



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 11:06 PM GMT

PDB ID : 2R6F
Title : Crystal Structure of Bacillus stearothermophilus UvrA
Authors : Inuzuka, Y.; Pakotiprapha, D.; Bowman, B.R.; Jeruzalmi, D.; Verdine, G.L.
Deposited on : 2007-09-05
Resolution : 3.20 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>

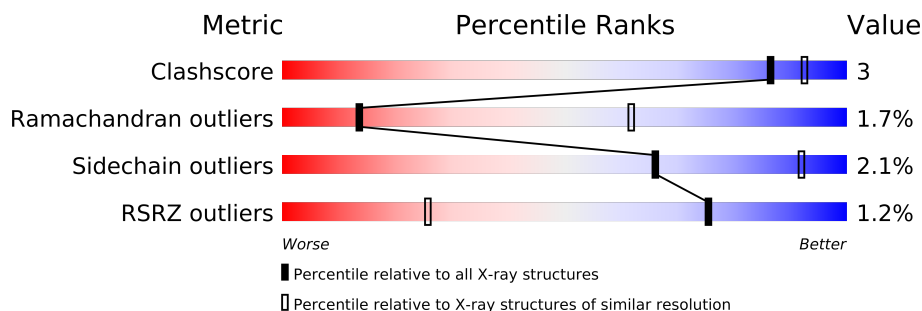
The following versions of software and data (see [references](#)) were used in the production of this report:

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 3.20 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	79885	1078 (3.26-3.14)
Ramachandran outliers	78287	1059 (3.26-3.14)
Sidechain outliers	78261	1058 (3.26-3.14)
RSRZ outliers	66119	1825 (3.30-3.10)

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. 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	A	972	
1	B	972	

2 Entry composition i

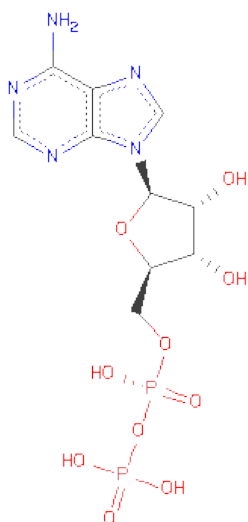
There are 4 unique types of molecules in this entry. The entry contains 13986 atoms, of which 0 are hydrogen and 0 are deuterium.

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 protein called Excinuclease ABC subunit A.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	899	Total	C	N	O	S	Se	0	0	0
			7006	4416	1231	1332	12	15			
1	B	879	Total	C	N	O	S	Se	0	0	0
			6862	4318	1212	1305	12	15			

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	3	Total 3	Zn 3	0	0
3	A	3	Total 3	Zn 3	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total 2	O 2	0	0
4	B	2	Total 2	O 2	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	102.71Å 94.72Å 130.48Å 90.00° 108.80° 90.00°	Depositor
Resolution (Å)	50.00 – 3.20 33.03 – 3.20	Depositor EDS
% Data completeness (in resolution range)	98.5 (50.00-3.20) 98.6 (33.03-3.20)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.57 (at 3.18Å)	Xtriage
Refinement program	REFMAC 5.3.0037	Depositor
R, R_{free}	0.253 , 0.292 0.257 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	82.0	Xtriage
Anisotropy	0.477	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 28.9	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 38742 reflections	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	13986	wwPDB-VP
Average B, all atoms (Å ²)	100.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.26% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, 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	A	0.38	0/7114	0.63	0/9597
1	B	0.36	0/6968	0.60	0/9396
All	All	0.37	0/14082	0.61	0/18993

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	A	7006	0	35	28	0
1	B	6862	0	60	8	0
2	A	54	0	24	0	0
2	B	54	0	24	0	0
3	A	3	0	0	0	0
3	B	3	0	0	0	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
All	All	13986	0	143	36	0

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 3.

