



wwPDB X-ray Structure Validation Summary Report ⓘ

May 13, 2020 – 10:40 am BST

PDB ID : 1E0U
Title : Structure R271L mutant of E. coli pyruvate kinase
Authors : Fortin, R.; Mattevi, A.
Deposited on : 2000-04-10
Resolution : 2.80 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

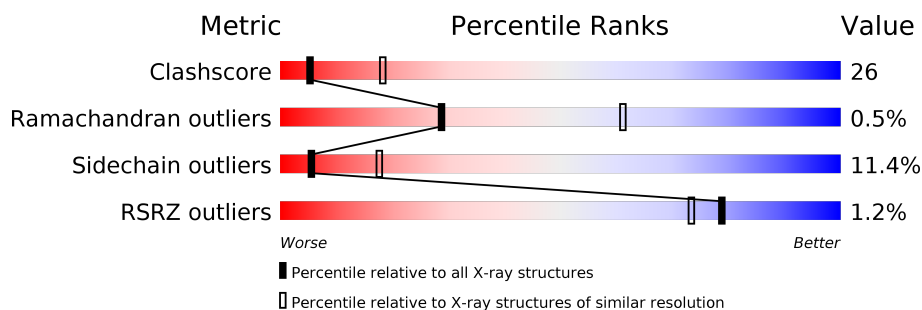
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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))
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	470	
1	B	470	
1	C	470	
1	D	470	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14000 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 Pyruvate kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	461	Total	C	N	O	S	0	0	0
			3445	2150	594	676	25			
1	B	461	Total	C	N	O	S	0	0	0
			3445	2150	594	676	25			
1	C	461	Total	C	N	O	S	11	0	0
			3445	2150	594	676	25			
1	D	461	Total	C	N	O	S	0	0	0
			3445	2150	594	676	25			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	271	LEU	ARG	engineered mutation	UNP A0A0A0G552
A	279	MET	GLN	engineered mutation	UNP A0A0A0G552
B	271	LEU	ARG	engineered mutation	UNP A0A0A0G552
B	279	MET	GLN	engineered mutation	UNP A0A0A0G552
C	271	LEU	ARG	engineered mutation	UNP A0A0A0G552
C	279	MET	GLN	engineered mutation	UNP A0A0A0G552
D	271	LEU	ARG	engineered mutation	UNP A0A0A0G552
D	279	MET	GLN	engineered mutation	UNP A0A0A0G552

- 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	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		

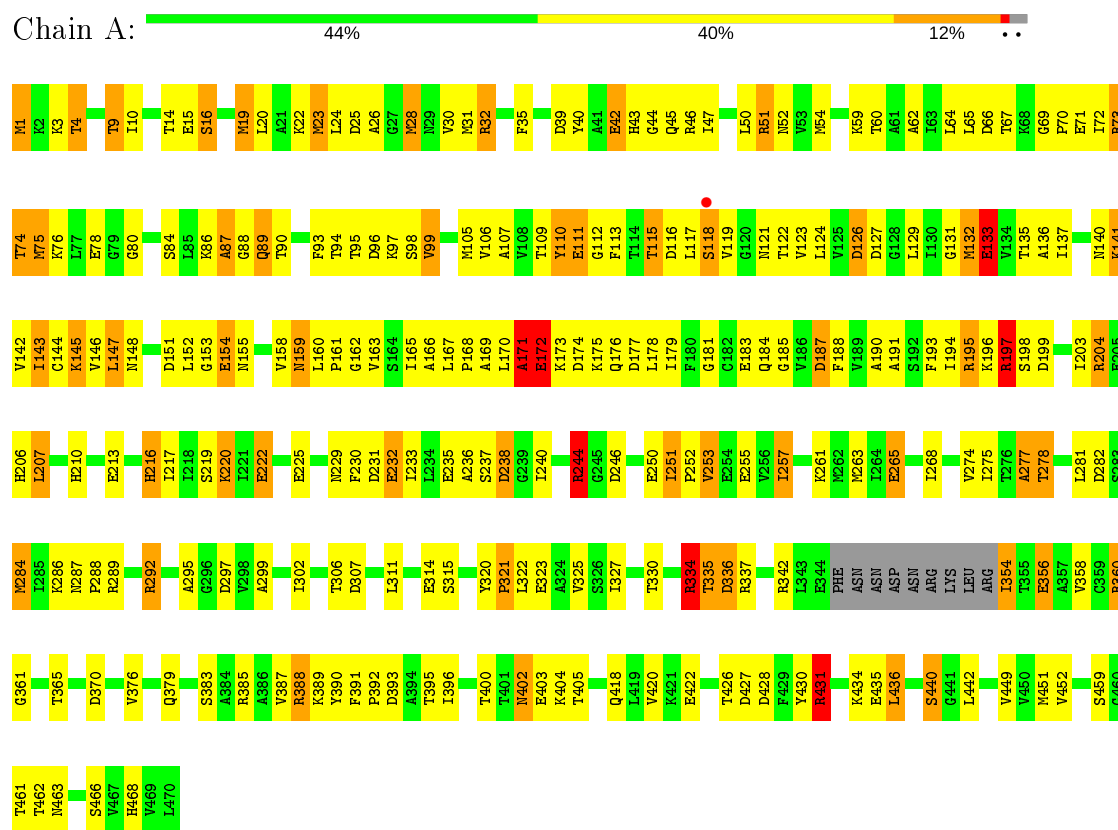
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	38	Total	O	0	0
			38	38		
3	B	55	Total	O	0	0
			55	55		
3	C	48	Total	O	0	0
			48	48		
3	D	59	Total	O	0	0
			59	59		

