W O R L D W I D E
wwPDB
PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 07:33 PM GMT

PDB ID	:	1G60
Title	:	Crystal Structure of Methyltransferase MboIIa (Moraxella bovis)
Authors	:	Osipiuk, J.; Walsh, M.A.; Joachimiak, A.; Midwest Center for Structural Genomics (MCSG)
Deposited on	:	2000-11-02
Resolution	:	1.74 Å(reported)

The following versions of software and data (see references (i)) 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 1.74 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.
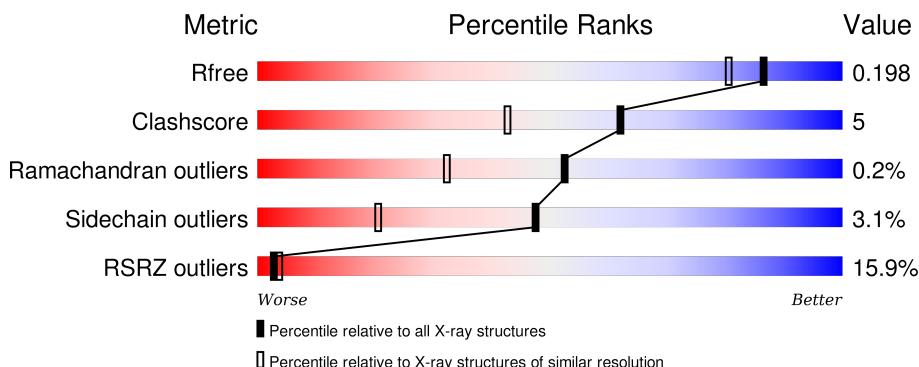
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2417 (1.76-1.72)
Clashscore	102246	2570 (1.76-1.72)
Ramachandran outliers	100387	2544 (1.76-1.72)
Sidechain outliers	100360	2544 (1.76-1.72)
RSRZ outliers	91569	2420 (1.76-1.72)

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 >=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 <=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	260	
1	B	260	
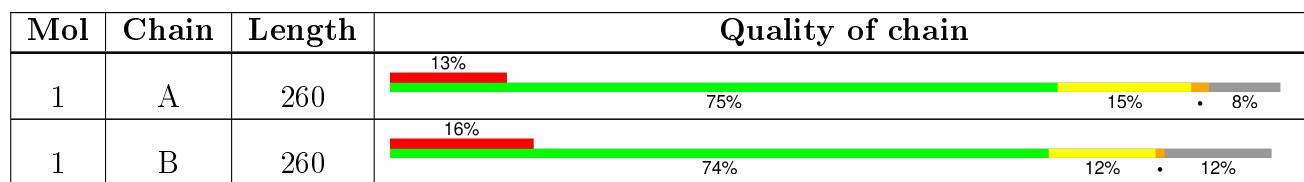
2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 4305 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 Adenine-specific Methyltransferase MboIIA.

| Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	238	Total	C	N	O	S	0	9	0
			1985	1271	343	359	12			
1	B	228	Total	C	N	O	S	0	8	0
			1903	1220	326	344	13			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	51	ALA	PRO	SEE REMARK 999	UNP P23192
A	111	ARG	GLY	SEE REMARK 999	UNP P23192
B	51	ALA	PRO	SEE REMARK 999	UNP P23192
B	111	ARG	GLY	SEE REMARK 999	UNP P23192

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Na	0	0
			1	1		
2	A	1	Total	Na	0	0
			1	1		

- Molecule 3 is S-ADENOSYLMETHIONINE (three-letter code: SAM) (formula: $C_{15}H_{22}N_6O_5S$).
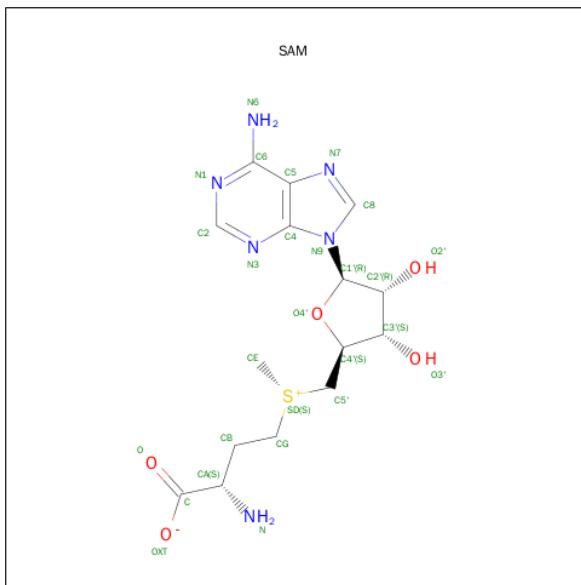
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	N	O	S		0	0
			27	15	6	5	1			
3	B	1	Total	C	N	O	S		0	0
			27	15	6	5	1			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	195	Total	O	0	0
			195	195		
4	B	166	Total	O	0	0
			166	166		

