



wwPDB X-ray Structure Validation Summary Report ⓘ

May 25, 2020 – 05:36 am BST

PDB ID : 3ZUR
Title : Crystal structure of an engineered botulinum neurotoxin type A- SNARE23 derivative, LC0-A-SNAP25-Hn-A
Authors : Masuyer, G.; Stancombe, P.; Chaddock, J.A.; Acharya, K.R.
Deposited on : 2011-07-19
Resolution : 2.71 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

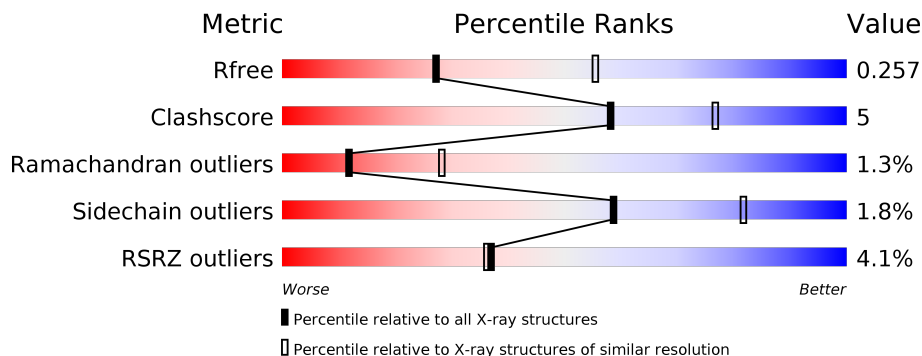
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.71 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}	130704	3359 (2.74-2.70)
Clashscore	141614	3686 (2.74-2.70)
Ramachandran outliers	138981	3622 (2.74-2.70)
Sidechain outliers	138945	3623 (2.74-2.70)
RSRZ outliers	127900	3276 (2.74-2.70)

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 on 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	960	 3% 76% 11% • 12%
1	B	960	 4% 75% 12% • 12%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 13823 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 BOTULINUM NEUROTOXIN TYPE A, SYNAPTOSOMA L-ASSOCIATED PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	848	6848	4401	1104	1324	19	0	0	1
1	B	844	6801	4371	1097	1314	19	0	0	1

There are 122 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	MET	-	expression tag	UNP P10845
A	-1	GLY	-	expression tag	UNP P10845
A	0	SER	-	expression tag	UNP P10845
A	1	MET	-	expression tag	UNP P10845
A	2	GLU	-	expression tag	UNP P10845
A	27	ALA	VAL	variant	UNP P10845
A	224	GLN	GLU	engineered mutation	UNP P10845
A	227	TYR	HIS	engineered mutation	UNP P10845
A	431	VAL	-	linker	UNP P10845
A	432	ASP	-	linker	UNP P10845
A	433	GLY	-	linker	UNP P10845
A	434	GLY	-	linker	UNP P10845
A	435	GLY	-	linker	UNP P10845
A	436	GLY	-	linker	UNP P10845
A	437	SER	-	linker	UNP P10845
A	438	GLY	-	linker	UNP P10845
A	439	GLY	-	linker	UNP P10845
A	440	GLY	-	linker	UNP P10845
A	441	GLY	-	linker	UNP P10845
A	442	SER	-	linker	UNP P10845
A	443	GLY	-	linker	UNP P10845
A	444	GLY	-	linker	UNP P10845
A	445	GLY	-	linker	UNP P10845
A	446	GLY	-	linker	UNP P10845

