



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 06:47 PM UTC

PDB ID : 8TI7 / pdb_00008ti7
Title : Crystal structure of profilin from *Dermatophagoides pteronyssinus* in complex with a poly(L-proline) peptide
Authors : O'Malley, A.; Sankaran, S.; Chruszcz, M.
Deposited on : 2023-07-19
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

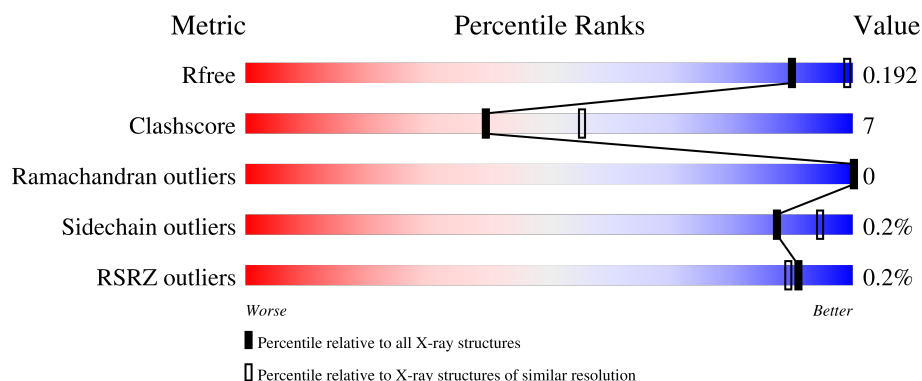
1 Overall quality at a glance

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	154	
1	C	154	
1	E	154	
1	G	154	
1	I	154	

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Mol	Chain	Length	Quality of chain
1	K	154	
1	M	154	
1	O	154	
2	B	12	
2	D	12	
2	F	12	
2	H	12	
2	J	12	
2	L	12	
2	N	12	
2	P	12	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8829 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 Profilin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	132	Total	C	N	O	S	0	0	0
			994	615	177	197	5			
1	C	130	Total	C	N	O	S	0	0	0
			988	615	176	192	5			
1	E	131	Total	C	N	O	S	0	0	0
			996	619	177	195	5			
1	G	132	Total	C	N	O	S	0	0	0
			983	608	175	195	5			
1	I	131	Total	C	N	O	S	0	0	0
			990	615	176	194	5			
1	K	132	Total	C	N	O	S	0	0	0
			997	619	177	196	5			
1	M	131	Total	C	N	O	S	0	0	0
			993	615	175	198	5			
1	O	130	Total	C	N	O	S	0	0	0
			987	613	175	194	5			

There are 200 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-23	MET	-	initiating methionine	UNP A0A2L0EBJ5
A	-22	HIS	-	expression tag	UNP A0A2L0EBJ5
A	-21	HIS	-	expression tag	UNP A0A2L0EBJ5
A	-20	HIS	-	expression tag	UNP A0A2L0EBJ5
A	-19	HIS	-	expression tag	UNP A0A2L0EBJ5
A	-18	HIS	-	expression tag	UNP A0A2L0EBJ5
A	-17	HIS	-	expression tag	UNP A0A2L0EBJ5
A	-16	SER	-	expression tag	UNP A0A2L0EBJ5
A	-15	SER	-	expression tag	UNP A0A2L0EBJ5
A	-14	GLY	-	expression tag	UNP A0A2L0EBJ5
A	-13	VAL	-	expression tag	UNP A0A2L0EBJ5
A	-12	ASP	-	expression tag	UNP A0A2L0EBJ5
A	-11	LEU	-	expression tag	UNP A0A2L0EBJ5

