



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2020 – 09:43 PM BST

PDB ID : 5X3V
Title : Structure of human SHMT2 protein mutant
Authors : Li, J.; Sheng, J.
Deposited on : 2017-02-09
Resolution : 2.85 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 ⓘ 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 : 2.13.1
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) : 2.13.1

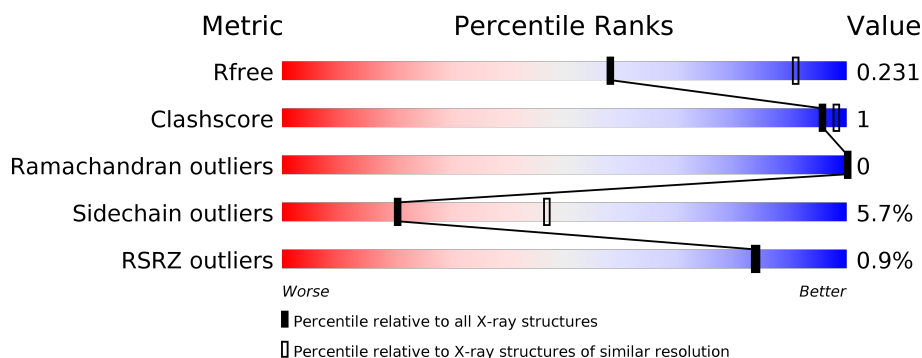
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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}	130704	3168 (2.90-2.82)
Clashscore	141614	3438 (2.90-2.82)
Ramachandran outliers	138981	3348 (2.90-2.82)
Sidechain outliers	138945	3351 (2.90-2.82)
RSRZ outliers	127900	3103 (2.90-2.82)

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	496	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 1%, green 82%, grey 10%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 82% 7% 10% </div> </div>
1	B	496	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 6%, green 83%, grey 11%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 83% 6% 11% </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6984 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 Serine hydroxymethyltransferase, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	445	Total	C	N	O	S	0	0	0
			3457	2179	622	641	15			
1	B	442	Total	C	N	O	S	0	2	0
			3433	2164	616	638	15			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	74	ARG	LYS	engineered mutation	UNP P34897
A	484	LYS	-	expression tag	UNP P34897
A	485	LEU	-	expression tag	UNP P34897
A	486	ALA	-	expression tag	UNP P34897
A	487	ALA	-	expression tag	UNP P34897
A	488	ALA	-	expression tag	UNP P34897
A	489	LEU	-	expression tag	UNP P34897
A	490	GLU	-	expression tag	UNP P34897
A	491	HIS	-	expression tag	UNP P34897
A	492	HIS	-	expression tag	UNP P34897
A	493	HIS	-	expression tag	UNP P34897
A	494	HIS	-	expression tag	UNP P34897
A	495	HIS	-	expression tag	UNP P34897
A	496	HIS	-	expression tag	UNP P34897
B	74	ARG	LYS	engineered mutation	UNP P34897
B	484	LYS	-	expression tag	UNP P34897
B	485	LEU	-	expression tag	UNP P34897
B	486	ALA	-	expression tag	UNP P34897
B	487	ALA	-	expression tag	UNP P34897
B	488	ALA	-	expression tag	UNP P34897
B	489	LEU	-	expression tag	UNP P34897
B	490	GLU	-	expression tag	UNP P34897
B	491	HIS	-	expression tag	UNP P34897
B	492	HIS	-	expression tag	UNP P34897
B	493	HIS	-	expression tag	UNP P34897

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	494	HIS	-	expression tag	UNP P34897
B	495	HIS	-	expression tag	UNP P34897
B	496	HIS	-	expression tag	UNP P34897

- 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	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	36	Total	O	0	0
			36	36		
3	B	28	Total	O	0	0
			28	28		

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.

