



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 03:33 PM GMT

PDB ID : 4CKK
Title : Apo structure of 55 kDa N-terminal domain of E. coli DNA gyrase A subunit
Authors : Hearnshaw, S.J.; Edwards, M.J.; Stevenson, C.E.M.; Lawson, D.M.; Maxwell, A.
Deposited on : 2014-01-07
Resolution : 1.90 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

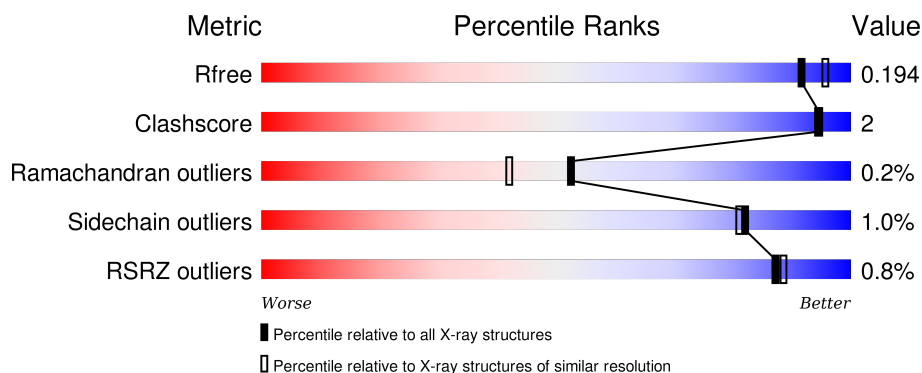
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	4755 (1.90-1.90)
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (1.90-1.90)

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	493	<div> <div></div> <div>94%</div> <div>••</div> </div>
1	B	493	<div> <div>%</div> <div>94%</div> <div>••</div> </div>
1	C	493	<div> <div>%</div> <div>92%</div> <div>6% •</div> </div>
1	D	493	<div> <div>%</div> <div>92%</div> <div>5% ••</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 16106 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 DNA GYRASE SUBUNIT A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	485	Total	C	N	O	S	0	2	0
			3788	2389	681	705	13			
1	B	484	Total	C	N	O	S	0	3	0
			3783	2391	676	703	13			
1	C	484	Total	C	N	O	S	0	0	0
			3710	2350	656	691	13			
1	D	484	Total	C	N	O	S	0	0	0
			3769	2378	666	712	13			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	279	Total	O	0	0
			279	279		
2	B	257	Total	O	0	0
			257	257		
2	C	281	Total	O	0	0
			281	281		
2	D	239	Total	O	0	0
			239	239		

3 Residue-property plots [i](#)

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.

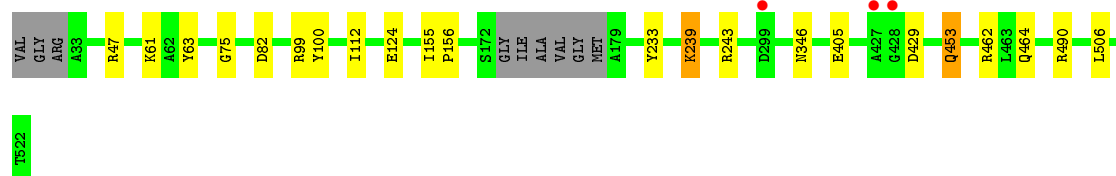
• Molecule 1: DNA GYRASE SUBUNIT A

Chain A: 



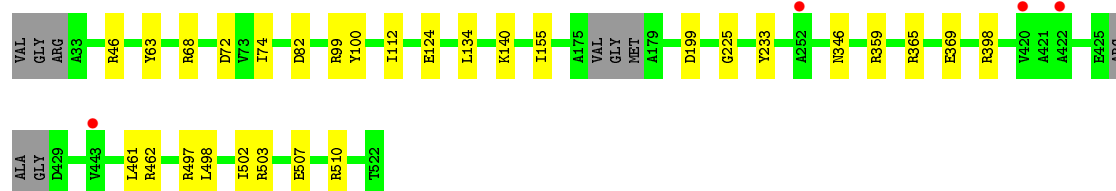
• Molecule 1: DNA GYRASE SUBUNIT A

Chain B: 

