



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 03:37 PM UTC

PDB ID : 1LXT / pdb_00001lxt
Title : STRUCTURE OF PHOSPHOTRANSFERASE PHOSPHOGLUCOMUTASE
FROM RABBIT
Authors : Ray Junior, W.J.; Baranidharan, S.; Liu, Y.
Deposited on : 1996-07-28
Resolution : 2.70 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

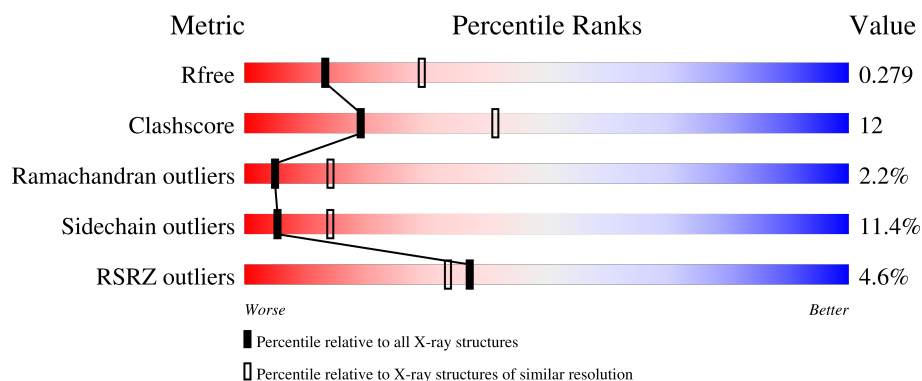
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	561	8% 48% 37% 13% .
1	B	561	% 50% 38% 11% .

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 9060 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.

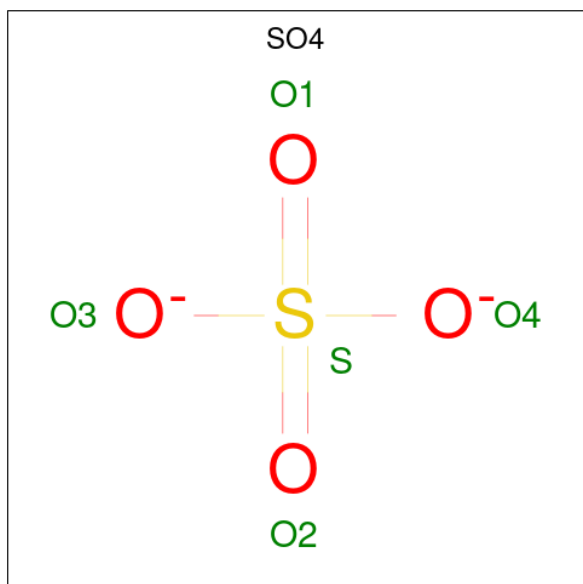
- Molecule 1 is a protein called PHOSPHOGLUCOMUTASE (DEPHOSPHO FORM).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	561	Total	C	N	O	S	0	0	0
			4329	2753	743	817	16			
1	B	561	Total	C	N	O	S	0	0	0
			4329	2753	743	817	16			

- Molecule 2 is CADMIUM ION (CCD ID: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Cd	0	0
			1	1		
2	B	1	Total	Cd	0	0
			1	1		

- 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	B	1	Total	O	S	0	0
			5	4	1		

