



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 13, 2016 – 08:16 AM EST

PDB ID : 5F7J  
Title : Crystal structure of Mutant N87T of adenosine/Methylthioadenosine phosphorylase from *Schistosoma mansoni* in complex with Adenine  
Authors : Torini, J.R.; Brandao-Neto, J.; DeMarco, R.; Pereira, H.M.  
Deposited on : 2015-12-08  
Resolution : 1.66 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

<http://wwpdb.org/validation/2016/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 : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20028442  
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) : rb-20028442

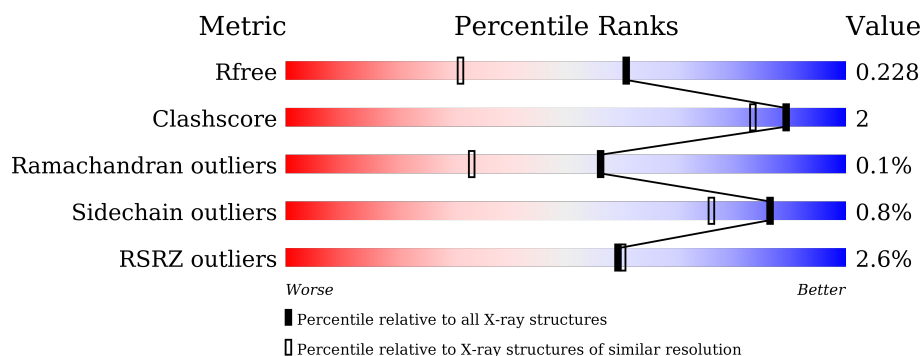
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.66 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	1226 (1.66-1.66)
Clashscore	102246	1323 (1.66-1.66)
Ramachandran outliers	100387	1295 (1.66-1.66)
Sidechain outliers	100360	1295 (1.66-1.66)
RSRZ outliers	91569	1227 (1.66-1.66)

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	320	<div> <div>0%</div> <div> <div></div> <div>82%</div> <div>7%</div> <div>12%</div> </div> </div>
1	B	320	<div> <div>3%</div> <div> <div></div> <div>83%</div> <div>8%</div> <div>9%</div> </div> </div>
1	C	320	<div> <div>2%</div> <div> <div></div> <div>83%</div> <div>6%</div> <div>10%</div> </div> </div>
1	D	320	<div> <div>2%</div> <div> <div></div> <div>86%</div> <div>•</div> <div>11%</div> </div> </div>
1	E	320	<div> <div>4%</div> <div> <div></div> <div>85%</div> <div>6%</div> <div>9%</div> </div> </div>
1	F	320	<div> <div>0%</div> <div> <div></div> <div>83%</div> <div>•</div> <div>15%</div> </div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14870 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
1	A	283	Total	C	N	O	S	0	1	0
			2171	1374	378	402	17			
1	B	291	Total	C	N	O	S	0	2	0
			2228	1413	386	412	17			
1	C	287	Total	C	N	O	S	0	1	0
			2192	1384	382	410	16			
1	D	286	Total	C	N	O	S	0	1	0
			2178	1377	380	404	17			
1	E	291	Total	C	N	O	S	0	2	0
			2235	1416	390	412	17			
1	F	273	Total	C	N	O	S	0	0	0
			2078	1318	359	385	16			

There are 132 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	87	THR	ASN	engineered mutation	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	87	THR	ASN	engineered mutation	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
C	-7	LEU	-	expression tag	UNP I0B503
C	-6	VAL	-	expression tag	UNP I0B503