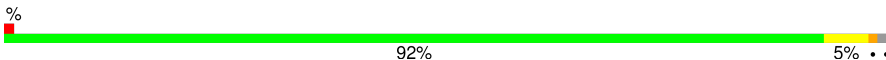


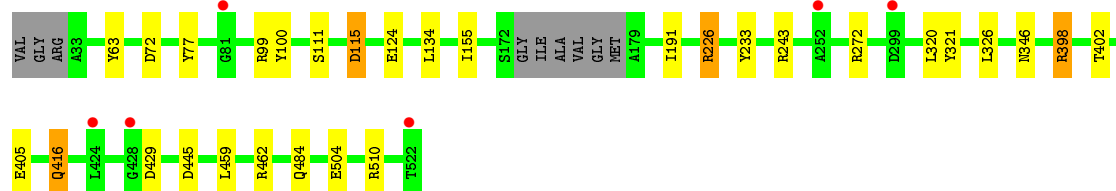
• Molecule 1: DNA GYRASE SUBUNIT A

Chain C: 



• Molecule 1: DNA GYRASE SUBUNIT A

Chain D: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	93.57Å 95.53Å 95.89Å 105.16° 118.81° 103.42°	Depositor
Resolution (Å)	81.51 – 1.90 81.51 – 1.90	Depositor EDS
% Data completeness (in resolution range)	97.0 (81.51-1.90) 82.9 (81.51-1.90)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.40 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.169 , 0.189 0.176 , 0.194	Depositor DCC
R_{free} test set	9799 reflections (5.31%)	DCC
Wilson B-factor (Å ²)	26.0	Xtriage
Anisotropy	0.062	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 40.9	EDS
Estimated twinning fraction	0.024 for h+k+l,-h,-k 0.024 for -k,-l,h+k+l 0.024 for k,h,-h-k-l 0.047 for l,-h-k-l,h 0.025 for -l,-k,-h 0.024 for -h-k-l,l,k 0.024 for -h,h+k+l,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 194496 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	16106	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.70% 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	0.66	0/3854	0.79	3/5220 (0.1%)
1	B	0.69	0/3853	0.78	4/5217 (0.1%)
1	C	0.69	0/3770	0.79	7/5114 (0.1%)
1	D	0.67	0/3830	0.79	4/5192 (0.1%)
All	All	0.67	0/15307	0.79	18/20743 (0.1%)

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	510	ARG	NE-CZ-NH1	9.80	125.20	120.30
1	B	243	ARG	NE-CZ-NH2	-7.69	116.45	120.30
1	C	497	ARG	NE-CZ-NH1	7.31	123.95	120.30
1	B	243	ARG	NE-CZ-NH1	7.25	123.93	120.30
1	A	490	ARG	NE-CZ-NH1	6.41	123.51	120.30
1	D	226	ARG	N-CA-CB	6.05	121.48	110.60
1	D	398	ARG	CA-CB-CG	5.65	125.83	113.40
1	C	134	LEU	CA-CB-CG	5.52	128.01	115.30
1	B	47	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	A	461	LEU	CA-CB-CG	5.35	127.60	115.30
1	C	46	ARG	NE-CZ-NH1	5.33	122.97	120.30
1	C	365	ARG	NE-CZ-NH1	5.29	122.95	120.30
1	C	498	LEU	CB-CG-CD2	-5.29	102.00	111.00
1	D	134	LEU	CA-CB-CG	5.25	127.37	115.30
1	C	461	LEU	CA-CB-CG	5.17	127.20	115.30
1	D	398	ARG	CB-CA-C	-5.15	100.09	110.40
1	B	239	LYS	N-CA-CB	-5.06	101.49	110.60
1	A	46	ARG	NE-CZ-NH1	5.05	122.83	120.30

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	3788	0	3787	12	0
1	B	3783	0	3801	14	0
1	C	3710	0	3673	16	0
1	D	3769	0	3757	18	0
2	A	279	0	0	2	0
2	B	257	0	0	5	0
2	C	281	0	0	3	0
2	D	239	0	0	4	0
All	All	16106	0	15018	51	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 2.

