



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2018 – 11:30 pm GMT

PDB ID : 2Y1O  
Title : Dual-target Inhibitor of MurD and MurE Ligases: Design, Synthesis and Binding Mode Studies  
Authors : Tomasic, T.; Sink, R.; Kovac, A.; Turk, S.; Contreras-Martel, C.; Dessen, A.; Blanot, D.; Gobec, S.; Zega, A.; Kikelj, D.; Peterlin-Masic, L.  
Deposited on : 2010-12-09  
Resolution : 1.49 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](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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : 1.13  
EDS : trunk30967  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk30967

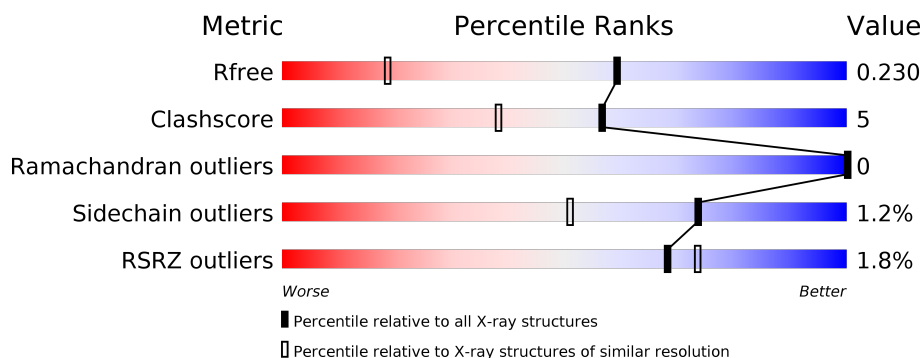
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.49 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))
$R_{free}$	111664	2534 (1.50-1.50)
Clashscore	122126	2727 (1.50-1.50)
Ramachandran outliers	120053	2661 (1.50-1.50)
Sidechain outliers	120020	2659 (1.50-1.50)
RSRZ outliers	108989	2481 (1.50-1.50)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	445	

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 3835 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.

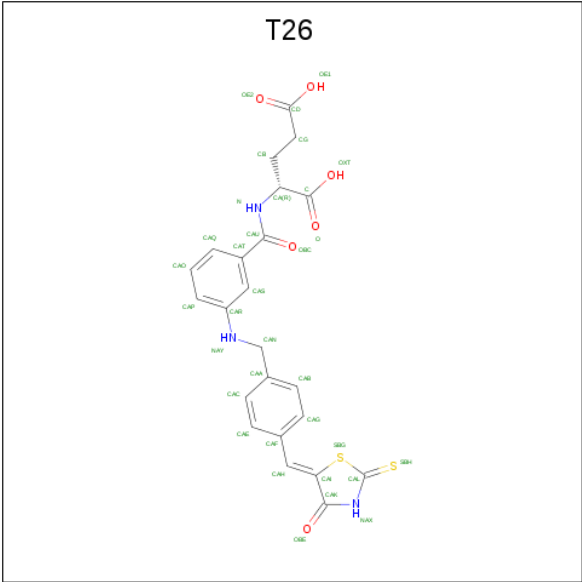
- Molecule 1 is a protein called UDP-N-ACETYLMURAMOYLALANINE--D-GLUTAMATE LIGASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	435	Total	C	N	O	S	0	14	0
			3350	2109	583	634	24			

There are 7 discrepancies between the modelled and reference sequences:

