



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 12:24 AM GMT

PDB ID : 2A8Y  
Title : Crystal structure of 5'-deoxy-5'methylthioadenosine phosphorylase complexed with 5'-deoxy-5'methylthioadenosine and sulfate  
Authors : Zhang, Y.; Porcelli, M.; Cacciapuoti, G.; Ealick, S.E.  
Deposited on : 2005-07-10  
Resolution : 1.45 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  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

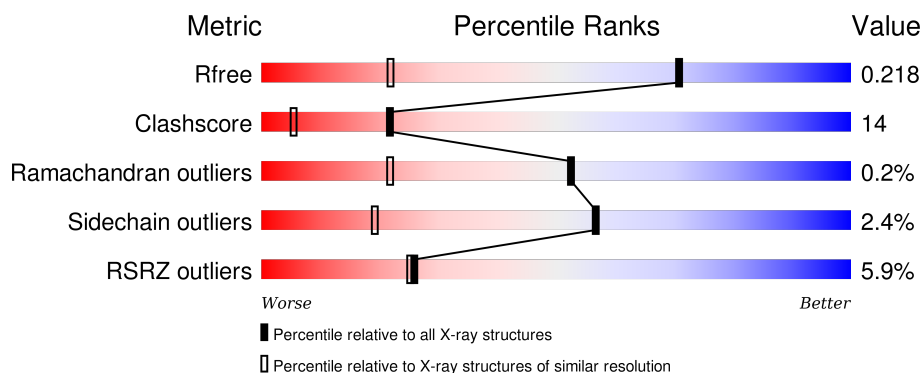
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.45 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))
$R_{free}$	91344	1278 (1.48-1.44)
Clashscore	102246	1336 (1.48-1.44)
Ramachandran outliers	100387	1320 (1.48-1.44)
Sidechain outliers	100360	1320 (1.48-1.44)
RSRZ outliers	91569	1279 (1.48-1.44)

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	270	<div> <div>5%</div> <div>78%</div> <div>19%</div> <div>..</div> </div>
1	B	270	<div> <div>5%</div> <div>77%</div> <div>20%</div> <div>..</div> </div>
1	C	270	<div> <div>6%</div> <div>78%</div> <div>19%</div> <div>..</div> </div>
1	D	270	<div> <div>6%</div> <div>75%</div> <div>22%</div> <div>..</div> </div>
1	E	270	<div> <div>6%</div> <div>76%</div> <div>20%</div> <div>..</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	270	
1	G	270	
1	H	270	
1	I	270	
1	J	270	
1	K	270	
1	L	270	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	A	4001	-	-	-	X
2	SO4	D	4011	-	-	-	X
2	SO4	H	4017	-	-	-	X
2	SO4	I	4026	-	-	-	X
2	SO4	L	4035	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 29330 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 5'-methylthioadenosine phosphorylase (mtaP).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	263	Total	C	N	O	S	0	16	0
			2113	1361	350	384	18			
1	B	263	Total	C	N	O	S	0	16	0
			2135	1370	354	393	18			
1	C	263	Total	C	N	O	S	0	16	0
			2136	1372	356	391	17			
1	D	263	Total	C	N	O	S	0	16	0
			2116	1363	350	385	18			
1	E	263	Total	C	N	O	S	0	16	0
			2138	1376	358	386	18			
1	F	263	Total	C	N	O	S	0	16	0
			2127	1370	352	388	17			
1	G	263	Total	C	N	O	S	0	16	0
			2130	1372	352	388	18			
1	H	263	Total	C	N	O	S	0	16	0
			2129	1370	355	386	18			
1	I	263	Total	C	N	O	S	0	16	0
			2146	1380	358	390	18			
1	J	263	Total	C	N	O	S	0	16	0
			2127	1369	356	385	17			
1	K	263	Total	C	N	O	S	0	16	0
			2136	1373	356	389	18			
1	L	263	Total	C	N	O	S	0	16	0
			2132	1369	355	391	17			

