



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 20, 2023 – 09:24 PM EDT

PDB ID : 5FAK  
Title : Crystal structure of Double Mutant S12T and N87T of Adenosine/Methylthio adenosine Phosphorylase from Schistosoma mansoni in complex with Adenine  
Authors : Torini, J.R.; Brandao-Neto, J.; DeMarco, R.; Pereira, H.M.  
Deposited on : 2015-12-11  
Resolution : 1.87 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 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 : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.35.1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.35.1

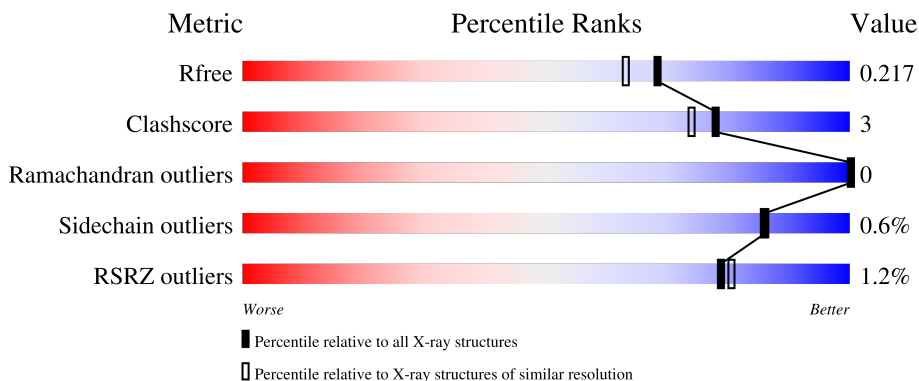
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.87 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.



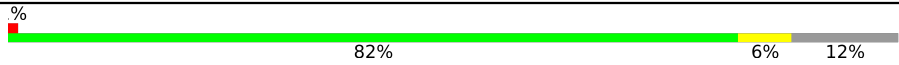
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	9470 (1.90-1.86)
Clashscore	141614	10282 (1.90-1.86)
Ramachandran outliers	138981	10152 (1.90-1.86)
Sidechain outliers	138945	10152 (1.90-1.86)
RSRZ outliers	127900	9303 (1.90-1.86)

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	320	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 81%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 8%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 11%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">81% 8% 12%</p>
1	B	320	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 80%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 9%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 11%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">80% 9% 11%</p>
1	C	320	<div style="display: flex; align-items: center;"> <div style="width: 86%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 11%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">86% 11%</p>
1	D	320	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 83%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 5%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 12%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">83% 5% 12%</p>
1	E	320	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 83%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 5%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 12%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">83% 5% 12%</p>

Continued on next page...

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
1	F	320	 <p>A horizontal bar chart representing the quality of chain. The bar is divided into three segments: a green segment representing 82%, a yellow segment representing 6%, and a grey segment representing 12%. A small red square is located at the beginning of the bar, and a '%' symbol is positioned above it.</p>

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 14268 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 Methylthioadenosine phosphorylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	283	Total 2162	C 1369	N 377	O 399	S 17	0	1	0
1	B	286	Total 2161	C 1371	N 378	O 397	S 15	0	1	0
1	C	286	Total 2175	C 1380	N 374	O 405	S 16	0	0	0
1	D	282	Total 2130	C 1350	N 369	O 394	S 17	0	1	0
1	E	283	Total 2144	C 1361	N 371	O 397	S 15	0	0	0
1	F	283	Total 2149	C 1364	N 370	O 398	S 17	0	0	0

There are 138 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	initiating methionine	UNP I0B503
A	-19	GLY	-	expression tag	UNP I0B503
A	-18	SER	-	expression tag	UNP I0B503
A	-17	SER	-	expression tag	UNP I0B503
A	-16	HIS	-	expression tag	UNP I0B503
A	-15	HIS	-	expression tag	UNP I0B503
A	-14	HIS	-	expression tag	UNP I0B503
A	-13	HIS	-	expression tag	UNP I0B503
A	-12	HIS	-	expression tag	UNP I0B503
A	-11	HIS	-	expression tag	UNP I0B503
A	-10	SER	-	expression tag	UNP I0B503
A	-9	SER	-	expression tag	UNP I0B503
A	-8	GLY	-	expression tag	UNP I0B503
A	-7	LEU	-	expression tag	UNP I0B503
A	-6	VAL	-	expression tag	UNP I0B503
A	-5	PRO	-	expression tag	UNP I0B503
A	-4	ARG	-	expression tag	UNP I0B503

