wwPDB X-ray Structure Validation Summary Report (i)

Sep 18, 2023 – 02:42 PM EDT

PDB ID	:	1LDB
Title	:	STRUCTURE DETERMINATION AND REFINEMENT OF BACILLUS STEAROTHERMOPHILUS LACTATE DEHYDROGENASE
Authors	:	Piontek, K.; Rossmann, M.G.
Deposited on	:	1989-03-27
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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

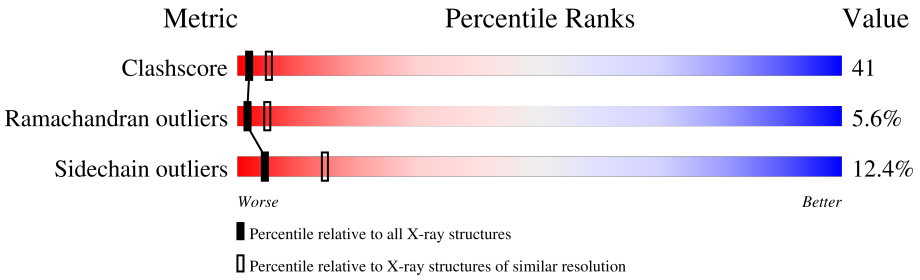
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

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)

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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	317	28% 36% 20% 9% 7%
1	B	317	28% 34% 21% 9% 7%
1	C	317	27% 37% 21% 8% 7%
1	D	317	27% 36% 21% 8% 7%

2 Entry composition (i)

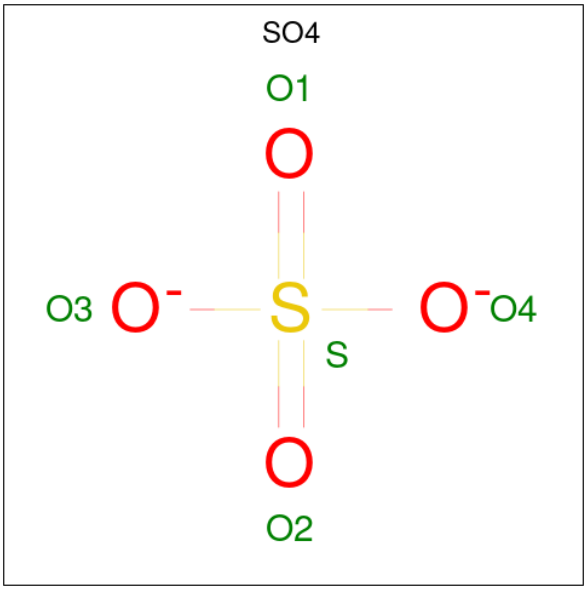
There are 3 unique types of molecules in this entry. The entry contains 9119 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 APO-L-LACTATE DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	294	Total	C	N	O	S	0	0	0
			2277	1457	390	422	8			
1	B	294	Total	C	N	O	S	0	0	0
			2277	1457	390	422	8			
1	C	294	Total	C	N	O	S	0	0	0
			2277	1457	390	422	8			
1	D	294	Total	C	N	O	S	0	0	0
			2277	1457	390	422	8			

- 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			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O 1 1	0	0

