1.98	0.45
1:A:405:SER:HB3	1:B:326:GLU:OE2	2.16	0.45
1:D:252:GLY:O	1:D:298:TYR:HA	2.17	0.45
1:A:251:VAL:CG1	1:A:343:ILE:HD11	2.47	0.45
1:A:290:ASN:O	1:A:293:ASP:HB2	2.16	0.45
1:C:254:VAL:HG22	1:C:271:ILE:CD1	2.47	0.45
1:B:370:ILE:HG23	1:B:383:TYR:HE1	1.81	0.44
1:A:269:LEU:HD12	1:A:269:LEU:N	2.32	0.44
1:D:300:LEU:HD12	1:D:300:LEU:N	2.32	0.44
1:D:305:LEU:HD11	1:D:318:MET:HG2	1.99	0.44
1:C:300:LEU:HD12	1:C:300:LEU:N	2.32	0.44
1:C:243:ASP:O	1:C:370:ILE:HD11	2.17	0.44
1:D:259:ILE:HG23	1:D:286:ARG:NH1	2.33	0.44
1:A:244:ILE:CD1	1:A:383:TYR:HB2	2.48	0.43
1:B:260:HIS:HB3	1:B:263:ALA:HB3	2.00	0.43
1:D:346:GLU:OE2	1:D:387:LYS:CG	2.66	0.43
1:B:328:ILE:HG23	1:B:328:ILE:O	2.18	0.43
1:B:266:LEU:HD22	1:B:282:CYS:HB3	2.01	0.43
1:D:305:LEU:HD12	1:D:317:GLY:HA2	2.01	0.42
1:C:365:ASN:HA	1:C:366:PRO:HD2	1.85	0.42
1:D:285:LEU:HD11	1:D:321:CYS:SG	2.59	0.42
1:C:254:VAL:HG22	1:C:271:ILE:HD12	2.00	0.42
1:A:260:HIS:CG	1:A:263:ALA:HB3	2.54	0.42
1:B:244:ILE:HG23	1:B:348:MET:HE1	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:334:PRO:HG2	1:C:392:LYS:HB2	2.02	0.41
1:A:356:LYS:HA	1:A:356:LYS:HD2	1.88	0.41
1:B:246:ARG:HA	1:B:354:PRO:HA	2.03	0.41
1:B:370:ILE:HG23	1:B:383:TYR:CE1	2.55	0.41
1:B:244:ILE:HB	1:B:383:TYR:CE1	2.55	0.41
1:D:241:LEU:CD2	1:D:369:HIS:CE1	3.04	0.40
1:D:343:ILE:C	1:D:344:ILE:HG23	2.41	0.40

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	163/204 (80%)	159 (98%)	4 (2%)	0	100	100
1	B	163/204 (80%)	160 (98%)	3 (2%)	0	100	100
1	C	163/204 (80%)	157 (96%)	6 (4%)	0	100	100
1	D	163/204 (80%)	161 (99%)	2 (1%)	0	100	100
All	All	652/816 (80%)	637 (98%)	15 (2%)	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	147/179 (82%)	145 (99%)	2 (1%)	67 84
1	B	148/179 (83%)	145 (98%)	3 (2%)	55 77
1	C	148/179 (83%)	148 (100%)	0	100 100
1	D	148/179 (83%)	147 (99%)	1 (1%)	84 93
All	All	591/716 (82%)	585 (99%)	6 (1%)	76 89

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	323	SER
1	A	346	GLU
1	B	262	ASP
1	B	313	ARG
1	B	320	LEU
1	D	297	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides 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, 95^{th} 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	165/204 (80%)	-0.11	0	100	100	34, 49, 71, 82	0
1	B	165/204 (80%)	-0.09	0	100	100	34, 47, 72, 89	0
1	C	165/204 (80%)	-0.14	0	100	100	31, 46, 68, 83	0
1	D	165/204 (80%)	-0.07	0	100	100	35, 51, 75, 95	0
All	All	660/816 (80%)	-0.10	0	100	100	31, 48, 72, 95	0

There are no RSRZ outliers to report.

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

There are no monosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.