wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 08:34 PM GMT

PDB ID	:	4TMA
Title	:	Crystal structure of gyrase bound to its inhibitor YacG
Authors	:	Vos, S.M.; Lyubimov, A.Y.; Hershey, D.M.; Schoeffler, A.J.; Berger, J.M.
Deposited on	:	2014-05-31
Resolution	:	3.30 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

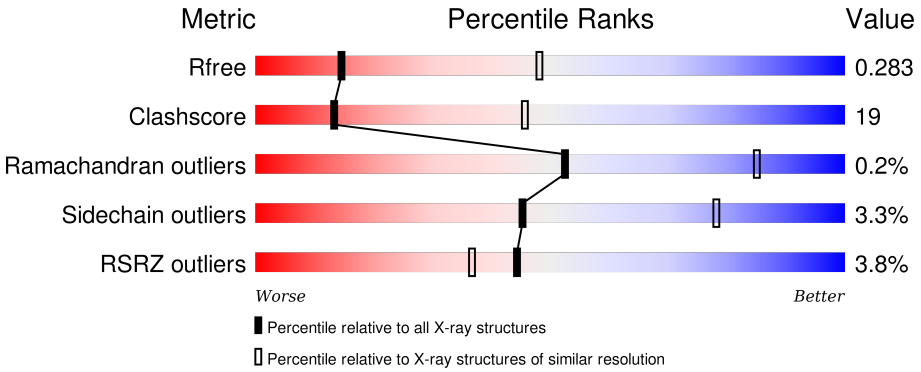
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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	2060 (3.40-3.20)
Clashscore	102246	1058 (3.38-3.22)
Ramachandran outliers	100387	1038 (3.38-3.22)
Sidechain outliers	100360	1037 (3.38-3.22)
RSRZ outliers	91569	2070 (3.40-3.20)

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 <=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	525	3% 58% 34%
1	C	525	5% 57% 31% 10%
1	E	525	3% 67% 25% 7%
1	G	525	3% 65% 25% 8%
2	B	417	% 53% 32% 10%

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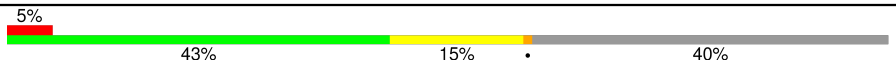
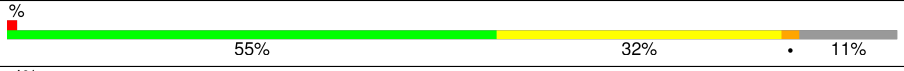
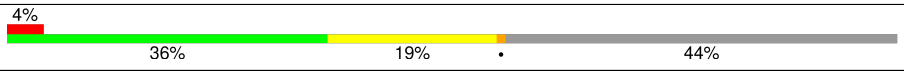
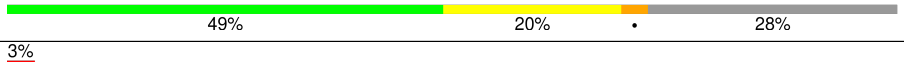
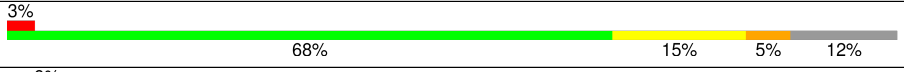
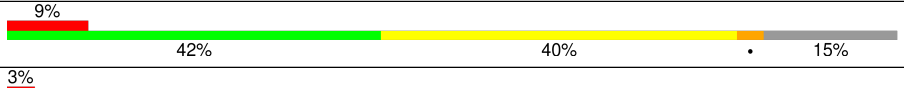
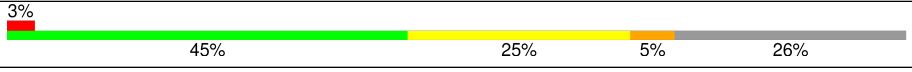
Mol	Chain	Length	Quality of chain
2	D	417	
2	F	417	
2	H	417	
3	I	65	
3	J	65	
3	K	65	
3	L	65	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 26792 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	505	Total	C	N	O	S	0	0	0
			3983	2510	711	747	15			
1	C	475	Total	C	N	O	S	0	0	0
			3733	2345	672	701	15			
1	E	486	Total	C	N	O	S	0	1	0
			3841	2413	698	715	15			
1	G	483	Total	C	N	O	S	0	0	0
			3800	2391	682	713	14			

