



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 08:14 PM UTC

PDB ID : 4KDF / pdb\_00004kdf  
Title : Crystal Structure of Thermus thermophilus Malate Dehydrogenase in Complex with NAD  
Authors : Hsu, C.-H.; Hong, C.-H.; Chang, Y.-Y.  
Deposited on : 2013-04-25  
Resolution : 2.36 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](mailto: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) : 2.0  
EDS : 3.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

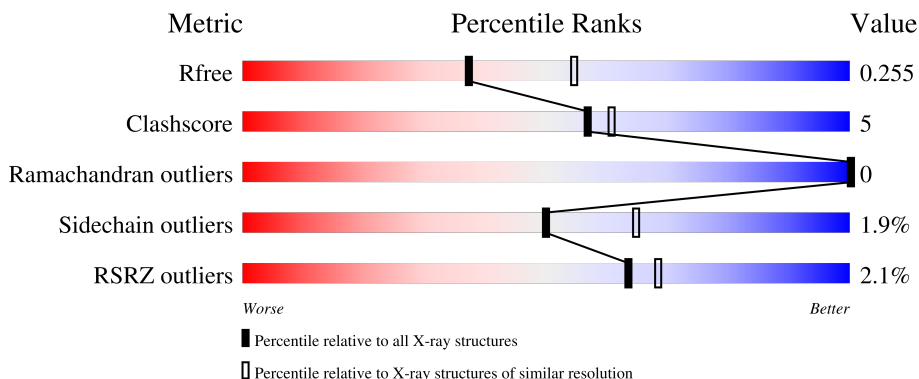
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*



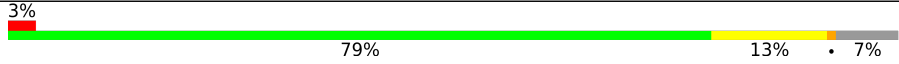
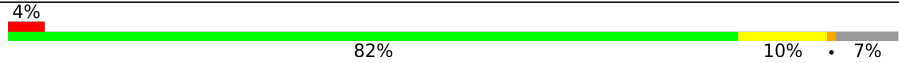
The reported resolution of this entry is 2.36 Å.

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))
$R_{free}$	180053	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

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  $\geq 3$ , 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	341	
1	B	341	
1	C	341	
1	D	341	

## 2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 10013 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 Malate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	317	2404	1527	417	448	12	0	0	0
1	B	317	2404	1527	417	448	12	0	0	0
1	C	318	2415	1533	421	449	12	0	0	0
1	D	318	2415	1533	421	449	12	0	0	0

There are 56 discrepancies between the modelled and reference sequences:

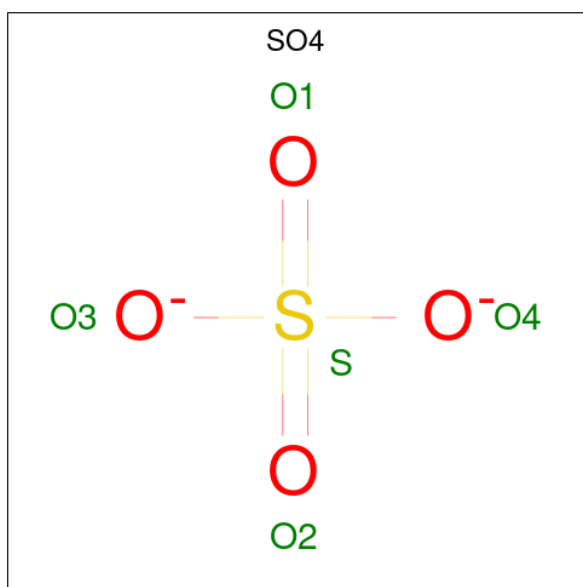
Chain	Residue	Modelled	Actual	Comment	Reference
A	328	ARG	-	expression tag	UNP P10584
A	329	LYS	-	expression tag	UNP P10584
A	330	LEU	-	expression tag	UNP P10584
A	331	ALA	-	expression tag	UNP P10584
A	332	ALA	-	expression tag	UNP P10584
A	333	ALA	-	expression tag	UNP P10584
A	334	LEU	-	expression tag	UNP P10584
A	335	GLU	-	expression tag	UNP P10584
A	336	HIS	-	expression tag	UNP P10584
A	337	HIS	-	expression tag	UNP P10584
A	338	HIS	-	expression tag	UNP P10584
A	339	HIS	-	expression tag	UNP P10584
A	340	HIS	-	expression tag	UNP P10584
A	341	HIS	-	expression tag	UNP P10584
B	328	ARG	-	expression tag	UNP P10584
B	329	LYS	-	expression tag	UNP P10584
B	330	LEU	-	expression tag	UNP P10584
B	331	ALA	-	expression tag	UNP P10584
B	332	ALA	-	expression tag	UNP P10584
B	333	ALA	-	expression tag	UNP P10584
B	334	LEU	-	expression tag	UNP P10584

