



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2018 – 09:04 pm GMT

PDB ID : 2D7D
Title : Structural insights into the cryptic DNA dependent ATP-ase activity of UvrB
Authors : Barrett, T.E.
Deposited on : 2005-11-18
Resolution : 2.10 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/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 : 1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30686

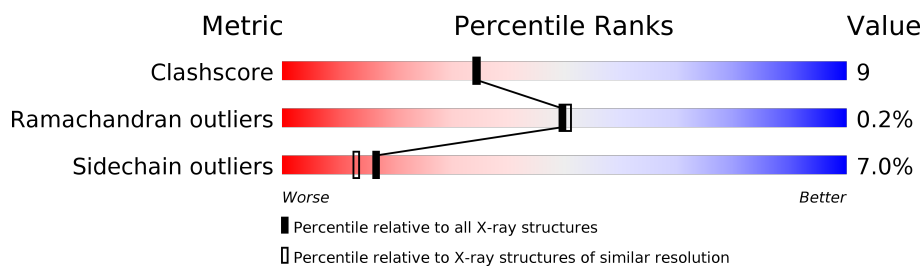
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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))
Clashscore	122078	5107 (2.10-2.10)
Ramachandran outliers	120005	5057 (2.10-2.10)
Sidechain outliers	119972	5058 (2.10-2.10)

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 $\leq 5\%$. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	D	3	
2	A	661	
3	B	40	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 5491 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(P*TP*TP*T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	3	Total	C	N	O	P	0	0	0
			61	30	6	22	3			

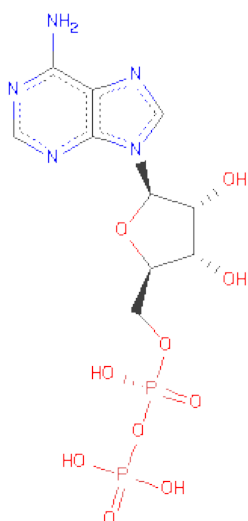
- Molecule 2 is a protein called UvrABC system protein B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	621	Total	C	N	O	S	0	0	0
			4898	3086	852	942	18			

- Molecule 3 is a protein called 40-mer from UvrABC system protein B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	B	38	Total	C	N	O	S	0	0	0
			301	187	53	59	2			

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	1	Total	O	0	0
			1	1		
5	A	191	Total	O	0	0
			191	191		
5	B	12	Total	O	0	0
			12	12		

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 the various outlier classes 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.

Note EDS was not executed.

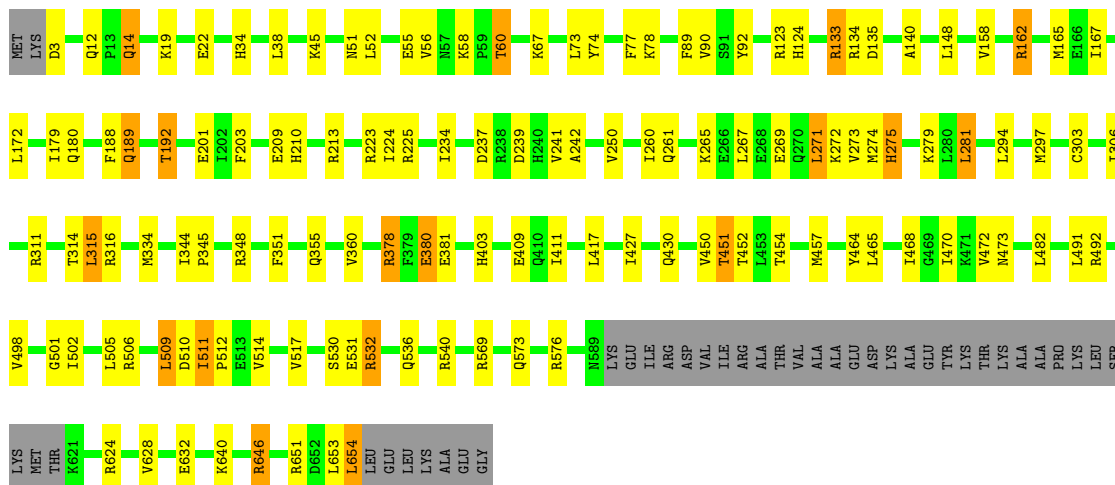
- Molecule 1: 5'-D(P*TP*TP*T)-3'