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP I0B503
A	-2	SER	-	expression tag	UNP I0B503
A	-1	HIS	-	expression tag	UNP I0B503
A	0	MET	-	expression tag	UNP I0B503
A	12	THR	SER	conflict	UNP I0B503
A	87	THR	ASN	conflict	UNP I0B503
B	-20	MET	-	initiating methionine	UNP I0B503
B	-19	GLY	-	expression tag	UNP I0B503
B	-18	SER	-	expression tag	UNP I0B503
B	-17	SER	-	expression tag	UNP I0B503
B	-16	HIS	-	expression tag	UNP I0B503
B	-15	HIS	-	expression tag	UNP I0B503
B	-14	HIS	-	expression tag	UNP I0B503
B	-13	HIS	-	expression tag	UNP I0B503
B	-12	HIS	-	expression tag	UNP I0B503
B	-11	HIS	-	expression tag	UNP I0B503
B	-10	SER	-	expression tag	UNP I0B503
B	-9	SER	-	expression tag	UNP I0B503
B	-8	GLY	-	expression tag	UNP I0B503
B	-7	LEU	-	expression tag	UNP I0B503
B	-6	VAL	-	expression tag	UNP I0B503
B	-5	PRO	-	expression tag	UNP I0B503
B	-4	ARG	-	expression tag	UNP I0B503
B	-3	GLY	-	expression tag	UNP I0B503
B	-2	SER	-	expression tag	UNP I0B503
B	-1	HIS	-	expression tag	UNP I0B503
B	0	MET	-	expression tag	UNP I0B503
B	12	THR	SER	conflict	UNP I0B503
B	87	THR	ASN	conflict	UNP I0B503
C	-20	MET	-	initiating methionine	UNP I0B503
C	-19	GLY	-	expression tag	UNP I0B503
C	-18	SER	-	expression tag	UNP I0B503
C	-17	SER	-	expression tag	UNP I0B503
C	-16	HIS	-	expression tag	UNP I0B503
C	-15	HIS	-	expression tag	UNP I0B503
C	-14	HIS	-	expression tag	UNP I0B503
C	-13	HIS	-	expression tag	UNP I0B503
C	-12	HIS	-	expression tag	UNP I0B503
C	-11	HIS	-	expression tag	UNP I0B503
C	-10	SER	-	expression tag	UNP I0B503
C	-9	SER	-	expression tag	UNP I0B503
C	-8	GLY	-	expression tag	UNP I0B503

