



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:39 AM GMT

PDB ID : 3FK9
Title : Crystal structure of mMutator MutT protein from *Bacillus halodurans*
Authors : Bonanno, J.B.; Freeman, J.; Bain, K.T.; Hu, S.; Romero, R.; Wasserman, S.; Sauder, J.M.; Burley, S.K.; Almo, S.C.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on : 2008-12-16
Resolution : 2.50 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
<http://wwpdb.org/validation/2016/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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

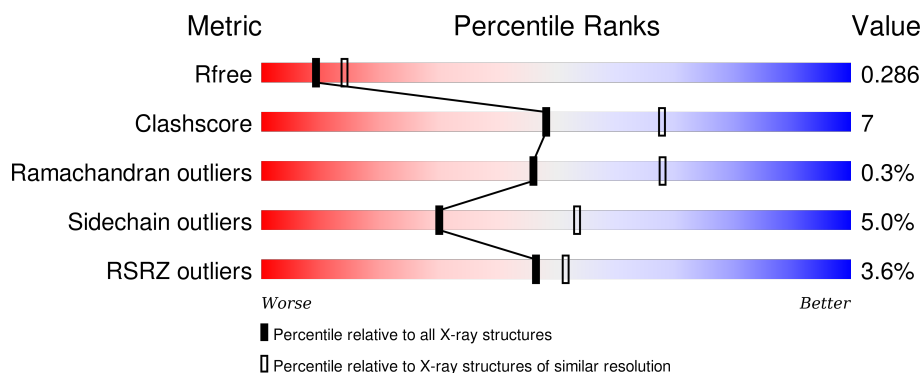
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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.

Mol	Chain	Length	Quality of chain
1	A	188	
1	B	188	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2457 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 Mutator MutT protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	153	Total	C	N	O	S	0	0	0
			1239	805	201	227	6			
1	B	153	Total	C	N	O	S	0	0	0
			1213	791	197	219	6			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	expression tag	UNP Q9K704
A	0	SER	-	expression tag	UNP Q9K704
A	1	LEU	-	expression tag	UNP Q9K704
A	158	LYS	-	expression tag	UNP Q9K704
A	159	GLY	-	expression tag	UNP Q9K704
A	160	ILE	-	expression tag	UNP Q9K704
A	161	ILE	-	expression tag	UNP Q9K704
A	162	THR	-	expression tag	UNP Q9K704
A	163	ILE	-	expression tag	UNP Q9K704
A	164	THR	-	expression tag	UNP Q9K704
A	165	THR	-	expression tag	UNP Q9K704
A	166	ASP	-	expression tag	UNP Q9K704
A	167	PRO	-	expression tag	UNP Q9K704
A	168	ASN	-	expression tag	UNP Q9K704
A	169	SER	-	expression tag	UNP Q9K704
A	170	SER	-	expression tag	UNP Q9K704
A	171	SER	-	expression tag	UNP Q9K704
A	172	VAL	-	expression tag	UNP Q9K704
A	173	ASP	-	expression tag	UNP Q9K704
A	174	LYS	-	expression tag	UNP Q9K704
A	175	LEU	-	expression tag	UNP Q9K704
A	176	ALA	-	expression tag	UNP Q9K704
A	177	ALA	-	expression tag	UNP Q9K704
A	178	ALA	-	expression tag	UNP Q9K704
A	179	LEU	-	expression tag	UNP Q9K704

Continued on next page...

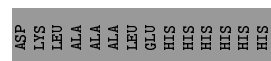
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	180	GLU	-	expression tag	UNP Q9K704
A	181	HIS	-	expression tag	UNP Q9K704
A	182	HIS	-	expression tag	UNP Q9K704
A	183	HIS	-	expression tag	UNP Q9K704
A	184	HIS	-	expression tag	UNP Q9K704
A	185	HIS	-	expression tag	UNP Q9K704
A	186	HIS	-	expression tag	UNP Q9K704
B	-1	MET	-	expression tag	UNP Q9K704
B	0	SER	-	expression tag	UNP Q9K704
B	1	LEU	-	expression tag	UNP Q9K704
B	158	LYS	-	expression tag	UNP Q9K704
B	159	GLY	-	expression tag	UNP Q9K704
B	160	ILE	-	expression tag	UNP Q9K704
B	161	ILE	-	expression tag	UNP Q9K704
B	162	THR	-	expression tag	UNP Q9K704
B	163	ILE	-	expression tag	UNP Q9K704
B	164	THR	-	expression tag	UNP Q9K704
B	165	THR	-	expression tag	UNP Q9K704
B	166	ASP	-	expression tag	UNP Q9K704
B	167	PRO	-	expression tag	UNP Q9K704
B	168	ASN	-	expression tag	UNP Q9K704
B	169	SER	-	expression tag	UNP Q9K704
B	170	SER	-	expression tag	UNP Q9K704
B	171	SER	-	expression tag	UNP Q9K704
B	172	VAL	-	expression tag	UNP Q9K704
B	173	ASP	-	expression tag	UNP Q9K704
B	174	LYS	-	expression tag	UNP Q9K704
B	175	LEU	-	expression tag	UNP Q9K704
B	176	ALA	-	expression tag	UNP Q9K704
B	177	ALA	-	expression tag	UNP Q9K704
B	178	ALA	-	expression tag	UNP Q9K704
B	179	LEU	-	expression tag	UNP Q9K704
B	180	GLU	-	expression tag	UNP Q9K704
B	181	HIS	-	expression tag	UNP Q9K704
B	182	HIS	-	expression tag	UNP Q9K704
B	183	HIS	-	expression tag	UNP Q9K704
B	184	HIS	-	expression tag	UNP Q9K704
B	185	HIS	-	expression tag	UNP Q9K704
B	186	HIS	-	expression tag	UNP Q9K704