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



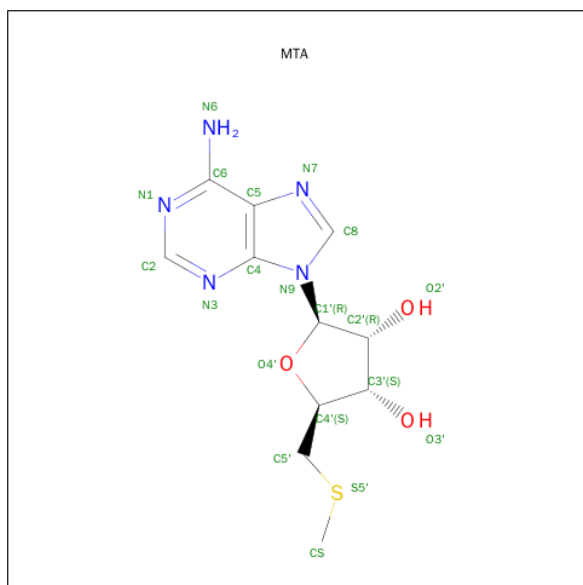
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	L	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	K	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	I	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		
2	H	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	H	1	Total	O	S	0	0
			5	4	1		
2	H	1	Total	O	S	0	0
			5	4	1		
2	I	1	Total	O	S	0	0
			5	4	1		
2	I	1	Total	O	S	0	0
			5	4	1		
2	J	1	Total	O	S	0	0
			5	4	1		
2	J	1	Total	O	S	0	0
			5	4	1		
2	K	1	Total	O	S	0	0
			5	4	1		
2	K	1	Total	O	S	0	0
			5	4	1		
2	L	1	Total	O	S	0	0
			5	4	1		
2	L	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is 5'-DEOXY-5'-METHYLTHIOADENOSINE (three-letter code: MTA) (formula: C<sub>11</sub>H<sub>15</sub>N<sub>5</sub>O<sub>3</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			20	11	5	3	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	N	O	S	0	0
			20	11	5	3	1		
3	C	1	Total	C	N	O	S	0	0
			20	11	5	3	1		
3	D	1	Total	C	N	O	S	0	0
			20	11	5	3	1		
3	E	1	Total	C	N	O	S	0	0
			20	11	5	3	1		
3	F	1	Total	C	N	O	S	0	0
			20	11	5	3	1		
3	G	1	Total	C	N	O	S	0	0
			20	11	5	3	1		
3	H	1	Total	C	N	O	S	0	0
			20	11	5	3	1		
3	I	1	Total	C	N	O	S	0	0
			20	11	5	3	1		
3	J	1	Total	C	N	O	S	0	0
			20	11	5	3	1		
3	K	1	Total	C	N	O	S	0	0
			20	11	5	3	1		
3	L	1	Total	C	N	O	S	0	0
			20	11	5	3	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	266	Total	O	0	0
			266	266		
4	B	311	Total	O	0	0
			311	311		
4	C	265	Total	O	0	0
			265	265		
4	D	293	Total	O	0	0
			293	293		
4	E	281	Total	O	0	0
			281	281		
4	F	275	Total	O	0	0
			275	275		
4	G	273	Total	O	0	0
			273	273		
4	H	283	Total	O	0	0
			283	283		

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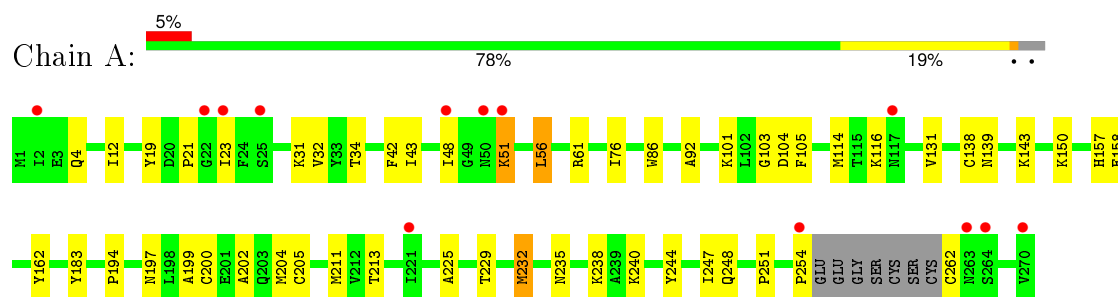
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	I	288	Total 288	O 288	0	0
4	J	261	Total 261	O 261	0	0
4	K	293	Total 293	O 293	0	0
4	L	316	Total 316	O 316	0	0



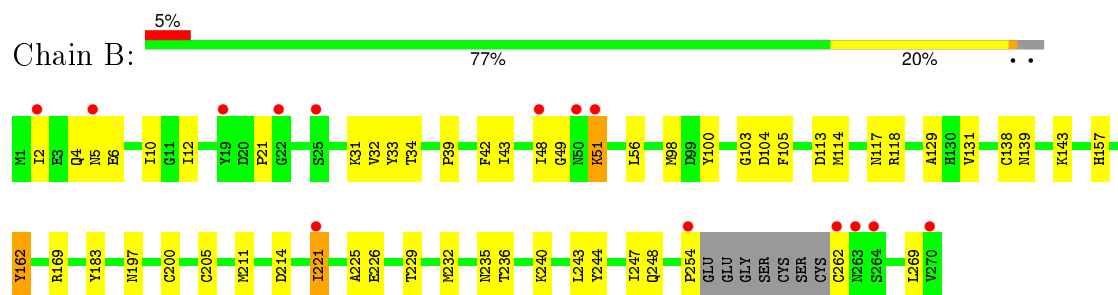
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 ( $\text{RSRZ} > 2$ ). 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.

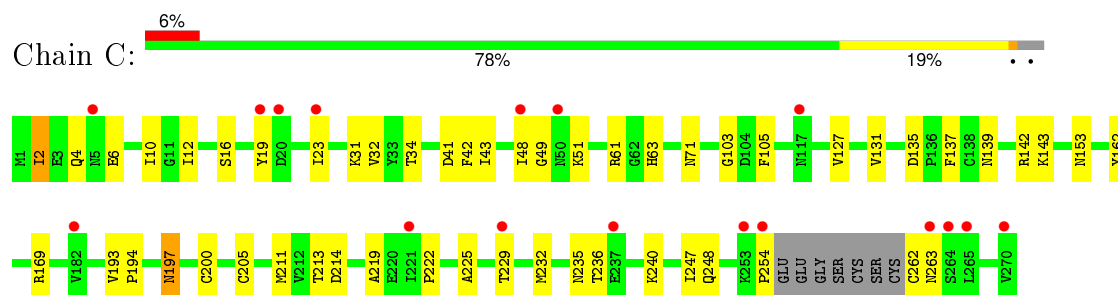
- Molecule 1: 5'-methylthioadenosine phosphorylase (mtaP)