*Continued on next page...*

*Continued from previous page...*

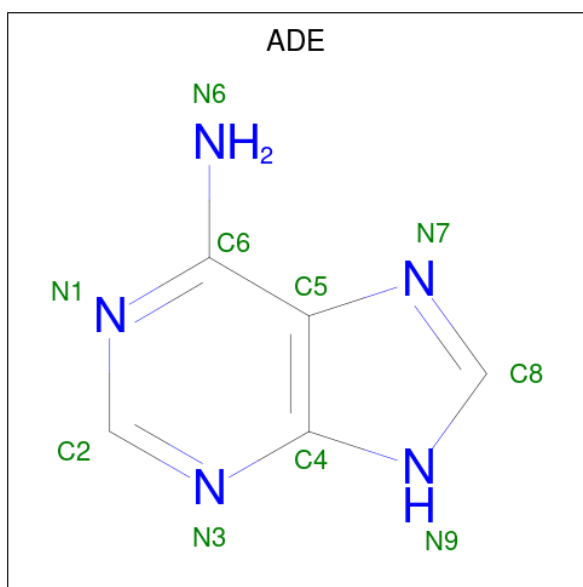
Chain	Residue	Modelled	Actual	Comment	Reference
C	-7	LEU	-	expression tag	UNP I0B503
C	-6	VAL	-	expression tag	UNP I0B503
C	-5	PRO	-	expression tag	UNP I0B503
C	-4	ARG	-	expression tag	UNP I0B503
C	-3	GLY	-	expression tag	UNP I0B503
C	-2	SER	-	expression tag	UNP I0B503
C	-1	HIS	-	expression tag	UNP I0B503
C	0	MET	-	expression tag	UNP I0B503
C	12	THR	SER	conflict	UNP I0B503
C	87	THR	ASN	conflict	UNP I0B503
D	-20	MET	-	initiating methionine	UNP I0B503
D	-19	GLY	-	expression tag	UNP I0B503
D	-18	SER	-	expression tag	UNP I0B503
D	-17	SER	-	expression tag	UNP I0B503
D	-16	HIS	-	expression tag	UNP I0B503
D	-15	HIS	-	expression tag	UNP I0B503
D	-14	HIS	-	expression tag	UNP I0B503
D	-13	HIS	-	expression tag	UNP I0B503
D	-12	HIS	-	expression tag	UNP I0B503
D	-11	HIS	-	expression tag	UNP I0B503
D	-10	SER	-	expression tag	UNP I0B503
D	-9	SER	-	expression tag	UNP I0B503
D	-8	GLY	-	expression tag	UNP I0B503
D	-7	LEU	-	expression tag	UNP I0B503
D	-6	VAL	-	expression tag	UNP I0B503
D	-5	PRO	-	expression tag	UNP I0B503
D	-4	ARG	-	expression tag	UNP I0B503
D	-3	GLY	-	expression tag	UNP I0B503
D	-2	SER	-	expression tag	UNP I0B503
D	-1	HIS	-	expression tag	UNP I0B503
D	0	MET	-	expression tag	UNP I0B503
D	12	THR	SER	conflict	UNP I0B503
D	87	THR	ASN	conflict	UNP I0B503
E	-20	MET	-	initiating methionine	UNP I0B503
E	-19	GLY	-	expression tag	UNP I0B503
E	-18	SER	-	expression tag	UNP I0B503
E	-17	SER	-	expression tag	UNP I0B503
E	-16	HIS	-	expression tag	UNP I0B503
E	-15	HIS	-	expression tag	UNP I0B503
E	-14	HIS	-	expression tag	UNP I0B503
E	-13	HIS	-	expression tag	UNP I0B503
E	-12	HIS	-	expression tag	UNP I0B503

*Continued on next page...*

*Continued from previous page...*

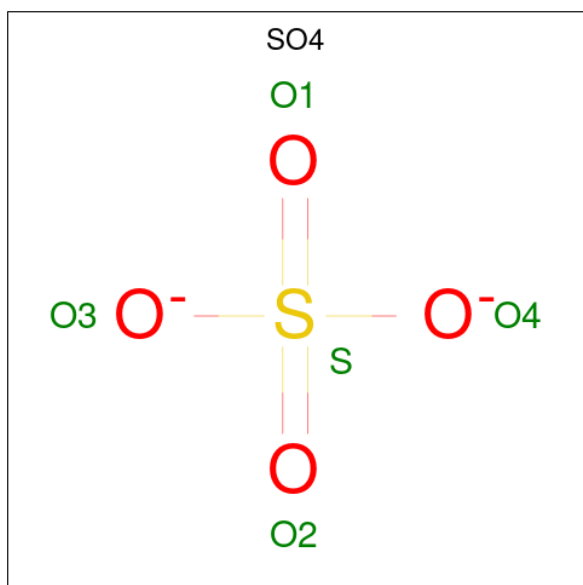
Chain	Residue	Modelled	Actual	Comment	Reference
E	-11	HIS	-	expression tag	UNP I0B503
E	-10	SER	-	expression tag	UNP I0B503
E	-9	SER	-	expression tag	UNP I0B503
E	-8	GLY	-	expression tag	UNP I0B503
E	-7	LEU	-	expression tag	UNP I0B503
E	-6	VAL	-	expression tag	UNP I0B503
E	-5	PRO	-	expression tag	UNP I0B503
E	-4	ARG	-	expression tag	UNP I0B503
E	-3	GLY	-	expression tag	UNP I0B503
E	-2	SER	-	expression tag	UNP I0B503
E	-1	HIS	-	expression tag	UNP I0B503
E	0	MET	-	expression tag	UNP I0B503
E	12	THR	SER	conflict	UNP I0B503
E	87	THR	ASN	conflict	UNP I0B503
F	-20	MET	-	initiating methionine	UNP I0B503
F	-19	GLY	-	expression tag	UNP I0B503
F	-18	SER	-	expression tag	UNP I0B503
F	-17	SER	-	expression tag	UNP I0B503
F	-16	HIS	-	expression tag	UNP I0B503
F	-15	HIS	-	expression tag	UNP I0B503
F	-14	HIS	-	expression tag	UNP I0B503
F	-13	HIS	-	expression tag	UNP I0B503
F	-12	HIS	-	expression tag	UNP I0B503
F	-11	HIS	-	expression tag	UNP I0B503
F	-10	SER	-	expression tag	UNP I0B503
F	-9	SER	-	expression tag	UNP I0B503
F	-8	GLY	-	expression tag	UNP I0B503
F	-7	LEU	-	expression tag	UNP I0B503
F	-6	VAL	-	expression tag	UNP I0B503
F	-5	PRO	-	expression tag	UNP I0B503
F	-4	ARG	-	expression tag	UNP I0B503
F	-3	GLY	-	expression tag	UNP I0B503
F	-2	SER	-	expression tag	UNP I0B503
F	-1	HIS	-	expression tag	UNP I0B503
F	0	MET	-	expression tag	UNP I0B503
F	12	THR	SER	conflict	UNP I0B503
F	87	THR	ASN	conflict	UNP I0B503

