



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 11:11 AM UTC

PDB ID : 1LDB / pdb_00001ldb
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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

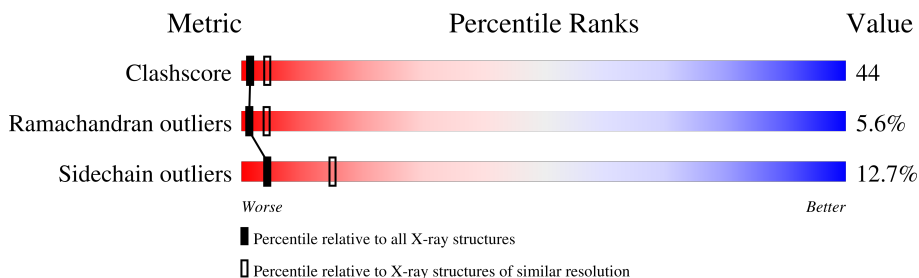
1 Overall quality at a glance

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	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (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 $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	317	16% 35% 32% 10% 7%
1	B	317	15% 34% 33% 10% 7%
1	C	317	16% 33% 33% 10% 7%
1	D	317	15% 33% 33% 11% 7%

2 Entry composition [i](#)

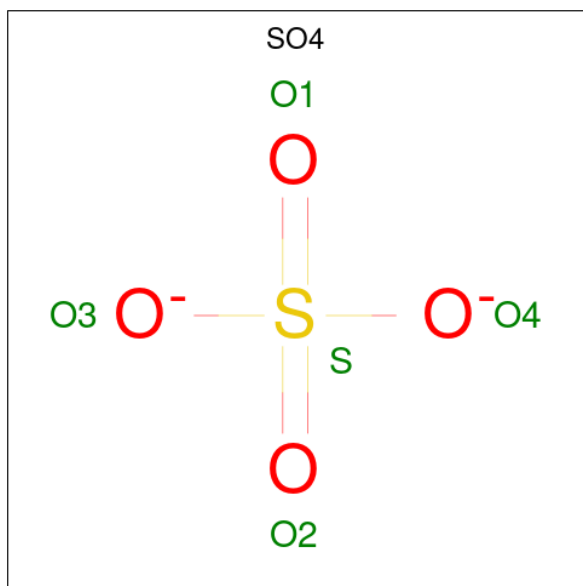
There are 3 unique types of molecules in this entry. The entry contains 9119 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (CCD ID: 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		

- Molecule 3 is water.

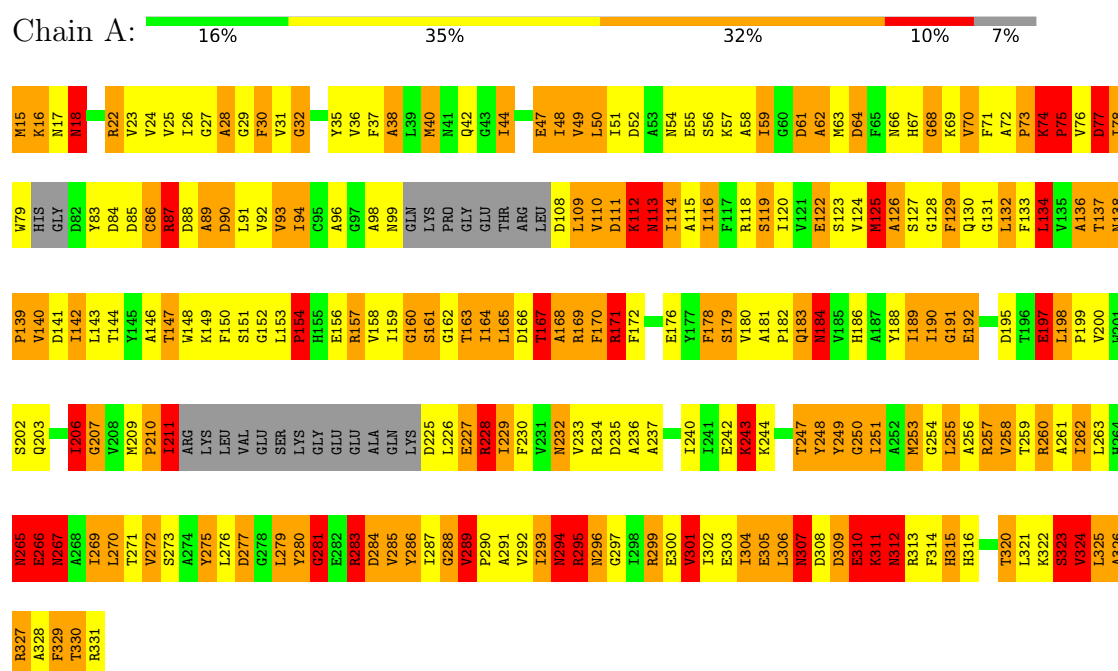
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	O	0	0
			1	1		