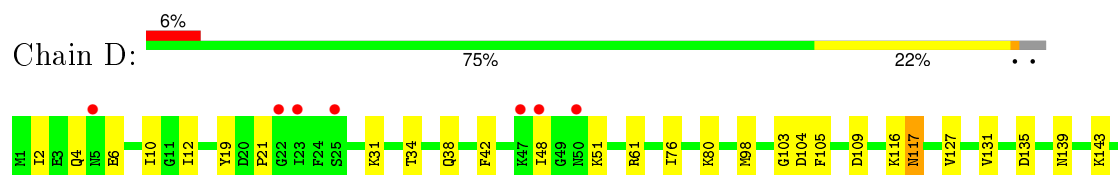
- Molecule 1: 5'-methylthioadenosine phosphorylase (mtaP)

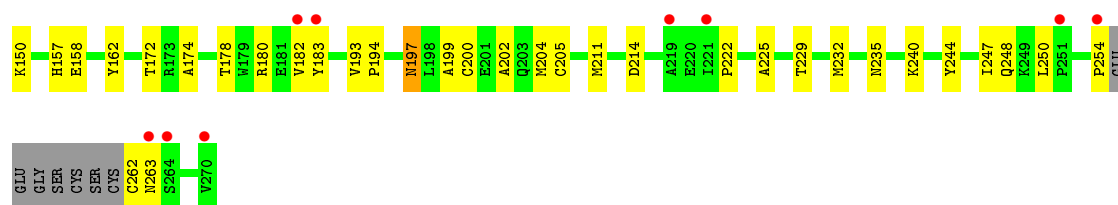


- Molecule 1: 5'-methylthioadenosine phosphorylase (mtaP)

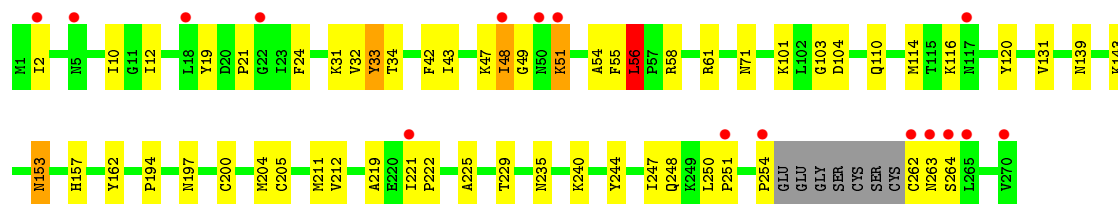
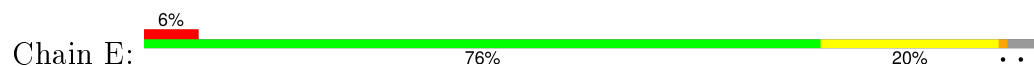


- Molecule 1: 5'-methylthioadenosine phosphorylase (mtaP)

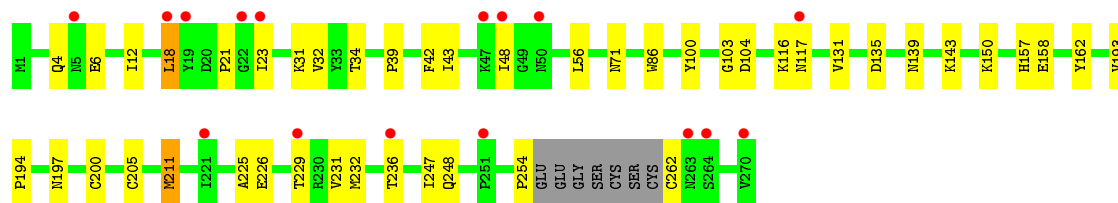
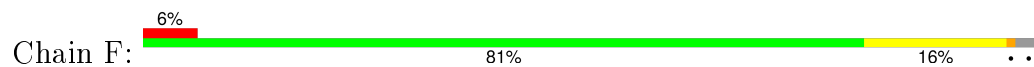




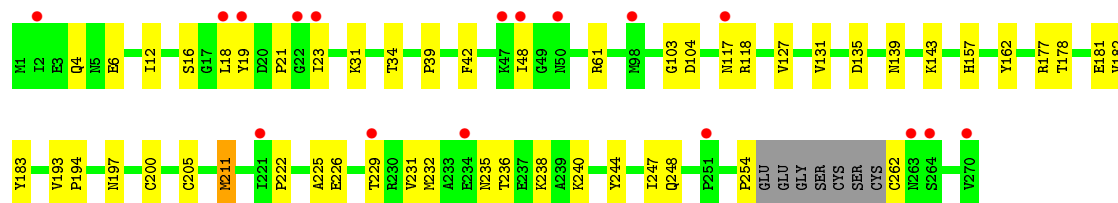
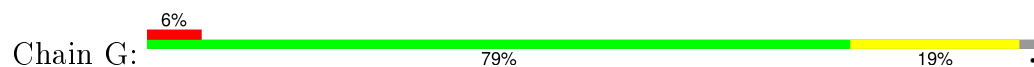
- Molecule 1: 5'-methylthioadenosine phosphorylase (mtaP)



