



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 10, 2014 – 02:10 PM EDT

PDB ID : 4C5M  
Title : Structure of the pyridoxal kinase from Staphylococcus aureus in complex with AMP-PCP  
Authors : Nodwell, M.; Alte, F.; Sieber, S.A.; Schneider, S.  
Deposited on : 2013-09-12  
Resolution : 1.45 Å(reported)

This is a full wwPDB validation 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 <http://wwpdb.org/ValidationPDFNotes.html>

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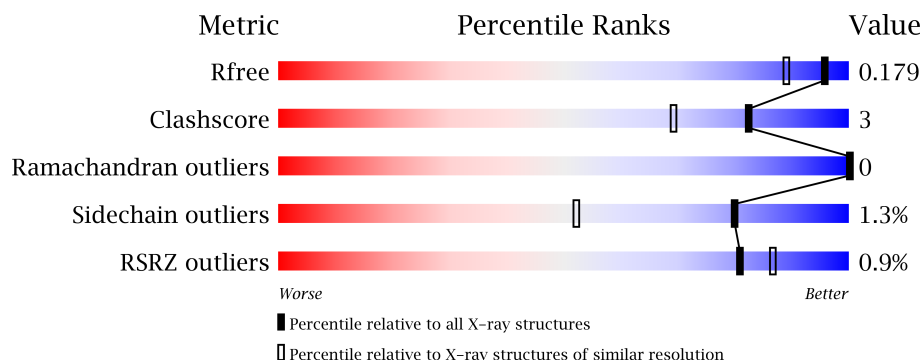
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : **FAILED**  
Xtriage (Phenix) : dev-1439  
EDS : stable22978  
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) : stable22978

# 1 Overall quality at a glance

The reported resolution of this entry is 1.45 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	2476 (1.50-1.42)
Clashscore	79885	2834 (1.50-1.42)
Ramachandran outliers	78287	2769 (1.50-1.42)
Sidechain outliers	78261	2767 (1.50-1.42)
RSRZ outliers	66119	2477 (1.50-1.42)

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. 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	276	
1	B	276	
1	C	276	
1	D	276	

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	ACP	B	500[A]	-	X
2	ACP	B	500[B]	-	X
2	ACP	B	500[C]	-	X
2	ACP	C	500[A]	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
2	ACP	C	500[B]	-	X
2	ACP	C	500[C]	-	X
3	SO4	A	1277	-	X
3	SO4	A	1278	-	X
3	SO4	A	1279	-	X
3	SO4	A	1280	-	X
3	SO4	B	1277	-	X
3	SO4	B	1278	-	X
3	SO4	B	1279	-	X
3	SO4	B	1280	-	X
3	SO4	C	1277	-	X
3	SO4	C	1278	-	X
3	SO4	C	1279	-	X
3	SO4	D	1277	-	X
3	SO4	D	1278	-	X
3	SO4	D	1279	-	X
3	SO4	D	1280	-	X
3	SO4	D	1281	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9733 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.

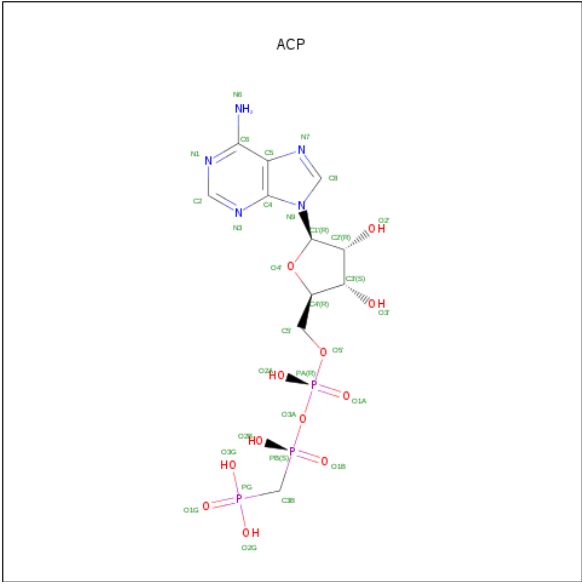
- Molecule 1 is a protein called PHOSPHOMETHYLPYRIMIDINEKINASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	273	Total	C	N	O	S	0	4	0
			2084	1327	338	407	12			
1	B	276	Total	C	N	O	S	0	14	0
			2154	1381	340	418	15			
1	C	273	Total	C	N	O	S	0	9	0
			2111	1349	339	408	15			
1	D	273	Total	C	N	O	S	0	10	0
			2112	1349	338	412	13			