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	GLY	-	expression tag	UNP A0A2L0EBJ5
A	-9	THR	-	expression tag	UNP A0A2L0EBJ5
A	-8	GLU	-	expression tag	UNP A0A2L0EBJ5
A	-7	ASN	-	expression tag	UNP A0A2L0EBJ5
A	-6	LEU	-	expression tag	UNP A0A2L0EBJ5
A	-5	TYR	-	expression tag	UNP A0A2L0EBJ5
A	-4	PHE	-	expression tag	UNP A0A2L0EBJ5
A	-3	GLN	-	expression tag	UNP A0A2L0EBJ5
A	-2	SER	-	expression tag	UNP A0A2L0EBJ5
A	-1	GLY	-	expression tag	UNP A0A2L0EBJ5
A	0	SER	-	expression tag	UNP A0A2L0EBJ5
A	1	GLY	-	expression tag	UNP A0A2L0EBJ5
C	-23	MET	-	initiating methionine	UNP A0A2L0EBJ5
C	-22	HIS	-	expression tag	UNP A0A2L0EBJ5
C	-21	HIS	-	expression tag	UNP A0A2L0EBJ5
C	-20	HIS	-	expression tag	UNP A0A2L0EBJ5
C	-19	HIS	-	expression tag	UNP A0A2L0EBJ5
C	-18	HIS	-	expression tag	UNP A0A2L0EBJ5
C	-17	HIS	-	expression tag	UNP A0A2L0EBJ5
C	-16	SER	-	expression tag	UNP A0A2L0EBJ5
C	-15	SER	-	expression tag	UNP A0A2L0EBJ5
C	-14	GLY	-	expression tag	UNP A0A2L0EBJ5
C	-13	VAL	-	expression tag	UNP A0A2L0EBJ5
C	-12	ASP	-	expression tag	UNP A0A2L0EBJ5
C	-11	LEU	-	expression tag	UNP A0A2L0EBJ5
C	-10	GLY	-	expression tag	UNP A0A2L0EBJ5
C	-9	THR	-	expression tag	UNP A0A2L0EBJ5
C	-8	GLU	-	expression tag	UNP A0A2L0EBJ5
C	-7	ASN	-	expression tag	UNP A0A2L0EBJ5
C	-6	LEU	-	expression tag	UNP A0A2L0EBJ5
C	-5	TYR	-	expression tag	UNP A0A2L0EBJ5
C	-4	PHE	-	expression tag	UNP A0A2L0EBJ5
C	-3	GLN	-	expression tag	UNP A0A2L0EBJ5
C	-2	SER	-	expression tag	UNP A0A2L0EBJ5
C	-1	GLY	-	expression tag	UNP A0A2L0EBJ5
C	0	SER	-	expression tag	UNP A0A2L0EBJ5
C	1	GLY	-	expression tag	UNP A0A2L0EBJ5
E	-23	MET	-	initiating methionine	UNP A0A2L0EBJ5
E	-22	HIS	-	expression tag	UNP A0A2L0EBJ5
E	-21	HIS	-	expression tag	UNP A0A2L0EBJ5
E	-20	HIS	-	expression tag	UNP A0A2L0EBJ5
E	-19	HIS	-	expression tag	UNP A0A2L0EBJ5

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-18	HIS	-	expression tag	UNP A0A2L0EBJ5
E	-17	HIS	-	expression tag	UNP A0A2L0EBJ5
E	-16	SER	-	expression tag	UNP A0A2L0EBJ5
E	-15	SER	-	expression tag	UNP A0A2L0EBJ5
E	-14	GLY	-	expression tag	UNP A0A2L0EBJ5
E	-13	VAL	-	expression tag	UNP A0A2L0EBJ5
E	-12	ASP	-	expression tag	UNP A0A2L0EBJ5
E	-11	LEU	-	expression tag	UNP A0A2L0EBJ5
E	-10	GLY	-	expression tag	UNP A0A2L0EBJ5
E	-9	THR	-	expression tag	UNP A0A2L0EBJ5
E	-8	GLU	-	expression tag	UNP A0A2L0EBJ5
E	-7	ASN	-	expression tag	UNP A0A2L0EBJ5
E	-6	LEU	-	expression tag	UNP A0A2L0EBJ5
E	-5	TYR	-	expression tag	UNP A0A2L0EBJ5
E	-4	PHE	-	expression tag	UNP A0A2L0EBJ5
E	-3	GLN	-	expression tag	UNP A0A2L0EBJ5
E	-2	SER	-	expression tag	UNP A0A2L0EBJ5
E	-1	GLY	-	expression tag	UNP A0A2L0EBJ5
E	0	SER	-	expression tag	UNP A0A2L0EBJ5
E	1	GLY	-	expression tag	UNP A0A2L0EBJ5
G	-23	MET	-	initiating methionine	UNP A0A2L0EBJ5
G	-22	HIS	-	expression tag	UNP A0A2L0EBJ5
G	-21	HIS	-	expression tag	UNP A0A2L0EBJ5
G	-20	HIS	-	expression tag	UNP A0A2L0EBJ5
G	-19	HIS	-	expression tag	UNP A0A2L0EBJ5
G	-18	HIS	-	expression tag	UNP A0A2L0EBJ5
G	-17	HIS	-	expression tag	UNP A0A2L0EBJ5
G	-16	SER	-	expression tag	UNP A0A2L0EBJ5
G	-15	SER	-	expression tag	UNP A0A2L0EBJ5
G	-14	GLY	-	expression tag	UNP A0A2L0EBJ5
G	-13	VAL	-	expression tag	UNP A0A2L0EBJ5
G	-12	ASP	-	expression tag	UNP A0A2L0EBJ5
G	-11	LEU	-	expression tag	UNP A0A2L0EBJ5
G	-10	GLY	-	expression tag	UNP A0A2L0EBJ5
G	-9	THR	-	expression tag	UNP A0A2L0EBJ5
G	-8	GLU	-	expression tag	UNP A0A2L0EBJ5
G	-7	ASN	-	expression tag	UNP A0A2L0EBJ5
G	-6	LEU	-	expression tag	UNP A0A2L0EBJ5
G	-5	TYR	-	expression tag	UNP A0A2L0EBJ5
G	-4	PHE	-	expression tag	UNP A0A2L0EBJ5
G	-3	GLN	-	expression tag	UNP A0A2L0EBJ5
G	-2	SER	-	expression tag	UNP A0A2L0EBJ5

