



Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 10:46 am BST

PDB ID : 1VL4
Title : CRYSTAL STRUCTURE OF A PUTATIVE MODULATOR OF A DNA GY-
RASE (TM0727) FROM THERMOTOGA MARITIMA MSB8 AT 1.95 Å
RESOLUTION
Authors : Joint Center for Structural Genomics (JCSG)
Deposited on : 2004-07-09
Resolution : 1.95 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
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

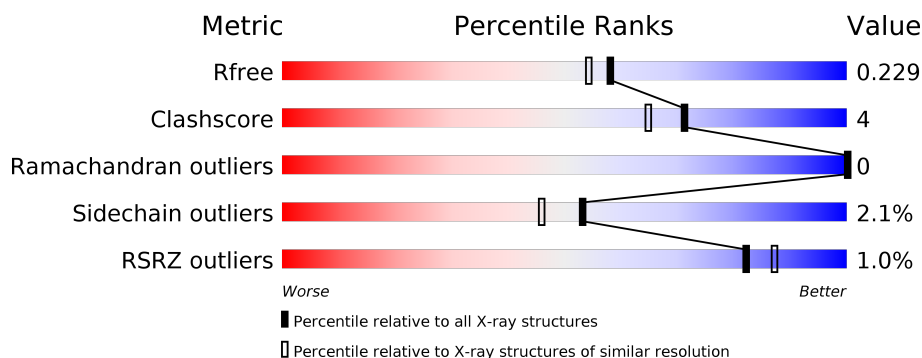
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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}	130704	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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 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	447	<div> <div>%</div> <div> <div></div> <div>87%</div> <div>8%</div> <div>• •</div> </div> </div>
1	B	447	<div> <div>%</div> <div> <div></div> <div>87%</div> <div>8%</div> <div>• •</div> </div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7177 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 pmbA-related protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	429	Total	C	N	O	S	0	6	1
			3345	2132	549	645	19			
1	B	429	Total	C	N	O	S	0	6	1
			3339	2126	546	649	18			

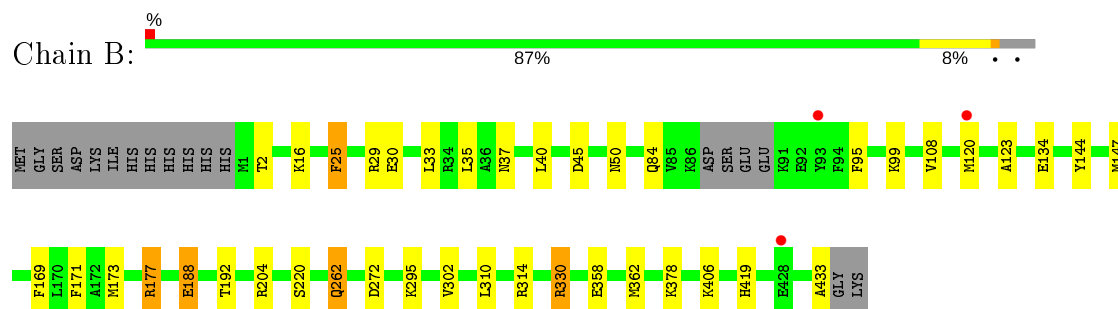
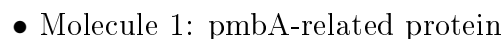
There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MET	-	LEADER SEQUENCE	UNP Q9WZI6
A	-10	GLY	-	LEADER SEQUENCE	UNP Q9WZI6
A	-9	SER	-	LEADER SEQUENCE	UNP Q9WZI6
A	-8	ASP	-	LEADER SEQUENCE	UNP Q9WZI6
A	-7	LYS	-	LEADER SEQUENCE	UNP Q9WZI6
A	-6	ILE	-	LEADER SEQUENCE	UNP Q9WZI6
A	-5	HIS	-	LEADER SEQUENCE	UNP Q9WZI6
A	-4	HIS	-	LEADER SEQUENCE	UNP Q9WZI6
A	-3	HIS	-	LEADER SEQUENCE	UNP Q9WZI6
A	-2	HIS	-	LEADER SEQUENCE	UNP Q9WZI6
A	-1	HIS	-	LEADER SEQUENCE	UNP Q9WZI6
A	0	HIS	-	LEADER SEQUENCE	UNP Q9WZI6
B	-11	MET	-	LEADER SEQUENCE	UNP Q9WZI6
B	-10	GLY	-	LEADER SEQUENCE	UNP Q9WZI6
B	-9	SER	-	LEADER SEQUENCE	UNP Q9WZI6
B	-8	ASP	-	LEADER SEQUENCE	UNP Q9WZI6
B	-7	LYS	-	LEADER SEQUENCE	UNP Q9WZI6
B	-6	ILE	-	LEADER SEQUENCE	UNP Q9WZI6
B	-5	HIS	-	LEADER SEQUENCE	UNP Q9WZI6
B	-4	HIS	-	LEADER SEQUENCE	UNP Q9WZI6
B	-3	HIS	-	LEADER SEQUENCE	UNP Q9WZI6
B	-2	HIS	-	LEADER SEQUENCE	UNP Q9WZI6
B	-1	HIS	-	LEADER SEQUENCE	UNP Q9WZI6
B	0	HIS	-	LEADER SEQUENCE	UNP Q9WZI6

