



Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 09:57 PM GMT

PDB ID : 3E9R
Title : Crystal structure of purine nucleoside phosphorylase from *Schistosoma mansoni* in complex with adenine
Authors : Pereira, H.M.; Rezende, M.M.; Oliva, G.; Garratt, R.C.
Deposited on : 2008-08-23
Resolution : 1.85 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

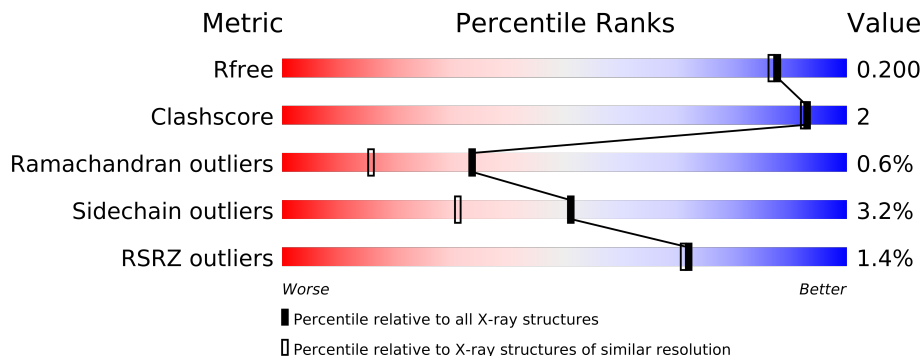
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 1.85 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}	66092	1269 (1.86-1.86)
Clashscore	79885	1470 (1.86-1.86)
Ramachandran outliers	78287	1451 (1.86-1.86)
Sidechain outliers	78261	1451 (1.86-1.86)
RSRZ outliers	66119	1269 (1.86-1.86)

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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	287	
1	B	287	
1	C	287	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	SO4	A	291	-	X
2	SO4	A	704	-	X
2	SO4	C	291	-	X
3	ACT	C	700	-	X

2 Entry composition

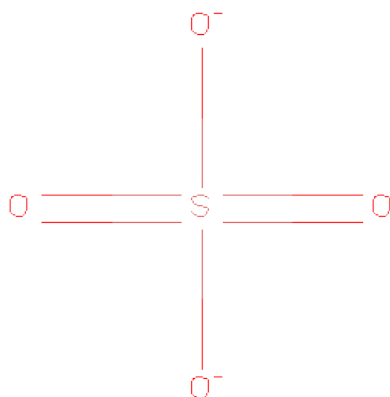
There are 6 unique types of molecules in this entry. The entry contains 7206 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Purine-nucleoside phosphorylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	285	Total	C	N	O	S	0	0	0
			2161	1376	372	399	14			
1	B	273	Total	C	N	O	S	0	1	0
			2066	1316	355	381	14			
1	C	284	Total	C	N	O	S	0	2	0
			2161	1378	373	396	14			

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



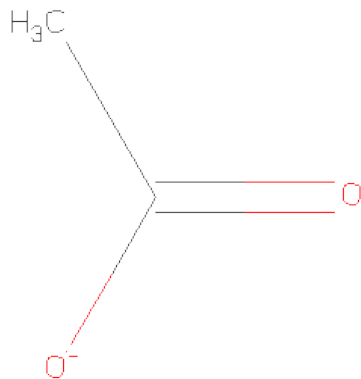
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

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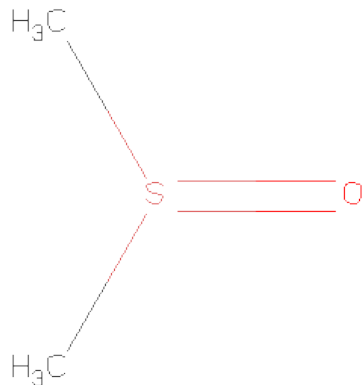
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is ACETATE ION (three-letter code: ACT) (formula: $\text{C}_2\text{H}_3\text{O}_2$).



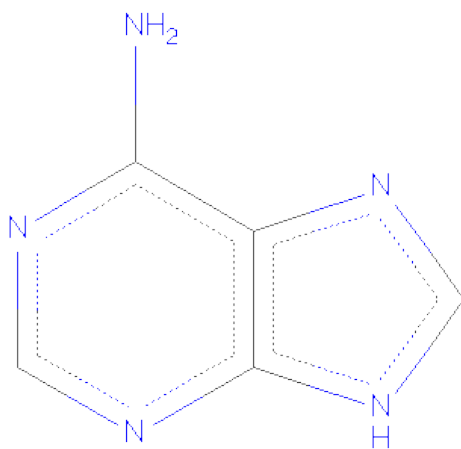
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: $\text{C}_2\text{H}_6\text{OS}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	S	0	0
			4	2	1	1		
4	B	1	Total	C	O	S	0	0
			4	2	1	1		
4	C	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 5 is ADENINE (three-letter code: ADE) (formula: C₅H₅N₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	N	0	0
			10	5	5		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	270	Total 270	O 270	0	0
6	B	240	Total 240	O 240	0	0
6	C	258	Total 258	O 258	0	0

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- Molecule 1: Purine-nucleoside phosphorylase

Diagram illustrating a protein structure with various domains and residues. The structure is composed of several colored blocks representing different regions: MET (grey), HIS (grey), E3 (green), S4 (green), V63 (yellow), V64 (yellow), L145 (yellow), V251 (yellow), E252 (yellow), N258 (yellow), K286 (yellow), and D287 (green). A red dot is positioned above the S4 block.

