wwPDB X-ray Structure Validation Summary Report (i)

Oct 16, 2023 – 12:48 PM EDT

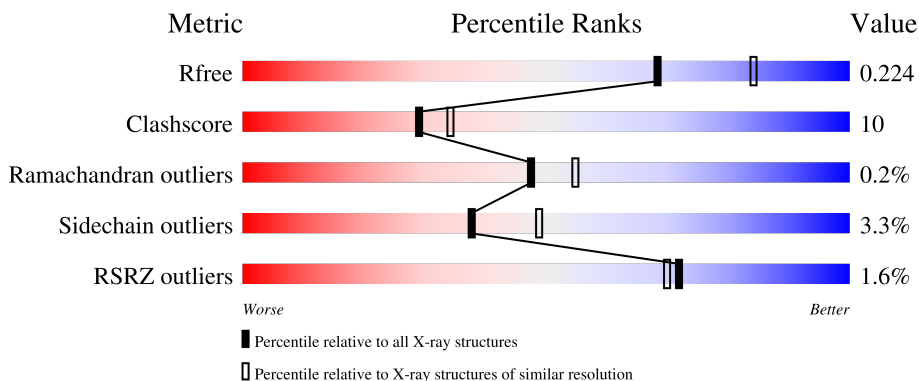|		
PDB ID	:	2E69
Title	:	Crystal structure of the stationary phase survival protein SurE from Thermus thermophilus HB8 in complex with sulfate
Authors	:	Iwasaki, W.; Miki, K.
Deposited on	:	2006-12-26
Resolution	:	2.20 Å(reported)

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 2.20 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	Percentile Ranks	Value
Rfree		0.224
Clashscore		10
Ramachandran outliers		0.2%
Sidechain outliers		3.3%
RSRZ outliers		1.6%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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	244	% 77% 19% · ·
1	B	244	2% 78% 16% · 5%
1	C	244	2% 75% 18% · 5%
1	D	244	% 80% 15% · ·

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	B	306	-	-	X	-
3	GOL	A	401	-	-	X	-

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 7550 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 5'-nucleotidase surE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	237	Total	C	N	O	S	0	0	0
			1837	1191	323	320	3			
1	B	232	Total	C	N	O	S	0	0	0
			1800	1168	314	315	3			
1	C	231	Total	C	N	O	S	0	0	0
			1796	1165	315	313	3			
1	D	234	Total	C	N	O	S	0	0	0
			1818	1180	318	317	3			

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).

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		

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

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).
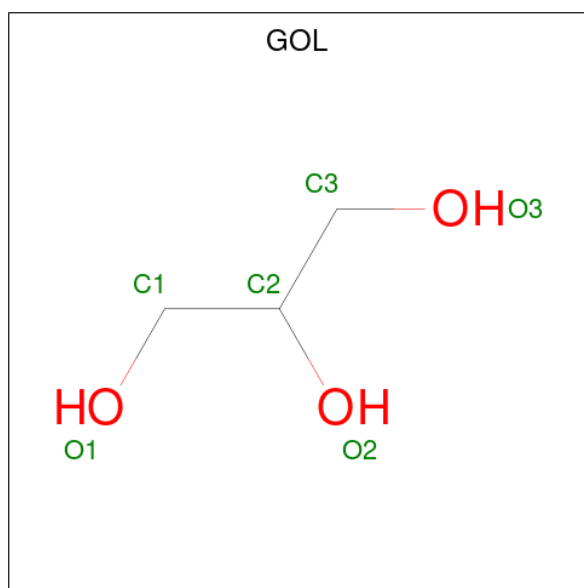
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 6	C 3	O 3	0	0
3	B	1	Total 6	C 3	O 3	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	69	Total 69	O 69	0	0
4	B	57	Total 57	O 57	0	0
4	C	46	Total 46	O 46	0	0
4	D	45	Total 45	O 45	0	0