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-1	GLY	-	expression tag	UNP A0A2L0EBJ5
G	0	SER	-	expression tag	UNP A0A2L0EBJ5
G	1	GLY	-	expression tag	UNP A0A2L0EBJ5
I	-23	MET	-	initiating methionine	UNP A0A2L0EBJ5
I	-22	HIS	-	expression tag	UNP A0A2L0EBJ5
I	-21	HIS	-	expression tag	UNP A0A2L0EBJ5
I	-20	HIS	-	expression tag	UNP A0A2L0EBJ5
I	-19	HIS	-	expression tag	UNP A0A2L0EBJ5
I	-18	HIS	-	expression tag	UNP A0A2L0EBJ5
I	-17	HIS	-	expression tag	UNP A0A2L0EBJ5
I	-16	SER	-	expression tag	UNP A0A2L0EBJ5
I	-15	SER	-	expression tag	UNP A0A2L0EBJ5
I	-14	GLY	-	expression tag	UNP A0A2L0EBJ5
I	-13	VAL	-	expression tag	UNP A0A2L0EBJ5
I	-12	ASP	-	expression tag	UNP A0A2L0EBJ5
I	-11	LEU	-	expression tag	UNP A0A2L0EBJ5
I	-10	GLY	-	expression tag	UNP A0A2L0EBJ5
I	-9	THR	-	expression tag	UNP A0A2L0EBJ5
I	-8	GLU	-	expression tag	UNP A0A2L0EBJ5
I	-7	ASN	-	expression tag	UNP A0A2L0EBJ5
I	-6	LEU	-	expression tag	UNP A0A2L0EBJ5
I	-5	TYR	-	expression tag	UNP A0A2L0EBJ5
I	-4	PHE	-	expression tag	UNP A0A2L0EBJ5
I	-3	GLN	-	expression tag	UNP A0A2L0EBJ5
I	-2	SER	-	expression tag	UNP A0A2L0EBJ5
I	-1	GLY	-	expression tag	UNP A0A2L0EBJ5
I	0	SER	-	expression tag	UNP A0A2L0EBJ5
I	1	GLY	-	expression tag	UNP A0A2L0EBJ5
K	-23	MET	-	initiating methionine	UNP A0A2L0EBJ5
K	-22	HIS	-	expression tag	UNP A0A2L0EBJ5
K	-21	HIS	-	expression tag	UNP A0A2L0EBJ5
K	-20	HIS	-	expression tag	UNP A0A2L0EBJ5
K	-19	HIS	-	expression tag	UNP A0A2L0EBJ5
K	-18	HIS	-	expression tag	UNP A0A2L0EBJ5
K	-17	HIS	-	expression tag	UNP A0A2L0EBJ5
K	-16	SER	-	expression tag	UNP A0A2L0EBJ5
K	-15	SER	-	expression tag	UNP A0A2L0EBJ5
K	-14	GLY	-	expression tag	UNP A0A2L0EBJ5
K	-13	VAL	-	expression tag	UNP A0A2L0EBJ5
K	-12	ASP	-	expression tag	UNP A0A2L0EBJ5
K	-11	LEU	-	expression tag	UNP A0A2L0EBJ5
K	-10	GLY	-	expression tag	UNP A0A2L0EBJ5

