wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 02:43 AM 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
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

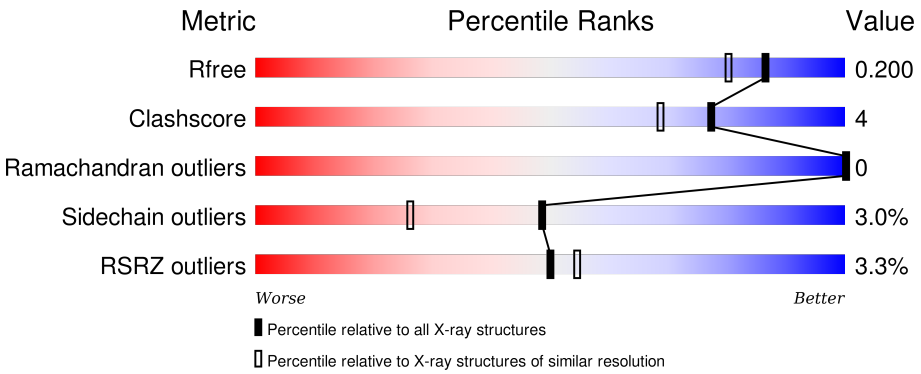
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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}	91344	3190 (1.70-1.70)
Clashscore	102246	3585 (1.70-1.70)
Ramachandran outliers	100387	3527 (1.70-1.70)
Sidechain outliers	100360	3527 (1.70-1.70)
RSRZ outliers	91569	3200 (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 >=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	B	10	60% 40%
1	E	10	40% 50% 10%
2	C	10	60% 10% 30%
2	F	10	50% 50%
3	A	421	3% 85% 7% • 7%

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Mol	Chain	Length	Quality of chain
3	D	421	3% 85% 7% • 7%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	GOL	D	3006	-	-	-	X

2 Entry composition (i)

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
			Total	C	N	O	P			
1	B	10	202	98	34	61	9	0	0	0
1	E	10	202	98	34	61	9	0	0	0

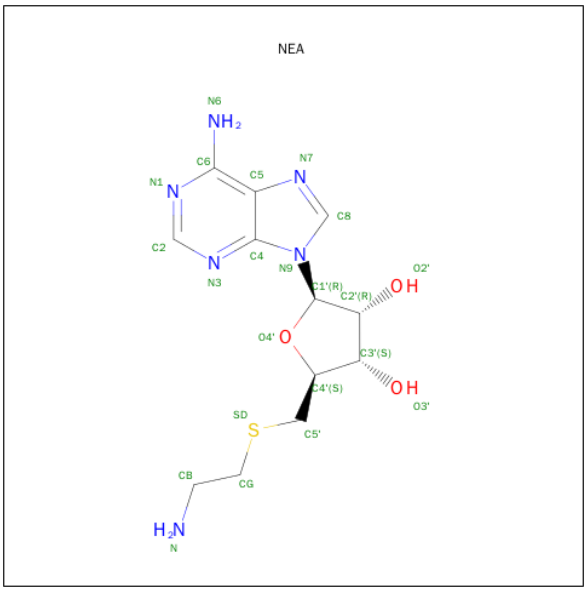
- Molecule 2 is a DNA chain called 5'-D(*GP*AP*CP*AP*(3DR)P*CP*GP*(6MA)P*AP*C)-3'.

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

- Molecule 3 is a protein called Modification methylase TaqI.

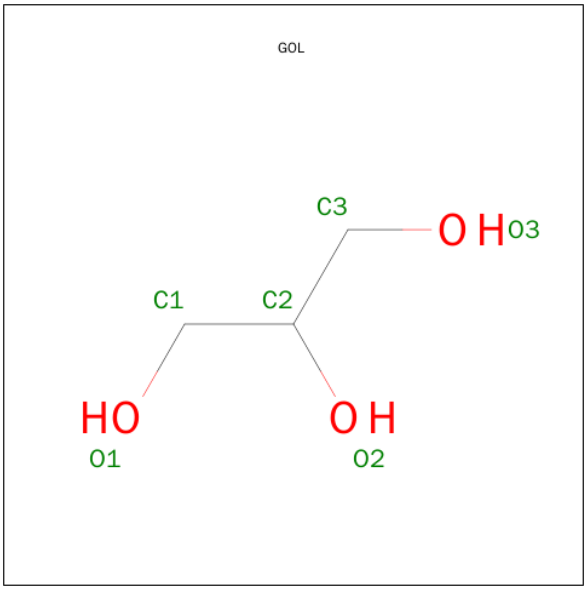
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	A	393	3189	2087	548	548	6	0	0	0
3	D	393	3189	2087	548	548	6	0	0	0

- Molecule 4 is 5'-DEOXY-5'-[2-(AMINO)ETHYLTHIO]ADENOSINE (three-letter code: NEA) (formula: $C_{12}H_{18}N_6O_3S$).