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
B	335	GLU	-	expression tag	UNP P10584
B	336	HIS	-	expression tag	UNP P10584
B	337	HIS	-	expression tag	UNP P10584
B	338	HIS	-	expression tag	UNP P10584
B	339	HIS	-	expression tag	UNP P10584
B	340	HIS	-	expression tag	UNP P10584
B	341	HIS	-	expression tag	UNP P10584
C	328	ARG	-	expression tag	UNP P10584
C	329	LYS	-	expression tag	UNP P10584
C	330	LEU	-	expression tag	UNP P10584
C	331	ALA	-	expression tag	UNP P10584
C	332	ALA	-	expression tag	UNP P10584
C	333	ALA	-	expression tag	UNP P10584
C	334	LEU	-	expression tag	UNP P10584
C	335	GLU	-	expression tag	UNP P10584
C	336	HIS	-	expression tag	UNP P10584
C	337	HIS	-	expression tag	UNP P10584
C	338	HIS	-	expression tag	UNP P10584
C	339	HIS	-	expression tag	UNP P10584
C	340	HIS	-	expression tag	UNP P10584
C	341	HIS	-	expression tag	UNP P10584
D	328	ARG	-	expression tag	UNP P10584
D	329	LYS	-	expression tag	UNP P10584
D	330	LEU	-	expression tag	UNP P10584
D	331	ALA	-	expression tag	UNP P10584
D	332	ALA	-	expression tag	UNP P10584
D	333	ALA	-	expression tag	UNP P10584
D	334	LEU	-	expression tag	UNP P10584
D	335	GLU	-	expression tag	UNP P10584
D	336	HIS	-	expression tag	UNP P10584
D	337	HIS	-	expression tag	UNP P10584
D	338	HIS	-	expression tag	UNP P10584
D	339	HIS	-	expression tag	UNP P10584
D	340	HIS	-	expression tag	UNP P10584
D	341	HIS	-	expression tag	UNP P10584

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O<sub>4</sub>S).



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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	85	Total O 85 85	0	0
3	B	85	Total O 85 85	0	0

*Continued on next page...*

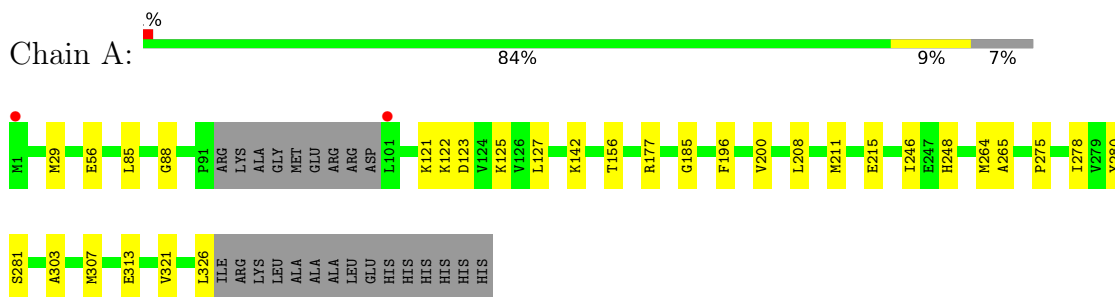
*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
3	C	75	Total 75	O 75	0	0
3	D	80	Total 80	O 80	0	0