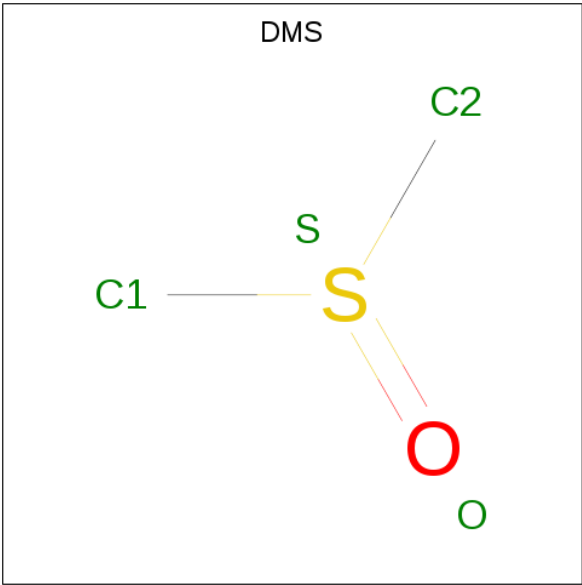
Chain	Residue	Modelled	Actual	Comment	Reference
A	438	SER	-	expression tag	UNP P14900
A	439	HIS	-	expression tag	UNP P14900
A	440	HIS	-	expression tag	UNP P14900
A	441	HIS	-	expression tag	UNP P14900
A	442	HIS	-	expression tag	UNP P14900
A	443	HIS	-	expression tag	UNP P14900
A	444	HIS	-	expression tag	UNP P14900

- Molecule 2 is (2R)-2-[[3-[[4-[(Z)-(4-OXO-2-SULFANYLIDENE-1,3-THIAZOLIDIN-5-YLIDENE)METHYL]PHENYL]METHYLAMINO]PHENYL]CARBONYLAMINO]PENTANED IOIC ACID (three-letter code: T26) (formula: C<sub>23</sub>H<sub>21</sub>N<sub>3</sub>O<sub>6</sub>S<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			34	23	3	6	2		

- Molecule 3 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C<sub>2</sub>H<sub>6</sub>OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	S	0	0
			4	2	1	1		
3	A	1	Total	C	O	S	0	0
			4	2	1	1		
3	A	1	Total	C	O	S	0	0
			4	2	1	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		

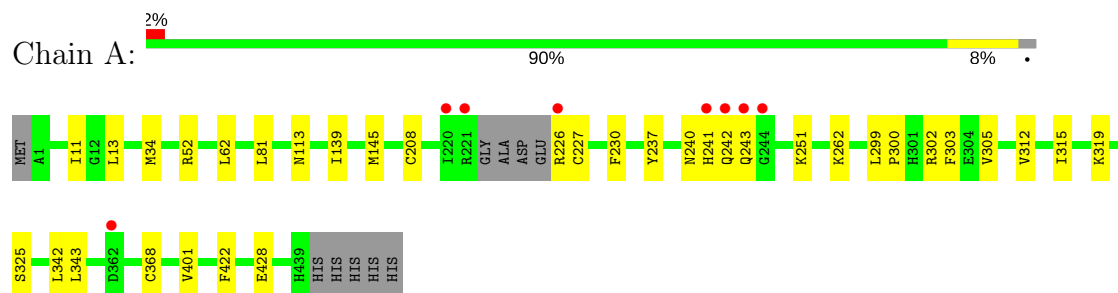
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	415	Total	O	0	0
			415	415		

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

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: UDP-N-ACETYLMURAMOYLALANINE--D-GLUTAMATE LIGASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	65.84Å 65.84Å 135.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.56 – 1.49 38.39 – 1.49	Depositor EDS
% Data completeness (in resolution range)	100.0 (46.56-1.49) 94.1 (38.39-1.49)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.04	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.28 (at 1.49Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.205 , 0.228 0.207 , 0.230	Depositor DCC
$R_{free}$ test set	8825 reflections (10.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	15.5	Xtriage
Anisotropy	0.118	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 41.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.046 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	3835	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.14% of the height of the origin peak. No significant pseudotranslation is detected.*

<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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: DMS, KCX, T26, 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	0.60	0/3433	0.73	0/4652

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	3350	0	3389	36	0
2	A	34	0	19	1	0
3	A	16	0	24	0	0
4	A	20	0	0	0	0
5	A	415	0	0	13	1
All	All	3835	0	3432	37	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 5.