- Molecule 2 is ADENINE (three-letter code: ADE) (formula: C<sub>5</sub>H<sub>5</sub>N<sub>5</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	N		
2	A	1	10	5	5	0	0
2	B	1	10	5	5	0	0
2	D	1	10	5	5	0	0
2	E	1	10	5	5	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		

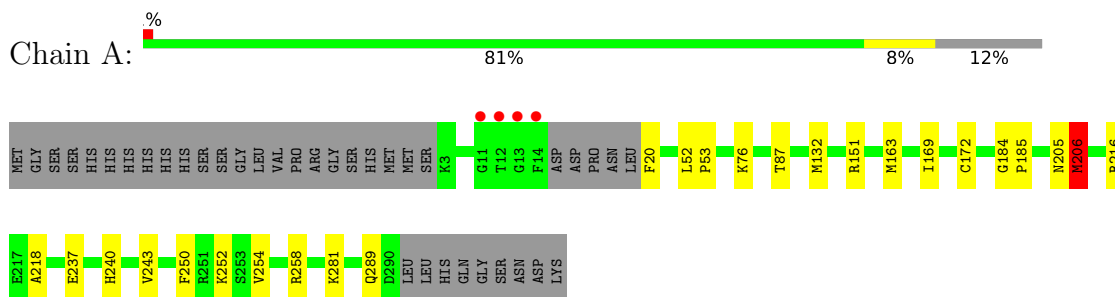
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	216	Total	O	0	0
			216	216		
4	B	191	Total	O	0	0
			191	191		
4	C	279	Total	O	0	0
			279	279		
4	D	201	Total	O	0	0
			201	201		
4	E	190	Total	O	0	0
			190	190		
4	F	200	Total	O	0	0
			200	200		

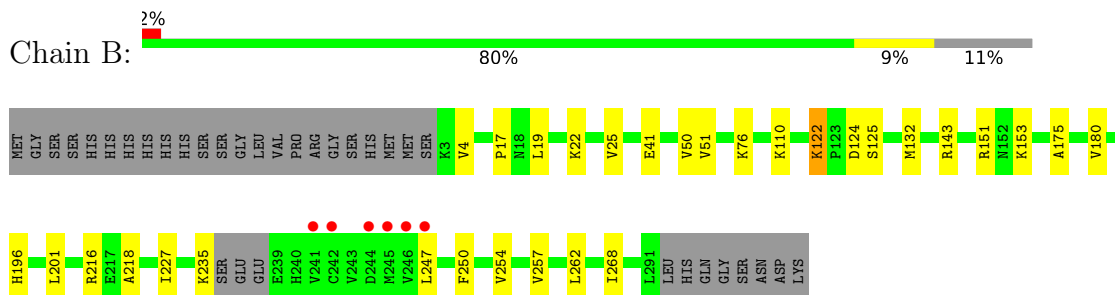
### 3 Residue-property plots

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 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.