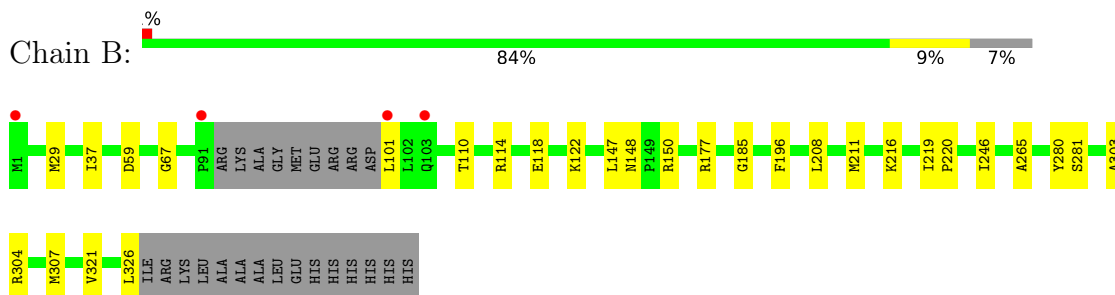
### 3 Residue-property plots [i](#)

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 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.

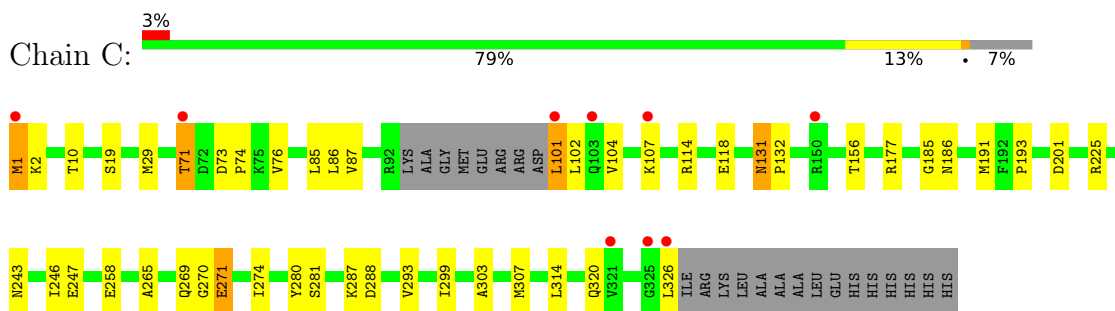
- Molecule 1: Malate dehydrogenase



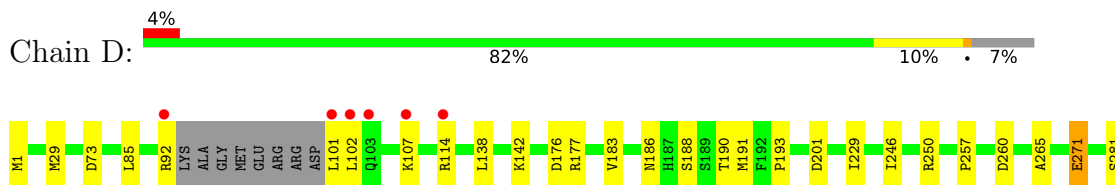
- Molecule 1: Malate dehydrogenase



- Molecule 1: Malate dehydrogenase



- Molecule 1: Malate dehydrogenase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	96.60Å 114.62Å 144.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.27 – 2.36 24.27 – 2.36	Depositor EDS
% Data completeness (in resolution range)	98.6 (24.27-2.36) 91.4 (24.27-2.36)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.98 (at 2.36Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, $R_{free}$	0.183 , 0.232 (Not available) , 0.255	Depositor DCC
$R_{free}$ test set	2000 reflections (2.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	33.1	Xtriage
Anisotropy	1.097	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 44.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	10013	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	50.0	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 90.67 % 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 2.0825e-08. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>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	0.48	0/2447	0.78	0/3317
1	B	0.46	0/2447	0.79	0/3317
1	C	0.50	0/2458	0.83	0/3331
1	D	0.52	0/2458	0.79	2/3331 (0.1%)
All	All	0.49	0/9810	0.80	2/13296 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	73	ASP	CA-C-N	5.51	125.34	119.28
1	D	73	ASP	C-N-CA	5.51	125.34	119.28

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	2404	0	2436	19	0
1	B	2404	0	2436	18	0
1	C	2415	0	2449	30	0
1	D	2415	0	2449	25	0
2	A	15	0	0	0	0

