Full wwPDB X-ray Structure Validation Report (i)

Oct 27, 2026 – 02:08 PM EDT

PDB ID	:	39CB / pdb_000039cb
Title	:	perdeuterated M379A tyrosine phenol lyase apoenzyme
Authors	:	Phillips, R.S.; Kovalevsky, A.
Deposited on	:	2026-09-29
Resolution	:	2.00 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 (i) 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 (1)) were used in the production of this report:

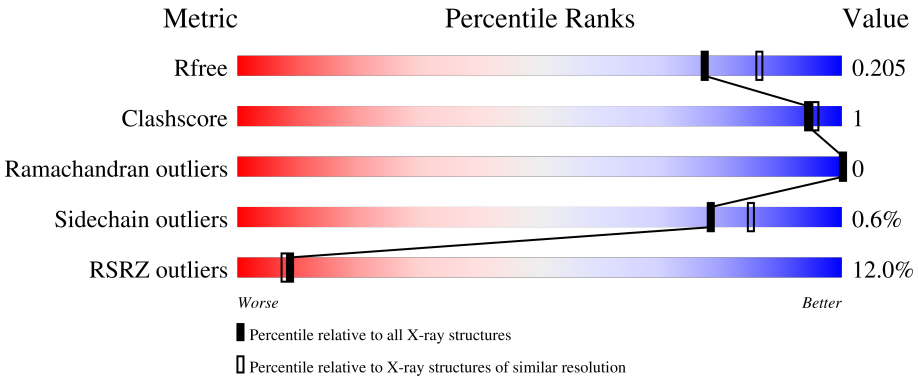
MolProbity	:	4-5-2 with Phenix2.2
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.2
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

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 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	456	13% 89% · 8%
1	B	456	9% 86% · 10%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 7184 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 Tyrosine phenol-lyase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	420	Total	C	N	O	S	0	17	0
			3434	2179	585	642	28			
1	B	412	Total	C	N	O	S	0	10	0
			3325	2110	568	622	25			

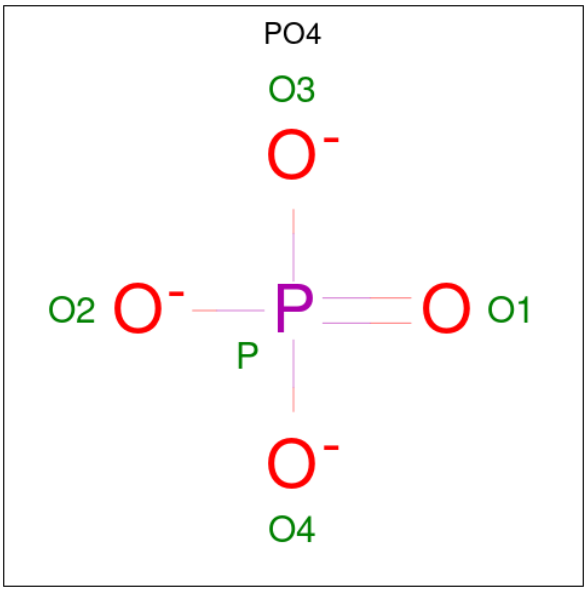
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	205	ALA	GLU	conflict	UNP P31013
A	379	ALA	MET	engineered mutation	UNP P31013
B	205	ALA	GLU	conflict	UNP P31013
B	379	ALA	MET	engineered mutation	UNP P31013

- Molecule 2 is POTASSIUM ION (CCD ID: K) (formula: K).

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

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O P 5 4 1	0	0
3	B	1	Total O P 5 4 1	0	0

- Molecule 4 is water.

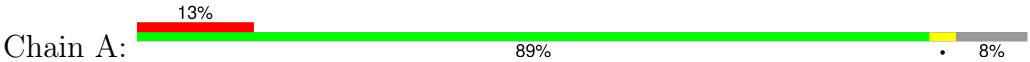
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	200	Total O 200 200	0	9
4	B	213	Total O 213 213	0	6

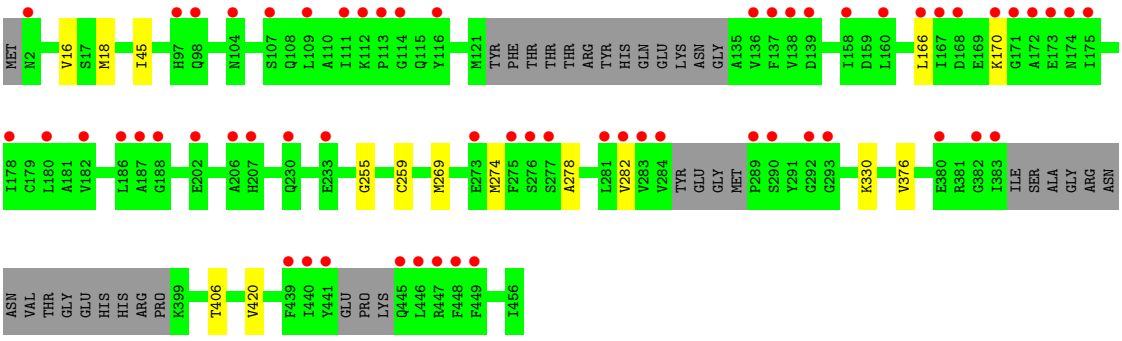
3 Residue-property plots (i)

