



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 08:04 PM UTC

PDB ID : 5N8J / pdb_00005n8j
Title : CRYSTAL STRUCTURE OF STREPTAVIDIN WITH PEPTIDE D-amino acid containing peptide GyGlanvdessG
Authors : Lyamichev, V.; Goodrich, L.; Sullivan, E.; Bannen, R.; Benz, J.; Albert, T.; Patel, J.
Deposited on : 2017-02-23
Resolution : 1.05 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
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

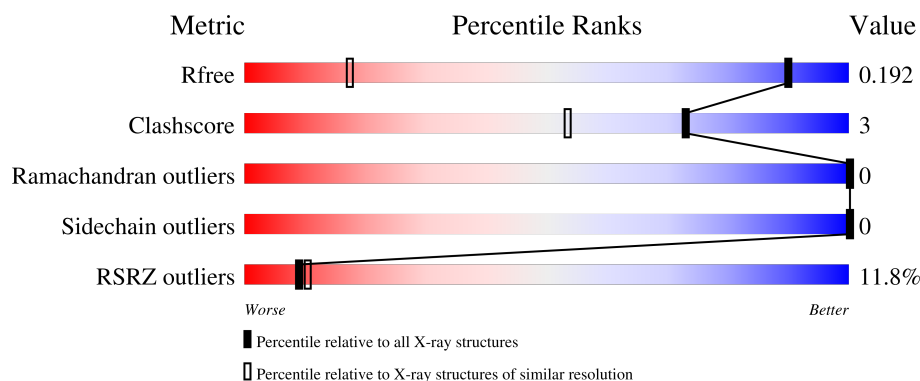
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.05 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	1182 (1.08-1.04)
Clashscore	190562	1204 (1.08-1.04)
Ramachandran outliers	187476	1175 (1.08-1.04)
Sidechain outliers	187428	1176 (1.08-1.04)
RSRZ outliers	180081	1181 (1.08-1.04)

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	183	9% 63% 33%
1	B	183	8% 62% 34%
1	C	183	5% 61% 34%
1	D	183	8% 64% 34%
2	E	12	8% 58% 8% 33%

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Mol	Chain	Length	Quality of chain
2	O	12	 58%42%
2	P	12	 67%8%25%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4571 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 Streptavidin.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	122	Total	C	N	O	0	7	0
			941	594	158	189			
1	B	120	Total	C	N	O	0	7	0
			926	584	156	186			
1	C	120	Total	C	N	O	0	6	0
			923	582	157	184			
1	D	120	Total	C	N	O	0	5	0
			917	578	156	183			

- Molecule 2 is a protein (with D amino acids) called GLY-DTY-GLY-DLE-DAL-DSG-DVA-DAS-DGL-DSN-DSN-GLY.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	P	9	Total	C	N	O	0	0	0
			61	35	10	16			
2	O	7	Total	C	N	O	0	0	0
			51	30	8	13			
2	E	8	Total	C	N	O	0	0	0
			55	32	9	14			

- Molecule 3 is ISOPROPYL ALCOHOL (CCD ID: IPA) (formula: C₃H₈O).

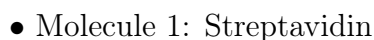
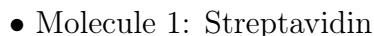
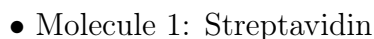


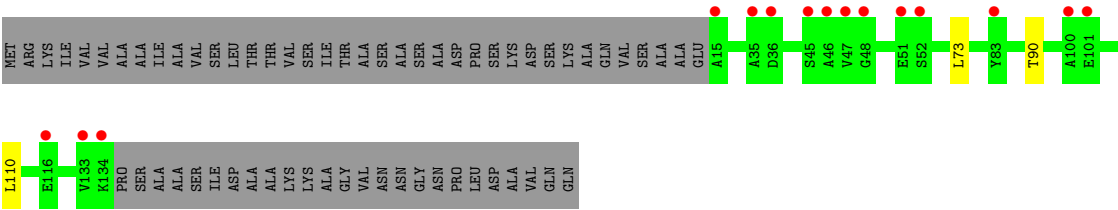
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total	C	O	0	0
			4	3	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	177	Total	O	0	0
			177	177		
4	B	154	Total	O	0	3
			157	157		
4	C	176	Total	O	0	1
			177	177		
4	D	161	Total	O	0	0
			161	161		
4	P	15	Total	O	0	0
			15	15		
4	O	3	Total	O	0	0
			3	3		
4	E	3	Total	O	0	0
			3	3		