*Continued on next page...*

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	15	0	0	0	0
2	C	10	0	0	0	0
2	D	10	0	0	1	0
3	A	85	0	0	3	0
3	B	85	0	0	4	0
3	C	75	0	0	3	0
3	D	80	0	0	3	0
All	All	10013	0	9770	90	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 90 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:A:215:GLU:OE2	3:A:567:HOH:O	1.82	0.96
1:D:326:LEU:O	3:D:569:HOH:O	1.84	0.95
1:C:1:MET:SD	3:C:567:HOH:O	2.35	0.84
1:C:177:ARG:NH1	1:C:201:ASP:OD2	2.12	0.82
1:C:2:LYS:NZ	3:C:561:HOH:O	2.18	0.75

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	313/341 (92%)	310 (99%)	3 (1%)	0	100 100
1	B	313/341 (92%)	310 (99%)	3 (1%)	0	100 100
1	C	314/341 (92%)	311 (99%)	3 (1%)	0	100 100
1	D	314/341 (92%)	313 (100%)	1 (0%)	0	100 100

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1254/1364 (92%)	1244 (99%)	10 (1%)	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	244/263 (93%)	242 (99%)	2 (1%)	73	84
1	B	244/263 (93%)	242 (99%)	2 (1%)	73	84
1	C	245/263 (93%)	234 (96%)	11 (4%)	24	32
1	D	245/263 (93%)	241 (98%)	4 (2%)	55	70
All	All	978/1052 (93%)	959 (98%)	19 (2%)	50	65

5 of 19 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	326	LEU
1	D	271	GLU
1	D	310	THR
1	D	102	LEU
1	C	104	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	131	ASN
1	A	166	GLN
1	A	248	HIS
1	B	166	GLN
1	C	312	GLN

### 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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

10 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	402	-	4,4,4	0.23	0	6,6,6	0.30	0
2	SO4	A	402	-	4,4,4	0.21	0	6,6,6	0.27	0
2	SO4	C	402	-	4,4,4	0.25	0	6,6,6	0.08	0
2	SO4	C	401	-	4,4,4	0.25	0	6,6,6	0.14	0
2	SO4	B	401	-	4,4,4	0.22	0	6,6,6	0.22	0
2	SO4	A	401	-	4,4,4	0.26	0	6,6,6	0.15	0
2	SO4	B	403	-	4,4,4	0.25	0	6,6,6	0.12	0
2	SO4	D	402	-	4,4,4	0.27	0	6,6,6	0.08	0
2	SO4	D	401	-	4,4,4	0.22	0	6,6,6	0.12	0
2	SO4	A	403	-	4,4,4	0.25	0	6,6,6	0.13	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	402	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	317/341 (92%)	-0.19	2 (0%) 85 89	32, 47, 69, 91	0
1	B	317/341 (92%)	-0.12	4 (1%) 75 79	34, 48, 72, 96	0
1	C	318/341 (93%)	0.32	9 (2%) 55 61	33, 48, 73, 100	0
1	D	318/341 (93%)	0.21	12 (3%) 44 50	32, 47, 74, 98	0
All	All	1270/1364 (93%)	0.06	27 (2%) 63 68	32, 48, 72, 100	0

The worst 5 of 27 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	101	LEU	6.8
1	C	326	LEU	5.5
1	C	325	GLY	4.9
1	D	325	GLY	4.6
1	C	1	MET	4.5

### 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 oligosaccharides 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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
2	SO4	D	402	5/5	0.83	0.11	96,97,98,99	0
2	SO4	A	403	5/5	0.87	0.13	86,86,91,96	0
2	SO4	C	402	5/5	0.88	0.10	91,93,98,99	0
2	SO4	B	403	5/5	0.90	0.12	86,88,90,92	0
2	SO4	C	401	5/5	0.91	0.14	75,75,78,81	0
2	SO4	A	402	5/5	0.92	0.09	64,68,72,76	0
2	SO4	B	402	5/5	0.92	0.10	60,67,70,77	0
2	SO4	D	401	5/5	0.95	0.11	74,74,78,78	0
2	SO4	A	401	5/5	0.96	0.08	54,61,64,65	0
2	SO4	B	401	5/5	0.97	0.07	59,60,65,65	0

## 6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.