WORLDWIDE PDB
PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Feb 27, 2014 – 03:29 PM GMT

PDB ID   :   3P4X
Title   :   Helicase domain of reverse gyrase from Thermotoga maritima
Authors   :   Rudolph, M.G.; Klostermeier, D.
Deposited on   :   2010-10-07
Resolution   :   2.41 Å(reported)

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 2.41 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	Percentile Ranks	Value
Rfree		0.258
Clashscore		3
Ramachandran outliers		0.2%
Sidechain outliers		5.8%
RSRZ outliers		3.3%

Worse — Better

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
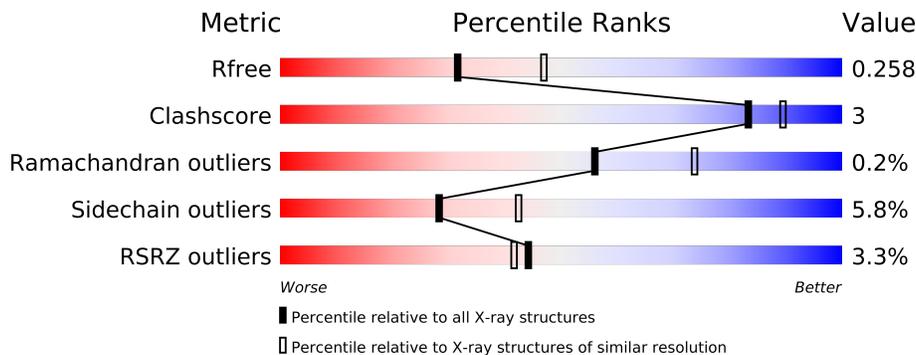
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	2496 (2.44-2.40)
Clashscore	79885	3124 (2.44-2.40)
Ramachandran outliers	78287	3067 (2.44-2.40)
Sidechain outliers	78261	3068 (2.44-2.40)
RSRZ outliers	66119	2499 (2.44-2.40)

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	413	
1	B	413	

2 Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 6729 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 reverse gyrase helicase-like domain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	399	Total	C	N	O	S	0	0	0
			3278	2123	554	595	6			
1	B	410	Total	C	N	O	S	0	0	0
			3370	2180	569	615	6			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).
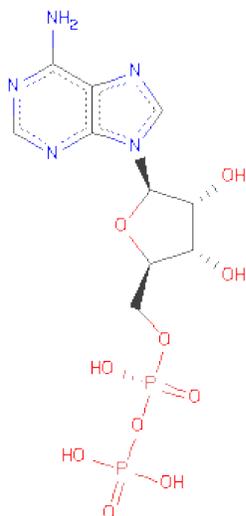
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total 1	Cl 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	20	Total 20	O 20	0	0
5	B	32	Total 32	O 32	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: reverse gyrase helicase-like domain

Chain A:
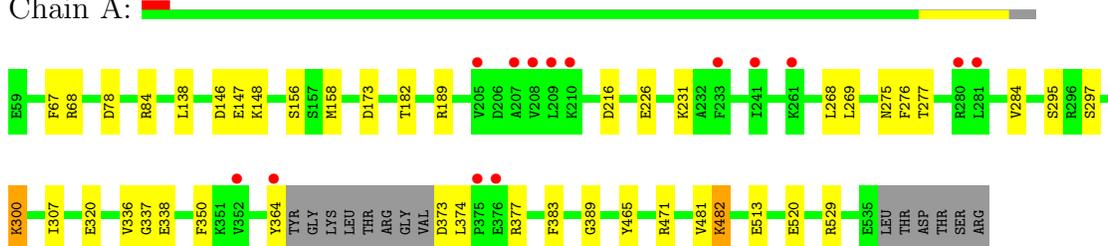
• Molecule 1: reverse gyrase helicase-like domain