All (37) 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:145[A]:MET:CE	5:A:2026:HOH:O	2.11	0.98
1:A:305:VAL:HG22	1:A:315[B]:ILE:CD1	2.17	0.74
1:A:299:LEU:HB2	1:A:302[B]:ARG:HD3	1.74	0.69
1:A:11[A]:ILE:HD13	1:A:34:MET:HG2	1.78	0.66
1:A:11[A]:ILE:HD11	1:A:62:LEU:HD21	1.78	0.64
1:A:113[B]:ASN:OD1	1:A:325:SER:HB2	1.99	0.63
1:A:208[B]:CYS:HB2	1:A:227:CYS:SG	2.39	0.62
2:A:500:T26:HAG	2:A:500:T26:SBG	2.41	0.60
1:A:428:GLU:HG3	5:A:2396:HOH:O	2.00	0.60
1:A:240:ASN:HD21	1:A:242:GLN:HE22	1.50	0.59
1:A:11[A]:ILE:HD13	1:A:34:MET:CG	2.34	0.57
1:A:303:PHE:CE1	1:A:315[A]:ILE:HD13	2.40	0.57
1:A:302[A]:ARG:NH2	5:A:2142:HOH:O	2.37	0.57
1:A:302[B]:ARG:NE	1:A:319:LYS:HG2	2.20	0.57
1:A:319:LYS:HE3	5:A:2310:HOH:O	2.06	0.55
1:A:241:HIS:HB3	5:A:2256:HOH:O	2.06	0.55
1:A:145[A]:MET:HE1	5:A:2026:HOH:O	1.96	0.54
1:A:262:LYS:NZ	5:A:2272:HOH:O	2.40	0.53
1:A:251:LYS:NZ	5:A:2258:HOH:O	2.42	0.52
1:A:305:VAL:HG22	1:A:315[B]:ILE:HD12	1.90	0.52
1:A:319:LYS:CE	5:A:2310:HOH:O	2.58	0.52
1:A:139:ILE:HG12	5:A:2154:HOH:O	2.12	0.49
1:A:240:ASN:HD21	1:A:242:GLN:NE2	2.09	0.49
1:A:262:LYS:HE3	5:A:2293:HOH:O	2.12	0.48
1:A:145[A]:MET:HE2	5:A:2026:HOH:O	1.96	0.47
1:A:319:LYS:HD3	1:A:422:PHE:CZ	2.50	0.47
1:A:11[A]:ILE:CD1	1:A:34:MET:CG	2.93	0.46
1:A:302[A]:ARG:NH2	1:A:319:LYS:HG3	2.32	0.45
1:A:302[A]:ARG:HD3	1:A:302[A]:ARG:HA	1.65	0.45
1:A:305:VAL:HG22	1:A:315[B]:ILE:HD11	1.97	0.44
1:A:242:GLN:O	1:A:243:GLN:HB2	2.17	0.44
1:A:230:PHE:HA	1:A:237:TYR:O	2.20	0.42
1:A:343:LEU:O	1:A:368:CYS:HA	2.20	0.41
1:A:312:VAL:HG11	1:A:401:VAL:HG11	2.02	0.41
1:A:11[B]:ILE:CD1	1:A:81:LEU:HD21	2.51	0.41
1:A:13:LEU:HA	1:A:13:LEU:HD12	1.94	0.40
1:A:242:GLN:HG3	5:A:2250:HOH:O	2.20	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)
5:A:2043:HOH:O	5:A:2370:HOH:O[4_464]	1.91	0.29

### 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	444/445 (100%)	435 (98%)	9 (2%)	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	358/352 (102%)	354 (99%)	4 (1%)	76	55

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	ARG
1	A	226	ARG
1	A	300	PRO
1	A	342	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	240	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

1 non-standard protein/DNA/RNA residue is 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	$\# Z  > 2$
1	KCX	A	198	1	8,11,12	1.84	1 (12%)	6,12,14	0.77	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	KCX	A	198	1	-	0/6/10/12	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	198	KCX	CA-C	4.74	1.56	1.50

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.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

