



Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 04:23 PM GMT

PDB ID : 2FJW
Title : d(CTTGAATGCATTCAAG) in complex with MMLV RT catalytic fragment
Authors : Goodwin, K.D.; Georgiadis, M.M
Deposited on : 2006-01-03
Resolution : 1.95 Å(reported)

This is a full wwPDB validation 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/ValidationPDFNotes.html>

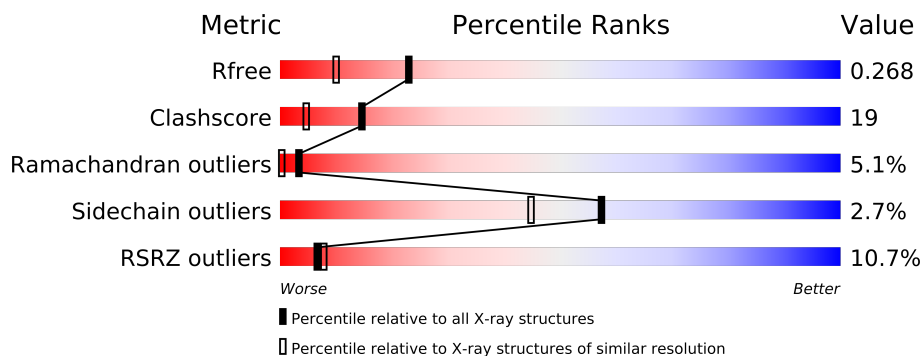
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 1.95 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}	66092	1321 (1.96-1.96)
Clashscore	79885	1488 (1.96-1.96)
Ramachandran outliers	78287	1475 (1.96-1.96)
Sidechain outliers	78261	1475 (1.96-1.96)
RSRZ outliers	66119	1321 (1.96-1.96)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	B	8	<div><div></div><div></div></div>
2	G	8	<div><div></div><div></div></div>
3	A	255	<div><div></div><div></div></div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 2579 atoms, of which 0 are hydrogen and 0 are deuterium.

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(*CP*TP*TP*GP*AP*AP*TP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	8	Total	C	N	O	P	0	0	0
			162	79	29	47	7			

- Molecule 2 is a DNA chain called 5'-D(P*CP*AP*TP*TP*CP*AP*AP*G)-3'.

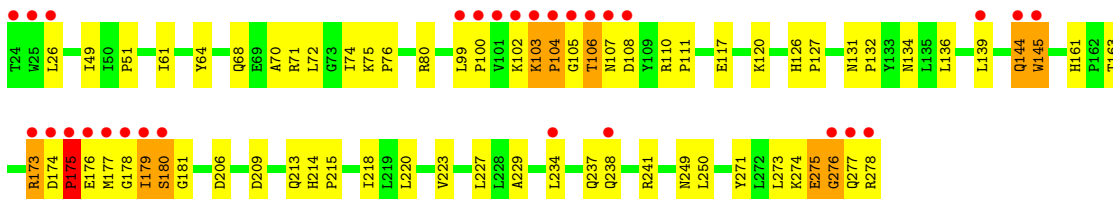
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	8	Total	C	N	O	P	0	0	0
			163	78	30	47	8			

- Molecule 3 is a protein called Reverse transcriptase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	255	Total	C	N	O	S	0	0	0
			2041	1311	356	367	7			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	209	Total	O	0	0
			209	209		
4	G	4	Total	O	0	0
			4	4		



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	54.95Å 145.65Å 46.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 1.95 46.81 – 1.95	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-1.95) 95.9 (46.81-1.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.78 (at 1.95Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.237 , 0.256 0.243 , 0.268	Depositor DCC
R_{free} test set	1323 reflections (4.87%)	DCC
Wilson B-factor (Å ²)	29.8	Xtriage
Anisotropy	0.200	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 44.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 28144 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	2579	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.72% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

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	0.24	0/181	0.66	0/278
2	G	0.24	0/182	0.67	0/278
3	A	0.32	0/2097	0.60	0/2858
All	All	0.31	0/2460	0.61	0/3414

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	162	0	93	8	1
2	G	163	0	91	17	1
3	A	2041	0	2056	65	1
4	A	209	0	0	6	0
4	G	4	0	0	1	0
All	All	2579	0	2240	89	2

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 19.