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: Tyrosine phenol-lyase

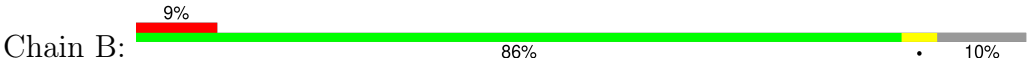
Chain A:

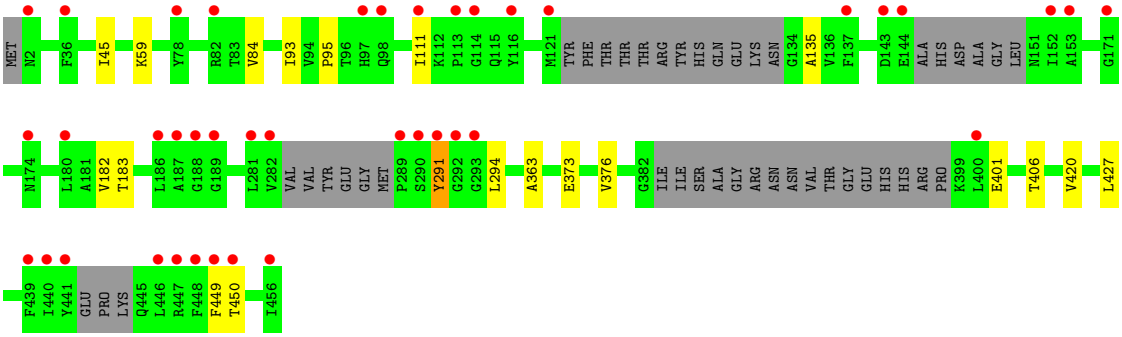




• Molecule 1: Tyrosine phenol-lyase

Chain B:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	137.99Å 75.94Å 94.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.81 – 2.00 29.81 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.0 (29.81-2.00) 99.0 (29.81-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.90 (at 2.00Å)	Xtriage
Refinement program	PHENIX 2.2.1_6174	Depositor
R, R_{free}	0.183 , 0.205 0.184 , 0.205	Depositor DCC
R_{free} test set	3402 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	26.8	Xtriage
Anisotropy	0.188	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 54.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	7184	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.25% of the height of the origin peak. No significant pseudotranslation is detected.*

[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

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, K

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	0.09	0/3514	0.26	0/4719
1	B	0.09	0/3393	0.27	0/4557
All	All	0.09	0/6907	0.27	0/9276

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

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	3434	0	3407	7	0
1	B	3325	0	3279	11	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	200	0	0	0	0
4	B	213	0	0	1	0
All	All	7184	0	6686	18	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 1.

All (18) 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:45:ILE:HB	1:A:376:VAL:HG22	1.85	0.58
1:A:376:VAL:HG21	1:A:420:VAL:HG22	1.88	0.56
1:B:45:ILE:HB	1:B:376:VAL:HG22	1.91	0.53
1:B:376:VAL:HG21	1:B:420:VAL:HG22	1.90	0.53
1:B:95:PRO:HG2	1:B:291[B]:TYR:HB3	1.91	0.52
1:A:166:LEU:HD12	1:A:170:LYS:HD3	1.94	0.49
1:B:363:ALA:HB2	1:B:401:GLU:HG3	1.94	0.48
1:A:16[A]:VAL:HG23	1:A:18[A]:MET:HG2	1.98	0.46
1:A:269:MET:HE2	1:A:274:MET:HG2	1.99	0.44
1:B:59:LYS:HD2	4:B:602[A]:HOH:O	2.17	0.44
1:B:449:PHE:CD2	1:B:450:THR:HG23	2.54	0.43
1:B:111:ILE:HG21	1:B:135:ALA:HB2	1.99	0.43
1:B:373:GLU:HG3	1:B:427:LEU:HD21	2.01	0.42
1:B:84:VAL:HG21	1:B:93:ILE:HD12	2.02	0.42
1:B:294:LEU:HD12	1:B:294:LEU:HA	1.89	0.41
1:A:278:ALA:O	1:A:282:VAL:HG23	2.20	0.41
1:B:182:VAL:HA	1:B:183:THR:HA	1.87	0.41
1:A:255:GLY:O	1:A:259:CYS:HB2	2.22	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	426/456 (93%)	418 (98%)	8 (2%)	0	100	100
1	B	410/456 (90%)	402 (98%)	8 (2%)	0	100	100
All	All	836/912 (92%)	820 (98%)	16 (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	363/377 (96%)	360 (99%)	3 (1%)	73 80
1	B	348/377 (92%)	345 (99%)	3 (1%)	70 78
All	All	711/754 (94%)	705 (99%)	6 (1%)	78 80