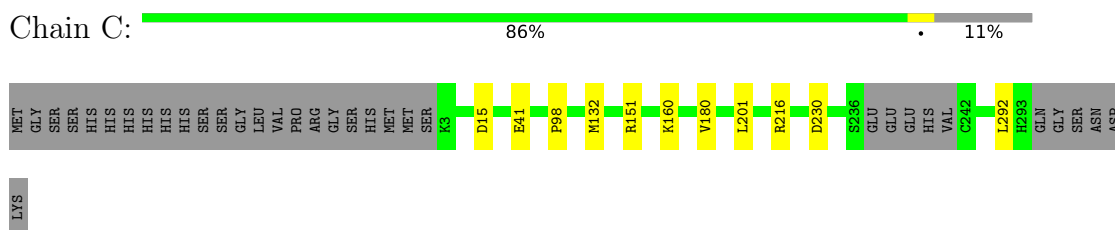
- Molecule 1: Methylthioadenosine phosphorylase



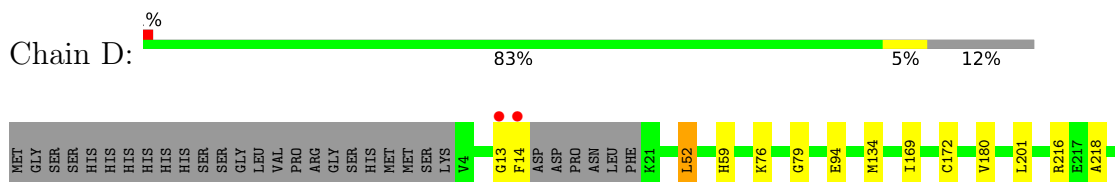
- Molecule 1: Methylthioadenosine phosphorylase

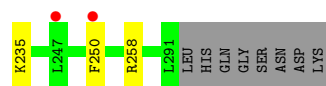


- Molecule 1: Methylthioadenosine phosphorylase

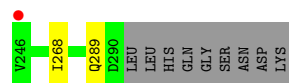
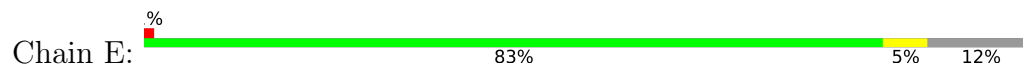


- Molecule 1: Methylthioadenosine phosphorylase

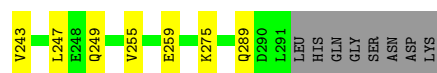
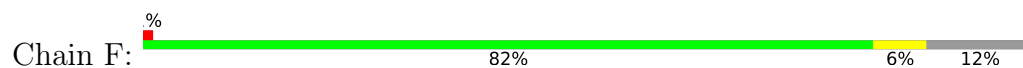




- Molecule 1: Methylthioadenosine phosphorylase



- Molecule 1: Methylthioadenosine phosphorylase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	81.06Å 82.09Å 150.15Å 90.00° 101.23° 90.00°	Depositor
Resolution (Å)	79.51 – 1.87 79.51 – 1.87	Depositor EDS
% Data completeness (in resolution range)	97.4 (79.51-1.87) 97.5 (79.51-1.87)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.86 (at 1.87Å)	Xtrriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.181 , 0.215 0.183 , 0.217	Depositor DCC
$R_{free}$ test set	7594 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	24.5	Xtrriage
Anisotropy	0.224	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 51.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	14268	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 51.91 % 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 5.2431e-05. 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, ADE

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	0.31	0/2208	0.51	1/2995 (0.0%)
1	B	0.32	0/2207	0.50	0/2996
1	C	0.34	0/2218	0.52	0/3011
1	D	0.31	0/2175	0.50	1/2955 (0.0%)
1	E	0.31	0/2187	0.50	0/2969
1	F	0.31	0/2192	0.50	0/2976
All	All	0.32	0/13187	0.51	2/17902 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	206	MET	CG-SD-CE	6.28	110.25	100.20
1	D	52	LEU	CA-CB-CG	5.10	127.03	115.30

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	2162	0	2148	18	0
1	B	2161	0	2131	19	0
1	C	2175	0	2162	8	0