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

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	435	435	435	0	0
			Total	O		
6	B	49	49	49	0	0
			Total	O		
6	C	41	41	41	0	0
			Total	O		
6	D	424	424	424	0	0
			Total	O		
6	E	56	56	56	0	0
			Total	O		
6	F	36	36	36	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: 5'-D(*GP*TP*TP*CP*GP*(2PR)P*TP*GP*TP*C)-3'

Chain B:

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

Chain E:

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

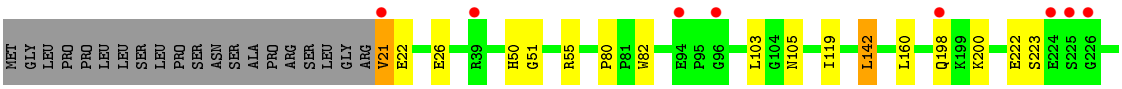
Chain C:

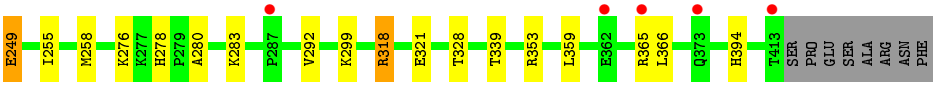
- Molecule 2: 5'-D(*GP*AP*CP*AP*(3DR)P*CP*GP*(6MA)P*AP*C)-3'

Chain F:

- Molecule 3: Modification methylase TaqI

Chain A:

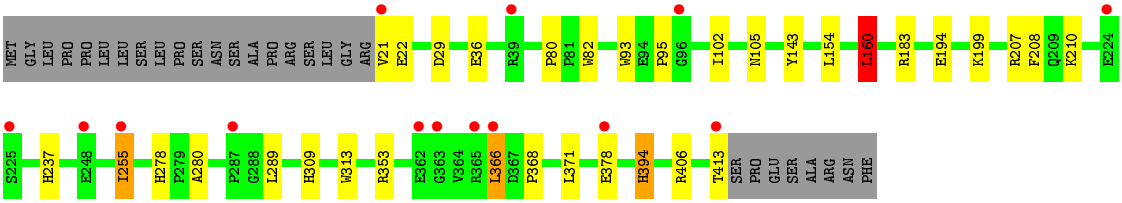




- Molecule 3: Modification methylase TaqI

Chain D:

3%
85%
7%
7%


MET GLY LEU PRO PRO LEU LEU SER LEU PRO SER ASN SER ALA PRO ARG SER LEU GLY ARG V21 E22 D29 E36 R39 P80 P81 W82 W93 E94 P95 G96 I102 N105 Y143 L154 L160 R183 E194 K199 R207 F208 Q209 K210 E224
S225 H237 E248 I255 H278 P279 A280 P287 G288 L289 H309 W313 R353 E362 G363 V364 R365 L366 D367 P368 L371 E378 H394 R406 T413 SER PRO GLU SER ALA ARG ASN PHE

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	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
$< I/\sigma(I) >$ [1]	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 (5.26%)	DCC
Wilson B-factor (Å^2)	15.6	Xtriage
Anisotropy	0.294	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.41 , 54.7	EDS
Estimated twinning fraction	0.036 for h,-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Outliers	0 of 98855 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	8297	wwPDB-VP
Average B, all atoms (Å^2)	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.*

[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: 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(^{o})	Ideal(^{o})
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 (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	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 (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	
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 (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	
3	A	332/356 (93%)	320 (96%)	12 (4%)	42	19
3	D	332/356 (93%)	324 (98%)	8 (2%)	57	36
All	All	664/712 (93%)	644 (97%)	20 (3%)	48	26

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 (i)

There are no RNA molecules in this entry.