*Continued on next page...*

*Continued from previous page...*

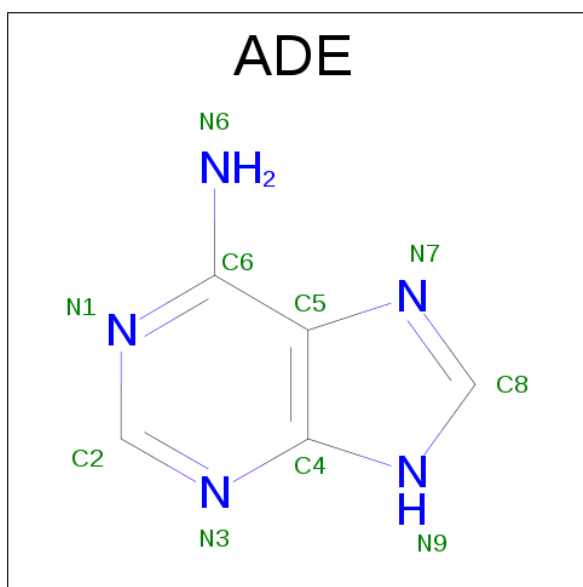
Chain	Residue	Modelled	Actual	Comment	Reference
C	-5	PRO	-	expression tag	UNP I0B503
C	-4	ARG	-	expression tag	UNP I0B503
C	-3	GLY	-	expression tag	UNP I0B503
C	-2	SER	-	expression tag	UNP I0B503
C	-1	HIS	-	expression tag	UNP I0B503
C	0	MET	-	expression tag	UNP I0B503
C	87	THR	ASN	engineered mutation	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	87	THR	ASN	engineered mutation	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
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

*Continued on next page...*

*Continued from previous page...*

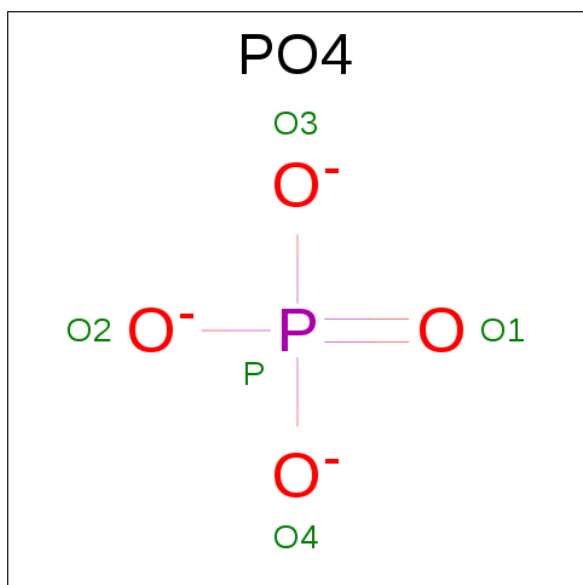
Chain	Residue	Modelled	Actual	Comment	Reference
E	-7	LEU	-	expression tag	UNP I0B503
E	-6	VAL	-	expression tag	UNP I0B503
E	-5	PRO	-	expression tag	UNP I0B503
E	-4	ARG	-	expression tag	UNP I0B503
E	-3	GLY	-	expression tag	UNP I0B503
E	-2	SER	-	expression tag	UNP I0B503
E	-1	HIS	-	expression tag	UNP I0B503
E	0	MET	-	expression tag	UNP I0B503
E	87	THR	ASN	engineered mutation	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	87	THR	ASN	engineered mutation	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
2	A	1	Total	C	N	0	0
			10	5	5		
2	B	1	Total	C	N	0	0
			10	5	5		
2	D	1	Total	C	N	0	0
			10	5	5		
2	E	1	Total	C	N	0	0
			10	5	5		

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



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

- Molecule 4 is water.

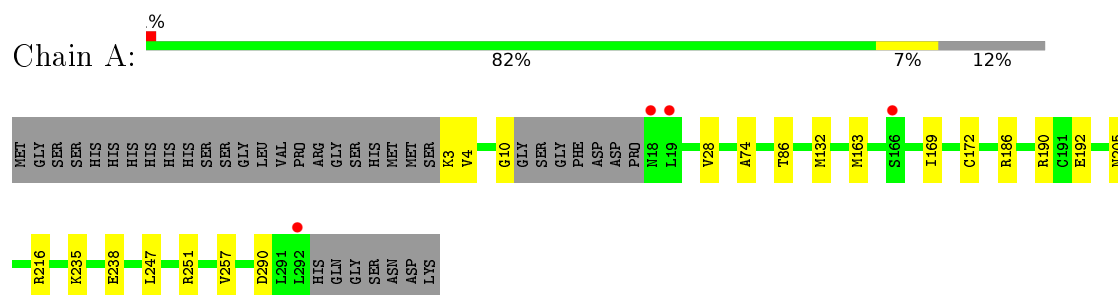
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	292	Total O 292 292	0	0
4	B	307	Total O 307 307	0	0
4	C	367	Total O 367 367	0	0
4	D	264	Total O 264 264	0	0
4	E	237	Total O 237 237	0	0
4	F	261	Total O 261 261	0	0