*Continued on next page...*

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2130	0	2107	10	0
1	E	2144	0	2121	11	0
1	F	2149	0	2137	12	0
2	A	10	0	4	0	0
2	B	10	0	4	0	0
2	D	10	0	4	0	0
2	E	10	0	4	0	0
3	A	5	0	0	1	0
3	B	5	0	0	0	0
3	C	5	0	0	0	0
3	D	5	0	0	0	0
3	E	5	0	0	0	0
3	F	5	0	0	0	0
4	A	216	0	0	5	0
4	B	191	0	0	4	0
4	C	279	0	0	4	0
4	D	201	0	0	1	0
4	E	190	0	0	1	0
4	F	200	0	0	3	0
All	All	14268	0	12822	76	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 3.

All (76) 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:134:MET:CE	1:D:216:ARG:HD2	2.15	0.76
1:D:134:MET:HE2	1:D:216:ARG:HD2	1.69	0.74
1:B:180:VAL:HB	1:B:201:LEU:HD13	1.71	0.73
1:E:243:VAL:N	4:E:401:HOH:O	2.20	0.73
1:B:41:GLU:HG2	1:B:50:VAL:HG22	1.71	0.72
1:E:41:GLU:HG2	1:E:50:VAL:HG22	1.74	0.69
1:B:153:LYS:NZ	4:B:402:HOH:O	2.25	0.69
1:C:160:LYS:NZ	4:C:403:HOH:O	2.32	0.62
1:F:180:VAL:HB	1:F:201:LEU:HD13	1.82	0.61
1:A:281:LYS:NZ	4:A:405:HOH:O	2.33	0.60
1:E:131:HIS:HD2	1:E:289:GLN:HG3	1.67	0.58
1:C:41:GLU:OE2	4:C:401:HOH:O	2.17	0.58
1:B:247:LEU:H	1:B:250:PHE:HB3	1.70	0.55
1:F:98:PRO:HG3	1:F:230:ASP:HA	1.88	0.54

Continued on next page...

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:132:MET:HE2	1:C:216:ARG:HG2	1.90	0.53
1:A:151[B]:ARG:NH2	4:A:409:HOH:O	2.42	0.53
1:E:190:ARG:HH12	1:E:236:SER:HA	1.72	0.53
1:C:151:ARG:NH2	4:C:405:HOH:O	2.41	0.53
1:C:180:VAL:HB	1:C:201:LEU:HD13	1.91	0.53
1:F:19:LEU:HD13	1:F:51:VAL:HG21	1.90	0.53
1:A:132:MET:HE2	1:A:216:ARG:HG2	1.91	0.52
1:D:180:VAL:HB	1:D:201:LEU:HD13	1.92	0.51
1:A:258:ARG:NH1	4:A:410:HOH:O	2.44	0.51
1:D:79:GLY:O	4:D:401:HOH:O	2.20	0.51
1:A:163:MET:O	4:A:401:HOH:O	2.19	0.51
1:A:87:THR:OG1	3:A:302:SO4:O2	2.17	0.51
1:B:151[A]:ARG:NH2	4:B:404:HOH:O	2.45	0.50
1:F:115:GLU:OE1	4:F:401:HOH:O	2.20	0.50
1:C:15:ASP:OD2	4:C:402:HOH:O	2.20	0.49
1:C:98:PRO:HG3	1:C:230:ASP:HA	1.95	0.49
1:A:184:GLY:CA	1:A:206:MET:HE3	2.43	0.49
1:F:249:GLN:NE2	4:F:402:HOH:O	2.20	0.48
1:F:275:LYS:NZ	4:F:408:HOH:O	2.44	0.48
1:F:255:VAL:O	1:F:259:GLU:HG3	2.14	0.48
1:D:14:PHE:HE1	1:D:258:ARG:HG2	1.79	0.48
1:A:76:LYS:HD2	1:A:218:ALA:HB1	1.96	0.47
1:A:52:LEU:HD12	1:A:53:PRO:HD2	1.96	0.47
1:A:250:PHE:O	1:A:254:VAL:HG13	2.15	0.47
1:A:169:ILE:O	1:A:172:CYS:HB3	2.14	0.47
1:E:122:LYS:H	1:E:122:LYS:CD	2.28	0.47
1:E:143:ARG:NH2	1:E:175:ALA:O	2.47	0.47
1:B:17:PRO:HG2	1:B:51:VAL:HG11	1.98	0.46
1:D:94:GLU:OE2	1:D:235:LYS:NZ	2.45	0.45
1:B:110:LYS:NZ	1:B:196:HIS:HE1	2.14	0.45
1:D:169:ILE:O	1:D:172:CYS:HB3	2.16	0.45
1:E:132:MET:HE2	1:E:216:ARG:HG2	1.97	0.45
1:B:132:MET:HE2	1:B:216:ARG:HG2	1.98	0.45
1:B:19:LEU:HB3	1:B:262:LEU:HD21	1.98	0.45
1:A:185:PRO:HA	1:A:206:MET:HE2	1.98	0.44
1:A:184:GLY:HA3	1:A:206:MET:HE3	1.99	0.44
1:D:76:LYS:HD2	1:D:218:ALA:HB1	1.99	0.44
1:A:243:VAL:HG12	1:C:292:LEU:HD22	1.99	0.44
1:E:17:PRO:HB2	1:E:19:LEU:HG	1.98	0.44
1:D:13:GLY:HA3	1:D:250:PHE:CE2	2.52	0.44
1:A:184:GLY:HA3	1:A:206:MET:CE	2.48	0.44