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Chain	Residue	Modelled	Actual	Comment	Reference
K	-9	THR	-	expression tag	UNP A0A2L0EBJ5
K	-8	GLU	-	expression tag	UNP A0A2L0EBJ5
K	-7	ASN	-	expression tag	UNP A0A2L0EBJ5
K	-6	LEU	-	expression tag	UNP A0A2L0EBJ5
K	-5	TYR	-	expression tag	UNP A0A2L0EBJ5
K	-4	PHE	-	expression tag	UNP A0A2L0EBJ5
K	-3	GLN	-	expression tag	UNP A0A2L0EBJ5
K	-2	SER	-	expression tag	UNP A0A2L0EBJ5
K	-1	GLY	-	expression tag	UNP A0A2L0EBJ5
K	0	SER	-	expression tag	UNP A0A2L0EBJ5
K	1	GLY	-	expression tag	UNP A0A2L0EBJ5
M	-23	MET	-	initiating methionine	UNP A0A2L0EBJ5
M	-22	HIS	-	expression tag	UNP A0A2L0EBJ5
M	-21	HIS	-	expression tag	UNP A0A2L0EBJ5
M	-20	HIS	-	expression tag	UNP A0A2L0EBJ5
M	-19	HIS	-	expression tag	UNP A0A2L0EBJ5
M	-18	HIS	-	expression tag	UNP A0A2L0EBJ5
M	-17	HIS	-	expression tag	UNP A0A2L0EBJ5
M	-16	SER	-	expression tag	UNP A0A2L0EBJ5
M	-15	SER	-	expression tag	UNP A0A2L0EBJ5
M	-14	GLY	-	expression tag	UNP A0A2L0EBJ5
M	-13	VAL	-	expression tag	UNP A0A2L0EBJ5
M	-12	ASP	-	expression tag	UNP A0A2L0EBJ5
M	-11	LEU	-	expression tag	UNP A0A2L0EBJ5
M	-10	GLY	-	expression tag	UNP A0A2L0EBJ5
M	-9	THR	-	expression tag	UNP A0A2L0EBJ5
M	-8	GLU	-	expression tag	UNP A0A2L0EBJ5
M	-7	ASN	-	expression tag	UNP A0A2L0EBJ5
M	-6	LEU	-	expression tag	UNP A0A2L0EBJ5
M	-5	TYR	-	expression tag	UNP A0A2L0EBJ5
M	-4	PHE	-	expression tag	UNP A0A2L0EBJ5
M	-3	GLN	-	expression tag	UNP A0A2L0EBJ5
M	-2	SER	-	expression tag	UNP A0A2L0EBJ5
M	-1	GLY	-	expression tag	UNP A0A2L0EBJ5
M	0	SER	-	expression tag	UNP A0A2L0EBJ5
M	1	GLY	-	expression tag	UNP A0A2L0EBJ5
O	-23	MET	-	initiating methionine	UNP A0A2L0EBJ5
O	-22	HIS	-	expression tag	UNP A0A2L0EBJ5
O	-21	HIS	-	expression tag	UNP A0A2L0EBJ5
O	-20	HIS	-	expression tag	UNP A0A2L0EBJ5
O	-19	HIS	-	expression tag	UNP A0A2L0EBJ5
O	-18	HIS	-	expression tag	UNP A0A2L0EBJ5

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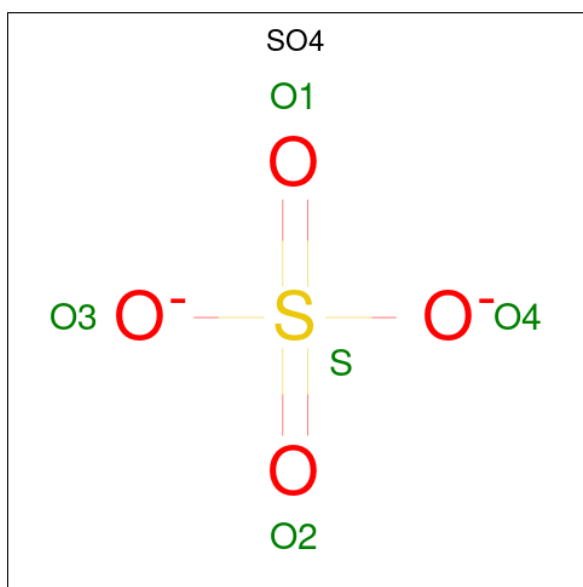
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Chain	Residue	Modelled	Actual	Comment	Reference
O	-17	HIS	-	expression tag	UNP A0A2L0EBJ5
O	-16	SER	-	expression tag	UNP A0A2L0EBJ5
O	-15	SER	-	expression tag	UNP A0A2L0EBJ5
O	-14	GLY	-	expression tag	UNP A0A2L0EBJ5
O	-13	VAL	-	expression tag	UNP A0A2L0EBJ5
O	-12	ASP	-	expression tag	UNP A0A2L0EBJ5
O	-11	LEU	-	expression tag	UNP A0A2L0EBJ5
O	-10	GLY	-	expression tag	UNP A0A2L0EBJ5
O	-9	THR	-	expression tag	UNP A0A2L0EBJ5
O	-8	GLU	-	expression tag	UNP A0A2L0EBJ5
O	-7	ASN	-	expression tag	UNP A0A2L0EBJ5
O	-6	LEU	-	expression tag	UNP A0A2L0EBJ5
O	-5	TYR	-	expression tag	UNP A0A2L0EBJ5
O	-4	PHE	-	expression tag	UNP A0A2L0EBJ5
O	-3	GLN	-	expression tag	UNP A0A2L0EBJ5
O	-2	SER	-	expression tag	UNP A0A2L0EBJ5
O	-1	GLY	-	expression tag	UNP A0A2L0EBJ5
O	0	SER	-	expression tag	UNP A0A2L0EBJ5
O	1	GLY	-	expression tag	UNP A0A2L0EBJ5