- Chain A: 
- | Residue | Type |
|---------|-----------|
| MET | Protein |
| ALA | Polar |
| ILE | Polar |
| ARG | Polar |
| ALA | Polar |
| GLN | Polar |
| HIS | Polar |
| SER | Polar |
| ASN | Polar |
| ALA | Polar |
| ALA | Polar |
| GLN | Polar |
| THR | Polar |
| THR | Polar |
| GLY | Polar |
| GLU | Polar |
| ALA | Polar |
| ASN | Polar |
| ARG | Polar |
| GLY | Polar |
| W22 | Polar |
| M35 | Polar |
| R41 | Polar |
| R45 | Polar |
| R74 | Polar |
| Q118 | Polar |
| P119 | Polar |
| Y120 | Polar |
| S121 | Polar |
| L127 | Non-polar |
| T131 | Polar |
| L143 | Non-polar |
| T152 | Polar |
| HIS | Polar |
| GLY | Polar |
| TYR | Polar |
| MET | Polar |
| SER | Polar |
| ASP | Polar |
| VAL | Polar |
| LYS | Polar |
| ARG | Polar |
| I162 | Polar |
| T165 | Polar |
| S171 | Polar |
| L176 | Polar |
- | Residue | Type |
|---------|-------|
| T191 | Polar |
| T204 | Polar |
| S205 | Polar |
| W216 | Polar |
| R224 | Polar |
| W231 | Polar |
| A242 | Polar |
| H253 | Polar |
| R248 | Polar |
| R265 | Polar |
| S266 | Polar |
| R272 | Polar |
| R276 | Polar |
| ALA | Polar |
| VAL | Polar |
| ASP | Polar |
| PRO | Polar |
| LYS | Polar |
| THR | Polar |
| GLY | Polar |
| ARG | Polar |
| E295 | Polar |
| A321 | Polar |
| F326 | Polar |
| R327 | Polar |
| E328 | Polar |
| D357 | Polar |
| N358 | Polar |
| V361 | Polar |
| E380 | Polar |
| N387 | Polar |
| S396 | Polar |
| T399 | Polar |
| A407 | Polar |
| P408 | Polar |
| R422 | Polar |
| S455 | Polar |
| E456 | Polar |
| R463 | Polar |
| L463 | Polar |

- Chain B:
-
- | Amino Acid | Frequency (%) |
|------------|---------------|
| MET | 1% |
| ALA | 1% |
| ILE | 1% |
| ARG | 1% |
| ALA | 1% |
| GLN | 1% |
| HIS | 1% |
| SER | 1% |
| ASN | 1% |
| ALA | 1% |
| ALA | 1% |
| GLN | 1% |
| THR | 1% |
| THR | 1% |
| GLY | 1% |
| GLU | 1% |
| ALA | 1% |
| ASN | 1% |
| ARG | 1% |
| GLY | 1% |
| W22 | 1% |
| E37 | 1% |
| L38 | 1% |
| L39 | 1% |
| S55 | 1% |
| K82 | 1% |
| L87 | 1% |
| S121 | 1% |
| H122 | 1% |
| S123 | 1% |
| L127 | 1% |
| T131 | 1% |
| I140 | 1% |
| L145 | 1% |
| L151 | 1% |
| THR | 1% |
| HIS | 1% |
| GLY | 1% |
| TYR | 1% |
| MET | 1% |
| SER | 1% |
| ASP | 1% |
| VAL | 1% |
| LYS | 1% |
| R161 | 1% |
| I162 | 1% |
| T165 | 1% |
| L176 | 1% |
| L188 | 1% |
| A199 | 1% |
| L190 | 1% |
| T204 | 1% |
| K246 | 1% |
| R262 | 1% |
| V275 | 1% |
| LYS | 1% |
| ALA | 1% |
| VAL | 1% |
| ASP | 1% |
| PRO | 1% |
| LYS | 1% |
| THR | 1% |
| GLY | 1% |
| ARG | 1% |
| GLU | 1% |
| L286 | 1% |
| P297 | 1% |
| M325 | 1% |
| E328 | 1% |
| L331 | 1% |
| D357 | 1% |
| N358 | 1% |
| H359 | 1% |
| L360 | 1% |
| D394 | 1% |
| ARG | 1% |
| S396 | 1% |
| A397 | 1% |
| I398 | 1% |
| V437 | 1% |
| T441 | 1% |
| F447 | 1% |
| E482 | 1% |
| H483 | 1% |
| LYS | 1% |
| LEU | 1% |
| ALA | 1% |
| ALA | 1% |
| ALA | 1% |
| LEU | 1% |
| GLU | 1% |
| HIS | 1% |
| HIS | 1% |
| HIS | 1% |
| HIS | 1% |

4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	158.66Å 158.66Å 209.36Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.85 29.98 – 2.85	Depositor EDS
% Data completeness (in resolution range)	75.7 (50.00-2.85) 75.8 (29.98-2.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.23 (at 2.85Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, R_{free}	0.177 , 0.231 0.181 , 0.231	Depositor DCC
R_{free} test set	1414 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	45.5	Xtriage
Anisotropy	0.169	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 30.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.36$, $\langle L^2 \rangle = 0.19$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6984	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.29% 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

5.1 Standard geometry

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	0.39	0/3525	0.68	2/4769 (0.0%)
1	B	0.40	0/3505	0.67	0/4742
All	All	0.40	0/7030	0.68	2/9511 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	265	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	A	41	ARG	NE-CZ-NH1	5.04	122.82	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	357	ASP	Peptide
1	B	357	ASP	Peptide