Chain D: 




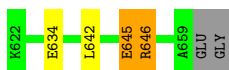
- Molecule 2: UvrABC system protein B

Chain A: 



- Molecule 3: 40-mer from UvrABC system protein B

Chain B: 



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	74.23Å 98.22Å 95.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.10	Depositor
% Data completeness (in resolution range)	96.1 (30.00-2.10)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.227 , 0.285	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5491	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

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: ADP

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	D	2.14	2/66 (3.0%)	2.56	4/98 (4.1%)
2	A	0.69	0/4979	0.80	2/6733 (0.0%)
3	B	0.67	0/302	0.75	0/402
All	All	0.72	2/5347 (0.0%)	0.85	6/7233 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	1	DT	OP3-P	-10.15	1.49	1.61
1	D	3	DT	C3'-O3'	9.02	1.55	1.44

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	1	DT	O4'-C4'-C3'	-12.21	98.67	106.00
1	D	3	DT	N3-C2-O2	-7.33	117.90	122.30
1	D	1	DT	C1'-O4'-C4'	-6.53	103.57	110.10
2	A	281	LEU	CA-CB-CG	6.22	129.61	115.30
1	D	1	DT	C4'-C3'-C2'	-5.52	98.13	103.10
2	A	315	LEU	CA-CB-CG	5.03	126.87	115.30

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	D	61	0	37	0	0
2	A	4898	0	4773	93	0
3	B	301	0	295	3	0
4	A	27	0	12	1	0
5	A	191	0	0	10	3
5	B	12	0	0	0	0
5	D	1	0	0	0	0
All	All	5491	0	5117	94	3

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 9.