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

Mol	Chain	Res	Type
1	A	330[A]	LYS
1	A	330[B]	LYS
1	A	406	THR
1	B	291[A]	TYR
1	B	291[B]	TYR
1	B	406	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	321	GLN

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	PO4	B	502	-	4,4,4	1.50	1 (25%)	6,6,6	0.44	0
3	PO4	A	502	-	4,4,4	1.53	1 (25%)	6,6,6	0.53	0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	502	PO4	P-O1	2.68	1.56	1.50
3	B	502	PO4	P-O1	2.64	1.56	1.50

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

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	420/456 (92%)	0.61	60 (14%) 6 5	9, 34, 84, 118	17 (4%)
1	B	412/456 (90%)	0.39	40 (9%) 13 12	11, 29, 67, 110	10 (2%)
All	All	832/912 (91%)	0.50	100 (12%) 9 8	9, 31, 77, 118	27 (3%)

All (100) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	441	TYR	6.1
1	B	441	TYR	5.6
1	A	440	ILE	5.5
1	A	383	ILE	5.4
1	B	448	PHE	5.0
1	A	289	PRO	4.9
1	B	290	SER	4.8
1	B	289	PRO	4.6
1	B	188	GLY	4.5
1	B	440	ILE	4.4
1	A	446	LEU	4.4
1	A	175	ILE	4.4
1	A	283	VAL	4.3
1	A	172	ALA	4.2
1	A	439	PHE	4.2
1	B	113	PRO	4.1
1	A	448	PHE	4.1
1	A	136	VAL	4.1
1	B	446	LEU	3.9
1	B	449	PHE	3.9
1	A	186	LEU	3.8
1	B	291[A]	TYR	3.7
1	A	166	LEU	3.7
1	A	206	ALA	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	173	GLU	3.6
1	A	137	PHE	3.5
1	A	97[A]	HIS	3.5
1	A	187	ALA	3.5
1	B	174	ASN	3.5
1	B	189	GLY	3.5
1	B	186	LEU	3.4
1	B	439	PHE	3.3
1	B	36	PHE	3.3
1	A	116	TYR	3.2
1	B	78	TYR	3.2
1	A	284	VAL	3.2
1	B	152	ILE	3.2
1	A	292	GLY	3.1
1	A	447	ARG	3.1
1	A	207	HIS	3.1
1	B	114	GLY	3.0
1	B	153	ALA	3.0
1	A	281	LEU	3.0
1	B	180[A]	LEU	2.9
1	A	282	VAL	2.8
1	B	111	ILE	2.8
1	A	113	PRO	2.8
1	A	382	GLY	2.8
1	B	456	ILE	2.8
1	B	292[A]	GLY	2.8
1	A	111	ILE	2.8
1	A	139	ASP	2.7
1	A	202[A]	GLU	2.7
1	A	98	GLN	2.7
1	A	276	SER	2.7
1	A	158	ILE	2.7
1	A	188	GLY	2.7
1	A	445	GLN	2.5
1	A	182	VAL	2.5
1	B	447	ARG	2.5
1	B	121	MET	2.5
1	A	112	LYS	2.4
1	B	144	GLU	2.4
1	A	168	ASP	2.4
1	A	171	GLY	2.4
1	A	293	GLY	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	449	PHE	2.4
1	B	116	TYR	2.4
1	A	2	ASN	2.3
1	A	160	LEU	2.3
1	B	2	ASN	2.3
1	A	114	GLY	2.3
1	B	293[A]	GLY	2.3
1	A	138	VAL	2.3
1	A	380	GLU	2.3
1	A	174	ASN	2.3
1	B	400	LEU	2.3
1	B	82	ARG	2.3
1	A	273	GLU	2.3
1	A	180	LEU	2.3
1	A	109	LEU	2.2
1	B	281	LEU	2.2
1	B	137	PHE	2.2
1	B	187	ALA	2.2
1	B	97[A]	HIS	2.2
1	A	277	SER	2.2
1	B	143	ASP	2.2
1	B	450	THR	2.2
1	A	275	PHE	2.1
1	B	282	VAL	2.1
1	B	171	GLY	2.1
1	A	170	LYS	2.1
1	A	107	SER	2.1
1	A	167	ILE	2.1
1	A	290	SER	2.1
1	A	230	GLN	2.1
1	A	178	ILE	2.1
1	A	104	ASN	2.0
1	B	98	GLN	2.0
1	A	233	GLU	2.0

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, 95^{th} 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
3	PO4	B	502	5/5	0.94	0.14	38,41,47,67	0
3	PO4	A	502	5/5	0.95	0.10	36,42,45,51	0
2	K	A	501	1/1	0.96	0.06	27,27,27,27	1
2	K	B	501	1/1	0.96	0.28	53,53,53,53	0

6.5 Other polymers (i)

There are no such residues in this entry.