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total 2	O 2	0	0
2	B	3	Total 3	O 3	0	0

- Molecule 1: Mutator MutT protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	54.34Å 59.08Å 108.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.50 40.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.3 (10.00-2.50) 99.3 (40.00-2.50)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.93 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.5.0066	Depositor
R, R_{free}	0.222 , 0.293 0.229 , 0.286	Depositor DCC
R_{free} test set	642 reflections (5.52%)	DCC
Wilson B-factor (Å ²)	41.8	Xtriage
Anisotropy	0.477	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 43.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	2 of 12512 reflections (0.016%)	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	2457	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.64% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

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	A	0.65	0/1274	0.67	0/1728
1	B	0.62	0/1248	0.70	0/1697
All	All	0.64	0/2522	0.69	0/3425

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-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 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	1239	0	1205	20	0
1	B	1213	0	1167	15	0
2	A	2	0	0	0	0
2	B	3	0	0	0	0
All	All	2457	0	2372	35	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 7.

All (35) 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:B:45:ARG:NH1	1:B:46:GLU:OE1	2.02	0.92

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:ARG:NH1	1:A:46:GLU:OE1	2.09	0.85
1:B:11:ASP:OD2	1:B:12:HIS:HD2	1.59	0.85
1:B:21:PRO:O	1:B:22:ARG:HB2	1.83	0.76
1:B:11:ASP:OD2	1:B:12:HIS:CD2	2.46	0.67
1:B:37:GLU:CD	1:B:45:ARG:HH21	2.00	0.65
1:A:1:LEU:HD23	1:A:1:LEU:O	1.96	0.64
1:B:70:ASP:HB3	1:B:75:VAL:HG11	1.80	0.63
1:B:1:LEU:HD12	1:B:77:GLU:HG2	1.81	0.63
1:B:106:LYS:NZ	1:B:126:LEU:O	2.33	0.62
1:A:45:ARG:O	1:A:49:GLU:HG3	2.03	0.58
1:B:21:PRO:O	1:B:22:ARG:CB	2.53	0.56
1:B:45:ARG:O	1:B:49:GLU:HG3	2.10	0.51
1:A:61:LYS:HA	1:A:131:LEU:HD12	1.92	0.51
1:A:21:PRO:O	1:A:22:ARG:HB2	2.11	0.49
1:B:6:ASN:HD22	1:B:6:ASN:C	2.17	0.48
1:A:106:LYS:HD2	1:A:126:LEU:HD22	1.96	0.48
1:A:6:ASN:C	1:A:6:ASN:HD22	2.17	0.47
1:A:66:MET:O	1:A:77:GLU:HA	2.14	0.47
1:A:68:ILE:HG13	1:A:78:TRP:HZ3	1.79	0.46
1:A:122:PHE:O	1:A:126:LEU:HB2	2.16	0.46
1:A:2:GLN:H	1:A:2:GLN:HG2	1.53	0.46
1:B:63:ILE:N	1:B:63:ILE:HD12	2.32	0.45
1:A:68:ILE:HB	1:A:76:SER:HB3	1.98	0.45
1:A:70:ASP:HB3	1:A:75:VAL:HG11	1.99	0.44
1:A:63:ILE:N	1:A:63:ILE:HD12	2.33	0.44
1:B:37:GLU:OE1	1:B:45:ARG:NH2	2.46	0.43
1:B:67:VAL:HG13	1:B:74:ILE:HG23	2.00	0.42
1:A:67:VAL:HG13	1:A:74:ILE:HG23	2.02	0.42
1:B:22:ARG:O	1:B:23:ARG:C	2.59	0.41
1:A:60:LEU:O	1:A:61:LYS:HD3	2.20	0.41
1:A:6:ASN:ND2	1:A:82:THR:HA	2.36	0.41
1:A:135:THR:O	1:A:147:TYR:HA	2.20	0.40
1:A:18:LEU:HD23	1:A:18:LEU:C	2.41	0.40
1:A:141:ASP:O	1:A:142:PHE:HB2	2.22	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	151/188 (80%)	146 (97%)	5 (3%)	0	100	100
1	B	151/188 (80%)	145 (96%)	5 (3%)	1 (1%)	26	46
All	All	302/376 (80%)	291 (96%)	10 (3%)	1 (0%)	46	68

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	22	ARG

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	132/168 (79%)	123 (93%)	9 (7%)	20	36
1	B	126/168 (75%)	122 (97%)	4 (3%)	46	74
All	All	258/336 (77%)	245 (95%)	13 (5%)	30	53

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	GLN
1	A	6	ASN
1	A	73	LYS
1	A	77	GLU
1	A	89	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	96	SER
1	A	98	GLU
1	A	127	HIS
1	A	131	LEU
1	B	6	ASN
1	B	75	VAL
1	B	77	GLU
1	B	96	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2	GLN
1	A	6	ASN
1	B	6	ASN
1	B	12	HIS
1	B	137	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](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

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 [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	153/188 (81%)	0.30	8 (5%) 31 35	47, 58, 70, 76	0
1	B	153/188 (81%)	0.18	3 (1%) 68 72	47, 58, 68, 73	0
All	All	306/376 (81%)	0.24	11 (3%) 46 51	47, 58, 70, 76	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	153	PRO	4.1
1	A	147	TYR	3.4
1	A	143	GLU	3.3
1	A	152	GLU	3.1
1	A	70	ASP	3.0
1	B	147	TYR	2.7
1	B	153	PRO	2.6
1	B	69	PHE	2.2
1	A	117	GLY	2.2
1	A	73	LYS	2.0
1	A	120	TRP	2.0

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 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.