



wwPDB X-ray Structure Validation Summary Report

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PDB ID : 1T5L
Title : Crystal structure of the DNA repair protein UvrB point mutant Y96A revealing a novel fold for domain 2
Authors : Truglio, J.J.; Croteau, D.L.; Skorvaga, M.; DellaVecchia, M.J.; Theis, K.; Mandavilli, B.S.; Van Houten, B.; Kisker, C.
Deposited on : 2004-05-04
Resolution : 2.60 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

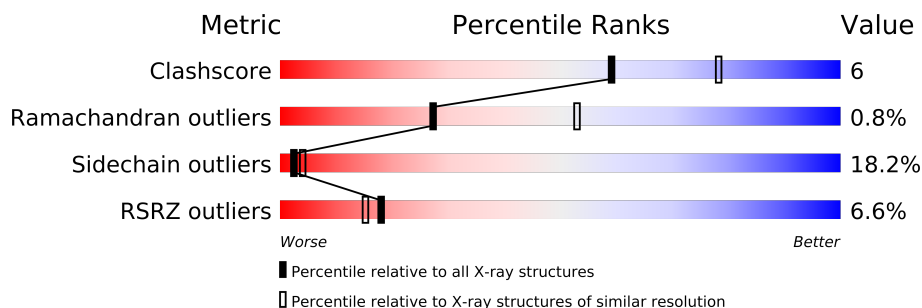
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.60 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	2154 (2.60-2.60)
Ramachandran outliers	78287	2113 (2.60-2.60)
Sidechain outliers	78261	2113 (2.60-2.60)
RSRZ outliers	66119	1718 (2.60-2.60)

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	658	
1	B	658	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	ZN	A	660	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9812 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 UvrABC system protein B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	595	Total	C	N	O	S	0	0	0
			4806	3027	858	909	12			
1	B	595	Total	C	N	O	S	0	0	0
			4806	3027	858	909	12			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	190	ARG	-	SEE REMARK 999	UNP P56981
A	233	GLU	LYS	SEE REMARK 999	UNP P56981
B	190	ARG	-	SEE REMARK 999	UNP P56981
B	233	GLU	LYS	SEE REMARK 999	UNP P56981

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Zn	0	0
			2	2		
2	A	2	Total	Zn	0	0
			2	2		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	80	Total	O	0	0
			80	80		
3	B	116	Total	O	0	0
			116	116		

GLN	R586	
LEU	R587	
ARG	R588	
ASP	R589	
ILE	R590	
ILE	R591	
PHE	R592	
GLU	R593	
LEU	R594	
LYS	R595	
ALA	ILE	
ALA	ARG	
GLU	ALA	
GLY	THR	
	TYR	
	ALA	
	ALA	
	GLU	
	GLU	
	GLU	
	MET	
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	TYR	
	GLU	
	ALA	
	LYS	
	PRO	
	ALA	
	ALA	
	ALA	
	MET	
	THR	
	LYS	
	GLN	
	GLU	
	ARG	
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	ALA	
	LYS	
	LYS	
	MET	
	GLU	
	ASP	
	PHE	
	GLU	
	ARG	
	ALA	
	ALA	

4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	150.81Å 150.81Å 159.83Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	25.00 – 2.60 24.83 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.9 (25.00-2.60) 99.9 (24.83-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.56 (at 2.60Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.230 , 0.287 0.232 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	47.8	Xtriage
Anisotropy	0.038	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 32.8	EDS
Estimated twinning fraction	0.026 for -h,-k,l	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 64639 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9812	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 64.43 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 8.2904e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

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	0.81	1/4887 (0.0%)	1.00	20/6604 (0.3%)
1	B	0.95	1/4887 (0.0%)	1.08	28/6604 (0.4%)
All	All	0.88	2/9774 (0.0%)	1.04	48/13208 (0.4%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	457	MET	SD-CE	5.12	2.06	1.77
1	A	457	MET	SD-CE	5.05	2.06	1.77

The worst 5 of 48 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	270	ARG	NE-CZ-NH1	8.46	124.53	120.30
1	B	134	ARG	NE-CZ-NH2	-8.20	116.20	120.30
1	A	94	ASP	CB-CG-OD2	7.84	125.36	118.30
1	B	185	ASP	CB-CG-OD2	7.73	125.26	118.30
1	B	270	ARG	NE-CZ-NH2	-7.70	116.45	120.30

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	4806	0	0	29	0
1	B	4806	0	0	30	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	80	0	0	5	0
3	B	116	0	0	6	0
All	All	9812	0	0	59	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 6.

The worst 5 of 59 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:457:MET:SD	1:A:457:MET:CE	2.06	1.44
1:B:457:MET:SD	1:B:457:MET:CE	2.06	1.42
1:A:130:LEU:O	3:A:729:HOH:O	2.02	0.77
1:B:43:THR:OG1	1:B:44:GLY:N	2.20	0.74
1:A:289:ARG:NH1	1:A:366:PHE:O	2.33	0.60

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	593/658 (90%)	552 (93%)	37 (6%)	4 (1%)	30	58
1	B	593/658 (90%)	565 (95%)	23 (4%)	5 (1%)	27	53
All	All	1186/1316 (90%)	1117 (94%)	60 (5%)	9 (1%)	27	53

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	112	ASP
1	B	115	ILE
1	B	186	ILE

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Mol	Chain	Res	Type
1	A	113	ALA
1	A	237	GLU

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	521/569 (92%)	419 (80%)	102 (20%)	2	3
1	B	521/569 (92%)	433 (83%)	88 (17%)	3	5
All	All	1042/1138 (92%)	852 (82%)	190 (18%)	2	4

5 of 190 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	495	LYS
1	B	57	ASN
1	B	493	LEU
1	A	507	GLU
1	A	568	LYS

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 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

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	595/658 (90%)	0.22	49 (8%) 12 9	29, 59, 161, 211	0
1	B	595/658 (90%)	-0.07	29 (4%) 28 25	26, 45, 98, 113	0
All	All	1190/1316 (90%)	0.08	78 (6%) 18 15	26, 53, 131, 211	0

The worst 5 of 78 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	VAL	9.4
1	A	95	TYR	7.5
1	B	95	TYR	7.2
1	A	230	LEU	7.1
1	A	223	ARG	5.6

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(\AA^2)	Q<0.9
2	ZN	A	660	1/1	0.88	16.50	89,89,89,89	1
2	ZN	B	660	1/1	0.18	0.91	72,72,72,72	1
2	ZN	A	659	1/1	0.10	-0.32	87,87,87,87	0
2	ZN	B	659	1/1	0.12	-0.45	83,83,83,83	0

6.5 Other polymers

There are no such residues in this entry.