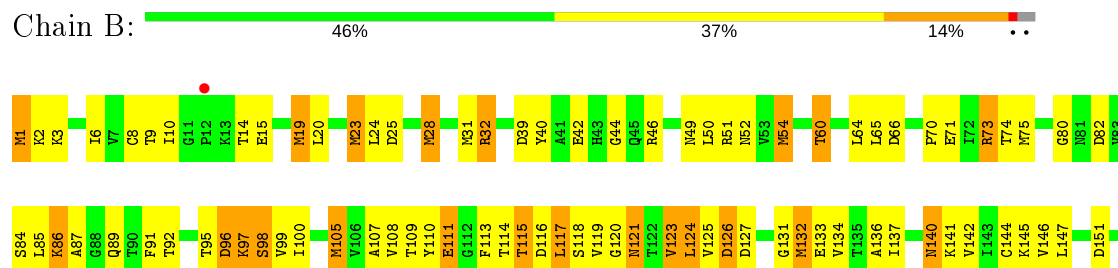
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: Pyruvate kinase



• Molecule 1: Pyruvate kinase





V376	V469	L303	L152	E78
A377	L470	D304	G153	G79
T378		D307	E154	G80
Q379			N155	
			K156	
K382		M310	N159	S84
		L311	L160	L85
R385		S312	P161	K86
A386			G162	A87
V387		S315	V163	G88
R388			S164	Q89
K389		Y320	L165	
Y390		P321	A166	T92
F391		L322	L167	F93
P392		A323	P168	T94
		A324	P169	T95
T395		V325	A170	D96
I396		S326	A171	K97
L397		I327	E172	S98
			K173	V99
T400		T330	D174	I100
T401		I331	K175	M105
E403		R334	Q176	
K404		T335	D177	Y110
T405		D386	L178	E111
		R337	I179	
L409		V338	E183	T114
V410		M339	V186	T115
			A190	D116
K413		R342	A191	L117
		E344	S192	S118
K421		PHE	F193	V119
E422		ASN	I194	G120
D427		ASN	R195	N121
		ASP	K196	T122
R431		ASN	R197	V123
		ARG	S198	
R434		LYS	D199	D127
		LEU	V200	M132
S440		ARG	I201	E133
G441		I354	E202	V134
L442		T355	R204	T135
		E356	E205	A136
D447		A357	H206	I137
V448		V358	E213	G139
V449		C359	H216	E138
V450		R360	I218	E141
M451		V363	K220	N140
V452		E367	E225	K141
S453		R368	G226	V142
		L369		I143
V457		D370		C144
P458		L373		K145
S459		I374		V146
G460		V375		L147
T461				N148
T462				N149
N463				G150
				D151

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	74.01Å 129.59Å 241.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.80 14.93 – 2.80	Depositor EDS
% Data completeness (in resolution range)	97.7 (15.00-2.80) 97.9 (14.93-2.80)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.83 (at 2.81Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.245 , 0.312 0.240 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	20.6	Xtriage
Anisotropy	0.367	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 47.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	14000	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 46.32 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.1649e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical 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	0.92	2/3479 (0.1%)	2.48	161/4695 (3.4%)
1	B	0.96	3/3479 (0.1%)	2.67	186/4695 (4.0%)
1	C	2.31	6/3479 (0.2%)	2.71	209/4695 (4.5%)
1	D	0.99	1/3479 (0.0%)	2.68	192/4695 (4.1%)
All	All	1.42	12/13916 (0.1%)	2.64	748/18780 (4.0%)

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	2
1	B	0	4
1	C	0	3
1	D	0	5
All	All	0	14