All (89) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:A:74:ILE:HG23	3:A:111:PRO:HG3	1.49	0.93
3:A:234:LEU:HG	3:A:238:GLN:HE21	1.34	0.90
1:B:7:DT:H2"	1:B:8:DG:H5'	1.57	0.85
3:A:139:LEU:HD13	3:A:278:ARG:OXT	1.78	0.84
3:A:102:LYS:HD3	3:A:106:THR:HA	1.62	0.81
3:A:173:ARG:HA	3:A:173:ARG:HE	1.47	0.79
3:A:103:LYS:HB2	3:A:104:PRO:HD3	1.65	0.78
3:A:174:ASP:HB3	3:A:178:GLY:HA2	1.65	0.77
3:A:161:HIS:HD2	3:A:163:THR:H	1.29	0.77
3:A:71:ARG:NH1	3:A:175:PRO:HG3	2.00	0.77
3:A:179:ILE:HG22	3:A:180:SER:H	1.49	0.76
3:A:274:LYS:HG2	3:A:275:GLU:HG3	1.67	0.76
3:A:234:LEU:HG	3:A:238:GLN:NE2	2.02	0.75
2:G:11:DT:H2"	2:G:12:DT:H5'	1.70	0.73
2:G:12:DT:H2"	2:G:13:DC:H5'	1.70	0.72
3:A:61:ILE:HD11	3:A:117:GLU:HG3	1.73	0.70
1:B:7:DT:H2"	1:B:8:DG:C5'	2.24	0.68
3:A:179:ILE:HG22	3:A:180:SER:N	2.09	0.67
3:A:68:GLN:O	3:A:72:LEU:HD13	1.94	0.67
3:A:234:LEU:O	3:A:237:GLN:HG2	1.96	0.66
3:A:70:ALA:HB1	3:A:100:PRO:HB3	1.78	0.65
2:G:11:DT:H2"	2:G:12:DT:C5'	2.28	0.64
3:A:218:ILE:HB	3:A:229:ALA:HB3	1.81	0.63
3:A:161:HIS:CD2	3:A:163:THR:H	2.15	0.62
3:A:26:LEU:O	3:A:26:LEU:HD23	1.99	0.62
3:A:249:ASN:HB2	4:A:479:HOH:O	2.01	0.60
2:G:10:DA:H2"	2:G:11:DT:C5'	2.32	0.60
1:B:6:DA:H2"	1:B:7:DT:H5"	1.83	0.59
3:A:103:LYS:NZ	3:A:110:ARG:HE	2.01	0.58
3:A:71:ARG:HH11	3:A:175:PRO:HG3	1.70	0.57
1:B:6:DA:H2"	1:B:7:DT:C5'	2.35	0.57
1:B:6:DA:C2'	1:B:7:DT:H5"	2.35	0.57
2:G:10:DA:H2"	2:G:11:DT:H5"	1.86	0.56
3:A:80:ARG:NH1	4:A:329:HOH:O	2.38	0.56
2:G:15:DA:H1'	4:G:164:HOH:O	2.06	0.56
2:G:16:DG:C2	3:A:99:LEU:HD21	2.41	0.56
3:A:131:ASN:HD21	3:A:134:ASN:ND2	2.05	0.55
1:B:2:DT:H2"	1:B:3:DT:H5'	1.91	0.53
3:A:277:GLN:HB2	4:A:394:HOH:O	2.09	0.53
3:A:275:GLU:O	3:A:277:GLN:HG2	2.10	0.52
3:A:71:ARG:HD3	4:A:352:HOH:O	2.09	0.51
3:A:139:LEU:HD11	3:A:227:LEU:CD2	2.40	0.51
2:G:10:DA:C2'	2:G:11:DT:H5"	2.39	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:G:12:DT:H1'	2:G:13:DC:H5''	1.93	0.50
2:G:10:DA:H1'	2:G:11:DT:H5''	1.93	0.50
3:A:80:ARG:HG2	3:A:80:ARG:HH11	1.77	0.49
3:A:132:PRO:O	3:A:136:LEU:HD23	2.12	0.49
3:A:139:LEU:HD11	3:A:227:LEU:HD23	1.94	0.49
1:B:6:DA:H1'	1:B:7:DT:H5''	1.95	0.48
3:A:214:HIS:N	3:A:215:PRO:HD3	2.29	0.47
3:A:139:LEU:HD13	3:A:278:ARG:C	2.33	0.47
3:A:273:LEU:HG	3:A:278:ARG:HB3	1.95	0.47
3:A:273:LEU:HG	3:A:278:ARG:CB	2.44	0.47
3:A:213:GLN:C	3:A:215:PRO:HD3	2.35	0.46
3:A:49:ILE:O	3:A:51:PRO:HD3	2.14	0.46
3:A:99:LEU:HA	3:A:100:PRO:HD3	1.76	0.46
2:G:11:DT:H1'	2:G:12:DT:H5''	1.98	0.46
3:A:61:ILE:HD11	3:A:117:GLU:CG	2.44	0.46
3:A:174:ASP:O	3:A:175:PRO:C	2.54	0.45
3:A:144:GLN:O	3:A:145:TRP:C	2.55	0.45
2:G:11:DT:H2'	2:G:12:DT:H71	1.98	0.45
3:A:179:ILE:CG2	3:A:180:SER:H	2.23	0.45
3:A:274:LYS:O	3:A:277:GLN:HG2	2.17	0.45
3:A:174:ASP:CG	3:A:175:PRO:HD2	2.37	0.45
3:A:213:GLN:HA	3:A:213:GLN:NE2	2.32	0.44
3:A:273:LEU:HG	3:A:278:ARG:OXT	2.18	0.44
3:A:237:GLN:O	3:A:241:ARG:HG3	2.18	0.44
2:G:14:DA:H1'	2:G:15:DA:H5''	1.99	0.44
3:A:206:ASP:HB3	3:A:250:LEU:HD13	2.00	0.44
3:A:104:PRO:HD2	3:A:107:ASN:O	2.18	0.43
1:B:3:DT:H2''	1:B:4:DG:C8	2.53	0.43
3:A:99:LEU:HD12	3:A:99:LEU:N	2.34	0.43
2:G:15:DA:H2''	2:G:16:DG:C8	2.54	0.43
2:G:14:DA:H2''	2:G:15:DA:H5'	1.99	0.42
3:A:144:GLN:HB3	3:A:145:TRP:H	1.61	0.42
3:A:75:LYS:HB3	3:A:76:PRO:HD3	2.02	0.42
3:A:173:ARG:NH2	3:A:179:ILE:O	2.52	0.41
2:G:12:DT:H2''	2:G:13:DC:C5'	2.44	0.41
3:A:71:ARG:HH12	3:A:175:PRO:HG3	1.77	0.41
3:A:120:LYS:HG3	4:A:435:HOH:O	2.20	0.41
3:A:126:HIS:HA	3:A:127:PRO:HD3	1.97	0.41
3:A:275:GLU:O	3:A:276:GLY:C	2.57	0.41
2:G:12:DT:H1'	2:G:13:DC:C5'	2.51	0.41
3:A:209:ASP:O	3:A:213:GLN:HG2	2.21	0.41
3:A:234:LEU:O	3:A:238:GLN:HG3	2.20	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:A:220:LEU:HD22	3:A:227:LEU:HD23	2.02	0.40
3:A:274:LYS:HE2	3:A:275:GLU:OE1	2.21	0.40
3:A:144:GLN:HE21	3:A:145:TRP:N	2.19	0.40
3:A:127:PRO:HG3	4:A:389:HOH:O	2.21	0.40