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	200	Total 200	O 200	0	0
2	B	293	Total 293	O 293	0	0

- Molecule 1: pmbA-related protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	80.37Å 106.64Å 120.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.75 – 1.95 48.75 – 1.95	Depositor EDS
% Data completeness (in resolution range)	94.0 (48.75-1.95) 94.1 (48.75-1.95)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.76 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.2.0001	Depositor
R, R_{free}	0.174 , 0.221 0.184 , 0.229	Depositor DCC
R_{free} test set	3584 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	23.0	Xtriage
Anisotropy	0.087	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 49.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7177	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.18% of the height of the origin peak. No significant pseudotranslation is detected.*

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](#)

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	1/3402 (0.0%)	0.80	1/4587 (0.0%)
1	B	0.92	1/3396 (0.0%)	0.87	6/4580 (0.1%)
All	All	0.86	2/6798 (0.0%)	0.84	7/9167 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	188	GLU	CG-CD	5.90	1.60	1.51
1	A	416	VAL	CB-CG2	-5.30	1.41	1.52

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	177	ARG	NE-CZ-NH1	11.18	125.89	120.30
1	B	177	ARG	NE-CZ-NH2	-9.31	115.64	120.30
1	B	330	ARG	NE-CZ-NH2	-6.48	117.06	120.30
1	B	272	ASP	CB-CG-OD1	6.09	123.78	118.30
1	B	362	MET	CG-SD-CE	5.50	108.99	100.20
1	A	166	ASP	CB-CG-OD1	5.35	123.11	118.30
1	B	84	GLN	CB-CA-C	-5.08	100.24	110.40

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	3345	0	3328	23	0
1	B	3339	0	3302	24	0
2	A	200	0	0	1	0
2	B	293	0	0	7	0
All	All	7177	0	6630	47	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 4.