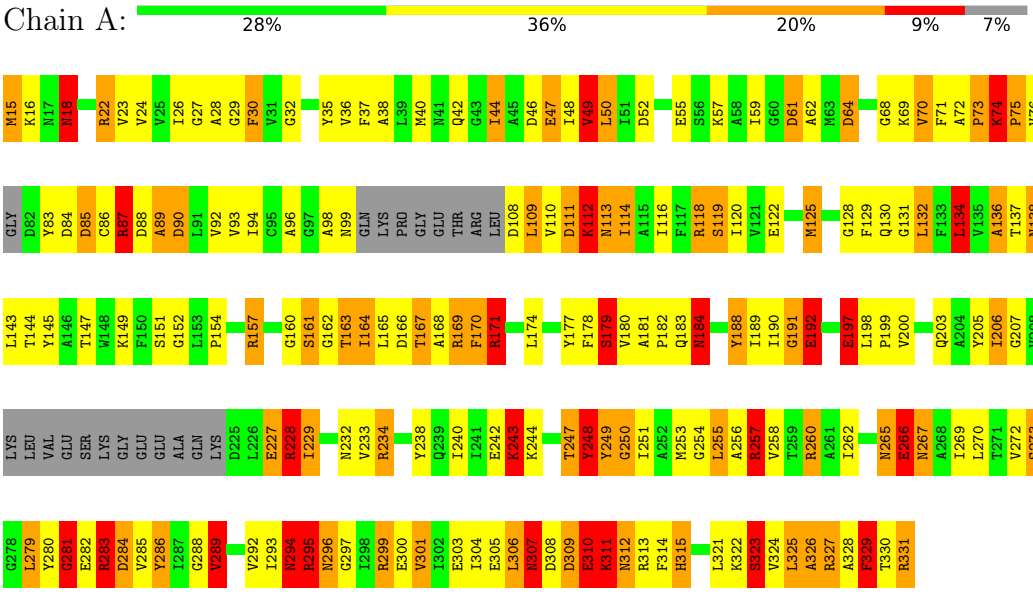
3 Residue-property plots (i)

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. 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. 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.

Note EDS was not executed.

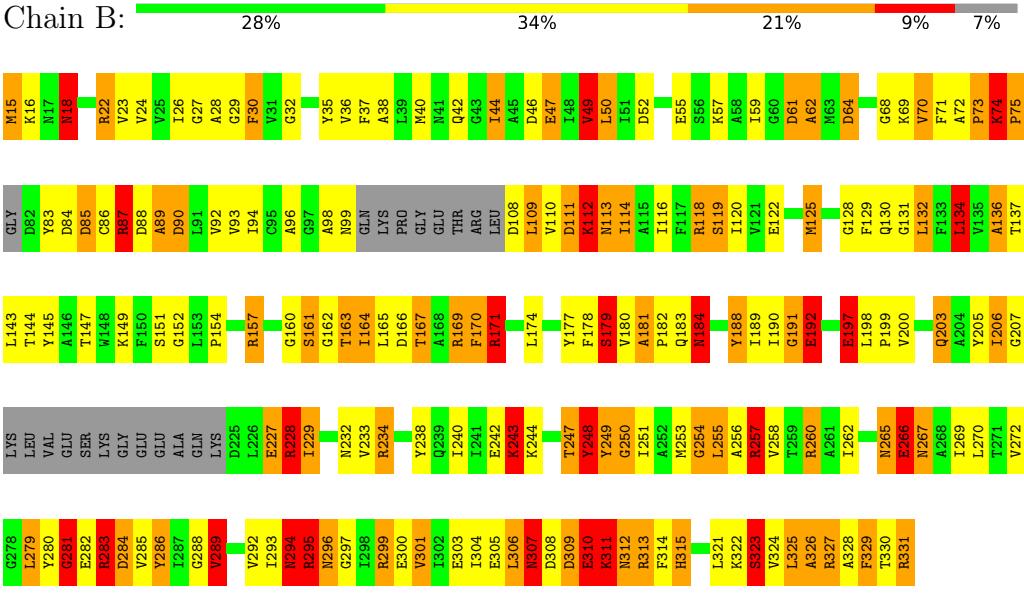
• Molecule 1: APO-L-LACTATE DEHYDROGENASE

Chain A:



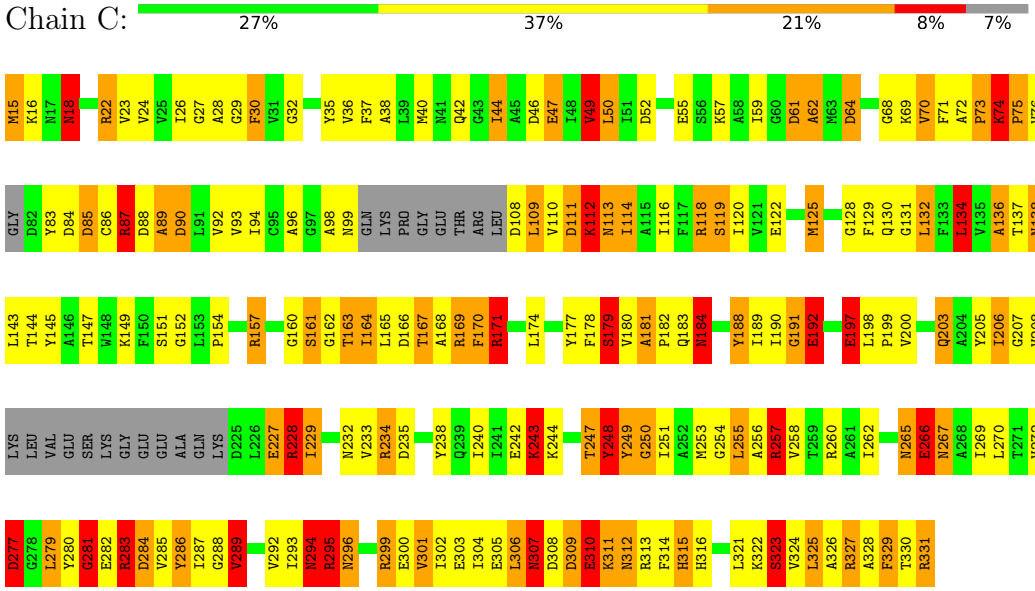
• Molecule 1: APO-L-LACTATE DEHYDROGENASE

Chain B:



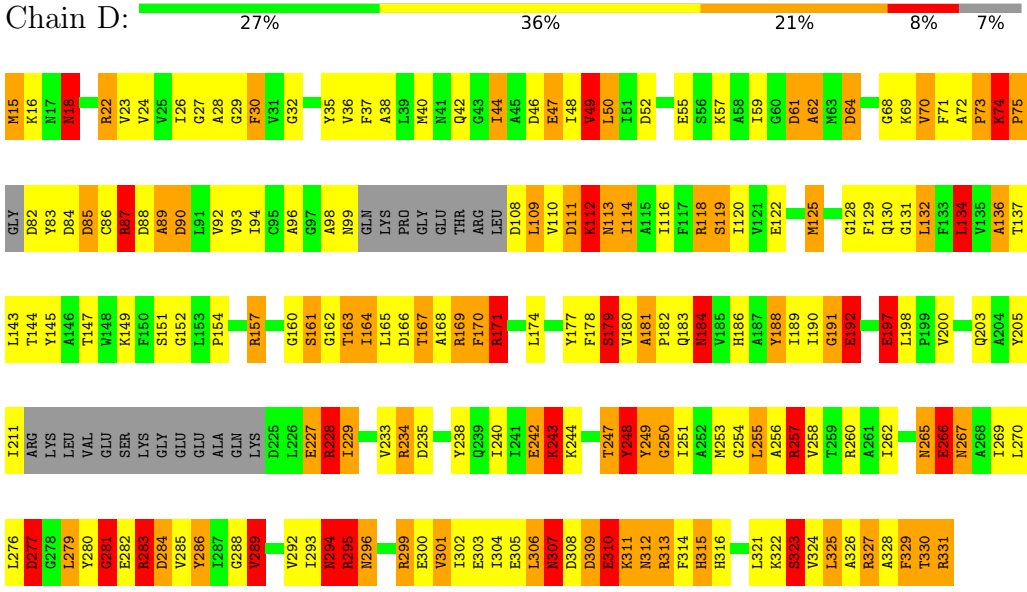
• Molecule 1: APO-L-LACTATE DEHYDROGENASE

Chain C:



• Molecule 1: APO-L-LACTATE DEHYDROGENASE

Chain D:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α, β, γ	86.90Å 86.90Å 357.30Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	6.00 – 2.80	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-2.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.286 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9119	wwPDB-VP
Average B, all atoms (Å^2)	18.0	wwPDB-VP

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	1.56	15/2320 (0.6%)	2.68	142/3146 (4.5%)
1	B	1.56	15/2320 (0.6%)	2.69	143/3146 (4.5%)
1	C	1.56	15/2320 (0.6%)	2.69	141/3146 (4.5%)
1	D	1.56	15/2320 (0.6%)	2.69	141/3146 (4.5%)
All	All	1.56	60/9280 (0.6%)	2.69	567/12584 (4.5%)