- Molecule 1: Streptavidin

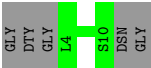




● Molecule 2: GLY-DTY-GLY-DLE-DAL-DSG-DVA-DAS-DGL-DSN-DSN-GLY



● Molecule 2: GLY-DTY-GLY-DLE-DAL-DSG-DVA-DAS-DGL-DSN-DSN-GLY



● Molecule 2: GLY-DTY-GLY-DLE-DAL-DSG-DVA-DAS-DGL-DSN-DSN-GLY



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	46.66Å 84.88Å 57.75Å 90.00° 99.10° 90.00°	Depositor
Resolution (Å)	57.09 – 1.05 57.03 – 1.05	Depositor EDS
% Data completeness (in resolution range)	99.9 (57.09-1.05) 99.9 (57.03-1.05)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.47 (at 1.05Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.169 , 0.193 (Not available) , 0.192	Depositor DCC
R_{free} test set	10213 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	12.1	Xtriage
Anisotropy	0.464	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 33.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	4571	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.39% 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: DAL, DSN, DSG, DGL, IPA, DVA, DAS, DLE

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	0.62	0/983	0.73	0/1347
1	B	0.64	0/967	0.74	0/1324
1	C	0.57	0/961	0.72	0/1315
1	D	0.60	0/952	0.75	0/1303
2	E	1.45	0/3	0.10	0/2
2	P	1.49	0/3	0.39	0/2
All	All	0.61	0/3869	0.73	0/5293

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	941	0	899	9	0
1	B	926	0	883	6	0
1	C	923	0	880	8	0
1	D	917	0	872	4	0
2	E	55	0	40	1	0
2	O	51	0	42	0	0
2	P	61	0	49	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	4	0	8	3	0
4	A	177	0	0	3	0
4	B	157	0	0	4	1
4	C	177	0	0	1	1
4	D	161	0	0	0	0
4	E	3	0	0	0	0
4	O	3	0	0	0	0
4	P	15	0	0	0	0
All	All	4571	0	3673	24	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 3.

All (24) 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:40[A]:THR:HG22	4:A:231:HOH:O	1.74	0.86
1:B:40[A]:THR:HG22	4:B:223:HOH:O	1.85	0.76
1:B:129[B]:THR:HG23	4:B:317:HOH:O	1.93	0.66
3:C:201:IPA:H32	4:C:341:HOH:O	2.00	0.60
1:A:40[A]:THR:CG2	4:A:231:HOH:O	2.40	0.59
1:A:57[A]:THR:HG21	1:C:57[A]:THR:OG1	2.07	0.55
1:A:57[A]:THR:HG23	4:A:231:HOH:O	2.06	0.54
1:A:57[A]:THR:CG2	1:C:57[A]:THR:OG1	2.56	0.53
1:B:40[A]:THR:CG2	4:B:223:HOH:O	2.52	0.52
1:B:103:ARG:HD3	1:B:131:THR:HG22	1.92	0.51
1:A:57[A]:THR:HG22	1:C:57[A]:THR:CG2	2.42	0.49
1:B:90:THR:OG1	2:E:6:DSG:ND2	2.47	0.47
1:A:84:ARG:HG2	1:A:85:ASN:N	2.30	0.46
1:A:110:LEU:C	1:A:110:LEU:HD23	2.40	0.46
1:B:24:GLN:NE2	4:B:204:HOH:O	2.50	0.45
1:D:90:THR:OG1	2:P:4:DSG:ND2	2.51	0.43
1:C:90:THR:OG1	3:C:201:IPA:H33	2.19	0.43
1:D:90:THR:HG1	1:D:110:LEU:HD13	1.85	0.42
1:D:90:THR:OG1	1:D:110:LEU:HD13	2.19	0.42
1:C:108:TRP:CE2	3:C:201:IPA:H11	2.55	0.41
1:C:23:ASN:HB3	1:C:130:PHE:CE2	2.56	0.41
1:C:131:THR:OG1	1:C:133:VAL:O	2.35	0.41
1:A:91:THR:HB	1:C:91:THR:HB	2.02	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:350:HOH:O	4:C:445:HOH:O[2_655]	2.16	0.04

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	126/183 (69%)	124 (98%)	2 (2%)	0	100	100
1	B	124/183 (68%)	122 (98%)	2 (2%)	0	100	100
1	C	123/183 (67%)	121 (98%)	2 (2%)	0	100	100
1	D	122/183 (67%)	120 (98%)	2 (2%)	0	100	100
All	All	495/732 (68%)	487 (98%)	8 (2%)	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	96/134 (72%)	96 (100%)	0	100	100
1	B	94/134 (70%)	94 (100%)	0	100	100
1	C	93/134 (69%)	93 (100%)	0	100	100
1	D	92/134 (69%)	92 (100%)	0	100	100
All	All	375/536 (70%)	375 (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 (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	82	ASN
1	B	82	ASN
1	C	82	ASN
1	D	82	ASN
1	D	127	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

22 non-standard protein/DNA/RNA residues are modelled in this entry.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

1 ligand is 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	IPA	C	201	-	3,3,3	1.63	1 (33%)	3,3,3	0.87	0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	201	IPA	O2-C2	2.19	1.56	1.42