- Molecule 1: Purine-nucleoside phosphorylase

Amino Acid Category	Count
MET	1
HIS	1
GLU	1
S4	2
V5	2
N8	3
C33	3
G34	3
S35	3
K39	4
L40	4
A41	4
D42	4
F55	5
P56	5
S62	5
VAL	6
GLY	6
HIS	6
S67	6
R86	6
L100	6
K106	6
K111	6
L242	6
N245	6
L249	6
D250	6
V251	6
E252	6
S253	6
ASP	6
LEU	6
LYS	6
PRO	6
ASN	6
HIS	6
E260	6
E261	6
V262	6
S263	6

- Molecule 1: Purine-nucleoside phosphorylase

Sequence logo for the 12th position. The y-axis represents information content in bits (0 to 1.5). The x-axis lists amino acids. The most frequent amino acids at this position are V63 and V64, both around 1.4 bits. Other significant contributors include S4, L70, L75, R86, F87, H88, N166, R170, E226, L242, and D254, all around 1.0-1.1 bits. MET, HIS, and GLU have very low frequencies. K286 and D287 have very low frequencies, with D287 being slightly higher than K286.

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	48.99Å 120.00Å 130.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.03 – 1.85 41.03 – 1.85	Depositor EDS
% Data completeness (in resolution range)	96.6 (41.03-1.85) 96.6 (41.03-1.85)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.96 (at 1.86Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.162 , 0.201 0.160 , 0.200	Depositor DCC
R_{free} test set	3268 reflections (5.06%)	DCC
Wilson B-factor (Å ²)	21.2	Xtriage
Anisotropy	0.539	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 44.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 64600 reflections	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	7206	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.08% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ADE, DMS, SO4, ACT

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	0.38	0/2199	0.54	0/2978
1	B	0.37	0/2100	0.56	0/2840
1	C	0.39	0/2206	0.56	0/2988
All	All	0.38	0/6505	0.55	0/8806

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2161	0	0	0	0
1	B	2066	0	0	4	0
1	C	2161	0	0	7	0
2	A	10	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	1	0
3	A	4	0	0	0	0
3	C	4	0	0	1	0
4	A	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	4	0	0	0	0
4	C	4	0	6	0	0
5	B	10	0	0	0	0
6	A	270	0	0	0	0
6	B	240	0	0	2	0
6	C	258	0	0	5	0
All	All	7206	0	6	11	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 2.

All (11) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:166:ASN:N	6:C:863:HOH:O	2.11	0.83
1:B:252:GLU:O	1:C:170:ARG:NE	2.36	0.58
1:B:39:LYS:C	1:B:41:ALA:N	2.63	0.51
1:C:88:HIS:NE2	2:C:291:SO4:O1	2.46	0.48
3:C:700:ACT:CH3	6:C:849:HOH:O	2.61	0.48
1:C:254:ASP:CB	6:C:820:HOH:O	2.63	0.47
1:B:35:SER:C	6:B:927:HOH:O	2.54	0.46
1:C:63:VAL:O	1:C:64:VAL:C	2.55	0.43
1:C:226:GLU:CD	6:C:810:HOH:O	2.57	0.43
1:C:286:LYS:CG	6:C:950:HOH:O	2.67	0.42
1:B:106:LYS:NZ	6:B:931:HOH:O	2.52	0.42

There are no symmetry-related clashes.

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	283/287 (99%)	277 (98%)	5 (2%)	1 (0%)	43 24
1	B	268/287 (93%)	258 (96%)	7 (3%)	3 (1%)	21 6
1	C	284/287 (99%)	279 (98%)	4 (1%)	1 (0%)	43 24

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	835/861 (97%)	814 (98%)	16 (2%)	5 (1%)	33	16

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	41	ALA
1	B	42	ASP
1	C	286	LYS
1	A	64	VAL
1	B	35	SER

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	238/242 (98%)	232 (98%)	6 (2%)	60	42
1	B	224/242 (93%)	213 (95%)	11 (5%)	35	14
1	C	238/242 (98%)	233 (98%)	5 (2%)	66	50
All	All	700/726 (96%)	678 (97%)	22 (3%)	51	32

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	63	VAL
1	A	145	LEU
1	A	251	VAL
1	A	252	GLU
1	A	258	ASN
1	A	286	LYS
1	B	5	VAL
1	B	8	ASN
1	B	33	CYS
1	B	39	LYS
1	B	86	ARG
1	B	100	LEU
1	B	111	LYS