3 Residue-property plots ⓘ

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: Adenine-specific Methyltransferase MboIIA
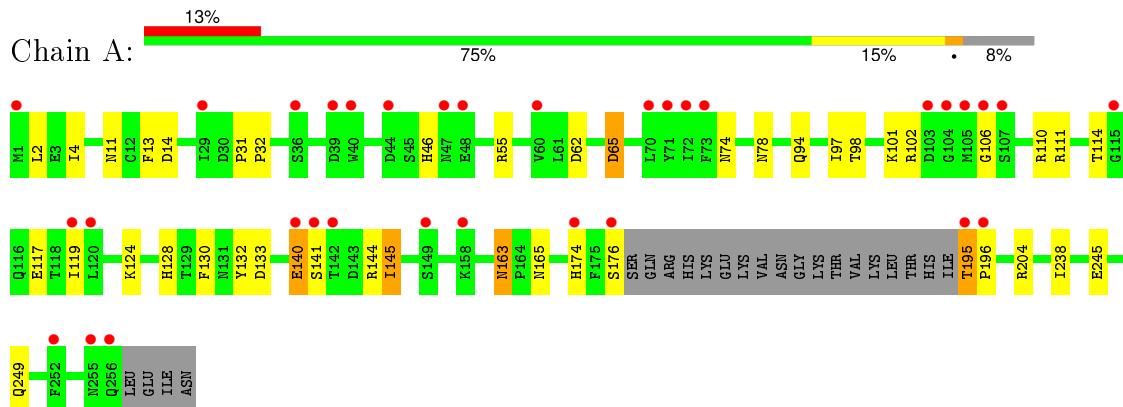
- Molecule 1: Adenine-specific Methyltransferase MboIIA
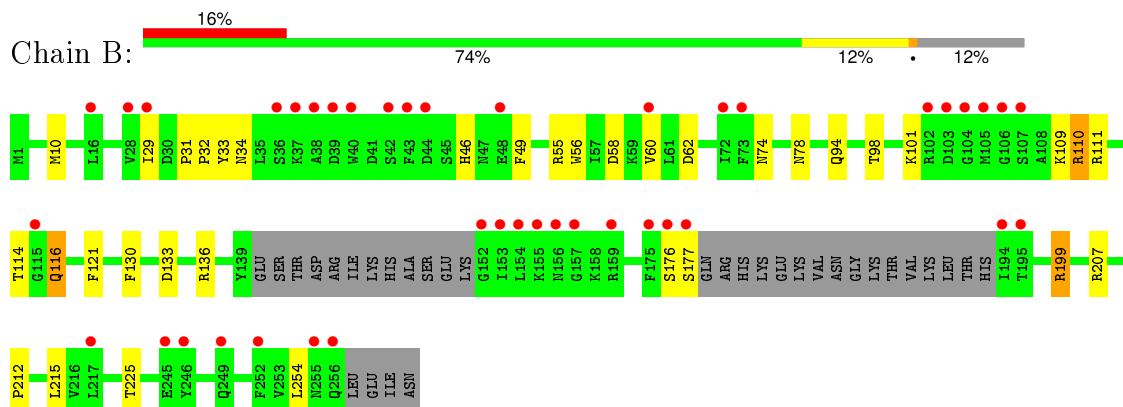
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	60.82Å 98.70Å 50.89Å 90.00° 101.93° 90.00°	Depositor
Resolution (Å)	29.75 – 1.74 28.79 – 1.74	Depositor EDS
% Data completeness (in resolution range)	99.6 (29.75-1.74) 99.7 (28.79-1.74)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	3.06 (at 1.74Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.198 , 0.221 0.188 , 0.198	Depositor DCC
R_{free} test set	2417 reflections (4.20%)	DCC
Wilson B-factor (Å^2)	21.9	Xtriage
Anisotropy	0.164	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 61.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$<|L|> = 0.50, <L^2> = 0.33$	Xtriage
Outliers	0 of 59974 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	4305	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.20% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $<|L|>$, $<L^2>$ 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: NA, SAM

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	0.61	0/2070	1.27	9/2790 (0.3%)
1	B	0.66	0/1982	1.32	19/2673 (0.7%)
All	All	0.64	0/4052	1.29	28/5463 (0.5%)

There are no bond length outliers.