Chain B:
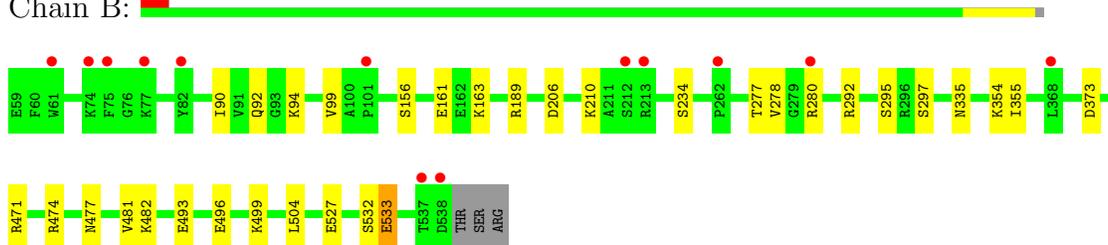
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	59.26Å 111.23Å 129.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	56.03 – 2.41 84.44 – 2.41	Depositor EDS
% Data completeness (in resolution range)	87.9 (56.03-2.41) 93.1 (84.44-2.41)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	1.27 (at 2.40Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6_289)	Depositor
R, R_{free}	0.186 , 0.256 0.192 , 0.258	Depositor DCC
R_{free} test set	1606 reflections (5.09%)	DCC
Wilson B-factor (Å^2)	50.1	Xtriage
Anisotropy	0.434	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 40.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Outliers	1 of 33607 reflections (0.003%)	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	6729	wwPDB-VP
Average B, all atoms (Å^2)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.94% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities 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: MG, ADP, CL

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	0.49	3/3342 (0.1%)	0.57	0/4485
1	B	0.45	0/3436	0.59	0/4613
All	All	0.47	3/6778 (0.0%)	0.58	0/9098

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	364	TYR	CD1-CE1	6.80	1.49	1.39
1	A	364	TYR	CD2-CE2	6.37	1.49	1.39
1	A	389	GLY	C-N	5.72	1.45	1.34

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	3278	0	24	11	0
1	B	3370	0	0	9	0
2	A	1	0	0	0	0
3	A	27	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	1	0	0	0	0
5	A	20	0	0	0	0
5	B	32	0	0	0	0
All	All	6729	0	24	20	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 (20) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:99:VAL:CG2	1:B:280:ARG:CG	2.72	0.67
1:B:373:ASP:OD2	1:B:474:ARG:NH1	2.31	0.64
1:B:278:VAL:O	1:B:278:VAL:CG2	2.55	0.55
1:A:78:ASP:O	3:A:800:ADP:N6	2.42	0.52
1:B:156:SER:O	1:B:163:LYS:NZ	2.43	0.51
1:A:300:LYS:NZ	1:A:513:GLU:OE1	2.46	0.49
1:A:68:ARG:NH2	1:A:84:ARG:NH2	2.61	0.49
1:A:373:ASP:O	1:A:374:LEU:CD2	2.62	0.47
1:B:335:ASN:ND2	1:B:354:LYS:O	2.47	0.47
1:A:374:LEU:O	1:A:377:ARG:N	2.50	0.45
1:B:206:ASP:O	1:B:210:LYS:N	2.50	0.45
1:A:482:LYS:O	1:A:529:ARG:NH1	2.50	0.45
1:A:67:PHE:CD1	1:A:67:PHE:C	2.91	0.43
1:B:92:GLN:NE2	1:B:94:LYS:NZ	2.67	0.43
1:A:146:ASP:O	1:A:148:LYS:N	2.52	0.42
1:A:336:VAL:CG2	1:A:337:GLY:N	2.82	0.42
1:B:477:ASN:ND2	1:B:532:SER:O	2.54	0.41
1:B:533:GLU:OE1	1:B:533:GLU:O	2.39	0.41
1:A:350:PHE:O	1:A:377:ARG:NE	2.54	0.41
1:A:383:PHE:CE2	1:A:465:TYR:CE1	3.09	0.41