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	201	IPA	3	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 ⓘ

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	122/183 (66%)	0.60	16 (13%) 7 8	6, 14, 25, 40	8 (6%)
1	B	120/183 (65%)	0.60	15 (12%) 8 9	5, 13, 28, 33	8 (6%)
1	C	120/183 (65%)	0.53	10 (8%) 17 20	6, 15, 26, 32	7 (5%)
1	D	120/183 (65%)	0.66	15 (12%) 8 9	6, 15, 25, 38	6 (5%)
2	E	1/12 (8%)	3.13	1 (100%) 0 0	32, 32, 32, 32	0
2	O	0/12	-	-	-	-
2	P	1/12 (8%)	1.21	0 100 100	15, 15, 15, 15	0
All	All	484/768 (63%)	0.60	57 (11%) 9 10	5, 14, 26, 40	29 (5%)

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	15	ALA	7.6
1	B	46	ALA	7.3
1	B	47	VAL	6.3
1	D	100	ALA	6.1
1	B	83	TYR	5.5
1	C	100	ALA	4.8
1	D	15	ALA	4.7
1	C	133	VAL	4.5
1	D	46	ALA	4.5
1	A	30	ILE	4.3
1	D	101	GLU	3.8
1	D	47	VAL	3.8
1	B	25	LEU	3.8
1	A	24	GLN	3.7
1	B	48	GLY	3.6
1	B	45	SER	3.4
1	A	15	ALA	3.4
1	A	100	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
1	D	35	ALA	3.3
1	A	99	GLY	3.3
1	D	51	GLU	3.2
2	E	3	GLY	3.1
1	C	47	VAL	3.1
1	D	45	SER	3.0
1	B	84	ARG	2.8
1	B	26	GLY	2.8
1	A	135	PRO	2.7
1	C	98	GLY	2.7
1	C	46	ALA	2.7
1	A	14	GLU	2.6
1	D	52	SER	2.6
1	B	66	THR	2.6
1	C	84	ARG	2.6
1	C	35	ALA	2.5
1	A	120	TRP	2.4
1	A	29	PHE	2.4
1	C	49	ASN	2.3
1	A	101	GLU	2.3
1	B	15	ALA	2.3
1	B	100	ALA	2.3
1	A	83	TYR	2.3
1	D	83	TYR	2.3
1	B	82	ASN	2.3
1	A	98	GLY	2.3
1	D	133	VAL	2.3
1	D	36	ASP	2.3
1	C	116	GLU	2.2
1	B	50	ALA	2.2
1	B	133	VAL	2.2
1	D	48	GLY	2.2
1	A	16	GLY	2.2
1	D	134	LYS	2.2
1	B	27	SER	2.1
1	A	116	GLU	2.1
1	A	97[A]	VAL	2.0
1	A	66	THR	2.0
1	D	116	GLU	2.0

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

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(Å ²)	Q<0.9
2	DAL	E	5	5/6	0.81	0.15	18,18,19,20	0
2	DSN	P	9	6/7	0.83	0.12	19,20,23,25	0
2	DAS	E	8	8/9	0.85	0.11	20,22,27,28	0
2	DSN	E	10	6/7	0.86	0.10	22,22,23,26	0
2	DLE	E	4	8/9	0.86	0.13	20,22,26,28	0
2	DVA	E	7	7/8	0.89	0.11	18,20,21,21	0
2	DGL	E	9	9/10	0.91	0.11	19,21,23,23	0
2	DAL	P	3	5/6	0.91	0.11	12,12,13,14	0
2	DVA	P	5	7/8	0.91	0.10	13,14,15,15	0
2	DAS	P	6	8/9	0.92	0.09	13,15,17,17	0
2	DLE	O	4	8/9	0.93	0.10	15,17,22,22	0
2	DSG	E	6	8/9	0.93	0.11	11,17,18,19	0
2	DGL	P	7	9/10	0.93	0.09	14,15,17,17	0
2	DLE	P	2	8/9	0.94	0.09	12,14,18,19	0
2	DSN	O	10	6/7	0.94	0.07	14,15,16,17	0
2	DSG	P	4	8/9	0.95	0.08	9,12,12,14	0
2	DAS	O	8	8/9	0.95	0.08	14,17,22,24	0
2	DSN	P	8	6/7	0.96	0.06	15,15,17,18	0
2	DGL	O	9	9/10	0.97	0.06	13,14,15,15	0
2	DVA	O	7	7/8	0.97	0.06	13,14,14,16	0
2	DAL	O	5	5/6	0.98	0.06	13,14,14,15	0
2	DSG	O	6	8/9	0.98	0.05	11,12,13,13	0

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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.

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	IPA	C	201	4/4	0.85	0.22	6,11,14,19	0

6.5 Other polymers [i](#)

There are no such residues in this entry.