- Molecule 2 is a protein called DNA gyrase subunit B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	374	Total	C	N	O	S	0	0	0
			2995	1875	527	579	14			
2	D	251	Total	C	N	O	S	0	0	0
			1990	1252	347	379	12			
2	F	371	Total	C	N	O	S	0	0	0
			2971	1863	523	571	14			
2	H	233	Total	C	N	O	S	0	1	0
			1863	1170	326	356	11			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	385	SER	-	expression tag	UNP U6NGU8
B	386	ASN	-	expression tag	UNP U6NGU8
B	387	ALA	-	expression tag	UNP U6NGU8
B	458	TYR	PHE	engineered mutation	UNP U6NGU8
D	385	SER	-	expression tag	UNP U6NGU8
D	386	ASN	-	expression tag	UNP U6NGU8
D	387	ALA	-	expression tag	UNP U6NGU8
D	458	TYR	PHE	engineered mutation	UNP U6NGU8

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Chain	Residue	Modelled	Actual	Comment	Reference
F	385	SER	-	expression tag	UNP U6NGU8
F	386	ASN	-	expression tag	UNP U6NGU8
F	387	ALA	-	expression tag	UNP U6NGU8
F	458	TYR	PHE	engineered mutation	UNP U6NGU8
H	385	SER	-	expression tag	UNP U6NGU8
H	386	ASN	-	expression tag	UNP U6NGU8
H	387	ALA	-	expression tag	UNP U6NGU8
H	458	TYR	PHE	engineered mutation	UNP U6NGU8

- Molecule 3 is a protein called DNA gyrase inhibitor YacG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	I	47	Total	C	N	O	S	0	0	0
			363	230	63	66	4			
3	J	57	Total	C	N	O	S	0	0	0
			446	279	74	89	4			
3	K	55	Total	C	N	O	S	0	0	0
			430	270	72	84	4			
3	L	48	Total	C	N	O	S	0	0	0
			371	234	64	69	4			

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

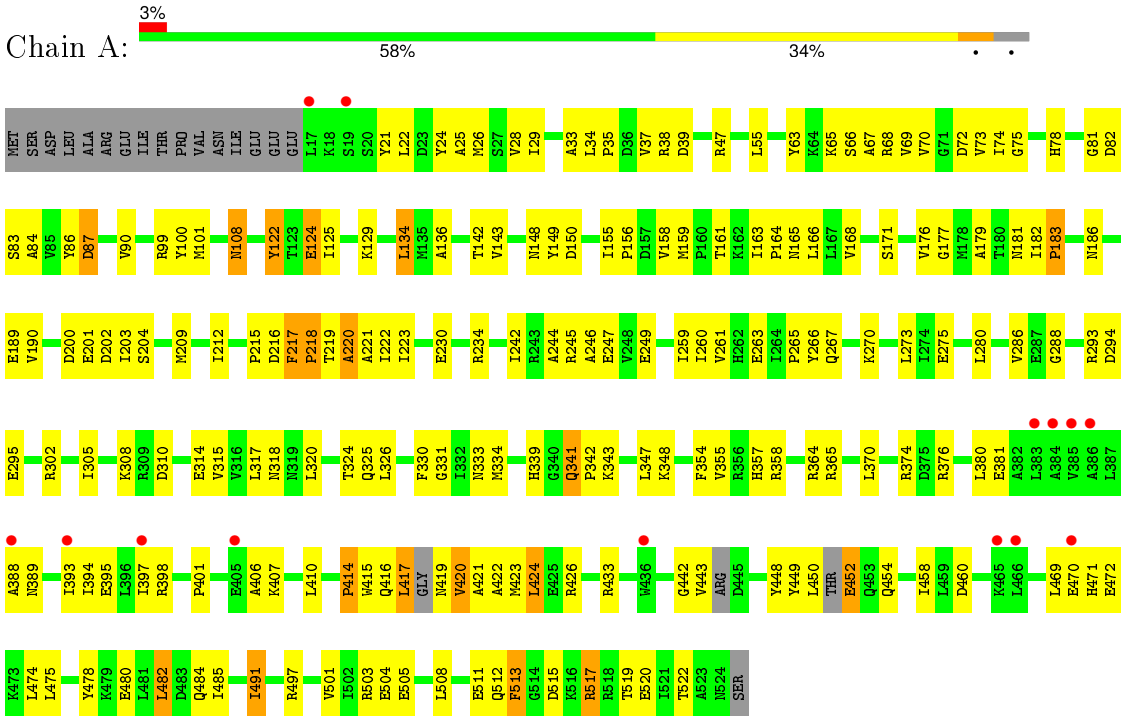
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	J	1	Total	Zn	0	0
			1	1		
4	K	1	Total	Zn	0	0
			1	1		
4	E	1	Total	Zn	0	0
			1	1		
4	B	1	Total	Zn	0	0
			1	1		
4	I	1	Total	Zn	0	0
			1	1		
4	L	1	Total	Zn	0	0
			1	1		

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.