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Chain	Residue	Modelled	Actual	Comment	Reference
A	447	SER	-	linker	UNP P10845
A	510	ALA	-	linker	UNP P10845
A	511	ASN	-	linker	UNP P10845
A	512	SER	-	linker	UNP P10845
A	513	ALA	-	linker	UNP P10845
A	514	LEU	-	linker	UNP P10845
A	515	ALA	-	linker	UNP P10845
A	516	GLY	-	linker	UNP P10845
A	517	GLY	-	linker	UNP P10845
A	518	GLY	-	linker	UNP P10845
A	519	GLY	-	linker	UNP P10845
A	520	SER	-	linker	UNP P10845
A	521	GLY	-	linker	UNP P10845
A	522	GLY	-	linker	UNP P10845
A	523	GLY	-	linker	UNP P10845
A	524	GLY	-	linker	UNP P10845
A	525	SER	-	linker	UNP P10845
A	526	GLY	-	linker	UNP P10845
A	527	GLY	-	linker	UNP P10845
A	528	GLY	-	linker	UNP P10845
A	529	GLY	-	linker	UNP P10845
A	530	SER	-	linker	UNP P10845
A	531	LEU	-	linker	UNP P10845
A	532	GLN	-	linker	UNP P10845
A	945	LEU	-	expression tag	UNP P10845
A	946	GLU	-	expression tag	UNP P10845
A	947	ALA	-	expression tag	UNP P10845
A	948	HIS	-	expression tag	UNP P10845
A	949	HIS	-	expression tag	UNP P10845
A	950	HIS	-	expression tag	UNP P10845
A	951	HIS	-	expression tag	UNP P10845
A	952	HIS	-	expression tag	UNP P10845
A	953	HIS	-	expression tag	UNP P10845
A	954	HIS	-	expression tag	UNP P10845
A	955	HIS	-	expression tag	UNP P10845
A	956	HIS	-	expression tag	UNP P10845
A	957	HIS	-	expression tag	UNP P10845
B	-2	MET	-	expression tag	UNP P10845
B	-1	GLY	-	expression tag	UNP P10845
B	0	SER	-	expression tag	UNP P10845
B	1	MET	-	expression tag	UNP P10845
B	2	GLU	-	expression tag	UNP P10845

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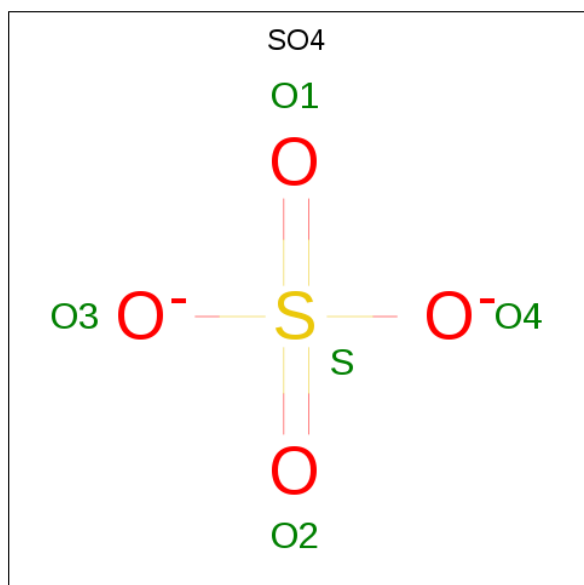
Chain	Residue	Modelled	Actual	Comment	Reference
B	27	ALA	VAL	variant	UNP P10845
B	224	GLN	GLU	engineered mutation	UNP P10845
B	227	TYR	HIS	engineered mutation	UNP P10845
B	431	VAL	-	linker	UNP P10845
B	432	ASP	-	linker	UNP P10845
B	433	GLY	-	linker	UNP P10845
B	434	GLY	-	linker	UNP P10845
B	435	GLY	-	linker	UNP P10845
B	436	GLY	-	linker	UNP P10845
B	437	SER	-	linker	UNP P10845
B	438	GLY	-	linker	UNP P10845
B	439	GLY	-	linker	UNP P10845
B	440	GLY	-	linker	UNP P10845
B	441	GLY	-	linker	UNP P10845
B	442	SER	-	linker	UNP P10845
B	443	GLY	-	linker	UNP P10845
B	444	GLY	-	linker	UNP P10845
B	445	GLY	-	linker	UNP P10845
B	446	GLY	-	linker	UNP P10845
B	447	SER	-	linker	UNP P10845
B	510	ALA	-	linker	UNP P10845
B	511	ASN	-	linker	UNP P10845
B	512	SER	-	linker	UNP P10845
B	513	ALA	-	linker	UNP P10845
B	514	LEU	-	linker	UNP P10845
B	515	ALA	-	linker	UNP P10845
B	516	GLY	-	linker	UNP P10845
B	517	GLY	-	linker	UNP P10845
B	518	GLY	-	linker	UNP P10845
B	519	GLY	-	linker	UNP P10845
B	520	SER	-	linker	UNP P10845
B	521	GLY	-	linker	UNP P10845
B	522	GLY	-	linker	UNP P10845
B	523	GLY	-	linker	UNP P10845
B	524	GLY	-	linker	UNP P10845
B	525	SER	-	linker	UNP P10845
B	526	GLY	-	linker	UNP P10845
B	527	GLY	-	linker	UNP P10845
B	528	GLY	-	linker	UNP P10845
B	529	GLY	-	linker	UNP P10845
B	530	SER	-	linker	UNP P10845
B	531	LEU	-	linker	UNP P10845