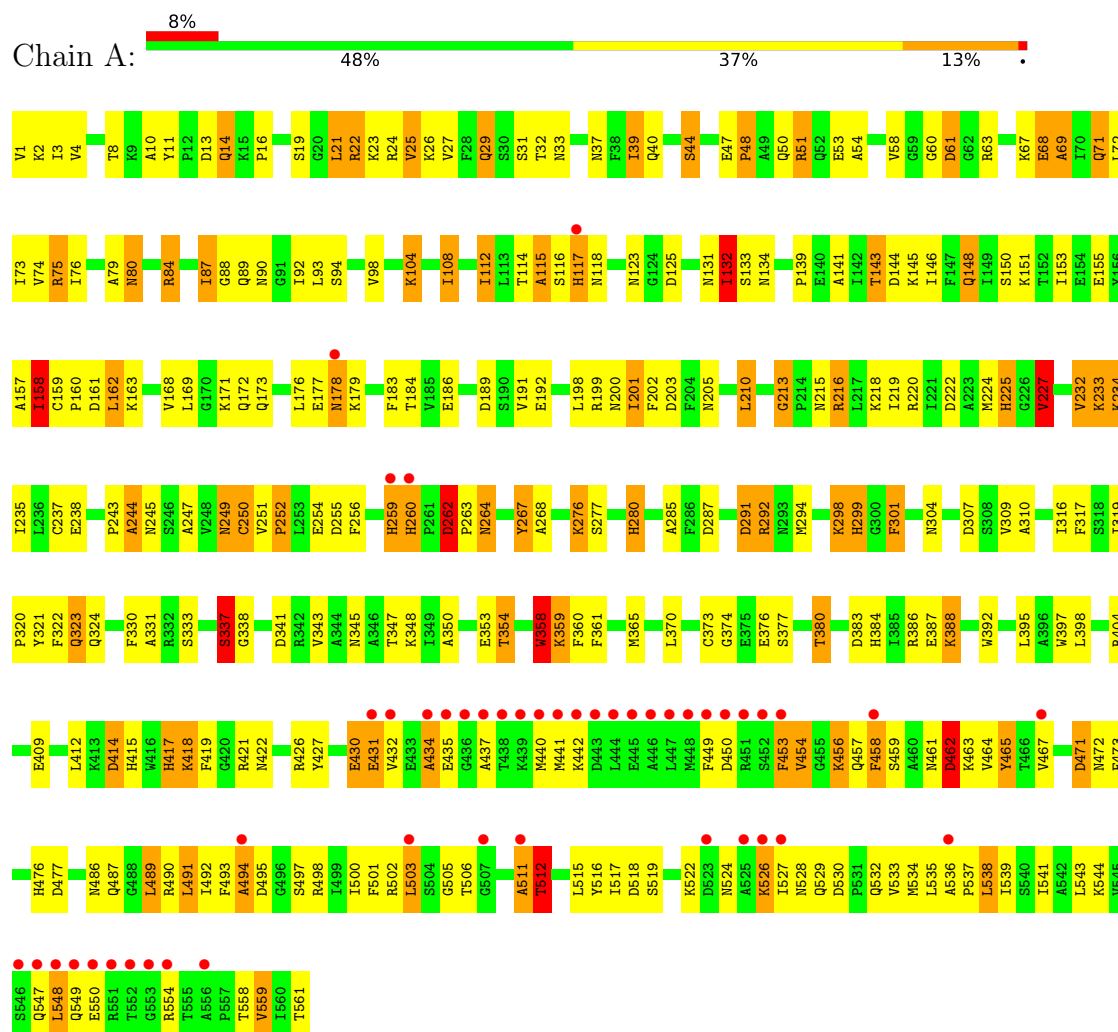
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	157	Total	O	0	0
			157	157		
4	B	233	Total	O	0	0
			233	233		

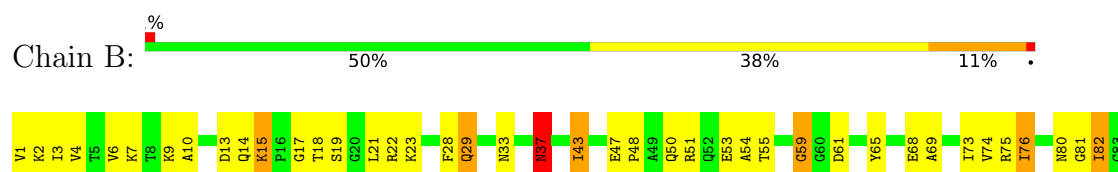
3 Residue-property plots

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: PHOSPHOGLUCOMUTASE (DEPHOSPHO FORM)



• Molecule 1: PHOSPHOGLUCOMUTASE (DEPHOSPHO FORM)



R84	G167	A247	V327	K413	G488
L85	V168	V248	R328	D414	L489
V86	L169	N249	G329	H415	R490
I87	G170	C250	S337	W416	L491
Q88	K171	E254	G338	H417	L492
N90	Q172			K418	F493
	Q173			F419	A494
		H259	D341	G420	
L93	L176	H260	R342	R421	S497
S94	E177	P261	V343	N422	R498
T95	N178	D262	A344		L499
P96	K179	P263	N345	T425	I500
A97	F180	N264	A346	R426	F501
V98	K181	L285	T347	Y427	R502
S99	P182	Y267	R348	D428	L503
	F183			Y429	S504
I102	T184	D270	T354	E430	G505
R103	V185	L271		F431	T506
K104			R358	Y432	G507
I105	V188		K359	F433	S508
K106	V191	K276	N363	A434	A509
A107	E192	E279	L364	E435	G510
I108		H280	N365	T438	A511
	T196	D281		K439	T512
I112		F282	S368		
L113			R369	K442	L515
		D287	L370		Y516
S116	R199		S371	M448	I517
H117	N200		L372	F449	D518
N118	T201			D450	S519
P119	L210	G290	E376	R451	Y520
	L211	D291	S377	F452	
N131	S212	R292	F378	F453	N524
I132	G213	N293	G379	R456	I527
S133	P214		T380	D457	G529
		L296	G381		
A138	R216	G297	S382	R461	M534
P139	L217	K298	D383	D462	L535
E140	T219	H299	H384	K463	A536
		V303	T385	V464	P537
T143	R220	N304	R386	Y465	L538
D144	T221	P305	E387		
	D222	S306	K388	K469	A542
F147	H225	D307	D389	D470	L543
Q148	G226	S308		D471	K544
I149	V227		W392	N472	
S150		V311		F473	O549
K151			V397	E474	R550
T152	V232		I398	Y475	R551
I153		N315	S399	H476	T552
E154	L236	F316	L400		G553
E155	C237	S318	L401	V479	R554
	E238	E239	A402		
P160	L240		T403	V483	
D161		F322	R404	S484	P557
I162		Q323	K405	K485	
K163	P243	G324	T325	N486	T561
V164	A244				
D165	S246				

