



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2018 – 07:22 pm GMT

PDB ID : 2IBT  
Title : Crystal structure of the adenine-specific DNA methyltransferase M.TaqI complexed with the cofactor analog AETA and a 10 bp DNA containing 2-aminopurine at the target position and an abasic site analog at the target base partner position  
Authors : Lenz, T.; Scheidig, A.J.; Weinhold, E.  
Deposited on : 2006-09-12  
Resolution : 1.70 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

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

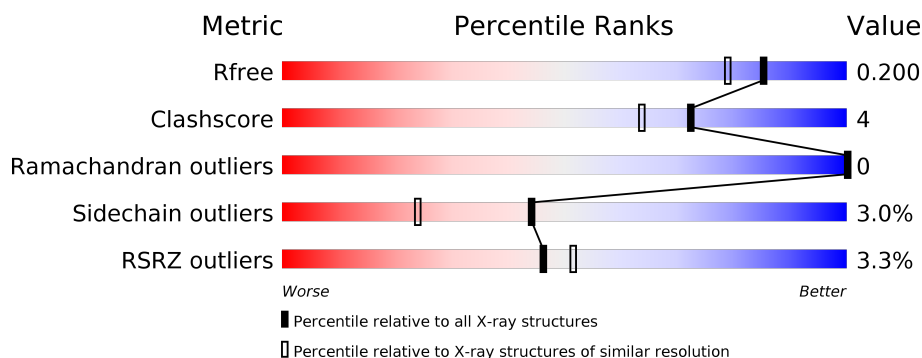
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	111664	3793 (1.70-1.70)
Clashscore	122126	4167 (1.70-1.70)
Ramachandran outliers	120053	4100 (1.70-1.70)
Sidechain outliers	120020	4100 (1.70-1.70)
RSRZ outliers	108989	3718 (1.70-1.70)

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	B	10	<div><div></div><div>60%40%</div></div>
1	E	10	<div><div></div><div>40%50%10%</div></div>
2	C	10	<div><div></div><div>60%10%30%</div></div>
2	F	10	<div><div></div><div>50%50%</div></div>
3	A	421	<div><div>3%</div><div>85%7%7%</div></div>
3	D	421	<div><div>3%</div><div>85%7%7%</div></div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8297 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 DNA chain called 5'-D(\*GP\*TP\*TP\*CP\*GP\*(2PR)P\*TP\*GP\*TP\*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	10	Total	C	N	O	P	0	0	0
			202	98	34	61	9			
1	E	10	Total	C	N	O	P	0	0	0
			202	98	34	61	9			

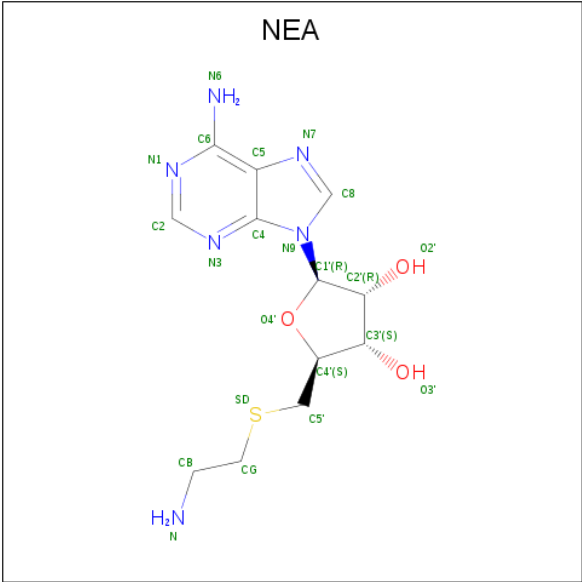
- Molecule 2 is a DNA chain called 5'-D(\*GP\*AP\*CP\*AP\*(3DR)P\*CP\*GP\*(6MA)P\*AP\*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	10	Total	C	N	O	P	0	0	0
			194	93	39	53	9			
2	F	10	Total	C	N	O	P	0	0	0
			194	93	39	53	9			

- Molecule 3 is a protein called Modification methylase TaqI.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	393	Total	C	N	O	S	0	0	0
			3189	2087	548	548	6			
3	D	393	Total	C	N	O	S	0	0	0
			3189	2087	548	548	6			