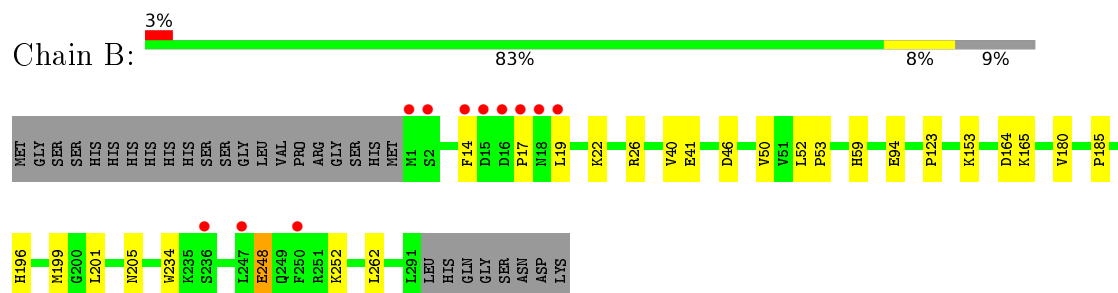
### 3 Residue-property plots [i](#)

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 ( $RSRZ > 2$ ). 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.

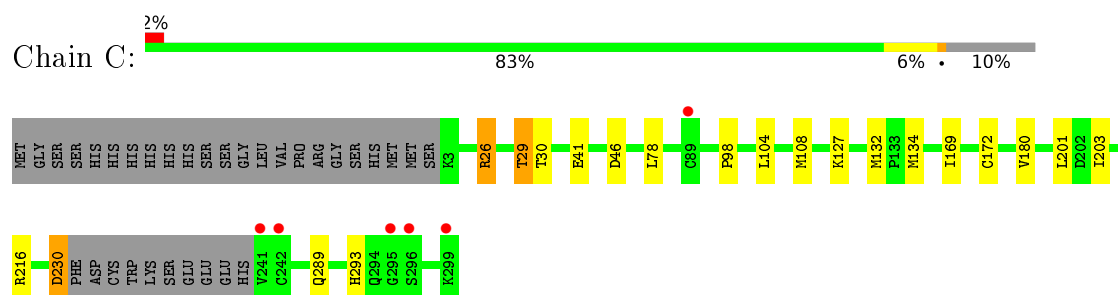
#### • Molecule 1: Methylthiadenosine phosphorylase



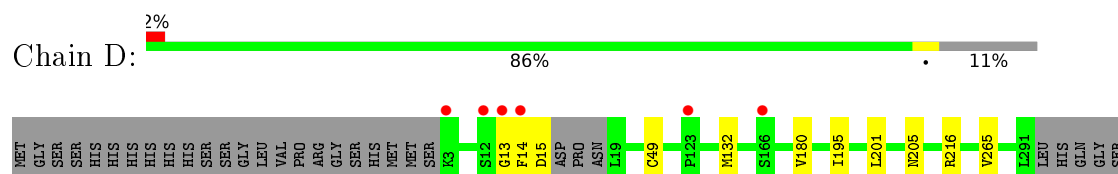
#### • Molecule 1: Methylthiadenosine phosphorylase