There are 4 discrepancies between the modelled and reference sequences:

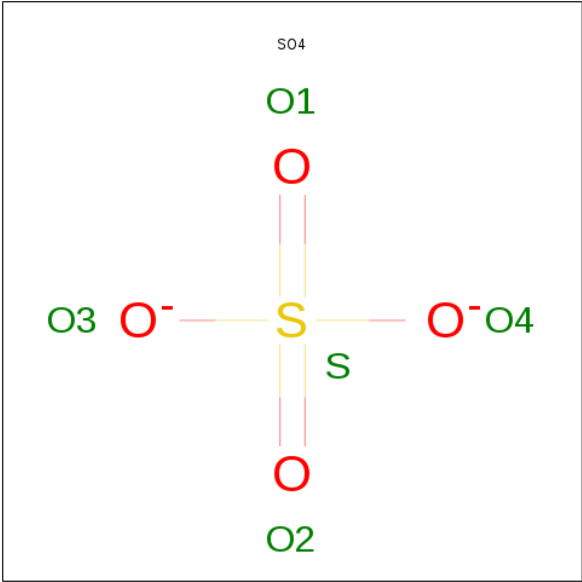
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	EXPRESSION TAG	UNP Q99W31
B	1	GLY	-	EXPRESSION TAG	UNP Q99W31
C	1	GLY	-	EXPRESSION TAG	UNP Q99W31
D	1	GLY	-	EXPRESSION TAG	UNP Q99W31

- Molecule 2 is PHOSPHOMETHYLPHOSPHONICACID ADENYLATE ESTER (three-letter code: ACP) (formula:  $C_{11}H_{18}N_5O_{12}P_3$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	1
			55	13	5	28	9		
2	B	1	Total	C	N	O	P	0	1
			55	13	5	28	9		
2	C	1	Total	C	N	O	P	0	1
			55	13	5	28	9		
2	D	1	Total	C	N	O	P	0	1
			43	12	5	20	6		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	275	Total O 276 276	0	1
4	B	249	Total O 249 249	0	0
4	C	200	Total O 200 200	0	0

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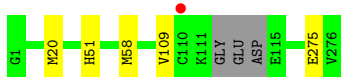
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	254	Total 254	O 254	0	0

### 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 errors 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.

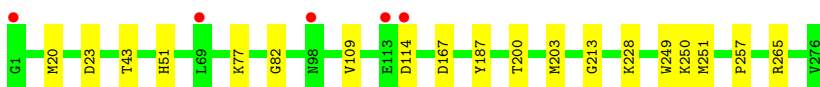
- Molecule 1: PHOSPHOMETHYLPYRIMIDINEKINASE

Chain A: 



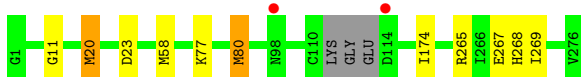
- Molecule 1: PHOSPHOMETHYLPYRIMIDINEKINASE

Chain B: 



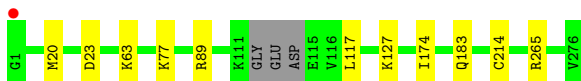
- Molecule 1: PHOSPHOMETHYLPYRIMIDINEKINASE

Chain C: 



- Molecule 1: PHOSPHOMETHYLPYRIMIDINEKINASE

Chain D: 





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	62.21Å 100.51Å 167.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.76 – 1.45 48.71 – 1.45	Depositor EDS
% Data completeness (in resolution range)	99.7 (48.76-1.45) 99.5 (48.71-1.45)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.13 (at 1.45Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, $R_{free}$	0.122 , 0.171 0.138 , 0.179	Depositor DCC
$R_{free}$ test set	9360 reflections (5.31%)	DCC
Wilson B-factor (Å <sup>2</sup> )	17.5	Xtriage
Anisotropy	0.254	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 36.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 185724 reflections	Xtriage
$F_o, F_c$ correlation	0.98	EDS
Total number of atoms	9733	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.46% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities 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: ACP, SO4

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	0.63	1/2133 (0.0%)	0.77	1/2887 (0.0%)
1	B	0.68	1/2234 (0.0%)	0.80	3/3023 (0.1%)
1	C	0.64	0/2172	0.83	5/2937 (0.2%)
1	D	0.64	0/2179	0.73	2/2949 (0.1%)
All	All	0.65	2/8718 (0.0%)	0.78	11/11796 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	275	GLU	CD-OE2	5.51	1.31	1.25
1	B	257	PRO	N-CD	5.30	1.55	1.47