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

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	15,23,24	0.80	1 (6%)	17,33,36	1.36	3 (17%)
2	3DR	C	15	2	7,11,12	0.65	0	8,14,17	1.45	1 (12%)
2	6MA	C	18	1,2	16,24,25	0.70	0	18,34,37	1.67	1 (5%)
1	2PR	E	6	1	15,23,24	0.73	1 (6%)	17,33,36	1.60	4 (23%)
2	3DR	F	15	2	7,11,12	0.66	0	8,14,17	0.82	0
2	6MA	F	18	1,2	16,24,25	0.80	0	18,34,37	1.72	4 (22%)

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	6	2PR	C6-N1	2.27	1.36	1.32
1	B	6	2PR	C6-N1	2.42	1.36	1.32

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	6	2PR	O4'-C1'-N9	-4.37	100.15	107.72
2	F	18	6MA	N6-C6-N1	-4.02	114.11	118.77
2	F	18	6MA	N3-C2-N1	-3.64	126.10	128.89
1	B	6	2PR	O4'-C1'-N9	-3.08	102.37	107.72
2	F	18	6MA	C1'-N9-C4	-2.01	123.74	127.16

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	-	19,24,24	1.16	2 (10%)	18,34,34	3.07	2 (11%)
5	GOL	A	3001	-	5,5,5	0.26	0	5,5,5	0.24	0
5	GOL	A	3002	-	5,5,5	0.36	0	5,5,5	0.37	0
5	GOL	A	3007	-	5,5,5	0.33	0	5,5,5	0.32	0
4	NEA	D	2002	-	19,24,24	1.05	2 (10%)	18,34,34	2.75	3 (16%)
5	GOL	D	3003	-	5,5,5	0.30	0	5,5,5	0.47	0
5	GOL	D	3004	-	5,5,5	0.44	0	5,5,5	0.47	0
5	GOL	D	3005	-	5,5,5	0.37	0	5,5,5	0.21	0
5	GOL	D	3006	-	5,5,5	0.43	0	5,5,5	0.29	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	2.14	1.38	1.33
4	A	2001	NEA	C2-N1	2.35	1.38	1.33
4	D	2002	NEA	C2-N3	3.24	1.37	1.32
4	A	2001	NEA	C2-N3	3.27	1.38	1.32

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	2001	NEA	N3-C2-N1	-12.14	119.60	128.89
4	D	2002	NEA	N3-C2-N1	-10.61	120.77	128.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	2001	NEA	C4-C5-N7	-2.57	107.12	109.48
4	D	2002	NEA	C1'-N9-C4	-2.22	123.59	126.94
4	D	2002	NEA	C5'-SD-CG	-2.11	96.08	102.41

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, 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(Å^2)	Q<0.9
1	B	9/10 (90%)	0.32	0	100	100	9, 10, 28, 30	0
1	E	9/10 (90%)	-0.25	0	100	100	10, 12, 23, 24	0
2	C	8/10 (80%)	0.18	0	100	100	10, 14, 26, 30	0
2	F	8/10 (80%)	-0.25	0	100	100	10, 17, 24, 25	0
3	A	393/421 (93%)	0.07	13 (3%)	50	54	8, 14, 25, 33	0
3	D	393/421 (93%)	0.09	14 (3%)	46	51	7, 14, 25, 35	0
All	All	820/882 (92%)	0.07	27 (3%)	50	54	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	A	225	SER	5.1
3	D	413	THR	5.1
3	A	226	GLY	4.3

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. 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
2	6MA	F	18	22/23	0.97	0.07	-	8,10,13,15	0
2	3DR	F	15	11/12	0.99	0.06	-	9,11,14,14	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
1	2PR	B	6	21/22	0.98	0.07	-	10,13,15,16	0
2	3DR	C	15	11/12	0.99	0.06	-	11,12,16,16	0
2	6MA	C	18	22/23	0.97	0.07	-	7,10,12,15	0
1	2PR	E	6	21/22	0.98	0.06	-	9,12,13,15	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. 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
5	GOL	D	3006	6/6	0.85	0.13	2.85	23,25,25,26	0
5	GOL	D	3004	6/6	0.87	0.17	1.66	19,25,26,26	0
5	GOL	D	3005	6/6	0.81	0.13	1.60	45,46,46,47	0
5	GOL	A	3002	6/6	0.92	0.12	0.72	16,23,26,27	0
5	GOL	D	3003	6/6	0.94	0.12	0.44	20,25,28,31	0
5	GOL	A	3001	6/6	0.95	0.09	0.07	20,21,22,23	0
5	GOL	A	3007	6/6	0.96	0.09	-0.33	19,20,22,24	0
4	NEA	D	2002	22/22	0.98	0.06	-0.58	9,11,14,15	0
4	NEA	A	2001	22/22	0.97	0.06	-0.59	11,13,14,14	0

6.5 Other polymers (i)

There are no such residues in this entry.