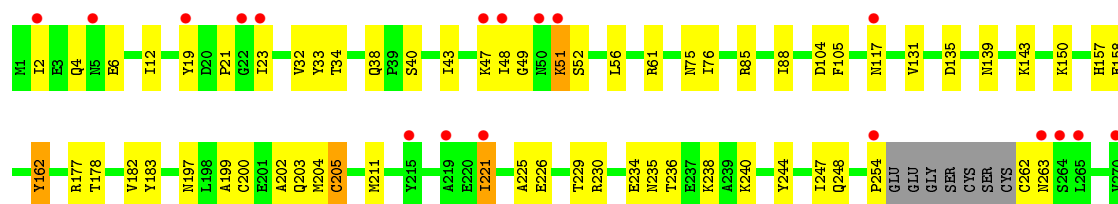
- Molecule 1: 5'-methylthioadenosine phosphorylase (mtaP)



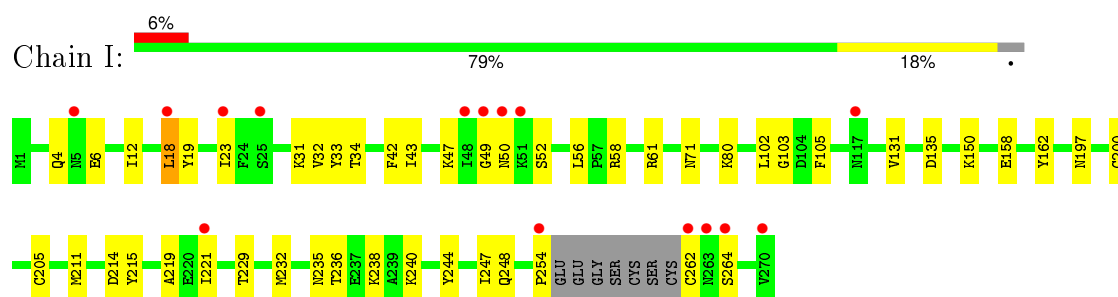
- Molecule 1: 5'-methylthioadenosine phosphorylase (mtaP)



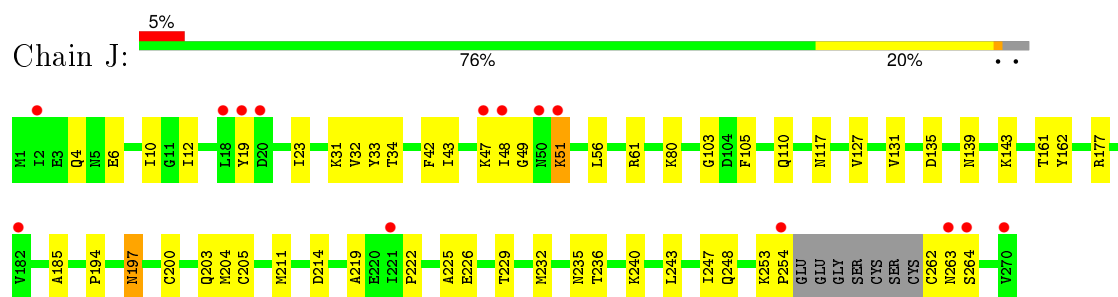
- Molecule 1: 5'-methylthioadenosine phosphorylase (mtaP)



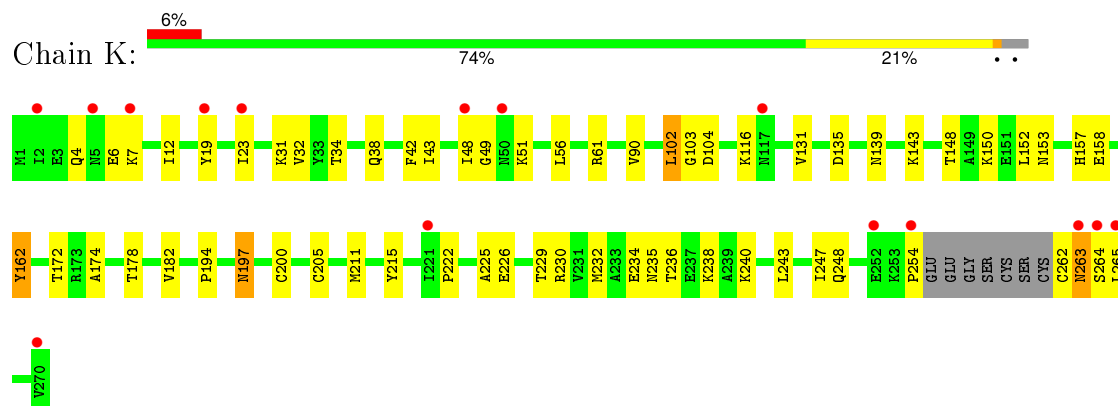
- Molecule 1: 5'-methylthioadenosine phosphorylase (mtaP)



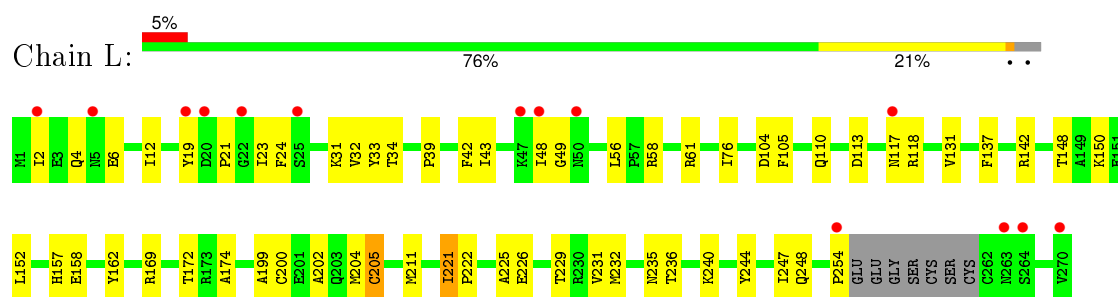
- Molecule 1: 5'-methylthioadenosine phosphorylase (mtaP)