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.
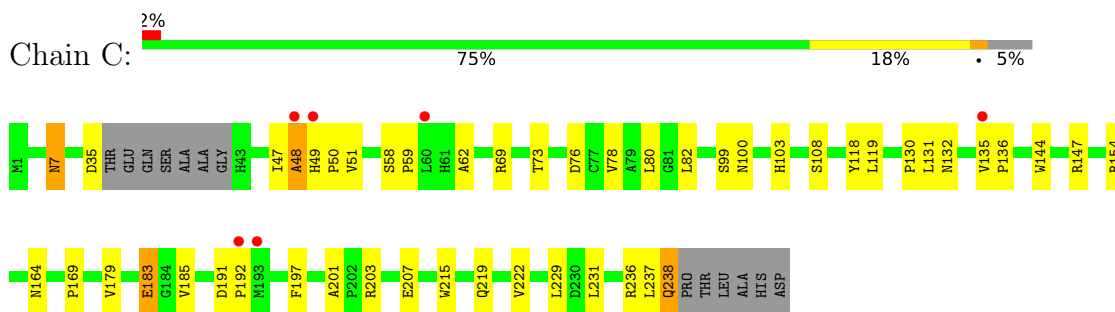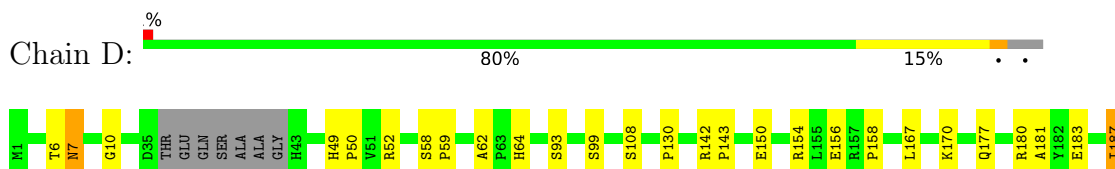
- Molecule 1: 5'-nucleotidase surE
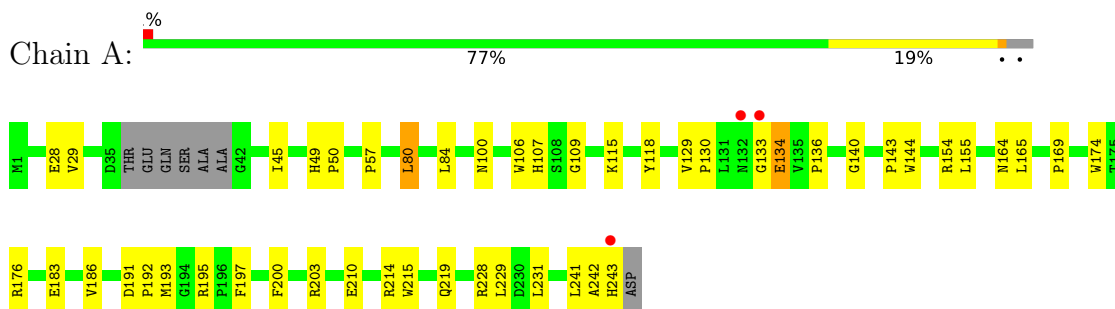
- Molecule 1: 5'-nucleotidase surE
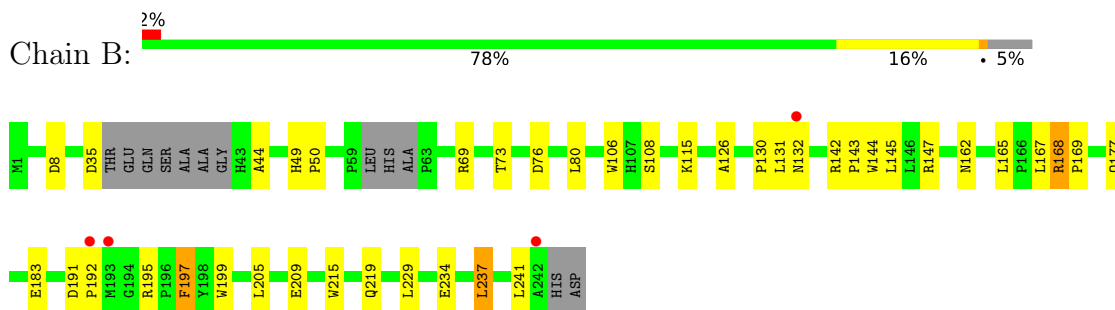
- Molecule 1: 5'-nucleotidase surE

- Molecule 1: 5'-nucleotidase surE

4   Data and refinement statistics   ⓘ

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	131.82Å 131.82Å 131.21Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	43.06 – 2.20 43.06 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.8 (43.06-2.20) 99.9 (43.06-2.20)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	7.93 (at 2.20Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.195 , 0.230 0.189 , 0.224	Depositor DCC
R_{free} test set	3412 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	32.7	Xtriage
Anisotropy	0.353	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 47.9	EDS
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.018 for -h,-k,l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	7550	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.39% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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: SO4, GOL

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	0.48	0/1897	0.70	0/2599
1	B	0.47	0/1857	0.72	0/2542
1	C	0.44	0/1854	0.69	0/2539
1	D	0.45	0/1877	0.70	0/2572
All	All	0.46	0/7485	0.70	0/10252

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	1837	0	1815	49	0
1	B	1800	0	1782	37	0
1	C	1796	0	1775	41	0
1	D	1818	0	1800	41	0
2	A	25	0	0	2	0
2	B	20	0	0	3	0
2	C	10	0	0	1	0
2	D	15	0	0	1	0
3	A	6	0	8	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	6	0	8	0	0
4	A	69	0	0	2	0
4	B	57	0	0	0	0
4	C	46	0	0	0	0
4	D	45	0	0	0	0
All	All	7550	0	7188	140	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 10.