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	395/413 (96%)	374 (95%)	19 (5%)	2 (0%)	38	52
1	B	408/413 (99%)	394 (97%)	14 (3%)	0	100	100
All	All	803/826 (97%)	768 (96%)	33 (4%)	2 (0%)	56	74

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	147	GLU
1	A	275	ASN

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	356/370 (96%)	332 (93%)	24 (7%)	23	34
1	B	367/370 (99%)	349 (95%)	18 (5%)	35	52
All	All	723/740 (98%)	681 (94%)	42 (6%)	28	42

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	138	LEU
1	A	156	SER
1	A	158	MET
1	A	173	ASP
1	A	182	THR
1	A	189	ARG
1	A	216	ASP
1	A	226	GLU
1	A	231	LYS
1	A	268	LEU
1	A	269	LEU
1	A	276	PHE
1	A	277	THR
1	A	284	VAL
1	A	295	SER

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Mol	Chain	Res	Type
1	A	297	SER
1	A	300	LYS
1	A	307	ILE
1	A	320	GLU
1	A	338	GLU
1	A	471	ARG
1	A	481	VAL
1	A	482	LYS
1	A	520	GLU
1	B	90	ILE
1	B	161	GLU
1	B	189	ARG
1	B	234	SER
1	B	277	THR
1	B	292	ARG
1	B	295	SER
1	B	297	SER
1	B	355	ILE
1	B	471	ARG
1	B	481	VAL
1	B	482	LYS
1	B	493	GLU
1	B	496	GLU
1	B	499	LYS
1	B	504	LEU
1	B	527	GLU
1	B	533	GLU

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 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 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	#$|Z| > 2$
3	ADP	A	800	2	29,29,29	1.11	2 (6%)	45,45,45	1.82	7 (15%)

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
3	ADP	A	800	2	-	0/16/32/32	0/1/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	800	ADP	C5-C4	3.28	1.47	1.40
3	A	800	ADP	C4-N9	-2.21	1.34	1.37

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	800	ADP	N3-C2-N1	-6.35	123.40	128.71
3	A	800	ADP	N3-C4-N9	5.72	135.76	125.43
3	A	800	ADP	C5-C4-N3	-3.29	118.54	125.70
3	A	800	ADP	C4-C5-N7	-3.13	106.84	109.52
3	A	800	ADP	C3'-C2'-C1'	2.71	105.15	100.91
3	A	800	ADP	C8-N9-C4	2.57	108.86	106.90
3	A	800	ADP	C2-N3-C4	2.49	121.09	114.01

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 (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	399/413 (96%)	-0.14	14 (3%)	42	39	30, 70, 128, 203	0
1	B	410/413 (99%)	-0.20	13 (3%)	45	43	24, 64, 116, 205	0
All	All	809/826 (97%)	-0.17	27 (3%)	44	41	24, 66, 124, 205	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	75	PHE	5.8
1	A	364	TYR	4.7
1	A	205	VAL	4.4
1	A	210	LYS	4.2
1	A	208	VAL	3.8
1	A	376	GLU	3.5
1	B	280	ARG	3.3
1	B	101	PRO	3.3
1	B	262	PRO	3.2
1	A	209	LEU	2.8
1	A	281	LEU	2.7
1	B	368	LEU	2.6
1	A	241	ILE	2.6
1	A	207	ALA	2.6
1	B	212	SER	2.5
1	B	538	ASP	2.5
1	A	261	LYS	2.4
1	B	77	LYS	2.4
1	A	280	ARG	2.3
1	B	61	TRP	2.3
1	B	213	ARG	2.3
1	A	352	VAL	2.3
1	B	82	TYR	2.2
1	B	537	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	233	PHE	2.1
1	B	74	LYS	2.1
1	A	375	PRO	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
4	CL	B	1	1/1	0.13	0.86	87,87,87,87	0
3	ADP	A	800	27/27	0.14	0.78	95,118,131,143	0
2	MG	A	799	1/1	0.10	-1.76	91,91,91,91	0

6.5 Other polymers ⓘ

There are no such residues in this entry.