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	138	GLU	CD-OE1	81.24	2.15	1.25
1	C	145	LYS	CD-CE	79.59	3.50	1.51
1	C	111	GLU	CD-OE2	50.21	1.80	1.25
1	D	225	GLU	CD-OE1	7.12	1.33	1.25
1	C	97	LYS	CE-NZ	-6.65	1.32	1.49

The worst 5 of 748 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	244	ARG	NE-CZ-NH1	35.92	138.26	120.30
1	C	385	ARG	CD-NE-CZ	34.00	171.20	123.60
1	B	385	ARG	NE-CZ-NH2	-32.17	104.22	120.30
1	D	265	GLU	OE1-CD-OE2	-30.92	86.20	123.30
1	B	360	ARG	NE-CZ-NH2	-28.51	106.04	120.30

There are no chirality outliers.

5 of 14 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	187	ASP	Mainchain
1	A	277	ALA	Mainchain
1	B	2	LYS	Mainchain
1	B	223	ASN	Mainchain
1	B	28	MET	Mainchain

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	3445	0	3533	176	0
1	B	3445	0	3533	134	0
1	C	3445	0	3533	300	1
1	D	3445	0	3533	142	1
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	1	0
3	A	38	0	0	4	0
3	B	55	0	0	2	0
3	C	48	0	0	10	0
3	D	59	0	0	5	0
All	All	14000	0	14132	736	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 26.

The worst 5 of 736 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:C:92:THR:HG22	1:C:105:MET:SD	1.35	1.62
1:C:136:ALA:CB	1:C:143:ILE:CG2	1.82	1.58
1:C:77:LEU:CD1	1:C:154:GLU:HB3	1.33	1.58
1:C:136:ALA:CB	1:C:143:ILE:HG21	1.36	1.51
1:C:92:THR:CG2	1:C:105:MET:SD	2.05	1.45

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)
1:C:115:THR:CG2	1:D:18:GLU:OE2[4_446]	1.86	0.34

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	457/470 (97%)	434 (95%)	19 (4%)	4 (1%)	17	46
1	B	457/470 (97%)	432 (94%)	24 (5%)	1 (0%)	47	78
1	C	457/470 (97%)	430 (94%)	24 (5%)	3 (1%)	22	53
1	D	457/470 (97%)	441 (96%)	15 (3%)	1 (0%)	47	78
All	All	1828/1880 (97%)	1737 (95%)	82 (4%)	9 (0%)	29	61

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	97	LYS
1	A	162	GLY
1	B	97	LYS
1	C	97	LYS
1	C	172	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	377/389 (97%)	337 (89%)	40 (11%)	6	20
1	B	377/389 (97%)	339 (90%)	38 (10%)	7	22
1	C	377/389 (97%)	322 (85%)	55 (15%)	3	9
1	D	377/389 (97%)	338 (90%)	39 (10%)	7	21
All	All	1508/1556 (97%)	1336 (89%)	172 (11%)	5	18

5 of 172 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	461	THR
1	C	117	LEU
1	D	312	SER
1	C	60	THR
1	C	92	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	224	GLN
1	B	402	ASN
1	C	224	GLN
1	A	402	ASN
1	C	206	HIS

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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

4 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	B	702	-	4,4,4	0.44	0	6,6,6	0.52	0
2	SO4	D	704	-	4,4,4	0.61	0	6,6,6	0.72	0
2	SO4	A	701	-	4,4,4	0.47	0	6,6,6	0.82	0
2	SO4	C	703	-	4,4,4	0.64	0	6,6,6	0.84	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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	704	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.

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	461/470 (98%)	-0.48	1 (0%) 95 94	5, 18, 50, 75	0
1	B	461/470 (98%)	-0.58	1 (0%) 95 94	5, 13, 37, 73	0
1	C	461/470 (98%)	-0.25	20 (4%) 35 25	5, 17, 71, 100	6 (1%)
1	D	461/470 (98%)	-0.64	0 100 100	4, 11, 33, 69	0
All	All	1844/1880 (98%)	-0.49	22 (1%) 79 73	4, 14, 53, 100	6 (0%)

The worst 5 of 22 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	77	LEU	5.0
1	C	36	SER	4.5
1	C	80	GLY	4.3
1	C	106	VAL	4.0
1	C	81	ASN	3.4

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	A	701	5/5	0.97	0.11	21,22,23,23	0
2	SO4	B	702	5/5	0.98	0.11	18,19,20,20	0
2	SO4	C	703	5/5	0.98	0.09	10,11,12,14	0
2	SO4	D	704	5/5	0.99	0.12	44,44,45,46	0

6.5 Other polymers [i](#)

There are no such residues in this entry.