- Molecule 2 is a protein called poly(L-proline).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	12	Total	C	N	O	0	0	0
			85	60	12	13			
2	D	12	Total	C	N	O	0	0	0
			85	60	12	13			
2	F	12	Total	C	N	O	0	0	0
			85	60	12	13			
2	H	12	Total	C	N	O	0	0	0
			85	60	12	13			
2	J	12	Total	C	N	O	0	0	0
			85	60	12	13			
2	L	12	Total	C	N	O	0	0	0
			85	60	12	13			
2	N	12	Total	C	N	O	0	0	0
			85	60	12	13			
2	P	12	Total	C	N	O	0	0	0
			85	60	12	13			

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	G	1	Total	O	S	0	0
			5	4	1		
3	I	1	Total	O	S	0	0
			5	4	1		
3	I	1	Total	O	S	0	0
			5	4	1		
3	K	1	Total	O	S	0	0
			5	4	1		
3	K	1	Total	O	S	0	0
			5	4	1		
3	M	1	Total	O	S	0	0
			5	4	1		
3	M	1	Total	O	S	0	0
			5	4	1		
3	O	1	Total	O	S	0	0
			5	4	1		
3	O	1	Total	O	S	0	0
			5	4	1		

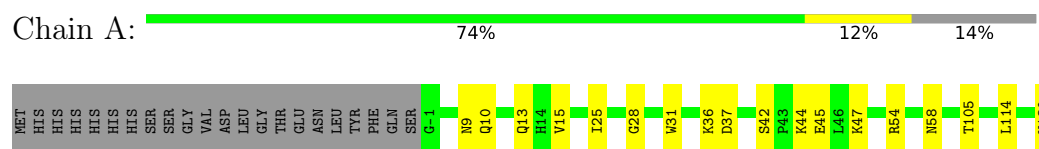
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	20	Total 20	O 20	0	0
4	C	22	Total 22	O 22	0	0
4	E	15	Total 15	O 15	0	0
4	G	23	Total 23	O 23	0	0
4	I	22	Total 22	O 22	0	0
4	K	20	Total 20	O 20	0	0
4	M	19	Total 19	O 19	0	0
4	O	14	Total 14	O 14	0	0
4	D	1	Total 1	O 1	0	0
4	F	1	Total 1	O 1	0	0
4	H	1	Total 1	O 1	0	0
4	J	2	Total 2	O 2	0	0
4	L	1	Total 1	O 1	0	0

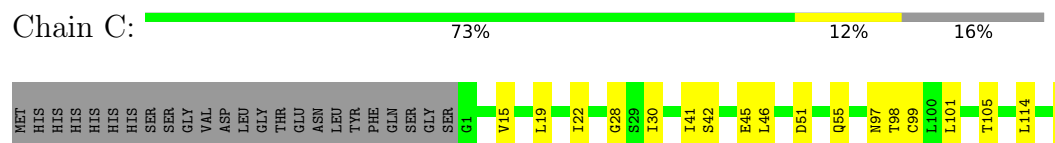
3 Residue-property plots [i](#)

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.