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	20	MET	CA-CB-CG	10.36	130.92	113.30
1	C	20	MET	CG-SD-CE	9.31	115.10	100.20
1	A	58	MET	CG-SD-CE	7.63	112.40	100.20
1	B	265	ARG	NE-CZ-NH1	6.82	123.71	120.30
1	B	167	ASP	CB-CG-OD1	5.71	123.44	118.30
1	D	89	ARG	NE-CZ-NH2	-5.68	117.46	120.30
1	C	265	ARG	NE-CZ-NH2	-5.17	117.71	120.30
1	B	203	MET	CG-SD-CE	-5.08	92.08	100.20
1	D	89	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	C	265	ARG	NE-CZ-NH1	5.07	122.84	120.30
1	C	20	MET	CB-CG-SD	5.03	127.50	112.40

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	2084	0	0	0	0
1	B	2154	0	0	9	0
1	C	2111	0	0	6	0
1	D	2112	0	0	7	0
2	A	55	0	0	1	0
2	B	55	0	0	3	0
2	C	55	0	0	1	0
2	D	43	0	0	0	0
3	A	20	0	0	0	0
3	B	20	0	0	1	0
3	C	20	0	0	2	0
3	D	25	0	0	1	0
4	A	276	0	0	1	0
4	B	249	0	0	5	0
4	C	200	0	0	2	0
4	D	254	0	0	6	0
All	All	9733	0	0	27	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 3.

All (27) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:214:CYS:SG	4:D:2193:HOH:O	2.07	1.12
3:D:1277:SO4:O1	4:D:2250:HOH:O	2.08	0.70
2:A:500[C]:ACP:O1B	4:A:2164:HOH:O	2.10	0.70
1:D:117:LEU:O	4:D:2111:HOH:O	2.14	0.64
2:B:500[B]:ACP:O2B	4:B:2177:HOH:O	2.15	0.62
1:B:82:GLY:N	4:B:2110:HOH:O	2.40	0.55
1:B:228[B]:LYS:NZ	4:B:2205:HOH:O	2.42	0.53
1:C:269:ILE:N	4:C:2170:HOH:O	2.41	0.52
3:C:1279:SO4:O3	4:C:2042:HOH:O	2.16	0.50
2:C:500[B]:ACP:O2G	2:C:500[B]:ACP:O1B	2.31	0.49
1:D:183[A]:GLN:NE2	4:D:2137:HOH:O	2.47	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:11:GLY:N	1:C:80[A]:MET:CG	2.78	0.47
2:B:500[A]:ACP:O1B	4:B:2177:HOH:O	2.20	0.47
1:C:23:ASP:OD1	1:C:77[A]:LYS:NZ	2.48	0.46
1:B:43:THR:OG1	1:D:63[B]:LYS:NZ	2.49	0.46
1:D:127:LYS:NZ	4:D:2121:HOH:O	2.48	0.46
1:B:249:TRP:CH2	1:B:251[B]:MET:SD	3.08	0.46
1:B:187:TYR:CD1	1:B:200[B]:THR:CG2	3.00	0.45
1:C:58:MET:N	3:C:1279:SO4:O4	2.50	0.45
1:B:250:LYS:NZ	3:B:1278:SO4:O1	2.50	0.45
1:C:267:GLU:CG	1:C:268:HIS:N	2.81	0.44
1:B:213:GLY:N	2:B:500[C]:ACP:C3B	2.82	0.43
1:B:23:ASP:OD1	1:B:77:LYS:NZ	2.53	0.42
1:C:80[A]:MET:N	1:C:80[A]:MET:SD	2.93	0.42
1:D:265[B]:ARG:NH2	4:D:2232:HOH:O	2.53	0.41
1:D:23:ASP:OD1	1:D:77:LYS:NZ	2.53	0.41
1:B:114:ASP:N	4:B:2135:HOH:O	2.55	0.40

