



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 25, 2020 – 12:15 am BST

PDB ID : 3BE6  
Title : Crystal structure of FitE (crystal form 2), a group III periplasmic siderophore binding protein  
Authors : Shi, R.; Matte, A.; Cygler, M.; Montreal-Kingston Bacterial Structural Genomics Initiative (BSGI)  
Deposited on : 2007-11-16  
Resolution : 1.82 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](mailto: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.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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)	:	2.11

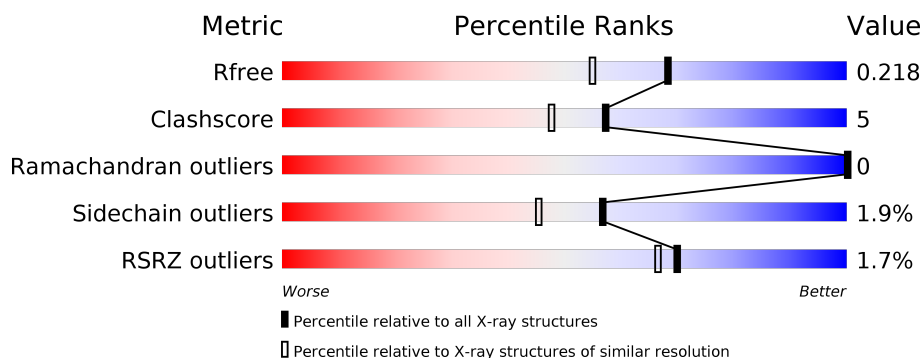
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.82 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	7484 (1.84-1.80)
Clashscore	141614	8401 (1.84-1.80)
Ramachandran outliers	138981	8290 (1.84-1.80)
Sidechain outliers	138945	8290 (1.84-1.80)
RSRZ outliers	127900	7371 (1.84-1.80)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	297	<div> <div>2%</div> <div>90%</div> <div>8%</div> <div>..</div> </div>
1	B	297	<div> <div>%</div> <div>86%</div> <div>12%</div> <div>..</div> </div>
1	C	297	<div> <div>%</div> <div>87%</div> <div>12%</div> <div>.</div> </div>
1	D	297	<div> <div>2%</div> <div>88%</div> <div>10%</div> <div>..</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	GOL	A	411	-	-	X	-
4	GOL	D	410	-	-	X	-

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9947 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 Putative iron compound-binding protein of ABC transporter family.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	294	Total	C	N	O	S	Se	0	8	0
			2303	1455	411	429	3	5			
1	B	292	Total	C	N	O	S	Se	0	6	0
			2271	1435	401	426	3	6			
1	C	294	Total	C	N	O	S	Se	0	4	0
			2278	1440	403	428	2	5			
1	D	292	Total	C	N	O	S	Se	0	4	0
			2262	1428	402	425	2	5			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	259	THR	ALA	SEE REMARK 999	UNP Q8XBR1
B	259	THR	ALA	SEE REMARK 999	UNP Q8XBR1
C	259	THR	ALA	SEE REMARK 999	UNP Q8XBR1
D	259	THR	ALA	SEE REMARK 999	UNP Q8XBR1

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Cl	0	0
			1	1		
2	D	4	Total	Cl	0	0
			4	4		
2	C	2	Total	Cl	0	0
			2	2		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Mg 1 1	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 6 3 3	0	0
4	C	1	Total C O 6 3 3	0	0
4	D	1	Total C O 6 3 3	0	0

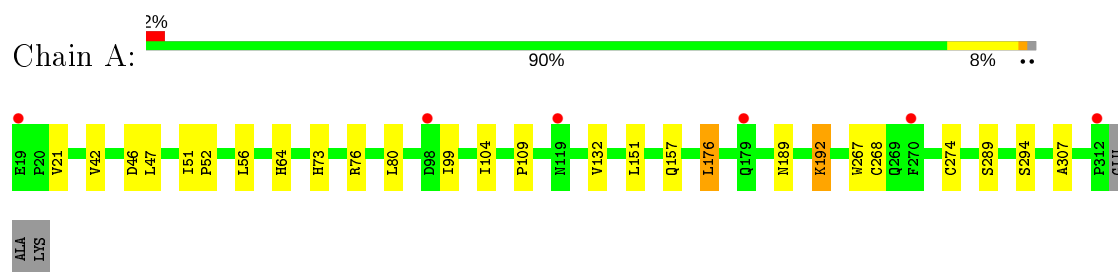
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	228	Total O 228 228	0	0
5	B	220	Total O 220 220	0	0
5	C	183	Total O 183 183	0	0
5	D	176	Total O 176 176	0	0

