



wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 1T5L / pdb_00001t5l
Title : Crystal structure of the DNA repair protein UvrB point mutant Y96A revealing a novel fold for domain 2
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Deposited on : 2004-05-04
Resolution : 2.60 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

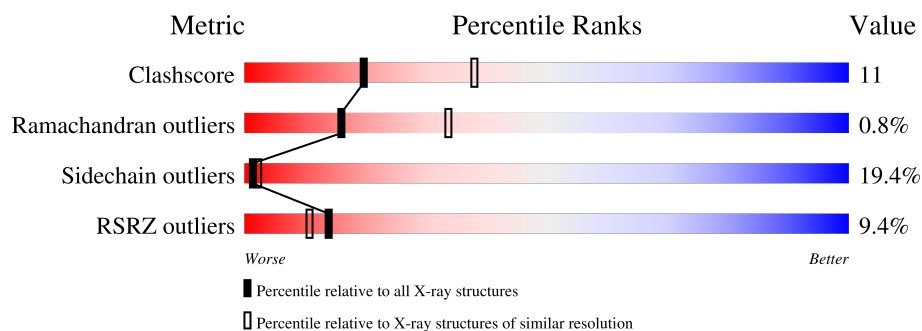
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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.

Mol	Chain	Length	Quality of chain
1	A	658	14% 58% 26% 6% 10%
1	B	658	3% 58% 25% 6% 10%

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
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 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 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

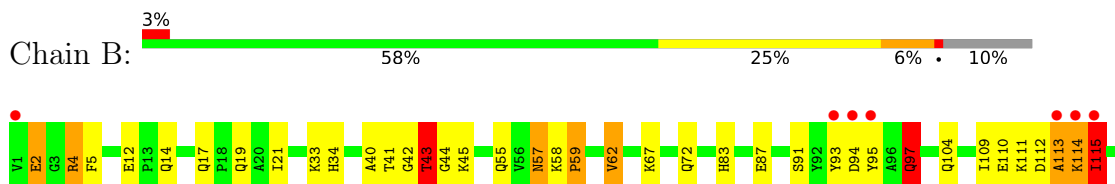
- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

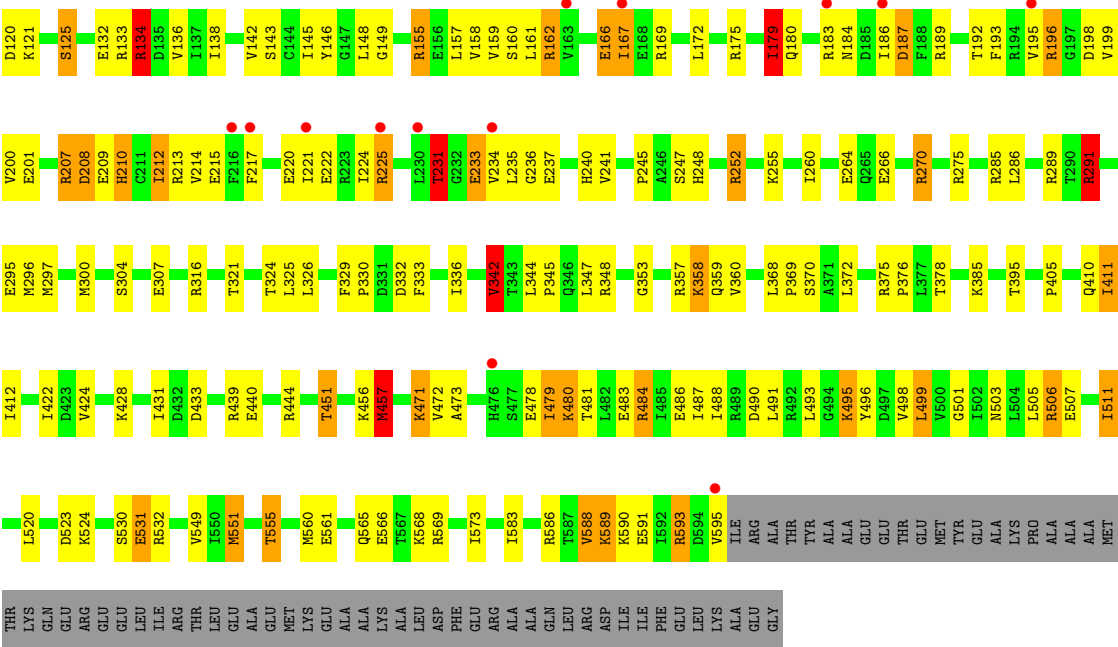
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Zn	0	0
			2	2		
2	B	2	Total	Zn	0	0
			2	2		