- Molecule 4 is 5'-DEOXY-5'-[2-(AMINO)ETHYLTHIO]ADENOSINE (three-letter code: NEA) (formula: C<sub>12</sub>H<sub>18</sub>N<sub>6</sub>O<sub>3</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			22	12	6	3	1		
4	D	1	Total	C	N	O	S	0	0
			22	12	6	3	1		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	D	1	Total	C	O	0	0
			6	3	3		
5	D	1	Total	C	O	0	0
			6	3	3		
5	D	1	Total	C	O	0	0
			6	3	3		
5	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	49	Total	O	0	0
			49	49		
6	C	41	Total	O	0	0
			41	41		
6	E	56	Total	O	0	0
			56	56		
6	F	36	Total	O	0	0
			36	36		
6	A	435	Total	O	0	0
			435	435		
6	D	424	Total	O	0	0
			424	424		



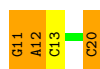
- Molecule 1: 5'-D(\*GP\*TP\*TP\*CP\*GP\*(2PR)P\*TP\*GP\*TP\*C)-3'



- Molecule 1: 5'-D(\*GP\*TP\*TP\*CP\*GP\*(2PR)P\*TP\*GP\*TP\*C)-3'



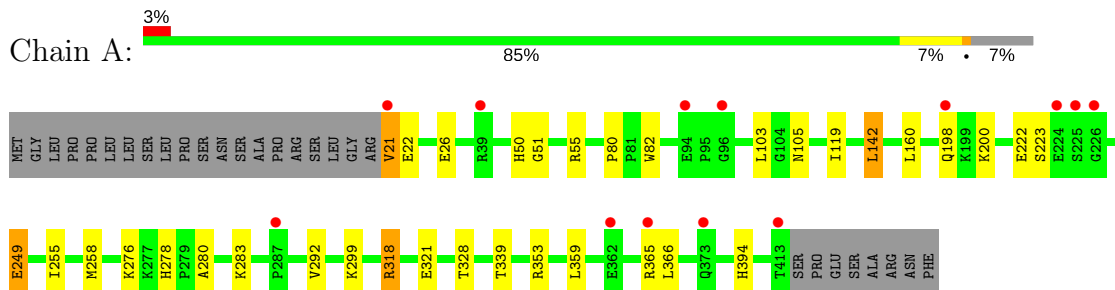
- Molecule 2: 5'-D(\*GP\*AP\*CP\*AP\*(3DR)P\*CP\*GP\*(6MA)P\*AP\*C)-3'



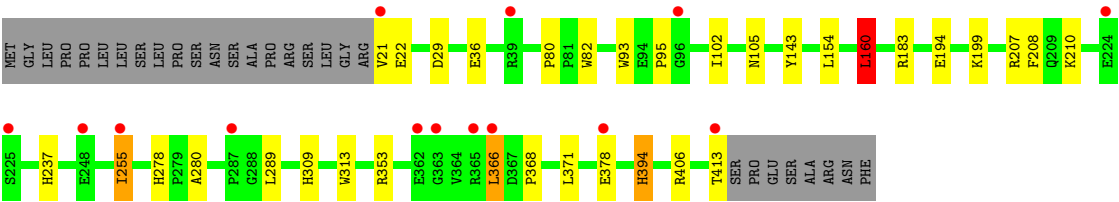
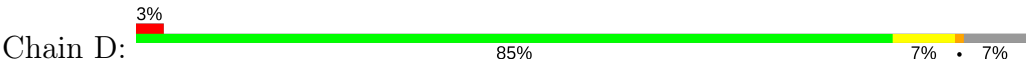
- Molecule 2: 5'-D(\*GP\*AP\*CP\*AP\*(3DR)P\*CP\*GP\*(6MA)P\*AP\*C)-3'



- Molecule 3: Modification methylase TaqI



- Molecule 3: Modification methylase TaqI



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	59.34Å 68.70Å 114.02Å 90.00° 92.09° 90.00°	Depositor
Resolution (Å)	19.92 – 1.70 19.92 – 1.70	Depositor EDS
% Data completeness (in resolution range)	98.1 (19.92-1.70) 98.1 (19.92-1.70)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.40 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.167 , 0.203 0.165 , 0.200	Depositor DCC
$R_{free}$ test set	4943 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	15.6	Xtriage
Anisotropy	0.294	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.41 , 54.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.036 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	8297	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.57% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NEA, GOL, 2PR, 3DR, 6MA

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	B	1.17	0/200	1.85	4/305 (1.3%)
1	E	1.07	0/200	1.89	4/305 (1.3%)
2	C	1.04	0/179	2.02	5/269 (1.9%)
2	F	1.05	0/179	1.78	4/269 (1.5%)
3	A	0.58	0/3293	0.69	3/4475 (0.1%)
3	D	0.60	0/3293	0.67	2/4475 (0.0%)
All	All	0.66	0/7344	0.90	22/10098 (0.2%)

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
3	D	0	1

There are no bond length outliers.