3 Residue-property plots

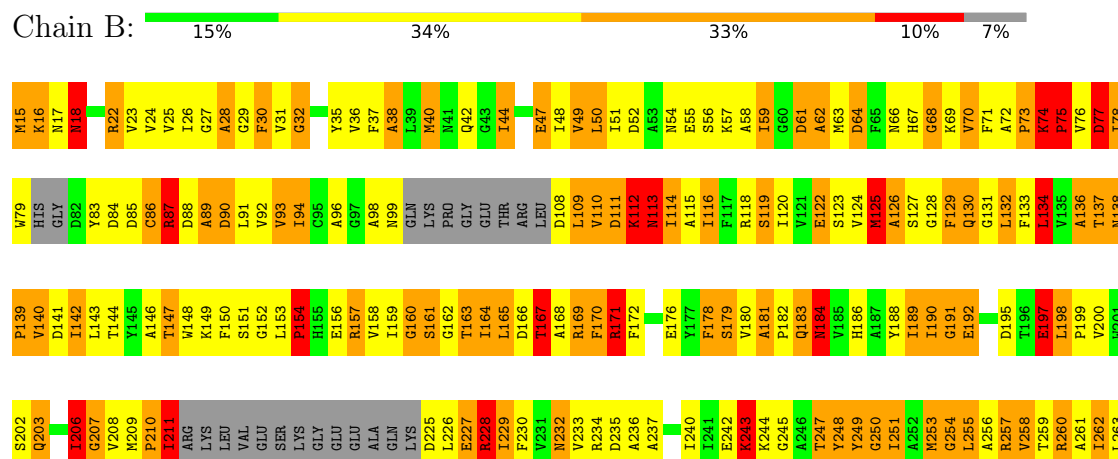
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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.

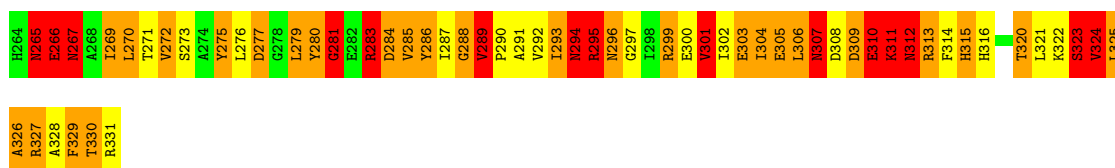
Note EDS was not executed.

• Molecule 1: APO-L-LACTATE DEHYDROGENASE



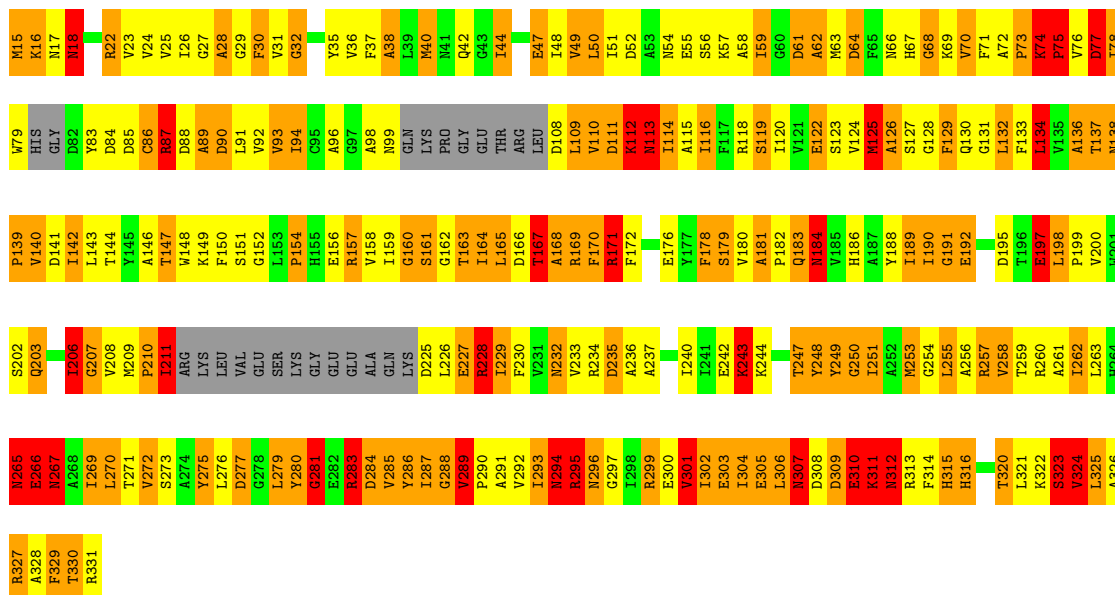
• Molecule 1: APO-L-LACTATE DEHYDROGENASE