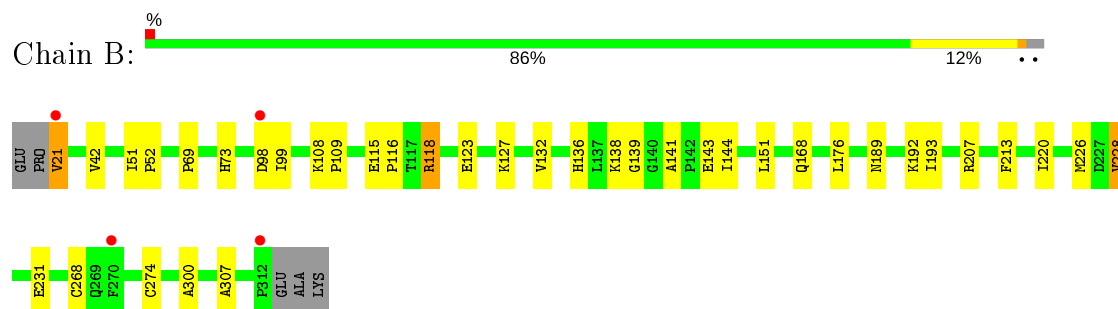
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

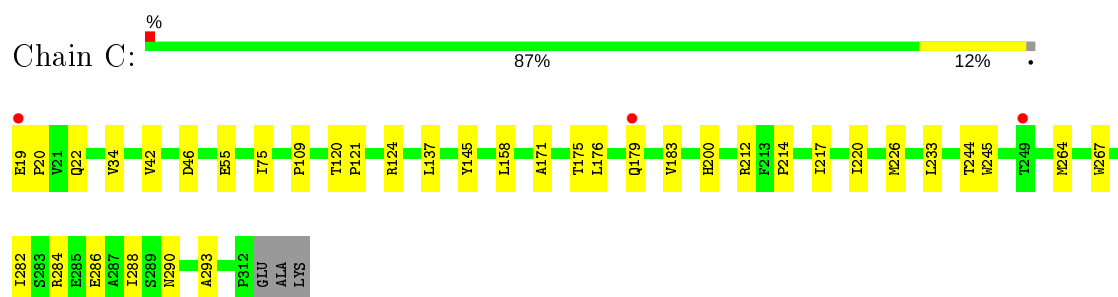
- Molecule 1: Putative iron compound-binding protein of ABC transporter family



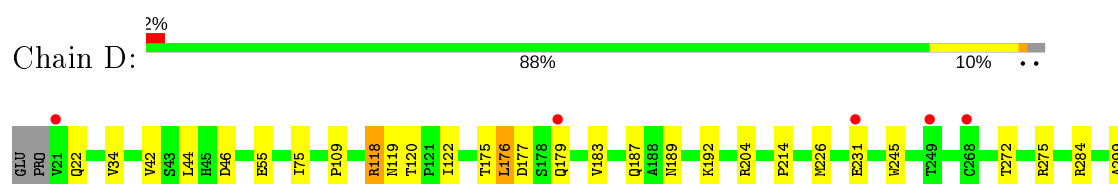
- Molecule 1: Putative iron compound-binding protein of ABC transporter family

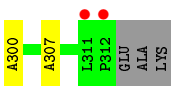


- Molecule 1: Putative iron compound-binding protein of ABC transporter family



- Molecule 1: Putative iron compound-binding protein of ABC transporter family





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	50.81Å 109.12Å 221.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.45 – 1.82 49.47 – 1.82	Depositor EDS
% Data completeness (in resolution range)	92.0 (49.45-1.82) 92.0 (49.47-1.82)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.77 (at 1.82Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.188 , 0.219 0.188 , 0.218	Depositor DCC
$R_{free}$ test set	5120 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	18.4	Xtriage
Anisotropy	0.848	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 50.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	9947	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.91% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, MG, CL

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	0.41	0/2363	0.54	0/3198
1	B	0.40	0/2321	0.51	0/3143
1	C	0.40	0/2329	0.52	0/3154
1	D	0.39	0/2312	0.52	0/3130
All	All	0.40	0/9325	0.52	0/12625

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	2303	0	2361	17	0
1	B	2271	0	2317	28	0
1	C	2278	0	2322	26	0
1	D	2262	0	2304	20	0
2	A	1	0	0	0	0
2	C	2	0	0	1	0
2	D	4	0	0	0	0
3	A	1	0	0	0	0
4	A	6	0	8	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	6	0	8	3	0
4	D	6	0	8	5	0
5	A	228	0	0	1	0
5	B	220	0	0	3	0
5	C	183	0	0	4	0
5	D	176	0	0	3	0
All	All	9947	0	9328	89	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 5.