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	E	10	DC	O4'-C1'-N1	12.32	116.63	108.00
2	C	20	DC	O4'-C1'-N1	11.79	116.25	108.00
2	F	20	DC	O4'-C1'-N1	8.97	114.28	108.00
2	C	12	DA	O4'-C1'-N9	-8.48	102.06	108.00
3	A	318	ARG	NE-CZ-NH2	-7.78	116.41	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	D	394	HIS	Peptide

## 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	B	202	0	116	1	0
1	E	202	0	116	5	0
2	C	194	0	111	4	0
2	F	194	0	111	1	0
3	A	3189	0	3184	25	0
3	D	3189	0	3184	21	0
4	A	22	0	18	1	0
4	D	22	0	18	0	0
5	A	18	0	24	1	0
5	D	24	0	32	0	0
6	A	435	0	0	13	0
6	B	49	0	0	0	0
6	C	41	0	0	6	0
6	D	424	0	0	8	0
6	E	56	0	0	1	0
6	F	36	0	0	0	0
All	All	8297	0	6914	53	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 4.

The worst 5 of 53 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)
3:A:318:ARG:HD2	3:A:321:GLU:OE2	1.83	0.78
3:A:223:SER:HB2	6:A:3442:HOH:O	1.85	0.77
2:C:11:DG:N3	6:C:1029:HOH:O	2.17	0.75
1:B:5:DG:N7	3:A:394:HIS:HE1	1.87	0.73
1:E:5:DG:N7	3:D:394:HIS:HE1	1.88	0.71

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	
3	A	391/421 (93%)	380 (97%)	11 (3%)	0	100	100
3	D	391/421 (93%)	378 (97%)	13 (3%)	0	100	100
All	All	782/842 (93%)	758 (97%)	24 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	
3	A	332/356 (93%)	320 (96%)	12 (4%)	38	17
3	D	332/356 (93%)	324 (98%)	8 (2%)	52	33
All	All	664/712 (93%)	644 (97%)	20 (3%)	44	24

5 of 20 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	359	LEU
3	A	365	ARG
3	D	255	ILE
3	A	258	MET
3	A	283	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
3	D	61	HIS
3	D	105	ASN
3	D	278	HIS
3	D	50	HIS
3	D	237	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

6 non-standard protein/DNA/RNA residues 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	$\# Z  > 2$
1	2PR	B	6	1	17,23,24	0.84	0	17,33,36	1.57	4 (23%)
2	3DR	C	15	2	8,11,12	0.70	0	9,14,17	1.21	1 (11%)
2	6MA	C	18	1,2	18,24,25	0.73	0	17,34,37	1.98	2 (11%)
1	2PR	E	6	1	17,23,24	0.64	0	17,33,36	1.75	3 (17%)
2	3DR	F	15	2	8,11,12	0.67	0	9,14,17	0.95	0
2	6MA	F	18	1,2	18,24,25	0.89	0	17,34,37	1.64	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
1	2PR	B	6	1	-	0/3/21/22	0/3/3/3
2	3DR	C	15	2	-	0/3/15/16	0/1/1/1
2	6MA	C	18	1,2	-	0/5/23/24	0/3/3/3
1	2PR	E	6	1	-	0/3/21/22	0/3/3/3
2	3DR	F	15	2	-	0/3/15/16	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	6MA	F	18	1,2	-	0/5/23/24	0/3/3/3

There are no bond length outliers.