#### • Molecule 1: Methylthiadenosine phosphorylase

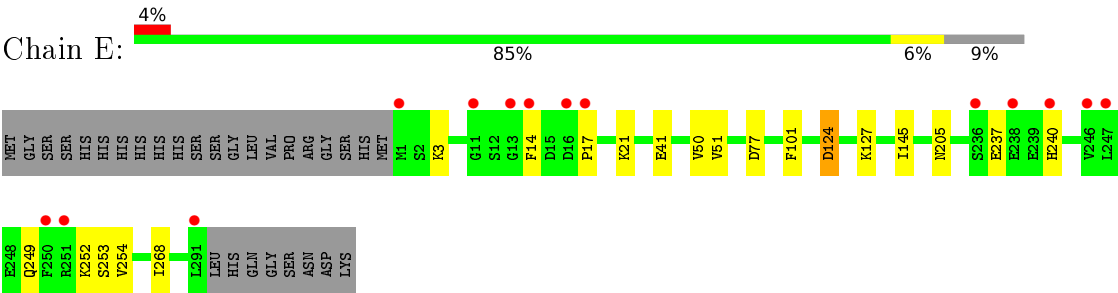


#### • Molecule 1: Methylthiadenosine phosphorylase

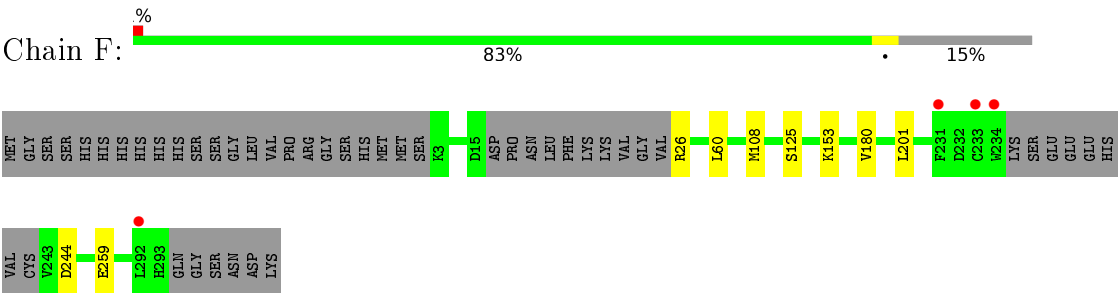


ASN  
ASP  
LYS

• 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, $\alpha$ , $\beta$ , $\gamma$	81.49 Å 82.11 Å 150.27 Å 90.00° 101.10° 90.00°	Depositor
Resolution (Å)	73.73 – 1.66 76.76 – 1.66	Depositor EDS
% Data completeness (in resolution range)	95.3 (73.73-1.66) 95.8 (76.76-1.66)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.65 (at 1.66 Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, $R_{free}$	0.195 , 0.226 0.197 , 0.228	Depositor DCC
$R_{free}$ test set	10766 reflections (4.91%)	DCC
Wilson B-factor (Å <sup>2</sup> )	17.0	Xtriage
Anisotropy	0.164	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 53.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	14870	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	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 55.38 % 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 3.1894e-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: PO4, 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	0.42	0/2216	0.58	0/3005
1	B	0.40	0/2279	0.58	0/3090
1	C	0.46	0/2235	0.61	0/3028
1	D	0.41	0/2223	0.56	0/3015
1	E	0.39	0/2286	0.56	0/3099
1	F	0.42	0/2118	0.58	0/2871
All	All	0.42	0/13357	0.58	0/18108

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 [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	2171	0	2162	14	0
1	B	2228	0	2231	17	0
1	C	2192	0	2196	14	0
1	D	2178	0	2160	6	0
1	E	2235	0	2237	11	0
1	F	2078	0	2071	7	0
2	A	10	0	4	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	10	0	4	0	0
2	D	10	0	4	0	0
2	E	10	0	4	0	0
3	B	5	0	0	0	0
3	C	5	0	0	0	0
3	E	5	0	0	0	0
3	F	5	0	0	0	0
4	A	292	0	0	3	0
4	B	307	0	0	4	1
4	C	367	0	0	1	0
4	D	264	0	0	0	0
4	E	237	0	0	1	0
4	F	261	0	0	1	1
All	All	14870	0	13073	64	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 2.