- 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		

- Molecule 1: UvrABC system protein B





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 25.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.9 (25.00-2.60) 99.7 (25.00-2.60)	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 0.229 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	47.8	Xtriage
Anisotropy	0.038	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 50.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.026 for -h,-k,l	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.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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: 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	1.05	6/4887 (0.1%)	1.25	16/6604 (0.2%)
1	B	1.13	9/4887 (0.2%)	1.32	29/6604 (0.4%)
All	All	1.09	15/9774 (0.2%)	1.28	45/13208 (0.3%)

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	457	MET	SD-CE	10.79	2.06	1.79
1	A	457	MET	SD-CE	10.63	2.06	1.79
1	B	551	MET	SD-CE	-10.58	1.53	1.79
1	A	551	MET	SD-CE	-9.73	1.55	1.79
1	B	300	MET	SD-CE	7.34	1.98	1.79

The worst 5 of 45 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	180	GLN	N-CA-C	9.24	123.86	112.58
1	B	111	LYS	N-CA-C	-9.08	96.84	110.28
1	A	495	LYS	N-CA-C	-8.30	102.19	111.82
1	B	179	ILE	N-CA-C	-8.02	104.55	112.17
1	B	207	ARG	N-CA-C	7.87	122.46	109.95

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	A	4806	0	4843	107	0
1	B	4806	0	4843	114	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	80	0	0	12	0
3	B	116	0	0	11	0
All	All	9812	0	9686	221	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 11.

The worst 5 of 221 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)
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:B:291:ARG:O	1:B:295:GLU:HG3	1.65	0.95
1:A:60:THR:HG22	1:A:334:LEU:HB3	1.48	0.93
1:B:157:LEU:O	1:B:179:ILE:HD11	1.70	0.91

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	
1	A	593/658 (90%)	552 (93%)	37 (6%)	4 (1%)	18	38
1	B	593/658 (90%)	565 (95%)	23 (4%)	5 (1%)	16	34
All	All	1186/1316 (90%)	1117 (94%)	60 (5%)	9 (1%)	16	34

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	112	ASP
1	B	115	ILE
1	B	186	ILE
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%)	414 (80%)	107 (20%)	1	2
1	B	521/569 (92%)	426 (82%)	95 (18%)	2	3
All	All	1042/1138 (92%)	840 (81%)	202 (19%)	1	2

5 of 202 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	93	TYR
1	B	220	GLU
1	B	591	GLU
1	B	114	LYS
1	B	167	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	210	HIS
1	B	288	GLN
1	B	565	GLN
1	A	374	ASN
1	A	536	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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.

No monomer is involved in short contacts.

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	A	595/658 (90%)	0.75	92 (15%) 5 4	29, 59, 161, 211	0
1	B	595/658 (90%)	0.11	20 (3%) 48 42	26, 45, 98, 113	0
All	All	1190/1316 (90%)	0.43	112 (9%) 14 11	26, 53, 131, 211	0

The worst 5 of 112 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	VAL	8.4
1	A	93	TYR	7.8
1	A	186	ILE	6.8
1	A	595	VAL	6.8
1	A	230	LEU	5.7

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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. 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	B-factors($\text{\AA}^2$)	Q<0.9
2	ZN	A	660	1/1	0.54	0.70	89,89,89,89	1
2	ZN	B	660	1/1	0.77	0.26	72,72,72,72	1
2	ZN	B	659	1/1	0.92	0.18	83,83,83,83	0
2	ZN	A	659	1/1	0.92	0.13	87,87,87,87	0

6.5 Other polymers [i](#)

There are no such residues in this entry.