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:235:LYS:NZ	4:B:405:HOH:O	2.48	0.44
1:A:252:LYS:NZ	4:A:411:HOH:O	2.45	0.43
1:B:250:PHE:O	1:B:254:VAL:HG23	2.17	0.43
1:A:237:GLU:HA	1:A:240:HIS:CE1	2.54	0.43
1:B:22:LYS:HD2	1:B:25:VAL:CG2	2.48	0.43
1:F:19:LEU:HD12	1:F:19:LEU:H	1.83	0.43
1:B:76:LYS:HD2	1:B:218:ALA:HB1	2.01	0.43
1:F:243:VAL:HG22	1:F:247:LEU:HD13	2.00	0.43
1:E:145:ILE:HG21	1:E:268:ILE:HG13	2.01	0.43
1:B:227:ILE:HD11	1:B:257:VAL:HG21	2.01	0.42
1:B:122:LYS:HG3	1:B:124:ASP:OD1	2.19	0.42
1:B:143:ARG:NH2	1:B:175:ALA:O	2.47	0.42
1:B:76:LYS:NZ	4:B:413:HOH:O	2.53	0.42
1:A:185:PRO:HA	1:A:206:MET:CE	2.50	0.42
1:E:122:LYS:H	1:E:122:LYS:HD3	1.85	0.41
1:F:104:LEU:HD21	1:F:203:ILE:HD11	2.02	0.41
1:F:25:VAL:HB	1:F:38:THR:HG21	2.01	0.41
1:E:34:LYS:HB3	1:E:34:LYS:HE3	1.81	0.41
1:B:122:LYS:NZ	1:B:125:SER:OG	2.54	0.40
1:D:59:HIS:CE1	1:F:289:GLN:HG2	2.56	0.40
1:B:4:VAL:HG11	1:B:268:ILE:HG22	2.03	0.40

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	280/320 (88%)	277 (99%)	3 (1%)	0	100	100
1	B	283/320 (88%)	278 (98%)	5 (2%)	0	100	100
1	C	282/320 (88%)	281 (100%)	1 (0%)	0	100	100
1	D	279/320 (87%)	277 (99%)	2 (1%)	0	100	100

Continued on next page...



Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	279/320 (87%)	277 (99%)	2 (1%)	0	100	100
1	F	279/320 (87%)	277 (99%)	2 (1%)	0	100	100
All	All	1682/1920 (88%)	1667 (99%)	15 (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	235/274 (86%)	231 (98%)	4 (2%)	60	54
1	B	229/274 (84%)	228 (100%)	1 (0%)	91	90
1	C	237/274 (86%)	237 (100%)	0	100	100
1	D	230/274 (84%)	229 (100%)	1 (0%)	91	90
1	E	230/274 (84%)	229 (100%)	1 (0%)	91	90
1	F	234/274 (85%)	232 (99%)	2 (1%)	78	76
All	All	1395/1644 (85%)	1386 (99%)	9 (1%)	86	86