All (64) 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:B:248:GLU:OE1	1:B:252:LYS:NZ	2.17	0.75
1:C:98:PRO:HG3	1:C:230[A]:ASP:HA	1.70	0.73
1:A:163:MET:SD	4:A:552:HOH:O	2.50	0.68
1:B:123:PRO:O	4:B:401:HOH:O	2.12	0.67
1:F:26:ARG:O	4:F:401:HOH:O	2.13	0.65
1:A:132:MET:HE2	1:A:216:ARG:HG2	1.80	0.64
1:B:180:VAL:HB	1:B:201:LEU:HD13	1.80	0.63
1:C:26:ARG:HD2	1:C:78:LEU:HD21	1.84	0.59
1:B:41:GLU:HG2	1:B:50:VAL:HG22	1.84	0.58
1:C:29:THR:HG22	1:C:30:THR:H	1.69	0.56
1:E:21:LYS:O	4:E:401:HOH:O	2.18	0.56
1:B:94:GLU:HG2	1:B:234:TRP:HH2	1.70	0.56
1:E:249:GLN:HA	1:E:252:LYS:HE2	1.88	0.55
1:C:104:LEU:HD21	1:C:203:ILE:HD11	1.89	0.55
1:C:46:ASP:OD1	4:C:401:HOH:O	2.18	0.54
4:A:485:HOH:O	1:B:59:HIS:HE1	1.91	0.53
1:B:14:PHE:HD1	1:B:17:PRO:HB3	1.75	0.51
1:E:41:GLU:HG2	1:E:50:VAL:HG22	1.93	0.51
1:D:49:CYS:SG	1:D:265:VAL:HG11	2.51	0.51
1:C:98:PRO:HG3	1:C:230[B]:ASP:HA	1.92	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:46:ASP:OD2	4:B:402:HOH:O	2.19	0.49
1:E:127:LYS:HD2	1:F:60:LEU:HD22	1.95	0.49
1:A:3:LYS:HE2	1:A:4:VAL:HG22	1.95	0.48
1:C:180:VAL:HB	1:C:201:LEU:HD13	1.95	0.48
1:E:17:PRO:HB3	1:E:51:VAL:HG11	1.96	0.48
1:F:244:ASP:N	1:F:244:ASP:OD1	2.44	0.47
1:D:180:VAL:HB	1:D:201:LEU:HD13	1.96	0.47
1:D:195:ILE:CD1	1:F:108:MET:HG3	2.44	0.47
1:B:52:LEU:HD12	1:B:53:PRO:HD2	1.96	0.47
1:A:169:ILE:O	1:A:172:CYS:HB3	2.13	0.47
1:A:192:GLU:HG2	1:C:108:MET:HG2	1.96	0.47
1:B:19:LEU:HB3	1:B:262:LEU:HD21	1.98	0.45
1:B:196:HIS:HA	1:B:199:MET:CE	2.46	0.45
1:A:238:GLU:H	1:A:238:GLU:CD	2.21	0.44
1:A:3:LYS:HD2	1:A:3:LYS:HA	1.72	0.44
1:A:28:VAL:HG21	1:A:74:ALA:HB1	1.99	0.44
1:C:132:MET:HE2	1:C:216:ARG:HG2	2.00	0.44
1:A:290:ASP:O	4:A:401:HOH:O	2.21	0.43
1:E:145:ILE:HG21	1:E:268:ILE:HG13	2.00	0.43
1:E:124:ASP:N	1:E:124:ASP:OD1	2.35	0.43
1:D:13:GLY:C	1:D:15:ASP:H	2.21	0.43
1:C:169:ILE:O	1:C:172:CYS:HB3	2.19	0.43
1:C:289:GLN:OE1	1:C:293:HIS:NE2	2.51	0.43
1:C:26:ARG:NH1	1:C:41:GLU:OE2	2.53	0.42
1:D:195:ILE:HD13	1:F:108:MET:HG3	2.02	0.42
1:F:153:LYS:HE2	1:F:259:GLU:HB3	2.02	0.42
1:B:185:PRO:HD2	4:B:591:HOH:O	2.20	0.41
1:B:153:LYS:HE3	4:B:509:HOH:O	2.21	0.41
1:E:237:GLU:HA	1:E:240:HIS:CE1	2.56	0.41
1:A:247:LEU:O	1:A:251:ARG:HG3	2.20	0.41
1:E:3:LYS:HA	1:E:3:LYS:HD2	1.85	0.41
1:B:26:ARG:NE	1:B:41:GLU:OE1	2.46	0.41
1:B:164:ASP:OD1	1:B:165:LYS:N	2.53	0.41
1:D:132:MET:HE2	1:D:216:ARG:HG2	2.03	0.41
1:F:180:VAL:HB	1:F:201:LEU:HD13	2.02	0.41
1:A:190:ARG:NH2	1:A:235:LYS:O	2.52	0.40
1:A:10:GLY:HA2	1:A:86:THR:HG22	2.02	0.40
1:B:22:LYS:HG2	1:B:40:VAL:HG11	2.02	0.40
1:C:127:LYS:HD2	1:C:127:LYS:N	2.35	0.40
1:A:186:ARG:HD2	1:C:134:MET:HG3	2.02	0.40
1:E:14:PHE:CE2	1:E:254:VAL:HG23	2.57	0.40