4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	174.42Å 174.42Å 101.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 2.70 6.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	82.0 (6.00-2.70) 84.6 (6.00-2.70)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.84 (at 2.69Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.201 , 0.260 0.246 , 0.279	Depositor DCC
R_{free} test set	3815 reflections (10.08%)	wwPDB-VP
Wilson B-factor (Å ²)	33.0	Xtriage
Anisotropy	0.700	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 100.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	9060	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.48% 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: SO4, CD

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	1.08	13/4416 (0.3%)	2.16	210/5969 (3.5%)
1	B	1.16	21/4416 (0.5%)	2.18	187/5969 (3.1%)
All	All	1.12	34/8832 (0.4%)	2.17	397/11938 (3.3%)

The worst 5 of 34 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	117	HIS	CD2-NE2	-10.79	1.25	1.37
1	A	117	HIS	CD2-NE2	-10.09	1.26	1.37
1	B	117	HIS	CG-ND1	-7.33	1.30	1.38
1	A	225	HIS	CD2-NE2	-6.98	1.30	1.37
1	B	102	ILE	CA-CB	6.76	1.61	1.54

The worst 5 of 397 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	291	ASP	CA-CB-CG	14.09	126.69	112.60
1	A	527	ILE	N-CA-C	11.16	121.99	110.72
1	A	547	GLN	OE1-CD-NE2	-10.93	111.67	122.60
1	B	192	GLU	N-CA-C	10.84	124.11	111.11
1	B	168	VAL	N-CA-C	10.43	124.00	107.73

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	4329	0	4332	105	0
1	B	4329	0	4332	98	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
4	A	157	0	0	6	0
4	B	233	0	0	12	0
All	All	9060	0	8664	203	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 12.

The worst 5 of 203 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:309:VAL:HG21	1:A:374:GLY:HA3	1.63	0.78
1:B:306:SER:HB3	1:B:337:SER:HB3	1.69	0.74
1:A:16:PRO:HB2	1:A:143:THR:HG22	1.68	0.74
1:A:292:ARG:HD3	1:A:377:SER:O	1.90	0.71
1:B:1:VAL:HG23	1:B:176:LEU:HD23	1.74	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	559/561 (100%)	499 (89%)	44 (8%)	16 (3%)	3 9
1	B	559/561 (100%)	505 (90%)	45 (8%)	9 (2%)	7 20

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1118/1122 (100%)	1004 (90%)	89 (8%)	25 (2%)	5	14

5 of 25 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	216	ARG
1	A	301	PHE
1	A	431	GLU
1	A	494	ALA
1	B	348	LYS

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	462/462 (100%)	404 (87%)	58 (13%)	4	11
1	B	462/462 (100%)	415 (90%)	47 (10%)	7	18
All	All	924/924 (100%)	819 (89%)	105 (11%)	5	14

5 of 105 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	561	THR
1	B	117	HIS
1	B	451	ARG
1	B	15	LYS
1	B	53	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	37	ASN
1	B	476	HIS
1	B	528	ASN

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Mol	Chain	Res	Type
1	B	487	GLN
1	A	249	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](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	$\# Z > 2$
3	SO4	B	563	2	4,4,4	0.33	0	6,6,6	0.16	0
3	SO4	A	563	2	4,4,4	0.60	0	6,6,6	0.75	0

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.

5.7 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, 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	561/561 (100%)	0.28	47 (8%) 17 14	0, 37, 91, 98	0
1	B	561/561 (100%)	-0.33	5 (0%) 81 80	3, 24, 56, 84	0
All	All	1122/1122 (100%)	-0.02	52 (4%) 37 34	0, 29, 81, 98	0

The worst 5 of 52 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	450	ASP	9.0
1	A	437	ALA	7.8
1	A	436	GLY	7.7
1	A	438	THR	7.6
1	A	452	SER	7.5

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	B	563	5/5	0.79	0.23	82,82,83,84	0
3	SO4	A	563	5/5	0.86	0.19	76,76,77,77	0
2	CD	A	562	1/1	0.97	0.25	2,2,2,2	0
2	CD	B	562	1/1	0.98	0.23	2,2,2,2	0

6.5 Other polymers [i](#)

There are no such residues in this entry.