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	273/276 (99%)	265 (97%)	8 (3%)	0	100	100
1	B	288/276 (104%)	280 (97%)	8 (3%)	0	100	100
1	C	278/276 (101%)	271 (98%)	7 (2%)	0	100	100
1	D	279/276 (101%)	270 (97%)	9 (3%)	0	100	100
All	All	1118/1104 (101%)	1086 (97%)	32 (3%)	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	220/221 (100%)	217 (99%)	3 (1%)	78	50
1	B	233/221 (105%)	230 (99%)	3 (1%)	80	52
1	C	226/221 (102%)	222 (98%)	4 (2%)	71	37
1	D	225/221 (102%)	223 (99%)	2 (1%)	87	68
All	All	904/884 (102%)	892 (99%)	12 (1%)	80	52

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	MET
1	A	51	HIS
1	A	109	VAL
1	B	20	MET
1	B	51	HIS
1	B	109	VAL
1	C	20	MET
1	C	80[A]	MET
1	C	80[B]	MET
1	C	174	ILE
1	D	20	MET
1	D	174	ILE

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 ⓘ

Mogul failed to run properly - this section will therefore be empty.

## 5.5 Carbohydrates ⓘ

Mogul failed to run properly - this section will therefore be empty.

## 5.6 Ligand geometry ⓘ

Mogul failed to run properly - this section will therefore be empty.

## 5.7 Other polymers ⓘ

Mogul failed to run properly - this section will therefore be empty.

## 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, 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	273/276 (98%)	-0.43	1 (0%) 90 94	12, 19, 36, 67	0
1	B	276/276 (100%)	-0.45	5 (1%) 65 72	12, 20, 39, 60	0
1	C	273/276 (98%)	-0.41	2 (0%) 84 90	13, 21, 40, 69	0
1	D	273/276 (98%)	-0.58	1 (0%) 90 94	11, 17, 33, 63	0
All	All	1095/1104 (99%)	-0.47	9 (0%) 81 88	11, 19, 38, 69	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	113	GLU	4.6
1	B	1	GLY	4.1
1	B	114	ASP	3.6
1	B	98	ASN	3.2
1	A	110	CYS	3.2
1	D	1	GLY	2.9
1	C	114	ASP	2.6
1	B	69	LEU	2.3
1	C	98	ASN	2.2

### 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, 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	SO4	C	1277	5/5	0.32	17.30	44,65,80,89	0
3	SO4	B	1279	5/5	0.17	13.42	22,33,42,49	5
3	SO4	D	1279	5/5	0.22	9.78	52,53,61,63	0
3	SO4	A	1280	5/5	0.16	7.92	21,29,44,46	5
3	SO4	A	1278	5/5	0.12	7.37	31,36,51,54	0
3	SO4	C	1279	5/5	0.23	6.78	53,64,73,93	0
3	SO4	C	1278	5/5	0.15	6.56	36,41,64,79	5
3	SO4	B	1278	5/5	0.17	5.17	27,37,52,54	5
3	SO4	A	1277	5/5	0.28	4.99	68,70,81,89	0
3	SO4	D	1281	5/5	0.14	4.85	29,39,43,46	5
3	SO4	B	1277	5/5	0.13	4.78	34,36,40,56	0
2	ACP	C	500[B]	12/31	0.10	4.56	16,23,37,38	12
3	SO4	D	1278	5/5	0.28	4.39	56,61,72,78	0
3	SO4	A	1279	5/5	0.21	4.25	30,44,51,52	5
3	SO4	D	1280	5/5	0.09	3.46	21,31,34,38	5
3	SO4	D	1277	5/5	0.14	3.45	24,24,38,43	0
2	ACP	B	500[B]	12/31	0.10	3.33	15,20,23,29	12
3	SO4	B	1280	5/5	0.36	3.23	51,60,84,86	0
2	ACP	B	500[A]	12/31	0.10	3.20	13,17,23,24	12
2	ACP	C	500[A]	12/31	0.10	2.94	19,20,26,32	12
2	ACP	C	500[C]	12/31	0.10	2.94	14,21,26,33	12
2	ACP	B	500[C]	12/31	0.10	2.66	7,24,26,30	12
3	SO4	C	1280	5/5	0.15	1.20	40,43,46,48	5
2	ACP	A	500[B]	12/31	0.07	1.13	18,22,33,33	12
2	ACP	A	500[A]	12/31	0.07	1.00	18,21,27,29	12
2	ACP	A	500[C]	12/31	0.07	0.89	11,17,22,23	12
2	ACP	D	500[A]	12/31	0.05	0.32	15,18,35,39	12
2	ACP	D	500[B]	12/31	0.05	0.32	15,19,24,29	12

## 6.5 Other polymers ⓘ

There are no such residues in this entry.