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:247:LEU:HA	1:A:247:LEU:HD23	1.89	0.40
1:B:14:PHE:CD1	1:B:17:PRO:HB3	2.55	0.40
1:E:101:PHE:HE1	1:E:253:SER:HB3	1.87	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)
4:B:402:HOH:O	4:F:609:HOH:O[2_645]	2.14	0.06

## 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	280/320 (88%)	276 (99%)	4 (1%)	0	100	100
1	B	291/320 (91%)	289 (99%)	2 (1%)	0	100	100
1	C	283/320 (88%)	280 (99%)	3 (1%)	0	100	100
1	D	283/320 (88%)	277 (98%)	5 (2%)	1 (0%)	39	18
1	E	291/320 (91%)	288 (99%)	3 (1%)	0	100	100
1	F	267/320 (83%)	267 (100%)	0	0	100	100
All	All	1695/1920 (88%)	1677 (99%)	17 (1%)	1 (0%)	56	33

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	14	PHE

### 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	237/274 (86%)	235 (99%)	2 (1%)	86	76
1	B	244/274 (89%)	242 (99%)	2 (1%)	86	76
1	C	242/274 (88%)	238 (98%)	4 (2%)	68	45
1	D	236/274 (86%)	235 (100%)	1 (0%)	93	89
1	E	244/274 (89%)	241 (99%)	3 (1%)	78	60
1	F	226/274 (82%)	225 (100%)	1 (0%)	93	89
All	All	1429/1644 (87%)	1416 (99%)	13 (1%)	86	72

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	205	ASN
1	A	257	VAL
1	B	205	ASN
1	B	248	GLU
1	C	26	ARG
1	C	29	THR
1	C	230[A]	ASP
1	C	230[B]	ASP
1	D	205	ASN
1	E	77	ASP
1	E	124	ASP
1	E	205	ASN
1	F	125	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	59	HIS
1	C	289	GLN



### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

8 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	ADE	A	301	-	9,11,11	1.31	1 (11%)	4,15,15	1.48	1 (25%)
2	ADE	B	301	-	9,11,11	0.95	1 (11%)	4,15,15	1.51	1 (25%)
3	PO4	B	302	-	4,4,4	0.42	0	6,6,6	0.24	0
3	PO4	C	301	-	4,4,4	0.67	0	6,6,6	0.25	0
2	ADE	D	301	-	9,11,11	1.29	1 (11%)	4,15,15	1.55	1 (25%)
2	ADE	E	301	-	9,11,11	1.24	1 (11%)	4,15,15	1.51	1 (25%)
3	PO4	E	302	-	4,4,4	0.43	0	6,6,6	0.24	0
3	PO4	F	301	-	4,4,4	0.47	0	6,6,6	0.25	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
2	ADE	A	301	-	-	0/0/0/0	0/2/2/2