- Molecule 1: 5'-methylthioadenosine phosphorylase (mtaP)



- Molecule 1: 5'-methylthioadenosine phosphorylase (mtaP)



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	96.60Å 96.56Å 96.63Å 91.57° 91.23° 91.52°	Depositor
Resolution (Å)	48.27 – 1.45 48.27 – 1.45	Depositor EDS
% Data completeness (in resolution range)	89.0 (48.27-1.45) 88.5 (48.27-1.45)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.41 (at 1.45Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.182 , 0.202 0.202 , 0.218	Depositor DCC
$R_{free}$ test set	37861 reflections (6.89%)	DCC
Wilson B-factor (Å <sup>2</sup> )	11.9	Xtriage
Anisotropy	0.126	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 51.4	EDS
Estimated twinning fraction	0.000 for l,k,-h 0.000 for -l,k,h 0.000 for h,-l,k 0.000 for h,l,-k 0.000 for -k,h,l 0.000 for k,-h,l 0.034 for l,h,k 0.034 for k,l,h 0.000 for -k,l,-h 0.000 for -l,-h,k 0.000 for -k,-l,h 0.000 for l,-h,-k 0.000 for -l,h,-k 0.000 for k,-l,-h 0.011 for -h,k,-l 0.000 for h,-k,-l 0.000 for -h,-k,l 0.000 for k,h,-l 0.033 for -k,-h,-l 0.000 for -h,l,k 0.036 for -h,-l,-k 0.011 for l,-k,h 0.467 for -l,-k,-h	Xtriage

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

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Property	Value	Source
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.53, \langle L^2 \rangle = 0.36$	Xtriage
Outliers	0 of 589654 reflections	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	29330	wwPDB-VP
Average B, all atoms ( $\text{\AA}^2$ )	18.0	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 45.63 % 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 1.2853e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: MTA, 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	0.62	0/2158	0.87	2/2929 (0.1%)
1	B	0.65	0/2180	0.88	2/2958 (0.1%)
1	C	0.61	0/2181	0.86	2/2958 (0.1%)
1	D	0.63	0/2161	0.86	4/2933 (0.1%)
1	E	0.64	0/2183	0.89	6/2959 (0.2%)
1	F	0.62	0/2172	0.84	2/2947 (0.1%)
1	G	0.61	0/2175	0.83	1/2950 (0.0%)
1	H	0.62	0/2174	0.86	4/2948 (0.1%)
1	I	0.63	0/2191	0.85	2/2969 (0.1%)
1	J	0.61	0/2172	0.87	2/2947 (0.1%)
1	K	0.62	0/2181	0.86	4/2957 (0.1%)
1	L	0.65	0/2177	0.89	3/2954 (0.1%)
All	All	0.63	0/26105	0.86	34/35409 (0.1%)

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	B	0	1
1	E	0	1
1	H	0	1
1	I	0	1
1	J	0	1
1	K	0	1
All	All	0	6

There are no bond length outliers.

The worst 5 of 34 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	56[A]	LEU	CA-CB-CG	6.61	130.50	115.30
1	L	56[B]	LEU	CA-CB-CG	6.61	130.50	115.30
1	E	56[A]	LEU	CA-CB-CG	6.44	130.10	115.30
1	E	56[B]	LEU	CA-CB-CG	6.44	130.10	115.30
1	K	56[A]	LEU	CA-CB-CG	6.32	129.84	115.30

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	162	TYR	Sidechain
1	E	33	TYR	Sidechain
1	H	162	TYR	Sidechain
1	I	33	TYR	Sidechain
1	J	33	TYR	Sidechain

## 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	2113	0	2080	79	0
1	B	2135	0	2099	68	0
1	C	2136	0	2110	53	0
1	D	2116	0	2085	65	0
1	E	2138	0	2131	72	0
1	F	2127	0	2106	43	0
1	G	2130	0	2109	60	0
1	H	2129	0	2107	63	0
1	I	2146	0	2139	45	0
1	J	2127	0	2107	64	0
1	K	2136	0	2115	58	0
1	L	2132	0	2099	66	0
2	A	10	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	10	0	0	0	0
2	E	5	0	0	0	0
2	F	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	G	10	0	0	0	0
2	H	15	0	0	0	0
2	I	15	0	0	0	0
2	J	10	0	0	0	0
2	K	15	0	0	0	0
2	L	15	0	0	0	0
3	A	20	0	15	1	0
3	B	20	0	15	2	0
3	C	20	0	15	2	0
3	D	20	0	15	2	0
3	E	20	0	15	1	0
3	F	20	0	15	1	0
3	G	20	0	15	1	0
3	H	20	0	15	1	0
3	I	20	0	15	2	0
3	J	20	0	15	2	0
3	K	20	0	15	1	0
3	L	20	0	15	0	0
4	A	266	0	0	13	0
4	B	311	0	0	18	0
4	C	265	0	0	8	0
4	D	293	0	0	12	0
4	E	281	0	0	21	0
4	F	275	0	0	9	0
4	G	273	0	0	5	0
4	H	283	0	0	10	0
4	I	288	0	0	16	0
4	J	261	0	0	11	0
4	K	293	0	0	13	0
4	L	316	0	0	11	0
All	All	29330	0	25467	723	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 14.