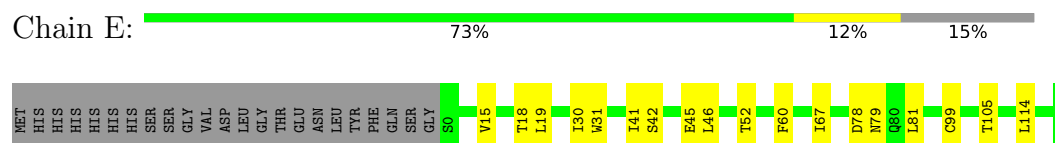
- Molecule 1: Profilin



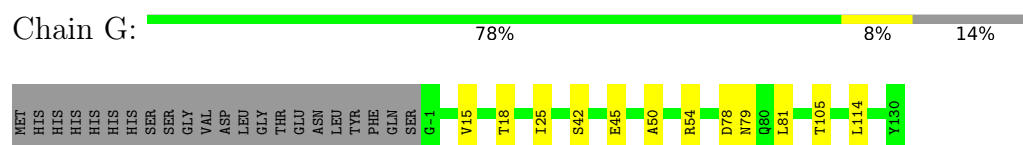
- Molecule 1: Profilin



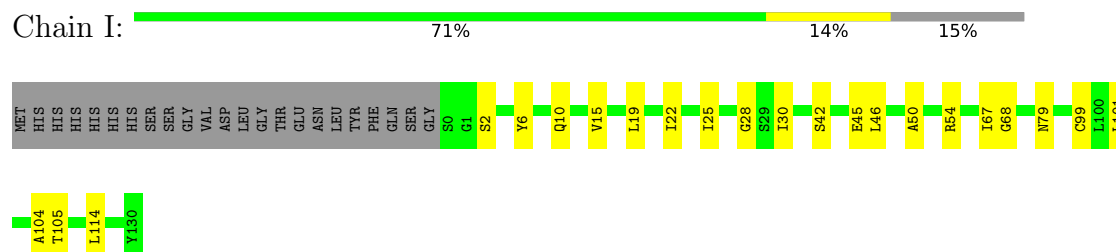
- Molecule 1: Profilin



- Molecule 1: Profilin

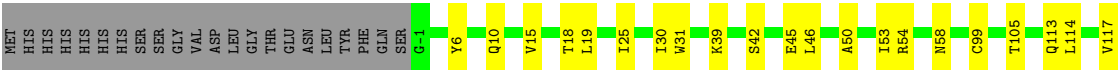


- Molecule 1: Profilin



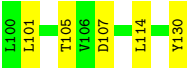
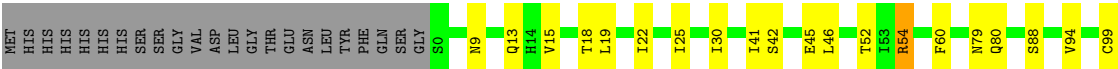
- Molecule 1: Profilin

Chain K: 71% 14% 14%



• Molecule 1: Profilin

Chain M: 69% 16% 15%



• Molecule 1: Profilin

Chain O: 70% 14% 16%



• Molecule 2: poly(L-proline)

Chain B: 75% 17% 8%



• Molecule 2: poly(L-proline)

Chain D: 92% 8%

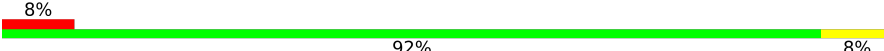


• Molecule 2: poly(L-proline)

Chain F: 75% 17% 8%



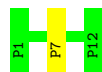
- Molecule 2: poly(L-proline)

Chain H:  8% 92% 8%



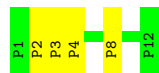
- Molecule 2: poly(L-proline)

Chain J:  92% 8%



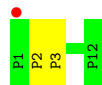
- Molecule 2: poly(L-proline)

Chain L:  67% 33%



- Molecule 2: poly(L-proline)

Chain N:  8% 83% 17%



- Molecule 2: poly(L-proline)

Chain P:  83% 17%



4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	152.80Å 152.80Å 186.85Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	34.16 – 2.40 34.16 – 2.40	Depositor EDS
% Data completeness (in resolution range)	98.8 (34.16-2.40) 98.8 (34.16-2.40)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.96 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.8.0415	Depositor
R, R_{free}	0.166 , 0.195 0.166 , 0.192	Depositor DCC
R_{free} test set	3205 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	60.8	Xtriage
Anisotropy	0.076	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 50.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.417 for -2/3*h-1/3*k+2/3*l,-1/3*h-2/3*k-2/3*l,2/3*h-2/3*k+1/3*l 0.447 for -h,1/3*h-1/3*k+2/3*l,2/3*h+4/3*k+1/3*l 0.440 for -1/3*h+1/3*k-2/3*l,-k,-4/3*h-2/3*k+1/3*l 0.430 for -h,2/3*h+1/3*k-2/3*l,-2/3*h-4/3*k-1/3*l 0.437 for 1/3*h+2/3*k+2/3*l,-k,4/3*h+2/3*k-1/3*l 0.458 for -1/3*h-2/3*k-2/3*l,-2/3*h-1/3*k+2/3*l,-2/3*h+2/3*k-1/3*l 0.418 for h,-h-k,-l	Xtriage

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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.

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Property	Value	Source
Reported twinning fraction	0.236 for H, K, L 0.084 for K, H, -L 0.161 for $-1/3H-2/3K-2/3L$, $-2/3H-1/3K+2/3L$, $-2/3H+2/3K-1/3L$ 0.122 for $-2/3H-1/3K+2/3L$, $-1/3H-2/3K-2/3L$, $2/3H-2/3K+1/3L$ 0.076 for $1/3H-1/3K+2/3L$, -H, $-2/3H-4/3K-1/3L$ 0.069 for -K, $-1/3H+1/3K-2/3L$, $4/3H+2/3K-1/3L$ 0.133 for $-1/3H+1/3K-2/3L$, -K, $-4/3H-2/3K+1/3L$ 0.120 for -H, $1/3H-1/3K+2/3L$, $2/3H+4/3K+1/3L$	Depositor
Outliers	0 of 63157 reflections	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	8829	wwPDB-VP
Average B, all atoms ($\text{\AA}^2$)	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.42% of the height of the origin peak. No significant pseudotranslation is detected.*