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ADE	B	301	-	-	0/0/0/0	0/2/2/2
3	PO4	B	302	-	-	0/0/0/0	0/0/0/0
3	PO4	C	301	-	-	0/0/0/0	0/0/0/0
2	ADE	D	301	-	-	0/0/0/0	0/2/2/2
2	ADE	E	301	-	-	0/0/0/0	0/2/2/2
3	PO4	E	302	-	-	0/0/0/0	0/0/0/0
3	PO4	F	301	-	-	0/0/0/0	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301	ADE	C4-N9	2.20	1.38	1.35
2	E	301	ADE	C4-N9	2.72	1.39	1.35
2	D	301	ADE	C4-N9	2.91	1.39	1.35
2	A	301	ADE	C4-N9	3.02	1.39	1.35

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	301	ADE	C5-C4-N9	-3.04	105.74	111.12
2	B	301	ADE	C5-C4-N9	-3.01	105.79	111.12
2	E	301	ADE	C5-C4-N9	-2.98	105.84	111.12
2	A	301	ADE	C5-C4-N9	-2.95	105.89	111.12

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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%)	-0.28	4 (1%) 78 80	13, 27, 49, 73	0
1	B	291/320 (90%)	-0.10	11 (3%) 44 44	15, 26, 60, 95	0
1	C	287/320 (89%)	-0.24	6 (2%) 67 70	13, 21, 47, 79	0
1	D	286/320 (89%)	-0.20	6 (2%) 67 70	15, 28, 55, 75	0
1	E	291/320 (90%)	0.05	14 (4%) 34 32	18, 30, 66, 100	0
1	F	273/320 (85%)	-0.17	4 (1%) 76 79	16, 28, 55, 75	0
All	All	1711/1920 (89%)	-0.16	45 (2%) 59 60	13, 27, 58, 100	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	14	PHE	7.6
1	F	233	CYS	7.4
1	E	17	PRO	6.8
1	E	250	PHE	6.5
1	E	291	LEU	5.8
1	B	250	PHE	5.4
1	E	247	LEU	4.8
1	B	1	MET	4.6
1	F	231	PHE	4.5
1	E	13	GLY	4.3
1	B	19	LEU	4.3
1	F	234	TRP	4.2
1	B	247	LEU	4.1
1	D	13	GLY	3.9
1	B	16	ASP	3.9
1	F	292	LEU	3.8
1	B	14	PHE	3.8
1	A	292	LEU	3.5
1	E	16	ASP	3.4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	C	241	VAL	3.4
1	D	166	SER	3.3
1	C	295	GLY	3.3
1	E	238	GLU	3.2
1	A	166	SER	3.1
1	B	18	ASN	3.0
1	B	17	PRO	3.0
1	D	12	SER	2.9
1	B	2	SER	2.8
1	E	11	GLY	2.8
1	D	14	PHE	2.5
1	E	1	MET	2.5
1	B	15	ASP	2.4
1	A	19	LEU	2.4
1	E	236	SER	2.3
1	C	242	CYS	2.3
1	B	236	SER	2.3
1	E	251	ARG	2.2
1	C	296	SER	2.2
1	D	3	LYS	2.1
1	A	18	ASN	2.1
1	C	89	CYS	2.1
1	C	299	LYS	2.0
1	D	123	PRO	2.0
1	E	240	HIS	2.0
1	E	246	VAL	2.0

## 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 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. 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( $\text{\AA}^2$ )	Q<0.9
2	ADE	B	301	10/10	0.94	0.14	1.83	33,35,38,40	0
2	ADE	E	301	10/10	0.93	0.12	1.29	34,36,38,38	0
3	PO4	B	302	5/5	0.98	0.12	0.27	27,27,29,30	0
2	ADE	D	301	10/10	0.97	0.07	-0.31	20,22,25,26	0
3	PO4	E	302	5/5	0.98	0.08	-0.43	29,31,32,33	0
3	PO4	C	301	5/5	0.99	0.06	-0.83	16,16,17,18	0
2	ADE	A	301	10/10	0.98	0.06	-1.37	17,18,20,21	0
3	PO4	F	301	5/5	0.99	0.04	-2.28	20,21,22,25	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.