The worst 5 of 723 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:L:48:ILE:HG22	1:L:248[B]:GLN:HE22	1.02	1.13
1:G:48:ILE:HG22	1:G:248[B]:GLN:HE22	1.15	1.11
1:D:48:ILE:HG22	1:D:248[B]:GLN:HE22	1.15	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:199:ALA:HA	1:L:204[A]:MET:HE3	1.34	1.09
1:E:51:LYS:NZ	1:E:51:LYS:HB3	1.67	1.09

There are no symmetry-related clashes.

## 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	275/270 (102%)	270 (98%)	5 (2%)	0	100	100
1	B	275/270 (102%)	271 (98%)	4 (2%)	0	100	100
1	C	275/270 (102%)	269 (98%)	6 (2%)	0	100	100
1	D	275/270 (102%)	269 (98%)	5 (2%)	1 (0%)	39	13
1	E	275/270 (102%)	268 (98%)	6 (2%)	1 (0%)	39	13
1	F	275/270 (102%)	270 (98%)	5 (2%)	0	100	100
1	G	275/270 (102%)	269 (98%)	6 (2%)	0	100	100
1	H	275/270 (102%)	267 (97%)	7 (2%)	1 (0%)	39	13
1	I	275/270 (102%)	270 (98%)	5 (2%)	0	100	100
1	J	275/270 (102%)	268 (98%)	6 (2%)	1 (0%)	39	13
1	K	275/270 (102%)	268 (98%)	6 (2%)	1 (0%)	39	13
1	L	275/270 (102%)	270 (98%)	5 (2%)	0	100	100
All	All	3300/3240 (102%)	3229 (98%)	66 (2%)	5 (0%)	52	22

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	263	ASN
1	H	263	ASN

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Mol	Chain	Res	Type
1	J	263	ASN
1	K	263	ASN
1	E	48	ILE

### 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	221/231 (96%)	216 (98%)	5 (2%)	58	21
1	B	226/231 (98%)	220 (97%)	6 (3%)	52	15
1	C	226/231 (98%)	219 (97%)	7 (3%)	47	12
1	D	222/231 (96%)	217 (98%)	5 (2%)	58	21
1	E	227/231 (98%)	217 (96%)	10 (4%)	35	5
1	F	225/231 (97%)	219 (97%)	6 (3%)	52	15
1	G	225/231 (97%)	221 (98%)	4 (2%)	66	30
1	H	224/231 (97%)	216 (96%)	8 (4%)	42	8
1	I	229/231 (99%)	223 (97%)	6 (3%)	54	17
1	J	224/231 (97%)	219 (98%)	5 (2%)	60	22
1	K	226/231 (98%)	220 (97%)	6 (3%)	52	15
1	L	225/231 (97%)	220 (98%)	5 (2%)	60	22
All	All	2700/2772 (97%)	2627 (97%)	73 (3%)	57	15

5 of 73 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	18	LEU
1	G	162	TYR
1	K	197[B]	ASN
1	F	211[A]	MET
1	G	211[B]	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 49 such

sidechains are listed below:

Mol	Chain	Res	Type
1	F	4	GLN
1	G	157	HIS
1	K	235	ASN
1	F	157	HIS
1	G	235	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