All (94) 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)
2:A:265:LYS:HG3	5:A:803:HOH:O	1.26	1.27
2:A:45:LYS:HD3	4:A:662:ADP:O3B	1.67	0.95
2:A:464:TYR:O	2:A:468:ILE:HG12	1.78	0.84
2:A:133:ARG:HD3	2:A:135:ASP:OD1	1.79	0.83
2:A:452:THR:HG21	2:A:457:MET:HB3	1.61	0.81
2:A:314:THR:HG22	2:A:316:ARG:HG3	1.60	0.81
2:A:452:THR:HG22	2:A:454:THR:H	1.46	0.81
2:A:260:ILE:HG23	2:A:294:LEU:HD22	1.65	0.78
2:A:492:ARG:HG2	2:A:511:ILE:HD12	1.65	0.76
2:A:314:THR:CG2	2:A:316:ARG:HG3	2.15	0.75
2:A:532:ARG:H	2:A:532:ARG:CD	2.00	0.73
2:A:201:GLU:OE2	2:A:213:ARG:HD3	1.87	0.73
2:A:452:THR:CG2	2:A:457:MET:HB3	2.19	0.73
2:A:58:LYS:O	2:A:60:THR:HG22	1.90	0.72
2:A:531:GLU:HB3	2:A:532:ARG:CZ	2.20	0.70
2:A:351:PHE:O	2:A:355:GLN:HG2	1.92	0.70
2:A:646:ARG:NH2	5:A:752:HOH:O	2.26	0.69
2:A:51:ASN:O	2:A:55:GLU:HG2	1.94	0.67
2:A:56:VAL:HG23	2:A:58:LYS:HG3	1.76	0.66
2:A:311:ARG:HD3	2:A:316:ARG:O	1.97	0.64
2:A:532:ARG:HD3	5:A:817:HOH:O	1.96	0.64
2:A:506:ARG:O	2:A:509:LEU:HD12	1.97	0.64
2:A:452:THR:HG21	2:A:457:MET:CB	2.29	0.63
2:A:124:HIS:HE1	5:A:746:HOH:O	1.81	0.63
2:A:532:ARG:H	2:A:532:ARG:HD2	1.62	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:452:THR:CG2	2:A:457:MET:HG2	2.31	0.60
2:A:209:GLU:HG2	2:A:210:HIS:N	2.18	0.58
2:A:269:GLU:O	2:A:273:VAL:HG23	2.03	0.58
2:A:189:GLN:H	2:A:192:THR:HG21	1.69	0.57
2:A:67:LYS:HD3	2:A:90:VAL:HG13	1.86	0.56
2:A:272:LYS:O	2:A:275:HIS:HD2	1.89	0.56
2:A:52:LEU:O	2:A:56:VAL:HG13	2.06	0.55
2:A:74:TYR:CZ	2:A:78:LYS:HD2	2.41	0.55
2:A:452:THR:HG23	2:A:457:MET:HG2	1.89	0.54
2:A:162:ARG:O	2:A:165:MET:HB3	2.06	0.54
2:A:378:ARG:CD	5:A:835:HOH:O	2.56	0.54
2:A:465:LEU:HD22	2:A:470:ILE:HD12	1.90	0.54
2:A:491:LEU:HD23	2:A:511:ILE:HD13	1.89	0.54
2:A:427:ILE:O	2:A:430:GLN:HB2	2.08	0.53
2:A:124:HIS:HD2	5:A:673:HOH:O	1.92	0.52
2:A:569:ARG:HH11	2:A:573:GLN:HE22	1.58	0.52
2:A:209:GLU:HG2	2:A:210:HIS:H	1.75	0.52
2:A:380:GLU:HG2	2:A:381:GLU:N	2.24	0.51
2:A:409:GLU:HG2	2:A:411:ILE:HG23	1.93	0.51
2:A:162:ARG:HG3	2:A:165:MET:HB2	1.93	0.50
2:A:378:ARG:NE	5:A:835:HOH:O	2.45	0.50
2:A:651:ARG:NH1	3:B:642:LEU:O	2.44	0.50
2:A:12:GLN:O	2:A:14:GLN:HG2	2.12	0.50
2:A:511:ILE:HG12	2:A:514:VAL:HG23	1.93	0.50
2:A:530:SER:HB2	2:A:532:ARG:HH11	1.76	0.50
2:A:56:VAL:HG22	5:A:666:HOH:O	2.11	0.50
2:A:267:LEU:HG	2:A:271:LEU:HD22	1.93	0.49
2:A:651:ARG:NH1	3:B:645:GLU:OE2	2.38	0.48
2:A:451:THR:HA	2:A:501:GLY:O	2.14	0.48
2:A:569:ARG:HH11	2:A:573:GLN:NE2	2.12	0.48
2:A:531:GLU:HB3	2:A:532:ARG:NH2	2.29	0.47
2:A:472:VAL:HG12	2:A:473:ASN:N	2.30	0.47
2:A:3:ASP:O	2:A:135:ASP:HB3	2.15	0.47
2:A:468:ILE:HG22	2:A:468:ILE:O	2.15	0.46
2:A:632:GLU:HG3	2:A:654:LEU:HD21	1.98	0.46
2:A:569:ARG:NH1	2:A:573:GLN:HE22	2.14	0.46
2:A:314:THR:O	2:A:314:THR:HG22	2.16	0.45
2:A:225:ARG:HH11	2:A:234:ILE:HD13	1.81	0.45
2:A:303:CYS:O	2:A:306:ILE:HB	2.17	0.45
2:A:464:TYR:CE1	2:A:468:ILE:HD11	2.51	0.45
3:B:634:GLU:OE2	3:B:646:ARG:NH1	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:90:VAL:O	2:A:123:ARG:HD2	2.15	0.45
2:A:344:ILE:HB	2:A:345:PRO:HD3	1.98	0.45
2:A:19:LYS:HE2	2:A:22:GLU:OE1	2.15	0.45
2:A:465:LEU:HB3	2:A:472:VAL:HG21	1.99	0.45
2:A:89:PHE:O	2:A:140:ALA:HA	2.17	0.44
2:A:348:ARG:NH1	5:A:830:HOH:O	2.52	0.43
2:A:470:ILE:HG22	2:A:472:VAL:HG23	1.99	0.43
2:A:73:LEU:O	2:A:77:PHE:HD1	2.02	0.43
2:A:472:VAL:HG22	2:A:498:VAL:HB	2.00	0.42
2:A:517:VAL:HG21	2:A:540:ARG:HB2	2.01	0.42
2:A:133:ARG:CD	2:A:135:ASP:OD1	2.58	0.42
2:A:189:GLN:O	2:A:192:THR:HB	2.20	0.42
2:A:224:ILE:HG21	2:A:241:VAL:CG2	2.50	0.42
2:A:260:ILE:HD11	2:A:297:MET:HB3	2.01	0.42
2:A:45:LYS:NZ	5:A:665:HOH:O	2.40	0.42
2:A:505:LEU:HD22	2:A:536:GLN:HB3	2.02	0.42
2:A:531:GLU:HB3	2:A:532:ARG:NE	2.34	0.42
2:A:274:MET:HB3	2:A:279:LYS:HB2	2.03	0.41
2:A:452:THR:O	2:A:502:ILE:HA	2.20	0.41
2:A:60:THR:HB	2:A:334:MET:HB3	2.02	0.41
2:A:188:PHE:HA	2:A:192:THR:HG21	2.03	0.41
2:A:179:ILE:O	2:A:180:GLN:HB2	2.21	0.41
2:A:624:ARG:O	2:A:628:VAL:HG23	2.20	0.41
2:A:511:ILE:HA	2:A:512:PRO:HD3	1.93	0.41
2:A:34:HIS:CG	2:A:403:HIS:HB3	2.56	0.40
2:A:491:LEU:HD23	2:A:511:ILE:CD1	2.50	0.40
2:A:158:VAL:HG11	2:A:242:ALA:HB1	2.03	0.40
2:A:510:ASP:OD1	2:A:540:ARG:NH1	2.55	0.40