All (36) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:892:LYS:NZ	1:A:939:ASP:OD2	2.24	0.70
1:B:559:GLY:N	1:B:568:GLU:O	2.25	0.68
1:A:559:GLY:N	1:A:568:GLU:O	2.33	0.62
1:A:901:GLY:N	1:A:910:GLN:O	2.36	0.59
1:B:379:VAL:CA	1:B:395:MSE:CE	2.89	0.50
1:B:589:TYR:OH	1:B:862:ASP:OD1	2.29	0.50
1:A:323:CYS:O	1:A:324:ARG:C	2.52	0.48
1:A:237:ILE:CG2	1:A:237:ILE:O	2.62	0.47
1:A:471:VAL:CG1	1:A:492:ARG:CB	2.92	0.47
1:A:619:ASN:ND2	1:A:905:GLY:O	2.47	0.47
1:A:379:VAL:CG1	1:A:395:MSE:CE	2.93	0.47
1:A:788:THR:CG2	1:A:815:GLY:O	2.63	0.46
1:A:696:ASN:O	1:A:697:PRO:C	2.53	0.46
1:A:499:ILE:CD1	1:A:532:MSE:CE	2.94	0.45
1:A:558:ILE:O	1:A:559:GLY:O	2.35	0.44
1:B:717:ALA:O	1:B:722:TYR:N	2.51	0.44
1:A:689:ILE:CG2	1:A:700:TYR:CD2	3.01	0.43
1:B:315:TYR:N	1:B:316:PRO:CD	2.81	0.43
1:A:315:TYR:N	1:A:316:PRO:CD	2.82	0.43
1:A:856:THR:O	1:A:857:THR:C	2.57	0.43
1:A:378:ASN:OD1	1:A:378:ASN:C	2.56	0.43
1:A:254:GLY:O	1:A:255:PHE:C	2.57	0.43
1:A:902:PRO:O	1:A:907:ARG:O	2.36	0.42
1:A:240:GLY:O	1:A:242:LEU:N	2.53	0.42
1:A:284:LEU:CD2	1:A:399:MSE:CE	2.98	0.42
1:B:216:ARG:O	1:B:220:SER:N	2.53	0.41
1:A:685:ASP:OD1	1:A:686:GLN:N	2.53	0.41
1:B:213:ILE:C	1:B:213:ILE:CD1	2.89	0.41
1:A:322:VAL:HG21	1:A:372:PHE:CZ	2.55	0.41
1:A:900:LEU:O	1:A:901:GLY:O	2.39	0.41
1:A:243:LEU:CD2	1:A:243:LEU:N	2.84	0.41
1:A:839:GLU:O	1:A:840:LEU:C	2.59	0.41
1:A:836:LEU:O	1:A:840:LEU:N	2.54	0.41
1:A:520:ARG:NH1	1:A:903:GLU:OE2	2.54	0.41
1:A:812:VAL:CG1	1:A:812:VAL:O	2.69	0.41
1:B:473:LEU:N	1:B:473:LEU:CD2	2.83	0.40

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	
1	A	893/972 (92%)	823 (92%)	56 (6%)	14 (2%)	14	63
1	B	873/972 (90%)	787 (90%)	70 (8%)	16 (2%)	13	60
All	All	1766/1944 (91%)	1610 (91%)	126 (7%)	30 (2%)	14	62

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	559	GLY
1	A	617	GLU
1	A	901	GLY
1	B	11	ALA
1	B	94	PRO
1	B	258	GLY
1	B	559	GLY
1	B	617	GLU
1	B	901	GLY
1	A	11	ALA
1	A	241	GLU
1	A	255	PHE
1	A	334	VAL
1	B	76	ILE
1	B	257	ILE
1	B	277	CYS
1	B	733	GLY
1	B	814	LEU
1	A	94	PRO
1	A	733	GLY
1	A	814	LEU
1	B	372	PHE
1	A	324	ARG
1	B	293	PRO
1	A	724	LYS
1	B	309	PRO
1	B	618	HIS

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Mol	Chain	Res	Type
1	A	618	HIS
1	A	766	ARG
1	B	8	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	
1	A	755/801 (94%)	736 (98%)	19 (2%)	60	90
1	B	739/801 (92%)	727 (98%)	12 (2%)	75	94
All	All	1494/1602 (93%)	1463 (98%)	31 (2%)	66	92

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	VAL
1	A	26	LEU
1	A	40	LEU
1	A	243	LEU
1	A	244	PHE
1	A	335	LYS
1	A	446	LEU
1	A	517	LEU
1	A	594	LYS
1	A	621	LYS
1	A	626	LYS
1	A	649	GLU
1	A	673	ARG
1	A	706	ASP
1	A	744	ILE
1	A	760	GLU
1	A	772	LEU
1	A	793	LEU
1	A	817	MSE
1	B	19	VAL
1	B	26	LEU
1	B	284	LEU

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Mol	Chain	Res	Type
1	B	335	LYS
1	B	464	ARG
1	B	476	LEU
1	B	538	THR
1	B	594	LYS
1	B	626	LYS
1	B	673	ARG
1	B	760	GLU
1	B	848	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 ⓘ

Of 10 ligands modelled in this entry, 6 are monoatomic - leaving 4 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	$\# Z > 2$
2	ADP	A	1000	-	29,29,29	1.13	2 (6%)	45,45,45	2.02	8 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ADP	A	1001	-	29,29,29	1.11	2 (6%)	45,45,45	1.93	9 (20%)
2	ADP	B	1002	-	29,29,29	1.03	2 (6%)	45,45,45	2.08	10 (22%)
2	ADP	B	1003	-	29,29,29	1.09	2 (6%)	45,45,45	1.85	9 (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
2	ADP	A	1000	-	-	0/16/32/32	0/1/3/3
2	ADP	A	1001	-	-	0/16/32/32	0/1/3/3
2	ADP	B	1002	-	-	0/16/32/32	0/1/3/3
2	ADP	B	1003	-	-	0/16/32/32	0/1/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1001	ADP	C4-N9	-3.08	1.33	1.37
2	B	1003	ADP	C4-N9	-3.01	1.33	1.37
2	A	1001	ADP	C5-C4	2.97	1.47	1.40
2	A	1000	ADP	C4-N9	-2.96	1.33	1.37
2	B	1003	ADP	C5-C4	2.86	1.46	1.40
2	A	1000	ADP	C5-C4	2.80	1.46	1.40
2	B	1002	ADP	C4-N9	-2.79	1.33	1.37
2	B	1002	ADP	C5-C4	2.77	1.46	1.40