36 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	4000	-	4,4,4	0.31	0	6,6,6	0.34	0
2	SO4	A	4001	-	4,4,4	0.24	0	6,6,6	0.42	0
3	MTA	A	4003	-	17,22,22	2.14	4 (23%)	17,32,32	2.08	4 (23%)
2	SO4	B	4004	-	4,4,4	0.21	0	6,6,6	0.41	0
3	MTA	B	4006	-	17,22,22	2.35	5 (29%)	17,32,32	1.98	4 (23%)
2	SO4	C	4007	-	4,4,4	0.38	0	6,6,6	0.73	0
3	MTA	C	4009	-	17,22,22	2.34	5 (29%)	17,32,32	2.13	4 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	SO4	D	4010	-	4,4,4	0.49	0	6,6,6	0.78	0
2	SO4	D	4011	-	4,4,4	0.22	0	6,6,6	0.19	0
3	MTA	D	4012	-	17,22,22	1.99	3 (17%)	17,32,32	2.02	5 (29%)
2	SO4	E	4013	-	4,4,4	0.47	0	6,6,6	1.05	1 (16%)
3	MTA	E	4015	-	17,22,22	2.32	4 (23%)	17,32,32	2.14	4 (23%)
2	SO4	F	4016	-	4,4,4	0.33	0	6,6,6	0.82	0
3	MTA	F	4018	-	17,22,22	2.09	5 (29%)	17,32,32	2.05	4 (23%)
2	SO4	G	4019	-	4,4,4	0.49	0	6,6,6	0.70	0
2	SO4	G	4020	-	4,4,4	0.40	0	6,6,6	0.13	0
3	MTA	G	4021	-	17,22,22	2.26	5 (29%)	17,32,32	1.90	3 (17%)
2	SO4	H	4017	-	4,4,4	0.24	0	6,6,6	0.21	0
2	SO4	H	4022	-	4,4,4	0.62	0	6,6,6	0.85	0
2	SO4	H	4023	-	4,4,4	0.34	0	6,6,6	0.10	0
3	MTA	H	4024	-	17,22,22	1.97	3 (17%)	17,32,32	2.13	6 (35%)
2	SO4	I	4014	-	4,4,4	0.12	0	6,6,6	0.38	0
2	SO4	I	4025	-	4,4,4	0.33	0	6,6,6	1.00	1 (16%)
2	SO4	I	4026	-	4,4,4	0.55	0	6,6,6	0.20	0
3	MTA	I	4027	-	17,22,22	2.04	5 (29%)	17,32,32	2.22	4 (23%)
2	SO4	J	4028	-	4,4,4	0.27	0	6,6,6	0.36	0
2	SO4	J	4029	-	4,4,4	0.23	0	6,6,6	0.10	0
3	MTA	J	4030	-	17,22,22	2.21	5 (29%)	17,32,32	1.90	4 (23%)
2	SO4	K	4008	-	4,4,4	0.25	0	6,6,6	0.20	0
2	SO4	K	4031	-	4,4,4	0.36	0	6,6,6	0.70	0
2	SO4	K	4032	-	4,4,4	0.45	0	6,6,6	0.12	0
3	MTA	K	4033	-	17,22,22	2.33	6 (35%)	17,32,32	2.05	4 (23%)
2	SO4	L	4005	-	4,4,4	0.12	0	6,6,6	0.39	0
2	SO4	L	4034	-	4,4,4	0.21	0	6,6,6	0.60	0
2	SO4	L	4035	-	4,4,4	0.54	0	6,6,6	0.26	0
3	MTA	L	4036	-	17,22,22	2.00	2 (11%)	17,32,32	2.13	4 (23%)

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
2	SO4	A	4000	-	-	0/0/0/0	0/0/0/0
2	SO4	A	4001	-	-	0/0/0/0	0/0/0/0
3	MTA	A	4003	-	-	0/3/23/23	0/3/3/3
2	SO4	B	4004	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MTA	B	4006	-	-	0/3/23/23	0/3/3/3
2	SO4	C	4007	-	-	0/0/0/0	0/0/0/0
3	MTA	C	4009	-	-	0/3/23/23	0/3/3/3
2	SO4	D	4010	-	-	0/0/0/0	0/0/0/0
2	SO4	D	4011	-	-	0/0/0/0	0/0/0/0
3	MTA	D	4012	-	-	0/3/23/23	0/3/3/3
2	SO4	E	4013	-	-	0/0/0/0	0/0/0/0
3	MTA	E	4015	-	-	0/3/23/23	0/3/3/3
2	SO4	F	4016	-	-	0/0/0/0	0/0/0/0
3	MTA	F	4018	-	-	0/3/23/23	0/3/3/3
2	SO4	G	4019	-	-	0/0/0/0	0/0/0/0
2	SO4	G	4020	-	-	0/0/0/0	0/0/0/0
3	MTA	G	4021	-	-	0/3/23/23	0/3/3/3
2	SO4	H	4017	-	-	0/0/0/0	0/0/0/0
2	SO4	H	4022	-	-	0/0/0/0	0/0/0/0
2	SO4	H	4023	-	-	0/0/0/0	0/0/0/0
3	MTA	H	4024	-	-	0/3/23/23	0/3/3/3
2	SO4	I	4014	-	-	0/0/0/0	0/0/0/0
2	SO4	I	4025	-	-	0/0/0/0	0/0/0/0
2	SO4	I	4026	-	-	0/0/0/0	0/0/0/0
3	MTA	I	4027	-	-	0/3/23/23	0/3/3/3
2	SO4	J	4028	-	-	0/0/0/0	0/0/0/0
2	SO4	J	4029	-	-	0/0/0/0	0/0/0/0
3	MTA	J	4030	-	-	0/3/23/23	0/3/3/3
2	SO4	K	4008	-	-	0/0/0/0	0/0/0/0
2	SO4	K	4031	-	-	0/0/0/0	0/0/0/0
2	SO4	K	4032	-	-	0/0/0/0	0/0/0/0
3	MTA	K	4033	-	-	0/3/23/23	0/3/3/3
2	SO4	L	4005	-	-	0/0/0/0	0/0/0/0
2	SO4	L	4034	-	-	0/0/0/0	0/0/0/0
2	SO4	L	4035	-	-	0/0/0/0	0/0/0/0
3	MTA	L	4036	-	-	0/3/23/23	0/3/3/3

The worst 5 of 52 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	K	4033	MTA	C8-N7	-3.66	1.27	1.34
3	D	4012	MTA	C8-N7	-3.51	1.27	1.34
3	H	4024	MTA	C8-N7	-3.27	1.28	1.34
3	A	4003	MTA	C8-N7	-3.13	1.28	1.34
3	F	4018	MTA	C8-N7	-3.12	1.28	1.34

The worst 5 of 52 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
3	I	4027	MTA	O4'-C1'-N9	-5.78	96.01	108.10
3	E	4015	MTA	O4'-C1'-N9	-5.73	96.10	108.10
3	A	4003	MTA	O4'-C1'-N9	-5.56	96.46	108.10
3	K	4033	MTA	O4'-C1'-N9	-5.51	96.56	108.10
3	B	4006	MTA	O4'-C1'-N9	-5.20	97.22	108.10