All (3) 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)
5:A:806:HOH:O	5:A:817:HOH:O[3_555]	1.98	0.22
5:A:722:HOH:O	5:A:757:HOH:O[3_455]	2.11	0.09
5:A:699:HOH:O	5:A:842:HOH:O[1_655]	2.13	0.07

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	
2	A	617/661 (93%)	603 (98%)	13 (2%)	1 (0%)	49	51
3	B	36/40 (90%)	36 (100%)	0	0	100	100
All	All	653/701 (93%)	639 (98%)	13 (2%)	1 (0%)	49	51

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	167	ILE

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	
2	A	517/586 (88%)	481 (93%)	36 (7%)	16	13
3	B	29/33 (88%)	27 (93%)	2 (7%)	17	13
All	All	546/619 (88%)	508 (93%)	38 (7%)	16	13

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	14	GLN
2	A	38	LEU
2	A	60	THR
2	A	92	TYR
2	A	133	ARG

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Mol	Chain	Res	Type
2	A	134	ARG
2	A	148	LEU
2	A	162	ARG
2	A	172	LEU
2	A	189	GLN
2	A	192	THR
2	A	203	PHE
2	A	223	ARG
2	A	237	ASP
2	A	239	ASP
2	A	250	VAL
2	A	261	GLN
2	A	271	LEU
2	A	275	HIS
2	A	281	LEU
2	A	315	LEU
2	A	360	VAL
2	A	378	ARG
2	A	380	GLU
2	A	417	LEU
2	A	450	VAL
2	A	451	THR
2	A	482	LEU
2	A	509	LEU
2	A	511	ILE
2	A	532	ARG
2	A	576	ARG
2	A	640	LYS
2	A	646	ARG
2	A	653	LEU
2	A	654	LEU
3	B	645	GLU
3	B	646	ARG

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

Mol	Chain	Res	Type
2	A	14	GLN
2	A	65	HIS
2	A	124	HIS
2	A	275	HIS
2	A	288	GLN

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Mol	Chain	Res	Type
2	A	374	ASN
2	A	388	ASN
2	A	536	GLN
2	A	573	GLN
2	A	581	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](#)

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](#)

1 ligand is 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	ADP	A	662	-	25,29,29	1.36	3 (12%)	25,45,45	1.82	5 (20%)

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	ADP	A	662	-	-	0/12/32/32	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	662	ADP	C2-N3	2.52	1.36	1.32
4	A	662	ADP	O4'-C1'	3.19	1.45	1.41
4	A	662	ADP	C5-C4	3.75	1.49	1.40

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	662	ADP	N3-C2-N1	-6.24	123.52	128.86
4	A	662	ADP	C4-C5-N7	-3.04	106.48	109.41
4	A	662	ADP	O3'-C3'-C4'	-2.09	105.01	111.06
4	A	662	ADP	C2-N1-C6	2.06	122.25	118.75
4	A	662	ADP	O3B-PB-O2B	2.15	116.11	107.59

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	662	ADP	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

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.