All (51) 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:453:GLN:NE2	2:B:2224:HOH:O	2.29	0.65
1:D:484:GLN:OE1	2:D:2216:HOH:O	2.14	0.65
1:D:416:GLN:HG2	2:D:2091:HOH:O	2.02	0.59
1:B:462:ARG:HH12	1:D:462:ARG:CZ	2.15	0.59
1:D:416:GLN:NE2	2:D:2190:HOH:O	2.35	0.59
1:B:462:ARG:HH12	1:D:462:ARG:NH2	2.02	0.57
1:A:74:ILE:HD11	1:A:82:ASP:HA	1.87	0.56
1:C:74:ILE:HD11	1:C:82:ASP:HA	1.86	0.56
1:B:462:ARG:NH1	1:D:462:ARG:CZ	2.69	0.56
1:D:402:THR:OG1	1:D:405:GLU:OE1	2.10	0.56
1:A:462:ARG:CZ	1:C:462:ARG:HH12	2.18	0.55
1:C:68:ARG:NH1	1:C:72:ASP:OD1	2.40	0.55
1:C:155:ILE:HD12	2:C:2018:HOH:O	2.10	0.50
1:C:63:TYR:HB3	1:C:124:GLU:HB3	1.94	0.50
1:A:356:ARG:HD3	2:A:2225:HOH:O	2.11	0.50
1:A:462:ARG:CZ	1:C:462:ARG:NH1	2.74	0.50
1:A:68[A]:ARG:NH1	1:A:72:ASP:OD1	2.44	0.49
1:B:63:TYR:HB3	1:B:124:GLU:HB3	1.94	0.49
1:A:63:TYR:HB3	1:A:124:GLU:HB3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:462:ARG:NH2	1:C:462:ARG:HH12	2.11	0.48
1:B:506:LEU:HD23	2:B:2100:HOH:O	2.13	0.48
1:B:155:ILE:HG13	1:B:156:PRO:HD2	1.95	0.48
1:B:464:GLN:HB3	1:D:459:LEU:HB3	1.95	0.47
1:C:199:ASP:OD1	1:C:503:ARG:NH1	2.48	0.46
1:D:63:TYR:HB3	1:D:124:GLU:HB3	1.96	0.46
1:A:275:GLU:OE1	2:A:2191:HOH:O	2.20	0.46
1:C:140:LYS:HE2	1:C:369:GLU:OE2	2.16	0.45
1:C:199:ASP:OD1	1:C:503:ARG:NH2	2.47	0.44
1:C:99:ARG:HG3	1:C:100:TYR:CE2	2.52	0.44
1:B:75:GLY:HA3	2:B:2038:HOH:O	2.18	0.44
1:B:99:ARG:HG3	1:B:100:TYR:CE2	2.53	0.44
1:C:507:GLU:HG3	2:C:2269:HOH:O	2.17	0.44
1:D:243:ARG:HG3	1:D:321:TYR:CE1	2.53	0.44
1:D:233:TYR:O	1:D:346:ASN:HB2	2.18	0.43
1:B:462:ARG:NH1	1:D:462:ARG:NH2	2.67	0.43
1:C:233:TYR:O	1:C:346:ASN:HB2	2.19	0.43
1:B:233:TYR:O	1:B:346:ASN:HB2	2.19	0.43
1:D:504:GLU:HG3	2:D:2222:HOH:O	2.19	0.43
1:C:359:ARG:HA	1:C:502:ILE:HD11	2.01	0.43
1:D:99:ARG:HG3	1:D:100:TYR:CE2	2.54	0.43
1:C:112:ILE:HD11	2:C:2189:HOH:O	2.19	0.42
1:D:191:ILE:HG21	1:D:510:ARG:HB2	2.02	0.42
1:D:111:SER:OG	1:D:115:ASP:OD2	2.37	0.42
1:B:61:LYS:HD3	2:B:2024:HOH:O	2.18	0.42
1:D:77:TYR:CE1	1:D:155:ILE:HG12	2.54	0.42
1:A:391:ASP:OD1	1:C:398:ARG:NH2	2.53	0.42
1:B:112:ILE:HD11	2:B:2157:HOH:O	2.19	0.42
1:A:74:ILE:HD11	1:A:82:ASP:CA	2.51	0.41
1:A:99:ARG:HG3	1:A:100:TYR:CE2	2.56	0.41
1:D:320:LEU:HB3	1:D:326:LEU:HD12	2.03	0.41
1:A:233:TYR:O	1:A:346:ASN: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	481/493 (98%)	474 (98%)	6 (1%)	1 (0%)	52	42
1	B	483/493 (98%)	476 (99%)	7 (1%)	0	100	100
1	C	478/493 (97%)	470 (98%)	7 (2%)	1 (0%)	52	42
1	D	480/493 (97%)	472 (98%)	7 (2%)	1 (0%)	52	42
All	All	1922/1972 (98%)	1892 (98%)	27 (1%)	3 (0%)	52	42