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

11 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	4003	MTA	1	0
3	B	4006	MTA	2	0
3	C	4009	MTA	2	0
3	D	4012	MTA	2	0
3	E	4015	MTA	1	0
3	F	4018	MTA	1	0
3	G	4021	MTA	1	0
3	H	4024	MTA	1	0
3	I	4027	MTA	2	0
3	J	4030	MTA	2	0
3	K	4033	MTA	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	263/270 (97%)	0.14	13 (4%)	33 33	8, 15, 33, 38	0
1	B	263/270 (97%)	0.14	14 (5%)	30 30	7, 13, 33, 44	0
1	C	263/270 (97%)	0.21	17 (6%)	22 22	7, 15, 33, 40	0
1	D	263/270 (97%)	0.22	16 (6%)	25 24	7, 15, 33, 37	0
1	E	263/270 (97%)	0.09	16 (6%)	25 24	7, 13, 32, 43	0
1	F	263/270 (97%)	0.24	16 (6%)	25 24	8, 15, 33, 42	0
1	G	263/270 (97%)	0.23	17 (6%)	22 22	8, 15, 33, 42	0
1	H	263/270 (97%)	0.22	18 (6%)	20 20	8, 15, 33, 38	0
1	I	263/270 (97%)	0.17	15 (5%)	27 27	7, 13, 33, 43	0
1	J	263/270 (97%)	0.18	14 (5%)	30 30	7, 14, 32, 40	0
1	K	263/270 (97%)	0.13	15 (5%)	27 27	7, 15, 32, 43	0
1	L	263/270 (97%)	0.24	14 (5%)	30 30	7, 14, 33, 43	0
All	All	3156/3240 (97%)	0.18	185 (5%)	26 25	7, 14, 33, 44	0

The worst 5 of 185 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	263	ASN	6.8
1	E	48	ILE	6.6
1	L	263	ASN	6.4
1	B	263	ASN	5.9
1	I	263	ASN	5.8

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	SO4	H	4017	5/5	0.86	0.17	7.88	51,52,52,53	0
2	SO4	A	4001	5/5	0.88	0.15	7.28	45,45,46,47	0
2	SO4	D	4011	5/5	0.89	0.15	6.29	50,51,51,52	0
2	SO4	L	4035	5/5	0.97	0.15	2.72	21,22,25,27	0
2	SO4	I	4026	5/5	0.97	0.14	2.10	22,22,25,27	0
2	SO4	J	4029	5/5	0.90	0.15	1.15	46,47,47,48	5
2	SO4	G	4020	5/5	0.88	0.14	0.61	28,28,29,29	5
2	SO4	H	4023	5/5	0.90	0.13	0.31	54,54,54,55	0
2	SO4	L	4034	5/5	0.99	0.07	-0.26	11,11,14,15	0
2	SO4	D	4010	5/5	0.99	0.07	-0.36	11,12,15,16	0
3	MTA	H	4024	20/20	0.98	0.06	-0.52	10,12,18,19	0
3	MTA	K	4033	20/20	0.98	0.06	-0.55	8,11,17,18	0
3	MTA	G	4021	20/20	0.98	0.06	-0.60	10,12,18,19	0
3	MTA	D	4012	20/20	0.97	0.06	-0.61	10,11,18,18	0
3	MTA	I	4027	20/20	0.98	0.06	-0.62	8,10,14,16	0
3	MTA	F	4018	20/20	0.98	0.06	-0.62	9,12,18,18	0
3	MTA	E	4015	20/20	0.98	0.06	-0.62	8,10,14,15	0
2	SO4	F	4016	5/5	0.99	0.07	-0.70	12,13,16,16	0
3	MTA	L	4036	20/20	0.98	0.07	-0.72	8,10,15,15	0
3	MTA	C	4009	20/20	0.98	0.06	-0.75	9,11,18,18	0
3	MTA	A	4003	20/20	0.98	0.05	-0.77	9,10,16,17	0
3	MTA	B	4006	20/20	0.98	0.06	-0.77	8,10,15,16	0
3	MTA	J	4030	20/20	0.98	0.06	-0.78	9,11,17,19	0
2	SO4	B	4004	5/5	0.99	0.06	-0.87	10,11,14,15	0
2	SO4	H	4022	5/5	0.99	0.06	-1.01	11,12,15,15	0
2	SO4	E	4013	5/5	0.99	0.06	-1.14	10,11,13,14	0
2	SO4	G	4019	5/5	0.99	0.06	-1.23	12,12,15,15	0
2	SO4	A	4000	5/5	0.99	0.05	-1.38	11,11,15,16	0
2	SO4	J	4028	5/5	0.99	0.05	-1.53	10,11,14,14	0
2	SO4	I	4025	5/5	1.00	0.06	-1.58	9,9,13,14	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	SO4	C	4007	5/5	0.99	0.06	-1.66	12,13,15,16	0
2	SO4	K	4031	5/5	0.99	0.05	-1.84	11,11,14,15	0
2	SO4	L	4005	5/5	0.90	0.17	-	46,47,48,49	0
2	SO4	I	4014	5/5	0.91	0.14	-	44,44,45,46	0
2	SO4	K	4008	5/5	0.90	0.15	-	43,43,44,45	0
2	SO4	K	4032	5/5	0.81	0.19	-	57,58,58,59	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.