All (47) 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:188:GLU:HG2	2:B:719:HOH:O	1.85	0.76
1:A:165[A]:MET:C	1:A:165[A]:MET:SD	2.70	0.70
1:A:49:PHE:O	1:A:67:GLN:HG2	1.94	0.68
1:B:40:LEU:CB	1:B:120[A]:MET:HE1	2.26	0.65
1:A:165[A]:MET:SD	1:A:165[A]:MET:O	2.55	0.64
1:A:356:ILE:HD13	1:A:396:ILE:HG21	1.86	0.57
1:A:165[B]:MET:SD	2:A:595:HOH:O	2.58	0.56
1:A:355:VAL:O	1:A:379:GLY:HA3	2.06	0.56
1:A:85:VAL:O	1:A:86:LYS:HB2	2.07	0.55
1:B:108:VAL:HG11	1:B:192:THR:CG2	2.37	0.54
1:B:108:VAL:HG11	1:B:192:THR:HG22	1.90	0.54
1:B:16:LYS:CE	2:B:632:HOH:O	2.56	0.54
1:B:419:HIS:HB3	2:B:614:HOH:O	2.07	0.54
1:A:53:ILE:HD13	1:A:75:CYS:HB3	1.90	0.53
1:A:356:ILE:CD1	1:A:396:ILE:HG21	2.40	0.52
1:B:314:ARG:HG2	2:B:559:HOH:O	2.09	0.52
1:A:330:ARG:HB2	1:A:331:PRO:HD2	1.93	0.51
1:B:220:SER:HB2	1:B:433:ALA:HA	1.93	0.50
1:B:134:GLU:O	1:B:177:ARG:NH2	2.45	0.50
1:B:40:LEU:CB	1:B:120[A]:MET:CE	2.91	0.49
1:B:95:PHE:HZ	1:B:99:LYS:HG3	1.77	0.49
1:A:25:PHE:CE2	1:A:49:PHE:HE1	2.30	0.49
1:B:33:LEU:HD11	1:B:123:ALA:CB	2.43	0.48
1:B:330:ARG:HD2	2:B:595:HOH:O	2.12	0.48
1:B:25:PHE:C	1:B:25:PHE:CD1	2.87	0.48
1:A:140:PRO:HD2	1:A:173:MET:O	2.13	0.48
1:B:310:LEU:O	1:B:314:ARG:HG2	2.15	0.47
1:B:358:GLU:OE2	2:B:640:HOH:O	2.20	0.47
1:B:35:LEU:HD21	1:B:120[A]:MET:HE1	1.97	0.47
1:B:30:GLU:HB3	1:B:147:MET:CE	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:95:PHE:CZ	1:B:99:LYS:HG3	2.49	0.47
1:A:173:MET:CE	1:A:183:SER:HB2	2.47	0.44
1:B:144:TYR:C	1:B:144:TYR:CD1	2.92	0.43
1:A:380:TYR:HB3	1:A:387:ILE:HG23	2.00	0.43
1:A:270:ILE:HD12	1:A:298:LEU:HD22	2.01	0.43
1:B:378:LYS:HD3	2:B:608:HOH:O	2.19	0.43
1:A:216:LYS:O	1:A:391:VAL:HA	2.20	0.42
1:A:188:GLU:HB2	1:A:201:ILE:HD11	2.02	0.42
1:A:173:MET:HE3	1:A:183:SER:HB2	2.02	0.42
1:A:298:LEU:HD12	1:A:303:LEU:HA	2.02	0.42
1:A:137:VAL:CG1	1:A:177:ARG:HB2	2.50	0.41
1:A:33:LEU:C	1:A:33:LEU:HD12	2.41	0.41
1:A:61:THR:C	1:A:83:LEU:HD23	2.40	0.41
1:A:73:GLU:O	1:A:77:GLU:HG2	2.21	0.41
1:B:262:GLN:HG2	1:B:302:VAL:HG22	2.02	0.41
1:B:169:PHE:CZ	1:B:171:PHE:HB2	2.56	0.41
1:B:29:ARG:NH1	1:B:45:ASP:OD1	2.54	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	431/447 (96%)	423 (98%)	8 (2%)	0	100	100
1	B	431/447 (96%)	426 (99%)	5 (1%)	0	100	100
All	All	862/894 (96%)	849 (98%)	13 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	359/382 (94%)	353 (98%)	6 (2%)	60	55
1	B	357/382 (94%)	348 (98%)	9 (2%)	47	38
All	All	716/764 (94%)	701 (98%)	15 (2%)	53	46

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	PHE
1	A	173	MET
1	A	217	THR
1	A	295	LYS
1	A	298	LEU
1	A	383	GLU
1	B	2	THR
1	B	25	PHE
1	B	37	ASN
1	B	50	ASN
1	B	173	MET
1	B	204	ARG
1	B	262	GLN
1	B	295	LYS
1	B	406	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	GLN

5.3.3 RNA ⓘ

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 [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	429/447 (95%)	0.26	6 (1%) 75 82	7, 17, 30, 40	0
1	B	429/447 (95%)	0.20	3 (0%) 87 92	8, 16, 30, 41	0
All	All	858/894 (95%)	0.23	9 (1%) 82 87	7, 16, 30, 41	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	93	TYR	3.6
1	A	217	THR	3.1
1	B	93	TYR	2.7
1	B	428	GLU	2.4
1	A	376	PHE	2.3
1	A	221	GLY	2.2
1	B	120[A]	MET	2.2
1	A	49	PHE	2.2
1	A	9	ARG	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 [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.