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	136	ARG	NE-CZ-NH1	11.94	126.27	120.30
1	B	199	ARG	NE-CZ-NH2	9.40	125.00	120.30
1	A	133	ASP	CB-CG-OD2	7.94	125.45	118.30
1	B	136	ARG	NE-CZ-NH2	-7.73	116.43	120.30
1	B	133	ASP	CB-CG-OD1	7.20	124.78	118.30
1	A	110	ARG	NE-CZ-NH1	7.14	123.87	120.30
1	A	144	ARG	CD-NE-CZ	7.01	133.41	123.60
1	A	130	PHE	CB-CG-CD1	-6.62	116.17	120.80
1	B	10[A]	MET	CA-CB-CG	6.51	124.36	113.30
1	B	10[B]	MET	CA-CB-CG	6.51	124.36	113.30
1	A	55	ARG	NE-CZ-NH2	-6.37	117.11	120.30
1	A	65	ASP	CB-CG-OD2	6.36	124.02	118.30
1	B	55[A]	ARG	NE-CZ-NH1	6.05	123.33	120.30
1	B	55[B]	ARG	NE-CZ-NH1	6.05	123.33	120.30
1	B	58	ASP	CB-CG-OD1	5.86	123.58	118.30
1	B	207	ARG	NE-CZ-NH2	-5.64	117.48	120.30
1	B	215	LEU	O-C-N	5.48	131.47	122.70
1	B	55[A]	ARG	NE-CZ-NH2	-5.44	117.58	120.30
1	B	55[B]	ARG	NE-CZ-NH2	-5.44	117.58	120.30
1	B	33	TYR	CA-CB-CG	5.36	123.59	113.40
1	A	62	ASP	CB-CG-OD2	5.34	123.11	118.30
1	A	110	ARG	NE-CZ-NH2	-5.25	117.67	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	204	ARG	NE-CZ-NH2	5.16	122.88	120.30
1	B	130	PHE	CB-CG-CD1	-5.12	117.22	120.80
1	B	55[A]	ARG	CD-NE-CZ	5.10	130.74	123.60
1	B	55[B]	ARG	CD-NE-CZ	5.10	130.74	123.60
1	B	110	ARG	NE-CZ-NH1	5.03	122.82	120.30
1	B	62	ASP	CB-CG-OD2	5.00	122.80	118.30