The worst 5 of 89 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:B:118:ARG:HD3	5:B:1087:HOH:O	1.73	0.89
1:A:268:CYS:HG	1:A:274[A]:CYS:HG	1.22	0.84
4:C:409:GOL:H12	5:C:525:HOH:O	1.85	0.74
1:C:171:ALA:HB3	4:C:409:GOL:O2	1.90	0.70
1:B:123:GLU:O	1:B:127:LYS:HE2	1.92	0.69

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	300/297 (101%)	296 (99%)	4 (1%)	0	100	100
1	B	296/297 (100%)	290 (98%)	6 (2%)	0	100	100
1	C	296/297 (100%)	293 (99%)	3 (1%)	0	100	100
1	D	294/297 (99%)	291 (99%)	3 (1%)	0	100	100
All	All	1186/1188 (100%)	1170 (99%)	16 (1%)	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	253/242 (104%)	250 (99%)	3 (1%)	71	64
1	B	249/242 (103%)	242 (97%)	7 (3%)	43	29
1	C	249/242 (103%)	247 (99%)	2 (1%)	81	77
1	D	247/242 (102%)	239 (97%)	8 (3%)	39	24
All	All	998/968 (103%)	978 (98%)	20 (2%)	57	43

5 of 20 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	231	GLU
1	C	137	LEU
1	D	122	ILE
1	B	138	LYS
1	B	228	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	168	GLN
1	B	170	ASN
1	C	290	ASN
1	B	157	GLN
1	C	170	ASN

### 5.3.3 RNA ⓘ

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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 8 are monoatomic - leaving 3 for Mogul analysis.

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	$\# Z  > 2$
4	GOL	A	411	-	5,5,5	0.39	0	5,5,5	0.41	0
4	GOL	C	409	-	5,5,5	0.52	0	5,5,5	0.60	0
4	GOL	D	410	-	5,5,5	0.53	0	5,5,5	0.51	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	A	411	-	-	1/4/4/4	-
4	GOL	C	409	-	-	2/4/4/4	-
4	GOL	D	410	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	410	GOL	O1-C1-C2-C3
4	C	409	GOL	O1-C1-C2-C3
4	D	410	GOL	O1-C1-C2-O2
4	C	409	GOL	O1-C1-C2-O2
4	A	411	GOL	O1-C1-C2-C3

There are no ring outliers.

3 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	411	GOL	4	0
4	C	409	GOL	3	0
4	D	410	GOL	5	0

## 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 [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	289/297 (97%)	-0.15	6 (2%) 63 59	12, 18, 31, 37	1 (0%)
1	B	287/297 (96%)	-0.14	4 (1%) 75 72	12, 19, 30, 34	1 (0%)
1	C	289/297 (97%)	-0.10	3 (1%) 82 80	12, 19, 31, 36	0
1	D	287/297 (96%)	-0.13	7 (2%) 59 54	13, 20, 32, 36	1 (0%)
All	All	1152/1188 (96%)	-0.13	20 (1%) 70 66	12, 19, 31, 37	3 (0%)

The worst 5 of 20 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	249	THR	5.3
1	B	312	PRO	3.7
1	A	312	PRO	3.7
1	D	312	PRO	3.4
1	B	98	ASP	3.4

### 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 carbohydrates 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, 95<sup>th</sup> 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
4	GOL	C	409	6/6	0.86	0.32	27,29,29,32	0
4	GOL	D	410	6/6	0.89	0.35	29,30,31,33	0
4	GOL	A	411	6/6	0.91	0.19	27,30,30,32	0
2	CL	C	401	1/1	0.95	0.07	30,30,30,30	0
2	CL	D	406	1/1	0.96	0.14	31,31,31,31	0
3	MG	A	408	1/1	0.97	0.26	30,30,30,30	0
2	CL	C	405	1/1	0.98	0.05	26,26,26,26	0
2	CL	D	402	1/1	0.98	0.04	27,27,27,27	0
2	CL	D	403	1/1	0.99	0.06	21,21,21,21	0
2	CL	A	404	1/1	0.99	0.03	27,27,27,27	0
2	CL	D	407	1/1	0.99	0.09	30,30,30,30	0

## 6.5 Other polymers

There are no such residues in this entry.