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Mol	Chain	Res	Type
1	B	242	LEU
1	B	245	ASN
1	B	249	LEU
1	B	250	ASP
1	C	70	LEU
1	C	75	LEU
1	C	86	ARG
1	C	242	LEU
1	C	286	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

10 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	$\# Z > 2$
2	SO4	A	291	-	4,4,4	5.46	4 (100%)	6,6,6	0.43	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ACT	A	700	-	1,3,3	3.19	1 (100%)	0,3,3	0.00	-
4	DMS	A	703	-	3,3,3	1.46	1 (33%)	3,3,3	0.48	0
2	SO4	A	704	-	4,4,4	5.77	4 (100%)	6,6,6	0.14	0
5	ADE	B	288	-	11,11,11	0.94	0	15,15,15	0.96	0
2	SO4	B	291	-	4,4,4	5.46	4 (100%)	6,6,6	0.17	0
4	DMS	B	703	-	3,3,3	1.34	0	3,3,3	0.59	0
2	SO4	C	291	-	4,4,4	5.43	4 (100%)	6,6,6	0.13	0
3	ACT	C	700	-	1,3,3	3.07	1 (100%)	0,3,3	0.00	-
4	DMS	C	703	-	3,3,3	1.43	1 (33%)	3,3,3	0.68	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
2	SO4	A	291	-	-	0/0/0/0	0/0/0/0
3	ACT	A	700	-	-	0/0/0/0	0/0/0/0
4	DMS	A	703	-	-	0/0/0/0	0/0/0/0
2	SO4	A	704	-	-	0/0/0/0	0/0/0/0
5	ADE	B	288	-	-	0/0/0/0	0/0/2/2
2	SO4	B	291	-	-	0/0/0/0	0/0/0/0
4	DMS	B	703	-	-	0/0/0/0	0/0/0/0
2	SO4	C	291	-	-	0/0/0/0	0/0/0/0
3	ACT	C	700	-	-	0/0/0/0	0/0/0/0
4	DMS	C	703	-	-	0/0/0/0	0/0/0/0

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	704	SO4	O1-S	6.01	1.66	1.47
2	A	704	SO4	O2-S	5.83	1.66	1.47
2	A	291	SO4	O1-S	5.77	1.65	1.47
2	A	704	SO4	O4-S	5.64	1.66	1.47
2	A	291	SO4	O2-S	5.63	1.65	1.47
2	A	704	SO4	O3-S	5.61	1.66	1.47
2	B	291	SO4	O3-S	5.56	1.66	1.47
2	C	291	SO4	O2-S	5.56	1.65	1.47
2	C	291	SO4	O1-S	5.53	1.65	1.47
2	B	291	SO4	O1-S	5.45	1.64	1.47
2	B	291	SO4	O4-S	5.42	1.65	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	291	SO4	O3-S	5.42	1.65	1.47
2	B	291	SO4	O2-S	5.40	1.64	1.47
2	A	291	SO4	O4-S	5.29	1.65	1.47
2	C	291	SO4	O4-S	5.22	1.65	1.47
2	A	291	SO4	O3-S	5.12	1.64	1.47
3	A	700	ACT	CH3-C	3.19	1.53	1.48
3	C	700	ACT	CH3-C	3.07	1.53	1.48
4	A	703	DMS	O-S	2.16	1.64	1.50
4	C	703	DMS	O-S	2.09	1.64	1.50

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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	285/287 (99%)	-0.34	1 (0%) 90 91	13, 24, 51, 102	0
1	B	273/287 (95%)	-0.07	10 (3%) 39 36	15, 26, 63, 147	1 (0%)
1	C	284/287 (98%)	-0.35	1 (0%) 90 91	13, 24, 51, 113	1 (0%)
All	All	842/861 (97%)	-0.26	12 (1%) 72 71	13, 25, 54, 147	2 (0%)

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	40	LEU	12.0
1	C	287	ASP	5.5
1	B	252	GLU	4.3
1	B	35	SER	3.7
1	B	56	PRO	3.2
1	B	262	VAL	2.7
1	B	5	VAL	2.7
1	B	260	GLU	2.7
1	B	4	SER	2.5
1	B	55	ILE	2.4
1	A	4	SER	2.2
1	B	62	SER	2.1

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	ACT	C	700	4/4	0.22	8.20	22,28,40,45	0
2	SO4	C	291	5/5	0.20	7.10	38,39,45,65	0
2	SO4	A	291	5/5	0.15	3.65	32,35,44,45	0
2	SO4	A	704	5/5	0.18	2.67	57,63,68,74	0
3	ACT	A	700	4/4	0.13	1.81	14,14,16,38	0
5	ADE	B	288	10/10	0.10	1.01	20,31,37,37	0
4	DMS	C	703	4/4	0.07	0.48	20,20,20,20	0
4	DMS	A	703	4/4	0.07	-0.17	14,15,17,18	0
2	SO4	B	291	5/5	0.09	-0.33	26,28,37,40	0
4	DMS	B	703	4/4	0.05	-1.19	17,17,19,21	0

6.5 Other polymers ⓘ

There are no such residues in this entry.