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	226	ARG
1	A	225	GLY
1	C	225	GLY

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	389/411 (95%)	386 (99%)	3 (1%)	86	86
1	B	390/411 (95%)	383 (98%)	7 (2%)	66	61
1	C	373/411 (91%)	373 (100%)	0	100	100
1	D	390/411 (95%)	383 (98%)	7 (2%)	66	61
All	All	1542/1644 (94%)	1525 (99%)	17 (1%)	82	79

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	272	ARG
1	A	398	ARG
1	A	497	ARG

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Mol	Chain	Res	Type
1	B	82[A]	ASP
1	B	82[B]	ASP
1	B	239	LYS
1	B	405	GLU
1	B	429	ASP
1	B	453	GLN
1	B	490	ARG
1	D	72	ASP
1	D	115	ASP
1	D	272	ARG
1	D	398	ARG
1	D	416	GLN
1	D	429	ASP
1	D	445	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	ASN
1	B	57	ASN
1	B	464	GLN
1	C	57	ASN
1	D	57	ASN
1	D	416	GLN

5.3.3 RNA ⓘ

There are no RNA molecules 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

There are no ligands in this entry.

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	485/493 (98%)	-0.11	2 (0%) 93 93	15, 29, 56, 84	0
1	B	484/493 (98%)	-0.16	3 (0%) 90 91	16, 28, 54, 85	0
1	C	484/493 (98%)	-0.14	4 (0%) 87 88	15, 28, 59, 89	0
1	D	484/493 (98%)	-0.06	6 (1%) 81 83	16, 31, 55, 77	0
All	All	1937/1972 (98%)	-0.12	15 (0%) 87 88	15, 29, 56, 89	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	81	GLY	5.3
1	A	175	ALA	4.5
1	D	522	THR	3.0
1	D	428	GLY	3.0
1	C	422	ALA	2.7
1	C	420	VAL	2.6
1	B	427	ALA	2.6
1	C	252	ALA	2.6
1	D	424	LEU	2.5
1	D	299	ASP	2.3
1	D	252	ALA	2.3
1	B	428	GLY	2.2
1	A	252	ALA	2.2
1	C	443	VAL	2.1
1	B	299	ASP	2.1

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 [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.