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	3457	0	3430	11	0
1	B	3433	0	3396	5	0
2	A	15	0	0	0	0
2	B	15	0	0	0	0
3	A	36	0	0	0	1
3	B	28	0	0	0	0
All	All	6984	0	6826	15	1

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 (15) 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:441:THR:HG21	1:B:447:PHE:HA	1.86	0.57
1:B:437:VAL:O	1:B:441:THR:HG22	2.11	0.51
1:A:205:SER:HB2	1:A:233:HIS:CE1	2.48	0.49
1:B:127:LEU:O	1:B:131:THR:HG23	2.17	0.44
1:A:118:GLN:N	1:A:119:PRO:CD	2.81	0.44
1:A:407:ALA:N	1:A:408:PRO:HD3	2.33	0.44
1:B:394:ASP:CB	1:B:398:ILE:HD12	2.48	0.44
1:A:143:LEU:HD21	1:A:176:LEU:HD13	2.00	0.43
1:A:45:ARG:NH2	1:A:380:GLU:OE1	2.52	0.42
1:A:143:LEU:HD12	1:A:204:THR:HG23	2.02	0.41
1:A:35:MET:CE	1:B:97:LEU:HD23	2.50	0.41
1:A:127:LEU:O	1:A:131:THR:HG23	2.20	0.41
1:A:165:THR:HG22	1:A:171:SER:HB3	2.01	0.41
1:A:407:ALA:N	1:A:408:PRO:CD	2.84	0.41
1:A:321:ALA:HA	1:A:326:PHE:CG	2.57	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:632:HOH:O	3:A:632:HOH:O[7_554]	1.95	0.25

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	439/496 (88%)	415 (94%)	24 (6%)	0	100	100
1	B	436/496 (88%)	417 (96%)	19 (4%)	0	100	100
All	All	875/992 (88%)	832 (95%)	43 (5%)	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	361/405 (89%)	343 (95%)	18 (5%)	24	53
1	B	358/405 (88%)	335 (94%)	23 (6%)	17	41
All	All	719/810 (89%)	678 (94%)	41 (6%)	20	47

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	74	ARG
1	A	121	SER
1	A	127	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	143	LEU
1	A	191	THR
1	A	216	MET
1	A	224	LYS
1	A	231	MET
1	A	248	LYS
1	A	266	SER
1	A	272	ARG
1	A	328	GLU
1	A	358	ASN
1	A	361	VAL
1	A	387	ASN
1	A	399	THR
1	A	422	ARG
1	A	456	GLU
1	B	37	GLU
1	B	39	LEU
1	B	55	SER
1	B	82	LYS
1	B	121	SER
1	B	123	SER
1	B	127	LEU
1	B	140	ILE
1	B	145	LEU
1	B	165	THR
1	B	176	LEU
1	B	188	LEU
1	B	190	LEU
1	B	204	THR
1	B	248	LYS
1	B	262	ARG
1	B	286	ILE
1	B	325	MET
1	B	328	GLU
1	B	331	LEU
1	B	358	ASN
1	B	360	LEU
1	B	482	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	112	GLN
1	B	387	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

6 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	501	-	4,4,4	0.31	0	6,6,6	0.13	0
2	SO4	B	501	-	4,4,4	0.29	0	6,6,6	0.27	0
2	SO4	B	502	-	4,4,4	0.34	0	6,6,6	0.23	0
2	SO4	A	503	-	4,4,4	0.32	0	6,6,6	0.19	0
2	SO4	A	502	-	4,4,4	0.34	0	6,6,6	0.13	0
2	SO4	B	503	-	4,4,4	0.31	0	6,6,6	0.16	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

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 [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	445/496 (89%)	-0.65	3 (0%) 87 87	22, 33, 54, 75	0
1	B	442/496 (89%)	-0.43	5 (1%) 80 80	24, 43, 68, 78	0
All	All	887/992 (89%)	-0.54	8 (0%) 84 84	22, 37, 62, 78	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	286	ILE	4.4
1	B	162	ILE	3.0
1	B	287	PRO	2.7
1	A	396	SER	2.5
1	A	152	THR	2.4
1	B	151	LEU	2.4
1	B	396	SER	2.2
1	A	455	SER	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 monosaccharides 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(Å ²)	Q<0.9
2	SO4	A	502	5/5	0.88	0.32	103,103,104,105	0
2	SO4	B	502	5/5	0.93	0.15	60,61,64,66	0
2	SO4	A	501	5/5	0.96	0.13	14,14,14,14	5
2	SO4	B	501	5/5	0.96	0.14	60,63,64,64	0
2	SO4	A	503	5/5	0.98	0.10	47,47,48,48	0
2	SO4	B	503	5/5	0.98	0.09	69,70,71,71	0

6.5 Other polymers [i](#)

There are no such residues in this entry.