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: 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	0.65	0/1009	1.03	1/1368 (0.1%)
1	C	0.66	0/1003	1.00	1/1359 (0.1%)
1	E	0.65	0/1011	1.02	1/1371 (0.1%)
1	G	0.65	0/998	1.03	1/1356 (0.1%)
1	I	0.63	0/1005	1.00	1/1363 (0.1%)
1	K	0.70	0/1012	1.05	1/1373 (0.1%)
1	M	0.68	0/1008	1.03	1/1368 (0.1%)
1	O	0.65	0/1002	1.03	1/1359 (0.1%)
2	B	0.91	0/96	1.18	1/140 (0.7%)
2	D	1.05	0/96	1.19	0/140
2	F	1.06	0/96	1.23	1/140 (0.7%)
2	H	1.06	0/96	1.31	1/140 (0.7%)
2	J	1.02	0/96	1.26	0/140
2	L	0.87	0/96	1.14	0/140
2	N	0.94	0/96	1.22	1/140 (0.7%)
2	P	0.93	0/96	1.17	0/140
All	All	0.69	0/8816	1.04	12/12037 (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	M	0	1
1	O	0	1
All	All	0	2

There are no bond length outliers.

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	18	THR	N-CA-C	-6.77	105.15	113.41
1	E	18	THR	N-CA-C	-6.65	105.20	113.38
2	F	11	PRO	N-CA-CB	6.51	106.61	103.22
1	M	18	THR	N-CA-C	-6.29	104.67	112.90
1	A	28	GLY	N-CA-C	-6.02	107.10	114.92

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	M	54	ARG	Sidechain
1	O	85	ARG	Sidechain

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	994	0	961	11	0
1	C	988	0	971	13	0
1	E	996	0	978	11	0
1	G	983	0	937	10	0
1	I	990	0	965	19	0
1	K	997	0	972	17	0
1	M	993	0	960	19	0
1	O	987	0	962	17	0
2	B	85	0	86	3	0
2	D	85	0	86	0	0
2	F	85	0	86	2	0
2	H	85	0	86	0	0
2	J	85	0	86	1	0
2	L	85	0	86	6	0
2	N	85	0	86	1	0
2	P	85	0	86	2	0
3	A	15	0	0	0	0
3	G	5	0	0	0	0
3	I	10	0	0	0	0
3	K	10	0	0	0	0
3	M	10	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	O	10	0	0	0	0
4	A	20	0	0	0	0
4	C	22	0	0	0	0
4	D	1	0	0	0	0
4	E	15	0	0	0	0
4	F	1	0	0	0	0
4	G	23	0	0	0	0
4	H	1	0	0	0	0
4	I	22	0	0	0	1
4	J	2	0	0	0	0
4	K	20	0	0	0	0
4	L	1	0	0	0	0
4	M	19	0	0	0	0
4	O	14	0	0	0	0
All	All	8829	0	8394	115	1

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.

The worst 5 of 115 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:G:105:THR:HG23	1:G:114:LEU:HD22	1.49	0.90
1:I:105:THR:HG23	1:I:114:LEU:HD22	1.50	0.90
1:C:105:THR:HG23	1:C:114:LEU:HD22	1.53	0.89
1:O:105:THR:HG23	1:O:114:LEU:HD22	1.52	0.89
1:O:98:THR:HG21	2:L:2:PRO:HG2	1.59	0.82

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:322:HOH:O	4:I:322:HOH:O[3_555]	1.93	0.27

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	130/154 (84%)	123 (95%)	7 (5%)	0	100	100
1	C	128/154 (83%)	123 (96%)	5 (4%)	0	100	100
1	E	129/154 (84%)	125 (97%)	4 (3%)	0	100	100
1	G	130/154 (84%)	124 (95%)	6 (5%)	0	100	100
1	I	129/154 (84%)	121 (94%)	8 (6%)	0	100	100
1	K	130/154 (84%)	124 (95%)	6 (5%)	0	100	100
1	M	129/154 (84%)	123 (95%)	6 (5%)	0	100	100
1	O	128/154 (83%)	122 (95%)	6 (5%)	0	100	100
2	B	10/12 (83%)	10 (100%)	0	0	100	100
2	D	10/12 (83%)	10 (100%)	0	0	100	100
2	F	10/12 (83%)	10 (100%)	0	0	100	100
2	H	10/12 (83%)	10 (100%)	0	0	100	100
2	J	10/12 (83%)	10 (100%)	0	0	100	100
2	L	10/12 (83%)	10 (100%)	0	0	100	100
2	N	10/12 (83%)	10 (100%)	0	0	100	100
2	P	10/12 (83%)	10 (100%)	0	0	100	100
All	All	1113/1328 (84%)	1065 (96%)	48 (4%)	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	
1	A	104/128 (81%)	104 (100%)	0	100	100
1	C	104/128 (81%)	104 (100%)	0	100	100
1	E	106/128 (83%)	106 (100%)	0	100	100
1	G	101/128 (79%)	101 (100%)	0	100	100
1	I	104/128 (81%)	104 (100%)	0	100	100
1	K	105/128 (82%)	105 (100%)	0	100	100
1	M	105/128 (82%)	105 (100%)	0	100	100
1	O	104/128 (81%)	104 (100%)	0	100	100
2	B	12/12 (100%)	12 (100%)	0	100	100
2	D	12/12 (100%)	11 (92%)	1 (8%)	10	17
2	F	12/12 (100%)	11 (92%)	1 (8%)	10	17
2	H	12/12 (100%)	12 (100%)	0	100	100
2	J	12/12 (100%)	12 (100%)	0	100	100
2	L	12/12 (100%)	12 (100%)	0	100	100
2	N	12/12 (100%)	12 (100%)	0	100	100
2	P	12/12 (100%)	12 (100%)	0	100	100
All	All	929/1120 (83%)	927 (100%)	2 (0%)	87	94