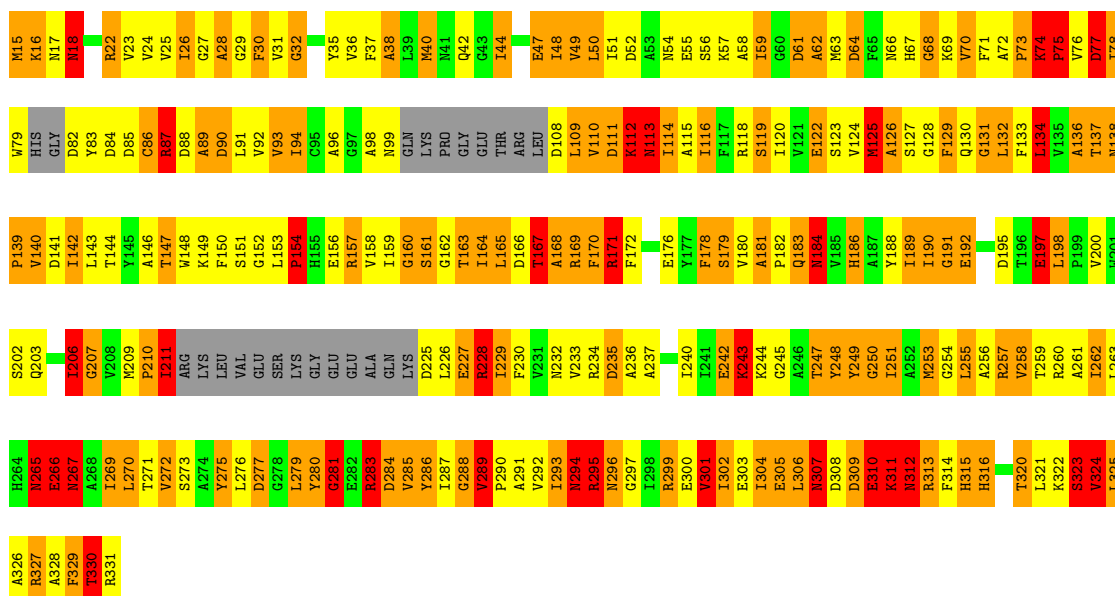
• Molecule 1: APO-L-LACTATE DEHYDROGENASE

Chain C: 16% 33% 33% 10% 7%



• Molecule 1: APO-L-LACTATE DEHYDROGENASE

Chain D: 15% 33% 33% 11% 7%



4 Data and refinement statistics

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 [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	2.05	62/2320 (2.7%)	3.16	308/3146 (9.8%)
1	B	2.05	64/2320 (2.8%)	3.16	313/3146 (9.9%)
1	C	2.05	62/2320 (2.7%)	3.16	317/3146 (10.1%)
1	D	2.05	65/2320 (2.8%)	3.16	313/3146 (9.9%)
All	All	2.05	253/9280 (2.7%)	3.16	1251/12584 (9.9%)

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 253 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	44	ILE	C-O	10.43	1.35	1.23
1	A	44	ILE	C-O	10.33	1.35	1.23
1	C	44	ILE	C-O	10.27	1.35	1.23
1	B	44	ILE	C-O	10.20	1.34	1.23
1	C	134	LEU	N-CA	9.98	1.58	1.46

The worst 5 of 1251 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	276	LEU	CA-C-N	22.07	157.57	120.72
1	A	276	LEU	C-N-CA	22.07	157.57	120.72
1	D	276	LEU	CA-C-N	22.06	157.57	120.72
1	D	276	LEU	C-N-CA	22.06	157.57	120.72
1	C	276	LEU	CA-C-N	22.05	157.54	120.72

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	2253	217	46
1	B	2277	0	2253	216	0
1	C	2277	0	2253	221	11
1	D	2277	0	2253	214	57
2	A	10	0	0	2	0
3	A	1	0	0	1	0
All	All	9119	0	9012	803	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 44.

The worst 5 of 803 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

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	286/317 (90%)	232 (81%)	38 (13%)	16 (6%)	1	4
1	B	286/317 (90%)	232 (81%)	38 (13%)	16 (6%)	1	4
1	C	286/317 (90%)	232 (81%)	38 (13%)	16 (6%)	1	4
1	D	286/317 (90%)	232 (81%)	38 (13%)	16 (6%)	1	4
All	All	1144/1268 (90%)	928 (81%)	152 (13%)	64 (6%)	1	4

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	15
1	B	236/255 (92%)	206 (87%)	30 (13%)	4	15
1	C	236/255 (92%)	206 (87%)	30 (13%)	4	15
1	D	236/255 (92%)	206 (87%)	30 (13%)	4	15
All	All	944/1020 (92%)	824 (87%)	120 (13%)	4	15

5 of 120 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	312	ASN
1	D	257	ARG
1	C	183	GLN
1	D	243	LYS
1	D	320	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 41 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	294	ASN
1	D	232	ASN
1	C	307	ASN
1	D	113	ASN
1	D	267	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	2	-	4,4,4	1.23	1 (25%)	6,6,6	1.03	1 (16%)
2	SO4	A	1	-	4,4,4	0.95	0	6,6,6	0.75	0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2	SO4	O2-S	2.12	1.57	1.44

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2	SO4	O4-S-O1	2.12	120.65	109.56

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	2	SO4	1	0
2	A	1	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.