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	1985	0	1944	31	0
1	B	1903	0	1849	23	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	27	0	22	0	0
3	B	27	0	22	0	0
4	A	195	0	0	2	0
4	B	166	0	0	2	0
All	All	4305	0	3837	42	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (42) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:ARG:HH21	1:B:94:GLN:HE22	1.32	0.77
1:A:111:ARG:HE	1:B:94:GLN:NE2	1.83	0.75
1:A:163:ASN:HD22	1:A:165:ASN:H	1.31	0.75
1:A:94:GLN:HE22	1:B:111:ARG:HH21	1.35	0.71
1:A:94:GLN:NE2	1:B:111:ARG:HE	1.93	0.66
1:A:111:ARG:HE	1:B:94:GLN:HE21	1.47	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:114:THR:HG23	4:B:619:HOH:O	1.98	0.62
1:B:199:ARG:HD3	1:B:225:THR:HG23	1.81	0.61
1:A:128:HIS:CD2	1:A:128:HIS:H	2.17	0.60
1:A:163:ASN:ND2	1:A:165:ASN:H	1.98	0.59
1:A:101:LYS:NZ	1:A:117:GLU:OE2	2.38	0.56
1:A:140:GLU:HG3	4:A:655:HOH:O	2.08	0.53
1:A:128:HIS:HE1	1:B:110:ARG:O	1.91	0.53
1:A:65:ASP:O	1:A:124[B]:LYS:HD3	2.08	0.53
1:A:94:GLN:HE21	1:B:111:ARG:HE	1.58	0.52
1:A:245:GLU:HG3	4:A:682:HOH:O	2.10	0.51
1:B:98:THR:HG23	1:B:116:GLN:HE21	1.76	0.51
1:B:31:PRO:HB2	1:B:32:PRO:HD2	1.93	0.51
1:B:29[B]:ILE:HD11	1:B:60:VAL:HG11	1.93	0.50
1:A:111:ARG:NH2	1:B:94:GLN:HE22	2.04	0.50
1:A:4:ILE:HG22	1:A:238[A]:ILE:CG2	2.42	0.50
1:A:141:SER:O	1:A:145:ILE:HD13	2.10	0.50
1:A:11:ASN:ND2	1:A:13:PHE:H	2.10	0.50
1:B:29[B]:ILE:HD13	1:B:56:TRP:HZ3	1.77	0.50
1:B:46:HIS:HE1	1:B:78:ASN:OD1	1.95	0.49
1:A:195:THR:N	1:A:196:PRO:CD	2.77	0.47
1:A:11:ASN:HD22	1:A:14:ASP:H	1.62	0.46
1:A:46:HIS:HE1	1:A:78:ASN:OD1	1.97	0.46
1:A:2:LEU:HD23	1:A:238[B]:ILE:HD11	1.97	0.45
1:B:34:ASN:HB2	1:B:49:PHE:CD1	2.52	0.45
1:A:31:PRO:HB2	1:A:32:PRO:HD2	2.00	0.44
1:B:29[B]:ILE:HD13	1:B:56:TRP:CZ3	2.52	0.44
1:A:98:THR:HG21	1:B:98:THR:HG21	2.00	0.44
1:A:94:GLN:HE22	1:B:111:ARG:NH2	2.11	0.43
1:A:102:ARG:NH2	1:A:174:HIS:CE1	2.86	0.43
1:A:97[A]:ILE:HB	1:A:119:ILE:HB	2.00	0.43
1:A:111:ARG:NE	1:B:94:GLN:NE2	2.62	0.42
1:B:101:LYS:HB2	4:B:614:HOH:O	2.19	0.41
1:A:102:ARG:HH21	1:A:174:HIS:CE1	2.39	0.41
1:A:132:TYR:CE2	1:B:109:LYS:HB3	2.56	0.41
1:B:31:PRO:HB2	1:B:32:PRO:CD	2.51	0.41
1:A:106:GLY:HA3	1:A:114:THR:O	2.21	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	243/260 (94%)	236 (97%)	7 (3%)	0	100	100
1	B	230/260 (88%)	219 (95%)	10 (4%)	1 (0%)	39	20
All	All	473/520 (91%)	455 (96%)	17 (4%)	1 (0%)	52	32

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	176	SER

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	223/235 (95%)	216 (97%)	7 (3%)	47	20
1	B	213/235 (91%)	207 (97%)	6 (3%)	51	25
All	All	436/470 (93%)	423 (97%)	13 (3%)	47	22

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

Mol	Chain	Res	Type
1	A	74	ASN
1	A	140	GLU
1	A	145	ILE
1	A	163	ASN
1	A	176	SER

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Mol	Chain	Res	Type
1	A	195	THR
1	A	249	GLN
1	B	74	ASN
1	B	116	GLN
1	B	121	PHE
1	B	177	SER
1	B	212	PRO
1	B	254	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	ASN
1	A	46	HIS
1	A	94	GLN
1	A	128	HIS
1	A	163	ASN
1	A	165	ASN
1	A	213	ASN
1	B	46	HIS
1	B	94	GLN
1	B	116	GLN
1	B	156	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)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

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	SAM	A	500	-	21,29,29	1.54	4 (19%)	17,42,42	2.14	6 (35%)
3	SAM	B	501	-	21,29,29	1.62	5 (23%)	17,42,42	1.43	3 (17%)

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
3	SAM	A	500	-	-	0/8/33/33	0/3/3/3
3	SAM	B	501	-	-	0/8/33/33	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	500	SAM	C2'-C3'	2.03	1.58	1.53
3	B	501	SAM	C2'-C3'	2.07	1.59	1.53
3	A	500	SAM	C2-N3	2.31	1.36	1.32
3	B	501	SAM	O2'-C2'	2.33	1.48	1.43
3	B	501	SAM	C2-N3	2.33	1.36	1.32
3	A	500	SAM	O4'-C1'	3.26	1.45	1.41
3	B	501	SAM	C4-N3	3.72	1.41	1.35
3	A	500	SAM	C4-N3	3.98	1.41	1.35
3	B	501	SAM	O4'-C1'	4.10	1.46	1.41