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	6	2PR	O4'-C1'-N9	-4.53	100.15	107.78
1	B	6	2PR	C2-N3-C4	-3.93	110.57	115.16
1	E	6	2PR	C2-N3-C4	-3.38	111.22	115.16
2	F	18	6MA	N3-C2-N1	-3.22	126.10	128.86
1	B	6	2PR	O4'-C1'-N9	-3.21	102.37	107.78

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	E	6	2PR	2	0
2	F	15	3DR	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

9 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
4	NEA	A	2001	-	21,24,24	1.16	2 (9%)	19,34,34	2.65	2 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	GOL	A	3001	-	5,5,5	0.29	0	5,5,5	0.25	0
5	GOL	A	3002	-	5,5,5	0.38	0	5,5,5	0.36	0
5	GOL	A	3007	-	5,5,5	0.35	0	5,5,5	0.31	0
4	NEA	D	2002	-	21,24,24	1.08	2 (9%)	19,34,34	2.39	2 (10%)
5	GOL	D	3003	-	5,5,5	0.32	0	5,5,5	0.46	0
5	GOL	D	3004	-	5,5,5	0.47	0	5,5,5	0.46	0
5	GOL	D	3005	-	5,5,5	0.38	0	5,5,5	0.26	0
5	GOL	D	3006	-	5,5,5	0.45	0	5,5,5	0.28	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NEA	A	2001	-	-	0/5/25/25	0/3/3/3
5	GOL	A	3001	-	-	0/4/4/4	0/0/0/0
5	GOL	A	3002	-	-	0/4/4/4	0/0/0/0
5	GOL	A	3007	-	-	0/4/4/4	0/0/0/0
4	NEA	D	2002	-	-	0/5/25/25	0/3/3/3
5	GOL	D	3003	-	-	0/4/4/4	0/0/0/0
5	GOL	D	3004	-	-	0/4/4/4	0/0/0/0
5	GOL	D	3005	-	-	0/4/4/4	0/0/0/0
5	GOL	D	3006	-	-	0/4/4/4	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	2002	NEA	C2-N1	2.15	1.38	1.33
4	A	2001	NEA	C2-N1	2.37	1.38	1.33
4	D	2002	NEA	C2-N3	3.55	1.37	1.32
4	A	2001	NEA	C2-N3	3.58	1.38	1.32

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	2001	NEA	N3-C2-N1	-10.82	119.60	128.86
4	D	2002	NEA	N3-C2-N1	-9.45	120.77	128.86
4	A	2001	NEA	C4-C5-N7	-2.37	107.12	109.41
4	D	2002	NEA	C5'-SD-CG	-2.06	96.08	102.27

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	2001	NEA	1	0
5	A	3007	GOL	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 [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, 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	B	9/10 (90%)	0.28	0 100 100	9, 10, 28, 30	0
1	E	9/10 (90%)	-0.29	0 100 100	10, 12, 23, 24	0
2	C	8/10 (80%)	0.16	0 100 100	10, 14, 26, 30	0
2	F	8/10 (80%)	-0.27	0 100 100	10, 17, 24, 25	0
3	A	393/421 (93%)	0.04	13 (3%) 46 51	8, 14, 25, 33	0
3	D	393/421 (93%)	0.06	14 (3%) 42 48	7, 14, 25, 35	0
All	All	820/882 (92%)	0.05	27 (3%) 46 51	7, 14, 26, 35	0

The worst 5 of 27 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	21	VAL	7.4
3	D	21	VAL	6.4
3	D	413	THR	5.0
3	A	225	SER	5.0
3	A	226	GLY	4.2

### 6.2 Non-standard residues in protein, DNA, RNA chains [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	6MA	F	18	22/23	0.97	0.07	8,10,13,15	0
2	6MA	C	18	22/23	0.97	0.07	7,10,12,15	0
1	2PR	B	6	21/22	0.98	0.07	10,13,15,16	0
1	2PR	E	6	21/22	0.98	0.06	9,12,13,15	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	3DR	F	15	11/12	0.99	0.06	9,11,14,14	0
2	3DR	C	15	11/12	0.99	0.06	11,12,16,16	0

### 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. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	GOL	D	3005	6/6	0.82	0.12	45,46,46,47	0
5	GOL	D	3006	6/6	0.85	0.13	23,25,25,26	0
5	GOL	D	3004	6/6	0.87	0.17	19,25,26,26	0
5	GOL	A	3002	6/6	0.92	0.12	16,23,26,27	0
5	GOL	D	3003	6/6	0.94	0.12	20,25,28,31	0
5	GOL	A	3001	6/6	0.95	0.08	20,21,22,23	0
5	GOL	A	3007	6/6	0.96	0.09	19,20,22,24	0
4	NEA	A	2001	22/22	0.97	0.06	11,13,14,14	0
4	NEA	D	2002	22/22	0.98	0.06	9,11,14,15	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.