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	31
1	B	0	32
1	C	0	31
1	D	0	31
All	All	0	125

The worst 5 of 60 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	188	TYR	CG-CD1	8.15	1.49	1.39
1	A	188	TYR	CG-CD1	8.14	1.49	1.39
1	C	188	TYR	CG-CD1	8.13	1.49	1.39
1	B	188	TYR	CG-CD1	8.03	1.49	1.39
1	C	192	GLU	CD-OE1	-6.89	1.18	1.25

The worst 5 of 567 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	169	ARG	NE-CZ-NH1	35.23	137.92	120.30
1	B	169	ARG	NE-CZ-NH1	35.19	137.90	120.30
1	D	169	ARG	NE-CZ-NH1	35.12	137.86	120.30
1	C	169	ARG	NE-CZ-NH1	35.09	137.84	120.30
1	C	260	ARG	NE-CZ-NH1	-24.25	108.17	120.30

There are no chirality outliers.

5 of 125 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	23	VAL	Mainchain
1	A	30	PHE	Sidechain
1	A	49	VAL	Mainchain
1	A	62	ALA	Mainchain
1	A	77	ASP	Mainchain

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	2277	0	2251	201	46
1	B	2277	0	2251	199	0
1	C	2277	0	2251	206	11
1	D	2277	0	2251	197	57
2	A	10	0	0	2	0
3	A	1	0	0	1	0
All	All	9119	0	9004	750	57

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 41.

The worst 5 of 750 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:D:87:ARG:HG3	1:D:88:ASP:H	1.12	1.13
1:B:87:ARG:HG3	1:B:88:ASP:H	1.11	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:142:ILE:HD13	1:D:324:VAL:HG11	1.31	1.11
1:C:142:ILE:HD13	1:C:324:VAL:HG11	1.31	1.10
1:B:142:ILE:HD13	1:B:324:VAL:HG11	1.32	1.09

The worst 5 of 57 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:A:326:ALA:N	1:D:331:ARG:CB[6_665]	0.71	1.49
1:A:326:ALA:C	1:D:331:ARG:C[6_665]	0.78	1.42
1:A:325:LEU:C	1:D:331:ARG:CB[6_665]	0.88	1.32
1:C:316:HIS:CE1	1:D:316:HIS:CE1[6_655]	1.07	1.13
1:C:316:HIS:NE2	1:D:316:HIS:CE1[6_655]	1.09	1.11

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	286/317 (90%)	232 (81%)	38 (13%)	16 (6%)	2 5
1	B	286/317 (90%)	232 (81%)	38 (13%)	16 (6%)	2 5
1	C	286/317 (90%)	232 (81%)	38 (13%)	16 (6%)	2 5
1	D	286/317 (90%)	232 (81%)	38 (13%)	16 (6%)	2 5
All	All	1144/1268 (90%)	928 (81%)	152 (13%)	64 (6%)	2 5

5 of 64 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	18	ASN
1	A	98	ALA
1	A	307	ASN

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Mol	Chain	Res	Type
1	A	311	LYS
1	A	329	PHE

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	236/255 (92%)	206 (87%)	30 (13%)	4	14
1	B	236/255 (92%)	207 (88%)	29 (12%)	4	15
1	C	236/255 (92%)	207 (88%)	29 (12%)	4	15
1	D	236/255 (92%)	207 (88%)	29 (12%)	4	15
All	All	944/1020 (92%)	827 (88%)	117 (12%)	4	14

5 of 117 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	295	ARG
1	D	266	GLU
1	C	183	GLN
1	D	265	ASN
1	D	179	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 43 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	265	ASN
1	D	138	ASN
1	C	267	ASN
1	D	18	ASN
1	D	232	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)

2 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	1	-	4,4,4	0.92	0	6,6,6	0.78	0
2	SO4	A	2	-	4,4,4	1.20	1 (25%)	6,6,6	1.03	1 (16%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2	SO4	O2-S	2.11	1.57	1.46

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	2	SO4	O4-S-O1	2.17	120.65	109.31

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1	SO4	1	0
2	A	2	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

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.