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	500	SAM	C1'-N9-C4	-3.31	121.95	126.94
3	A	500	SAM	O4'-C4'-C5'	-3.02	100.85	108.90
3	B	501	SAM	O4'-C4'-C5'	-3.02	100.86	108.90
3	A	500	SAM	C2'-C1'-N9	-2.08	111.12	114.29
3	B	501	SAM	O4'-C1'-N9	-2.05	103.81	108.10
3	A	500	SAM	N6-C6-N1	2.08	123.66	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	500	SAM	C4-C5-N7	2.27	111.57	109.48
3	B	501	SAM	C2-N1-C6	2.99	124.11	118.77
3	A	500	SAM	N3-C2-N1	5.12	132.82	128.89

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 (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th 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(Å²)	Q<0.9
1	A	238/260 (91%)	0.58	33 (13%)	4	5	15, 26, 47, 63	2 (0%)
1	B	228/260 (87%)	0.88	41 (17%)	2	3	14, 24, 54, 71	3 (1%)
All	All	466/520 (89%)	0.73	74 (15%)	3	4	14, 25, 53, 71	5 (1%)

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	104	GLY	16.0
1	A	104	GLY	8.9
1	B	105	MET	7.9
1	B	252	PHE	6.6
1	B	157	GLY	6.4
1	B	154	LEU	6.1
1	B	38	ALA	5.5
1	A	176	SER	5.3
1	B	106	GLY	5.0
1	A	115	GLY	4.9
1	A	105	MET	4.8
1	B	255	ASN	4.7
1	B	245[A]	GLU	4.6
1	B	103	ASP	4.6
1	B	195	THR	4.6
1	A	141	SER	4.2
1	B	249[A]	GLN	4.1
1	B	107	SER	4.1
1	B	177	SER	4.1
1	B	37	LYS	4.1
1	A	103	ASP	3.9
1	A	195	THR	3.9
1	B	152	GLY	3.8
1	A	252	PHE	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	43	PHE	3.7
1	B	40	TRP	3.7
1	B	156	ASN	3.7
1	A	142	THR	3.6
1	B	44	ASP	3.5
1	B	194	ILE	3.5
1	B	176	SER	3.4
1	A	196	PRO	3.4
1	A	107[A]	SER	3.4
1	B	36	SER	3.4
1	A	39	ASP	3.3
1	B	159	ARG	3.3
1	B	29[A]	ILE	3.3
1	A	29	ILE	3.2
1	B	256	GLN	3.2
1	A	72	ILE	3.2
1	B	115	GLY	3.2
1	A	106	GLY	3.1
1	B	102	ARG	3.1
1	A	44	ASP	3.1
1	A	149	SER	3.1
1	B	246	TYR	2.9
1	B	28	VAL	2.9
1	B	39	ASP	2.8
1	A	140	GLU	2.8
1	A	119	ILE	2.8
1	A	1	MET	2.7
1	B	217	LEU	2.6
1	B	16	LEU	2.6
1	B	153	ILE	2.6
1	A	48[A]	GLU	2.5
1	A	255	ASN	2.5
1	A	40	TRP	2.5
1	A	158	LYS	2.5
1	A	256	GLN	2.5
1	A	174	HIS	2.4
1	B	155	LYS	2.4
1	B	48[A]	GLU	2.3
1	A	71	TYR	2.3
1	A	60	VAL	2.3
1	B	42	SER	2.3
1	A	47[A]	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	73	PHE	2.2
1	A	36	SER	2.2
1	B	72	ILE	2.1
1	A	73	PHE	2.1
1	B	175	PHE	2.1
1	A	70	LEU	2.1
1	B	60	VAL	2.0
1	A	120	LEU	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, 95th 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($Å^2$)	Q<0.9
3	SAM	A	500	27/27	0.92	0.10	-0.12	27,32,39,40	0
3	SAM	B	501	27/27	0.90	0.12	-0.23	32,36,38,39	0
2	NA	A	401	1/1	0.80	0.12	-	39,39,39,39	0
2	NA	B	402	1/1	0.81	0.12	-	47,47,47,47	0

6.5 Other polymers (i)

There are no such residues in this entry.