9 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
4	SO4	A	1441	-	4,4,4	0.39	0	6,6,6	0.78	0
4	SO4	A	1442	-	4,4,4	0.19	0	6,6,6	0.44	0
4	SO4	A	1444	-	4,4,4	0.18	0	6,6,6	0.34	0
4	SO4	A	1445	-	4,4,4	0.27	0	6,6,6	0.19	0
2	T26	A	500	-	30,36,36	1.88	5 (16%)	42,49,49	2.74	8 (19%)
3	DMS	A	600	-	3,3,3	2.67	1 (33%)	3,3,3	0.33	0
3	DMS	A	601	-	3,3,3	1.99	1 (33%)	3,3,3	1.02	0
3	DMS	A	603	-	3,3,3	2.48	1 (33%)	3,3,3	0.49	0
3	DMS	A	604	-	3,3,3	2.55	1 (33%)	3,3,3	0.92	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	SO4	A	1441	-	-	0/0/0/0	0/0/0/0
4	SO4	A	1442	-	-	0/0/0/0	0/0/0/0
4	SO4	A	1444	-	-	0/0/0/0	0/0/0/0
4	SO4	A	1445	-	-	0/0/0/0	0/0/0/0
2	T26	A	500	-	-	0/18/38/38	0/3/3/3
3	DMS	A	600	-	-	0/0/0/0	0/0/0/0
3	DMS	A	601	-	-	0/0/0/0	0/0/0/0
3	DMS	A	603	-	-	0/0/0/0	0/0/0/0
3	DMS	A	604	-	-	0/0/0/0	0/0/0/0

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	500	T26	CAS-CAT	-2.96	1.35	1.39
2	A	500	T26	CAR-NAY	2.71	1.46	1.38
2	A	500	T26	OBE-CAK	2.81	1.28	1.23
3	A	601	DMS	O-S	3.23	1.72	1.50
3	A	603	DMS	O-S	4.14	1.78	1.50
3	A	604	DMS	O-S	4.25	1.79	1.50
3	A	600	DMS	O-S	4.46	1.80	1.50
2	A	500	T26	CAQ-CAT	5.27	1.48	1.39
2	A	500	T26	CAL-SBH	6.31	1.77	1.66

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	500	T26	CAL-NAX-CAK	-8.99	107.87	117.81
2	A	500	T26	CAL-SBG-CAI	-8.80	87.77	92.44
2	A	500	T26	OBE-CAK-CAI	-3.66	121.99	125.87
2	A	500	T26	SBG-CAL-SBH	-3.51	117.96	124.39
2	A	500	T26	SBH-CAL-NAX	-3.28	122.92	126.37
2	A	500	T26	CB-CA-N	-2.17	107.01	110.19
2	A	500	T26	CAI-CAK-NAX	6.52	115.87	110.21
2	A	500	T26	SBG-CAL-NAX	6.73	119.04	109.85

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	A	500	T26	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

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	434/445 (97%)	-0.39	8 (1%) 68 73	12, 20, 35, 61	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	221	ARG	5.0
1	A	243	GLN	4.9
1	A	220	ILE	4.2
1	A	244	GLY	4.0
1	A	242	GLN	3.0
1	A	226	ARG	2.9
1	A	241	HIS	2.1
1	A	362	ASP	2.1

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

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(Å <sup>2</sup> )	Q<0.9
1	KCX	A	198	12/13	0.98	0.08	12,14,17,17	0

### 6.3 Carbohydrates

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, 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
4	SO4	A	1444	5/5	0.83	0.12	50,51,53,54	0
3	DMS	A	603	4/4	0.93	0.14	26,32,34,36	0
3	DMS	A	604	4/4	0.94	0.11	37,38,40,45	0
3	DMS	A	600	4/4	0.94	0.12	32,35,36,37	0
4	SO4	A	1445	5/5	0.96	0.09	40,40,46,47	0
4	SO4	A	1442	5/5	0.97	0.08	54,54,54,57	0
2	T26	A	500	34/34	0.97	0.06	16,21,29,30	0
4	SO4	A	1441	5/5	0.98	0.09	24,28,31,32	0
3	DMS	A	601	4/4	0.98	0.10	18,19,25,26	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.