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	PHE
1	A	205	ASN
1	A	206	MET
1	A	289	GLN
1	B	122	LYS
1	D	52	LEU
1	E	122	LYS
1	F	22	LYS
1	F	77	ASP

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

Mol	Chain	Res	Type
1	B	196	HIS

### 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](#)

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	$\# Z  > 2$
3	SO4	C	301	-	4,4,4	0.11	0	6,6,6	0.25	0
3	SO4	B	302	-	4,4,4	0.18	0	6,6,6	0.35	0
2	ADE	B	301	-	9,11,11	1.06	0	7,15,15	1.09	1 (14%)
3	SO4	D	302	-	4,4,4	0.20	0	6,6,6	0.34	0
3	SO4	A	302	-	4,4,4	0.15	0	6,6,6	0.20	0
3	SO4	E	302	-	4,4,4	0.16	0	6,6,6	0.31	0
3	SO4	F	301	-	4,4,4	0.13	0	6,6,6	0.23	0
2	ADE	D	301	-	9,11,11	1.02	1 (11%)	7,15,15	1.13	1 (14%)
2	ADE	E	301	-	9,11,11	1.04	0	7,15,15	1.12	1 (14%)
2	ADE	A	301	-	9,11,11	1.02	0	7,15,15	1.12	1 (14%)

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	ADE	B	301	-	-	-	0/2/2/2
2	ADE	E	301	-	-	-	0/2/2/2
2	ADE	A	301	-	-	-	0/2/2/2
2	ADE	D	301	-	-	-	0/2/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	301	ADE	C4-N9	2.12	1.38	1.34

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	301	ADE	C5-C6-N6	2.15	123.62	120.35
2	B	301	ADE	C5-C6-N6	2.11	123.55	120.35
2	A	301	ADE	C5-C6-N6	2.09	123.52	120.35
2	E	301	ADE	C5-C6-N6	2.08	123.52	120.35

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
3	A	302	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

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	283/320 (88%)	-0.37	4 (1%) 75 77	19, 33, 57, 116	0
1	B	286/320 (89%)	-0.40	6 (2%) 63 65	22, 32, 65, 89	0
1	C	286/320 (89%)	-0.51	0 100 100	19, 28, 51, 81	0
1	D	282/320 (88%)	-0.40	4 (1%) 75 77	22, 35, 62, 86	0
1	E	283/320 (88%)	-0.41	3 (1%) 80 82	23, 35, 64, 89	0
1	F	283/320 (88%)	-0.45	3 (1%) 80 82	22, 33, 63, 109	0
All	All	1703/1920 (88%)	-0.42	20 (1%) 79 80	19, 33, 61, 116	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	13	GLY	14.1
1	B	246	VAL	6.3
1	A	11	GLY	4.9
1	A	14	PHE	4.6
1	E	245	MET	4.4
1	D	14	PHE	4.3
1	B	242	CYS	4.0
1	F	19	LEU	3.7
1	A	12	THR	3.7
1	E	246	VAL	3.4
1	E	243	VAL	3.3
1	D	13	GLY	3.3
1	F	242	CYS	3.3
1	B	241	VAL	3.1
1	B	245	MET	3.0
1	B	247	LEU	2.9
1	D	250	PHE	2.8
1	F	18	ASN	2.8
1	B	244	ASP	2.5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	D	247	LEU	2.4

## 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 monosaccharides 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(Å <sup>2</sup> )	Q<0.9
2	ADE	E	301	10/10	0.82	0.20	69,75,77,78	0
3	SO4	A	302	5/5	0.85	0.19	71,73,74,75	0
2	ADE	B	301	10/10	0.91	0.12	56,60,64,65	0
2	ADE	D	301	10/10	0.93	0.08	32,34,39,39	0
2	ADE	A	301	10/10	0.95	0.08	26,28,29,33	0
3	SO4	D	302	5/5	0.98	0.09	32,35,39,39	0
3	SO4	C	301	5/5	0.99	0.07	20,22,24,24	0
3	SO4	B	302	5/5	0.99	0.05	26,27,32,34	0
3	SO4	E	302	5/5	0.99	0.06	23,28,31,32	0
3	SO4	F	301	5/5	0.99	0.07	23,23,29,30	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.