All (2) 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	Distance(Å)	Clash(Å)
1:B:8:DG:O3'	2:G:9:DC:P[2_765]	1.61	0.59
3:A:271:TYR:OH	3:A:271:TYR:OH[2.665]	2.19	0.01

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	253/255 (99%)	233 (92%)	7 (3%)	13 (5%)	3 0

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	175	PRO
3	A	180	SER
3	A	104	PRO
3	A	145	TRP
3	A	275	GLU
3	A	276	GLY
3	A	106	THR
3	A	108	ASP
3	A	181	GLY
3	A	223	VAL
3	A	103	LYS
3	A	179	ILE
3	A	105	GLY

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	224/224 (100%)	218 (97%)	6 (3%)	57 45

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	64	TYR
3	A	144	GLN
3	A	173	ARG
3	A	175	PRO
3	A	176	GLU
3	A	177	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	31	GLN
3	A	77	HIS
3	A	84	GLN
3	A	134	ASN
3	A	144	GLN
3	A	161	HIS
3	A	213	GLN
3	A	238	GLN
3	A	245	GLN
3	A	277	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 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	8/8 (100%)	0.34	0 100 100	44, 60, 64, 68	0
2	G	8/8 (100%)	0.21	0 100 100	31, 66, 72, 73	0
3	A	255/255 (100%)	0.85	29 (11%) 6 6	18, 32, 77, 95	0
All	All	271/271 (100%)	0.82	29 (10%) 6 8	18, 33, 75, 95	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	106	THR	16.2
3	A	276	GLY	15.3
3	A	179	ILE	12.9
3	A	104	PRO	8.9
3	A	278	ARG	8.4
3	A	105	GLY	8.0
3	A	107	ASN	7.6
3	A	175	PRO	7.2
3	A	108	ASP	6.6
3	A	180	SER	6.2
3	A	101	VAL	4.3
3	A	144	GLN	4.3
3	A	177	MET	3.9
3	A	277	GLN	3.7
3	A	234	LEU	3.7
3	A	102	LYS	3.4
3	A	100	PRO	3.2
3	A	99	LEU	3.0
3	A	103	LYS	3.0
3	A	24	THR	2.8
3	A	176	GLU	2.7
3	A	238	GLN	2.6
3	A	145	TRP	2.6

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Mol	Chain	Res	Type	RSRZ
3	A	178	GLY	2.5
3	A	173	ARG	2.3
3	A	26	LEU	2.3
3	A	174	ASP	2.2
3	A	25	TRP	2.2
3	A	139	LEU	2.2

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.