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

Mol	Chain	Res	Type
2	D	1	PRO
2	F	1	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	M	13	GLN
1	M	14	HIS
1	M	79	ASN
1	I	79	ASN
1	C	9	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

12 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	$\# Z > 2$
3	SO4	A	202	-	4,4,4	0.39	0	6,6,6	0.09	0
3	SO4	A	203	-	4,4,4	0.39	0	6,6,6	0.09	0
3	SO4	I	201	-	4,4,4	0.43	0	6,6,6	0.24	0
3	SO4	M	202	-	4,4,4	0.42	0	6,6,6	0.23	0
3	SO4	M	201	-	4,4,4	0.37	0	6,6,6	0.33	0
3	SO4	O	201	-	4,4,4	0.40	0	6,6,6	0.07	0
3	SO4	A	201	-	4,4,4	0.44	0	6,6,6	0.27	0
3	SO4	O	202	-	4,4,4	1.04	0	6,6,6	1.39	1 (16%)
3	SO4	K	201	-	4,4,4	0.43	0	6,6,6	0.48	0
3	SO4	I	202	-	4,4,4	0.42	0	6,6,6	0.07	0
3	SO4	G	201	-	4,4,4	0.31	0	6,6,6	0.11	0
3	SO4	K	202	-	4,4,4	0.41	0	6,6,6	0.09	0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	O	202	SO4	O4-S-O3	3.06	125.39	108.54

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

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	132/154 (85%)	-0.64	0 100 100	57, 77, 108, 115	0
1	C	130/154 (84%)	-0.62	0 100 100	50, 74, 99, 128	0
1	E	131/154 (85%)	-0.62	0 100 100	52, 79, 109, 132	0
1	G	132/154 (85%)	-0.62	0 100 100	54, 76, 105, 128	0
1	I	131/154 (85%)	-0.58	0 100 100	49, 77, 108, 129	0
1	K	132/154 (85%)	-0.60	0 100 100	48, 71, 97, 137	0
1	M	131/154 (85%)	-0.63	0 100 100	60, 78, 110, 127	0
1	O	130/154 (84%)	-0.68	0 100 100	50, 75, 103, 131	0
2	B	12/12 (100%)	-0.72	0 100 100	75, 97, 106, 123	0
2	D	12/12 (100%)	-0.36	0 100 100	63, 78, 106, 130	0
2	F	12/12 (100%)	-0.70	0 100 100	56, 75, 92, 94	0
2	H	12/12 (100%)	-0.26	1 (8%) 17 14	61, 76, 111, 115	0
2	J	12/12 (100%)	-0.49	0 100 100	62, 78, 112, 119	0
2	L	12/12 (100%)	-0.65	0 100 100	65, 81, 100, 111	0
2	N	12/12 (100%)	-0.18	1 (8%) 17 14	64, 91, 130, 141	0
2	P	12/12 (100%)	-0.59	0 100 100	68, 77, 97, 125	0
All	All	1145/1328 (86%)	-0.61	2 (0%) 91 89	48, 77, 109, 141	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	1	PRO	3.1
2	N	1	PRO	3.1

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](#)

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	SO4	G	201	5/5	0.91	0.10	82,92,102,109	5
3	SO4	K	201	5/5	0.93	0.13	42,50,58,70	0
3	SO4	I	201	5/5	0.94	0.14	127,128,134,137	5
3	SO4	M	202	5/5	0.94	0.09	50,60,62,70	0
3	SO4	A	203	5/5	0.95	0.15	30,30,30,30	0
3	SO4	I	202	5/5	0.95	0.14	30,30,30,30	0
3	SO4	O	202	5/5	0.95	0.15	30,30,30,30	0
3	SO4	M	201	5/5	0.96	0.12	48,49,62,64	0
3	SO4	A	201	5/5	0.96	0.07	51,63,73,73	0
3	SO4	K	202	5/5	0.96	0.15	30,30,30,30	0
3	SO4	O	201	5/5	0.97	0.22	30,30,30,30	0
3	SO4	A	202	5/5	0.98	0.15	30,30,30,30	0

6.5 Other polymers [i](#)

There are no such residues in this entry.