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1000	ADP	N3-C2-N1	-7.42	122.50	128.71
2	B	1003	ADP	N3-C2-N1	-7.39	122.53	128.71
2	A	1001	ADP	N3-C2-N1	-7.23	122.67	128.71
2	B	1002	ADP	N3-C2-N1	-7.20	122.69	128.71
2	A	1000	ADP	O4'-C1'-N9	5.50	113.55	108.44
2	A	1001	ADP	N3-C4-N9	5.39	135.16	125.43
2	B	1002	ADP	N3-C4-N9	5.27	134.95	125.43
2	A	1000	ADP	N3-C4-N9	5.20	134.82	125.43
2	B	1003	ADP	N3-C4-N9	5.17	134.77	125.43
2	B	1002	ADP	PA-O3A-PB	-4.79	117.64	131.68
2	B	1002	ADP	C4-C5-N7	-3.81	106.26	109.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1001	ADP	C4-C5-N7	-3.48	106.54	109.52
2	B	1002	ADP	C8-N9-C4	3.38	109.48	106.90
2	A	1000	ADP	PA-O3A-PB	-3.35	121.86	131.68
2	A	1001	ADP	C8-N9-C4	3.30	109.42	106.90
2	A	1001	ADP	C5-C4-N3	-3.15	118.84	125.70
2	B	1002	ADP	C5-C4-N3	-3.14	118.86	125.70
2	A	1001	ADP	PA-O3A-PB	-3.12	122.53	131.68
2	A	1000	ADP	C5-C4-N3	-3.12	118.92	125.70
2	A	1000	ADP	C4-C5-N7	-3.07	106.89	109.52
2	B	1003	ADP	C5-C4-N3	-2.95	119.27	125.70
2	B	1002	ADP	C3'-C2'-C1'	2.76	105.23	100.91
2	B	1002	ADP	C2-N3-C4	2.72	121.75	114.01
2	B	1003	ADP	C4-C5-N7	-2.71	107.20	109.52
2	A	1001	ADP	C2-N3-C4	2.62	121.47	114.01
2	A	1000	ADP	C2-N3-C4	2.59	121.39	114.01
2	A	1001	ADP	O4'-C1'-N9	2.54	110.80	108.44
2	B	1003	ADP	O4'-C1'-N9	2.48	110.74	108.44
2	B	1003	ADP	C2-N3-C4	2.43	120.92	114.01
2	A	1000	ADP	C8-N9-C4	2.42	108.75	106.90
2	B	1003	ADP	C8-N9-C4	2.41	108.74	106.90
2	B	1003	ADP	PA-O3A-PB	-2.28	125.00	131.68
2	A	1001	ADP	O3B-PB-O2B	2.20	116.16	107.61
2	B	1002	ADP	O3B-PB-O2B	2.10	115.78	107.61
2	B	1002	ADP	O4'-C1'-N9	2.06	110.36	108.44
2	B	1003	ADP	O3B-PB-O2B	2.05	115.60	107.61

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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	A	899/972 (92%)	-0.02	4 (0%)	90 51	57, 86, 149, 198	0
1	B	879/972 (90%)	0.08	18 (2%)	62 17	66, 103, 156, 185	0
All	All	1778/1944 (91%)	0.03	22 (1%)	75 26	57, 95, 155, 198	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	135	MSE	4.7
1	B	130	GLN	4.1
1	B	206	ARG	3.6
1	B	142	TYR	3.3
1	B	149	GLN	3.1
1	B	139	LEU	3.0
1	B	132	ILE	2.9
1	B	221	LEU	2.9
1	B	140	LEU	2.8
1	A	330	MSE	2.6
1	B	148	MSE	2.6
1	B	663	LYS	2.5
1	B	136	VAL	2.4
1	B	727	PHE	2.4
1	B	661	ARG	2.3
1	B	138	ARG	2.3
1	A	227	LEU	2.1
1	A	283	LYS	2.1
1	B	729	PHE	2.1
1	A	226	LYS	2.1
1	B	227	LEU	2.1
1	B	711	PHE	2.0

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 ⓘ

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	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	ADP	A	1000	27/27	0.23	0.29	59,65,66,67	0
3	ZN	B	1009	1/1	0.18	0.20	99,99,99,99	0
2	ADP	A	1001	27/27	0.20	-0.45	57,68,70,70	0
2	ADP	B	1003	27/27	0.17	-0.62	68,71,72,72	0
2	ADP	B	1002	27/27	0.19	-0.71	75,81,82,82	0
3	ZN	B	1007	1/1	0.12	-0.82	94,94,94,94	0
3	ZN	A	1004	1/1	0.10	-0.91	96,96,96,96	0
3	ZN	A	1006	1/1	0.13	-1.01	89,89,89,89	0
3	ZN	A	1005	1/1	0.07	-1.59	92,92,92,92	0
3	ZN	B	1008	1/1	0.06	-1.68	103,103,103,103	0

6.5 Other polymers ⓘ

There are no such residues in this entry.