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Chain	Residue	Modelled	Actual	Comment	Reference
B	532	GLN	-	linker	UNP P10845
B	945	LEU	-	expression tag	UNP P10845
B	946	GLU	-	expression tag	UNP P10845
B	947	ALA	-	expression tag	UNP P10845
B	948	HIS	-	expression tag	UNP P10845
B	949	HIS	-	expression tag	UNP P10845
B	950	HIS	-	expression tag	UNP P10845
B	951	HIS	-	expression tag	UNP P10845
B	952	HIS	-	expression tag	UNP P10845
B	953	HIS	-	expression tag	UNP P10845
B	954	HIS	-	expression tag	UNP P10845
B	955	HIS	-	expression tag	UNP P10845
B	956	HIS	-	expression tag	UNP P10845
B	957	HIS	-	expression tag	UNP P10845

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



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

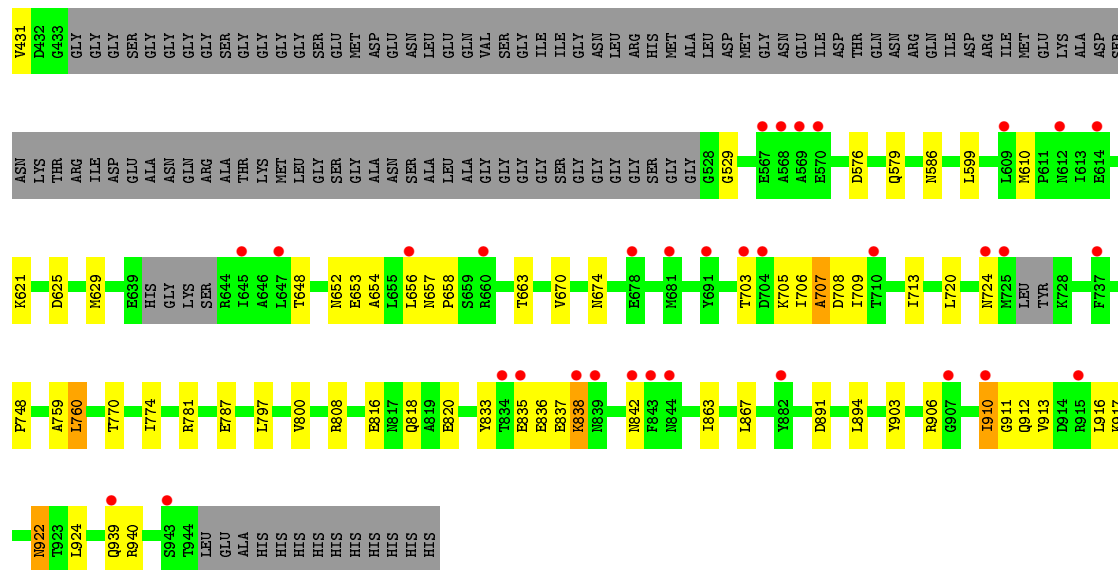
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	102	Total	O	0	0
			102	102		
3	B	47	Total	O	0	0
			47	47		