The worst 5 of 140 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:B:168:ARG:HB2	1:B:168:ARG:HH11	1.24	1.00
1:A:191:ASP:HB2	1:A:192:PRO:HD2	1.47	0.96
1:A:29:VAL:H	3:A:401:GOL:H31	1.33	0.92
1:A:49:HIS:HB2	1:A:50:PRO:HD2	1.59	0.83
1:C:237:LEU:O	1:C:238:GLN:HB2	1.80	0.82

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	233/244 (96%)	227 (97%)	5 (2%)	1 (0%)	34	37
1	B	226/244 (93%)	220 (97%)	6 (3%)	0	100	100
1	C	227/244 (93%)	221 (97%)	5 (2%)	1 (0%)	34	37
1	D	230/244 (94%)	227 (99%)	3 (1%)	0	100	100
All	All	916/976 (94%)	895 (98%)	19 (2%)	2 (0%)	47	55

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	48	ALA
1	A	134	GLU

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	189/194 (97%)	186 (98%)	3 (2%)	62	76
1	B	186/194 (96%)	179 (96%)	7 (4%)	33	42
1	C	185/194 (95%)	175 (95%)	10 (5%)	22	26
1	D	188/194 (97%)	183 (97%)	5 (3%)	44	57
All	All	748/776 (96%)	723 (97%)	25 (3%)	38	49

5 of 25 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	119	LEU
1	C	197	PHE
1	D	234	GLU
1	C	183	GLU
1	C	207	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 25 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	100	ASN
1	C	164	ASN
1	D	177	GLN
1	C	132	ASN
1	C	238	GLN

5.3.3 RNA ⓘ

There are no RNA molecules 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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

16 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	$\#|Z| > 2$
3	GOL	B	402	-	5,5,5	0.61	0	5,5,5	0.54	0
2	SO4	A	303	-	4,4,4	0.29	0	6,6,6	0.08	0
3	GOL	A	401	-	5,5,5	0.29	0	5,5,5	0.32	0
2	SO4	D	313	-	4,4,4	0.19	0	6,6,6	0.16	0
2	SO4	A	304	-	4,4,4	0.35	0	6,6,6	0.12	0
2	SO4	D	314	-	4,4,4	0.27	0	6,6,6	0.15	0
2	SO4	A	302	-	4,4,4	0.07	0	6,6,6	0.10	0
2	SO4	C	310	-	4,4,4	0.45	0	6,6,6	0.09	0
2	SO4	B	306	-	4,4,4	0.12	0	6,6,6	0.10	0
2	SO4	B	308	-	4,4,4	0.28	0	6,6,6	0.10	0
2	SO4	C	311	-	4,4,4	0.17	0	6,6,6	0.11	0
2	SO4	A	301	-	4,4,4	0.23	0	6,6,6	0.26	0
2	SO4	D	312	-	4,4,4	0.27	0	6,6,6	0.13	0
2	SO4	A	305	-	4,4,4	0.33	0	6,6,6	0.10	0
2	SO4	B	309	-	4,4,4	0.38	0	6,6,6	0.15	0
2	SO4	B	307	-	4,4,4	0.31	0	6,6,6	0.18	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
3	GOL	B	402	-	-	0/4/4/4	-
3	GOL	A	401	-	-	0/4/4/4	-

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.

7 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	401	GOL	4	0
2	A	304	SO4	1	0
2	B	306	SO4	2	0
2	C	311	SO4	1	0
2	A	301	SO4	1	0
2	D	312	SO4	1	0
2	B	309	SO4	1	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.

WORLDWIDE
wwPDB
PROTEIN DATA BANK

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	237/244 (97%)	-0.22	3 (1%)	77	75	18, 31, 55, 80	0
1	B	232/244 (95%)	-0.35	4 (1%)	70	68	21, 32, 61, 74	0
1	C	231/244 (94%)	-0.30	6 (2%)	56	53	22, 36, 60, 78	0
1	D	234/244 (95%)	-0.40	2 (0%)	84	83	21, 32, 57, 78	0
All	All	934/976 (95%)	-0.32	15 (1%)	72	70	18, 33, 59, 80	0

The worst 5 of 15 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	192	PRO	4.5
1	B	242	ALA	3.5
1	A	132	ASN	3.1
1	D	240	THR	3.1
1	A	133	GLY	3.1

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 monosaccharides 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.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	B	309	5/5	0.65	0.29	92,94,99,101	0
3	GOL	B	402	6/6	0.75	0.20	42,54,55,56	0
3	GOL	A	401	6/6	0.83	0.21	34,51,56,60	0
2	SO4	B	306	5/5	0.93	0.48	54,68,78,79	0
2	SO4	D	314	5/5	0.93	0.15	82,84,87,87	0
2	SO4	A	303	5/5	0.94	0.17	75,80,81,83	0
2	SO4	A	305	5/5	0.94	0.14	70,70,75,77	0
2	SO4	C	310	5/5	0.94	0.29	56,66,75,75	0
2	SO4	D	312	5/5	0.95	0.43	49,67,76,76	0
2	SO4	A	301	5/5	0.95	0.34	47,66,72,77	0
2	SO4	B	308	5/5	0.97	0.22	84,87,88,89	0
2	SO4	A	304	5/5	0.98	0.14	47,55,60,64	0
2	SO4	A	302	5/5	0.99	0.11	33,36,40,43	0
2	SO4	B	307	5/5	0.99	0.10	32,34,39,41	0
2	SO4	D	313	5/5	0.99	0.10	38,39,45,47	0
2	SO4	C	311	5/5	1.00	0.09	28,29,30,35	0

6.5 Other polymers ⓘ

There are no such residues in this entry.