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	78.96Å 157.50Å 209.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	125.86 – 2.71 29.58 – 2.71	Depositor EDS
% Data completeness (in resolution range)	96.5 (125.86-2.71) 96.6 (29.58-2.71)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.02 (at 2.72Å)	Xtrriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.212 , 0.266 0.207 , 0.257	Depositor DCC
R_{free} test set	3503 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	50.5	Xtrriage
Anisotropy	0.194	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 48.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	13823	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.63% 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

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	0.44	0/6991	0.56	0/9471
1	B	0.43	0/6941	0.55	0/9403
All	All	0.44	0/13932	0.55	0/18874

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 [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	6848	0	6742	63	0
1	B	6801	0	6692	71	0
2	A	20	0	0	0	0
2	B	5	0	0	0	0
3	A	102	0	0	1	0
3	B	47	0	0	0	0
All	All	13823	0	13434	131	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 5.

The worst 5 of 131 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:200:LEU:HD21	1:B:940:ARG:NH1	1.80	0.96
1:B:200:LEU:HD21	1:B:940:ARG:HH11	1.39	0.87
1:A:651:VAL:HG13	1:A:653:GLU:HG3	1.60	0.82
1:B:269:HIS:HE1	1:B:940:ARG:HE	1.25	0.82
1:A:346:THR:HG22	1:A:347:GLU:HG3	1.66	0.78

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	842/960 (88%)	795 (94%)	38 (4%)	9 (1%)	14	32
1	B	836/960 (87%)	780 (93%)	44 (5%)	12 (1%)	11	26
All	All	1678/1920 (87%)	1575 (94%)	82 (5%)	21 (1%)	12	28

5 of 21 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	910	ILE
1	A	609	LEU
1	A	645	ILE
1	B	199	SER
1	B	529	GLY

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	762/840 (91%)	747 (98%)	15 (2%)	55	80
1	B	755/840 (90%)	742 (98%)	13 (2%)	60	83
All	All	1517/1680 (90%)	1489 (98%)	28 (2%)	59	82

5 of 28 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	839	ASN
1	B	86	ASN
1	B	797	LEU
1	A	840	ASN
1	A	941	LEU

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

Mol	Chain	Res	Type
1	A	931	GLN
1	A	938	ASN
1	B	832	GLN
1	A	868	ASN
1	A	922	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

5 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	1944	-	4,4,4	0.15	0	6,6,6	0.27	0
2	SO4	A	1946	-	4,4,4	0.14	0	6,6,6	0.09	0
2	SO4	B	1939	-	4,4,4	0.19	0	6,6,6	0.18	0
2	SO4	A	1943	-	4,4,4	0.11	0	6,6,6	0.18	0
2	SO4	A	1945	-	4,4,4	0.14	0	6,6,6	0.22	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	848/960 (88%)	-0.05	32 (3%) 40 40	25, 43, 71, 88	0
1	B	844/960 (87%)	0.06	37 (4%) 34 33	28, 51, 87, 108	0
All	All	1692/1920 (88%)	0.00	69 (4%) 37 36	25, 47, 80, 108	0

The worst 5 of 69 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	727	TYR	6.4
1	B	839	ASN	6.3
1	A	726	LEU	6.0
1	B	609	LEU	5.8
1	B	1	MET	5.2

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 carbohydrates 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(\AA^2)	Q<0.9
2	SO4	B	1939	5/5	0.94	0.15	62,63,63,63	0
2	SO4	A	1945	5/5	0.94	0.17	68,68,69,69	0
2	SO4	A	1944	5/5	0.95	0.15	64,65,66,67	0
2	SO4	A	1946	5/5	0.96	0.14	79,79,79,79	0
2	SO4	A	1943	5/5	0.98	0.09	47,48,48,49	0

6.5 Other polymers [i](#)

There are no such residues in this entry.