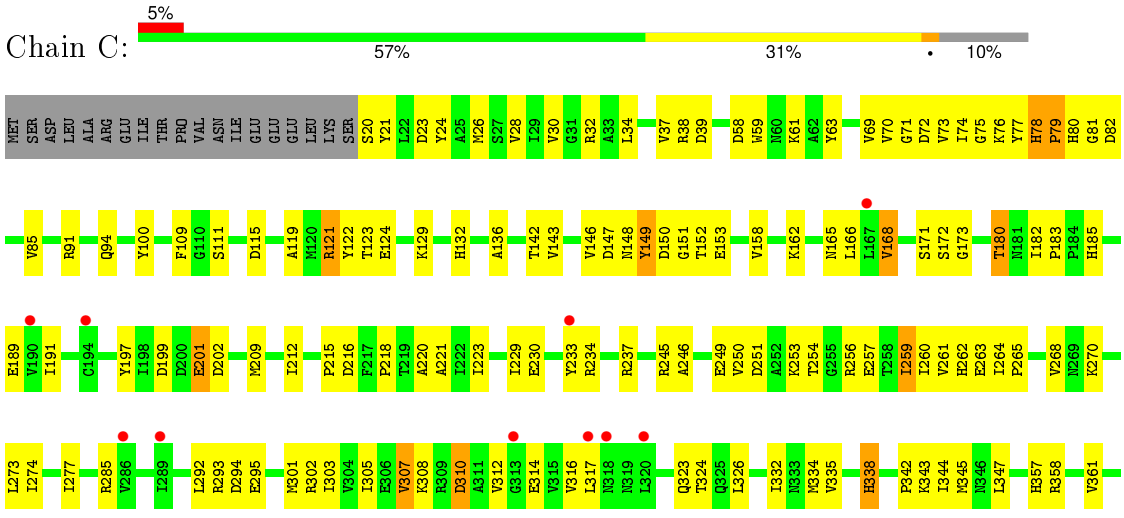
- Molecule 1: DNA gyrase subunit A

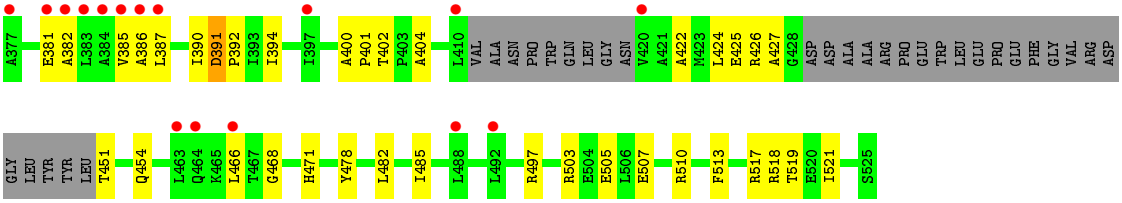
Chain A:



- Molecule 1: DNA gyrase subunit A

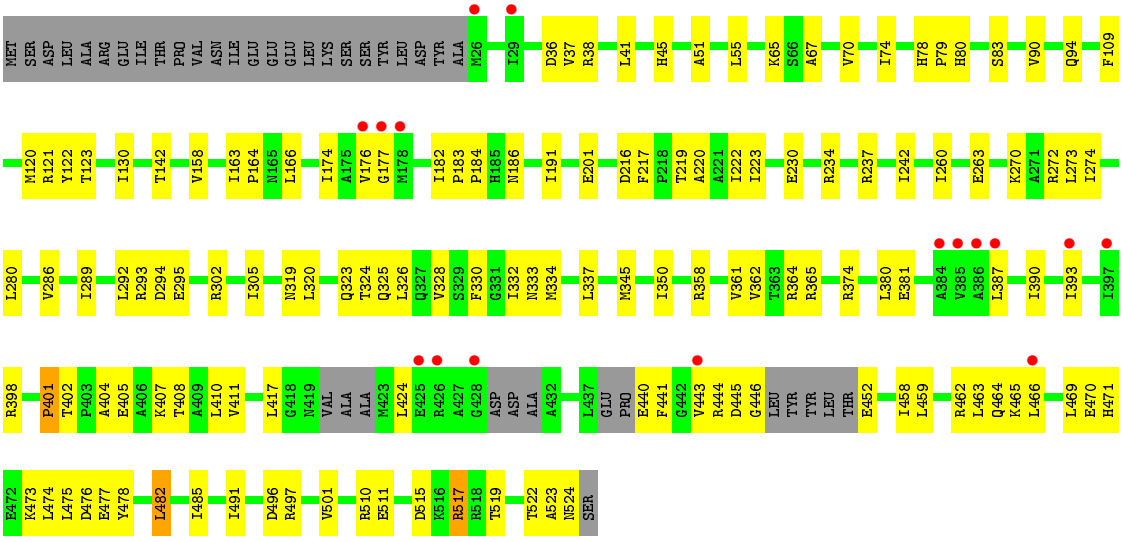
Chain C:





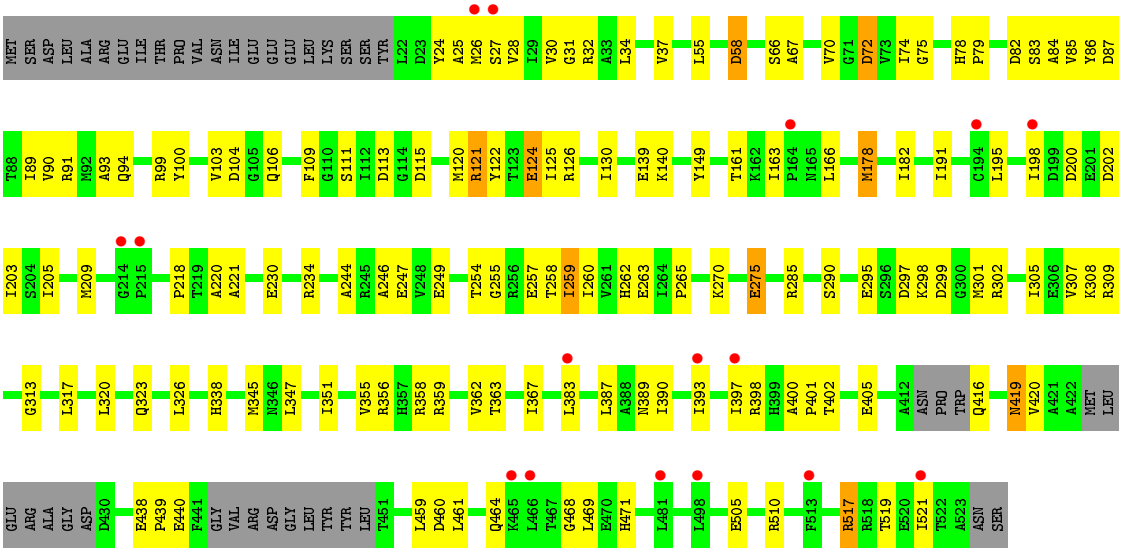
• Molecule 1: DNA gyrase subunit A

Chain E:



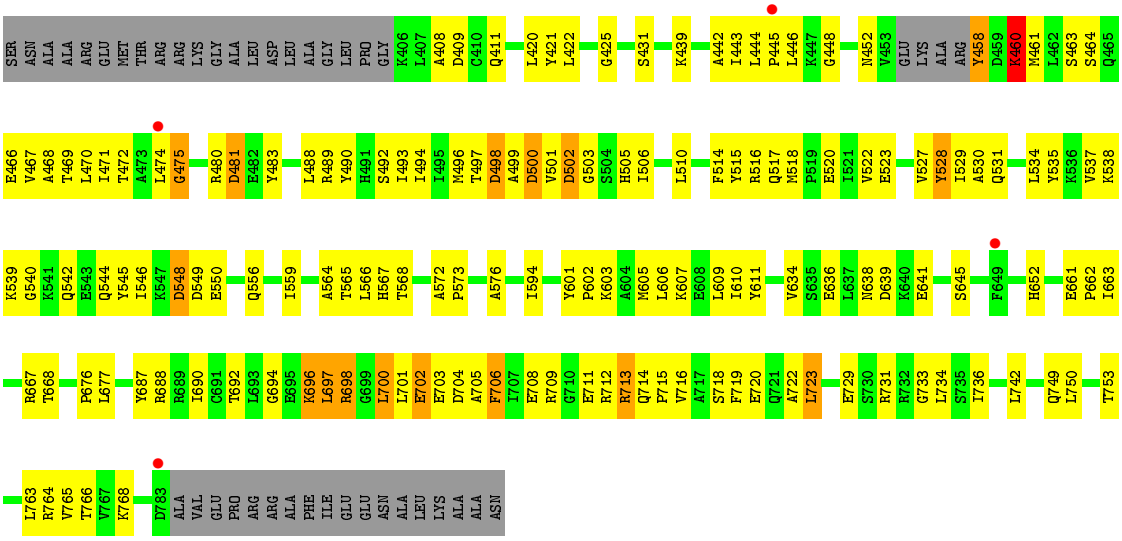
• Molecule 1: DNA gyrase subunit A

Chain G:



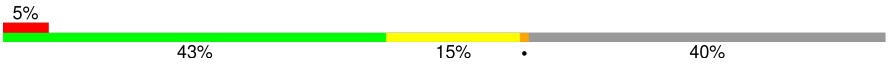
• Molecule 2: DNA gyrase subunit B

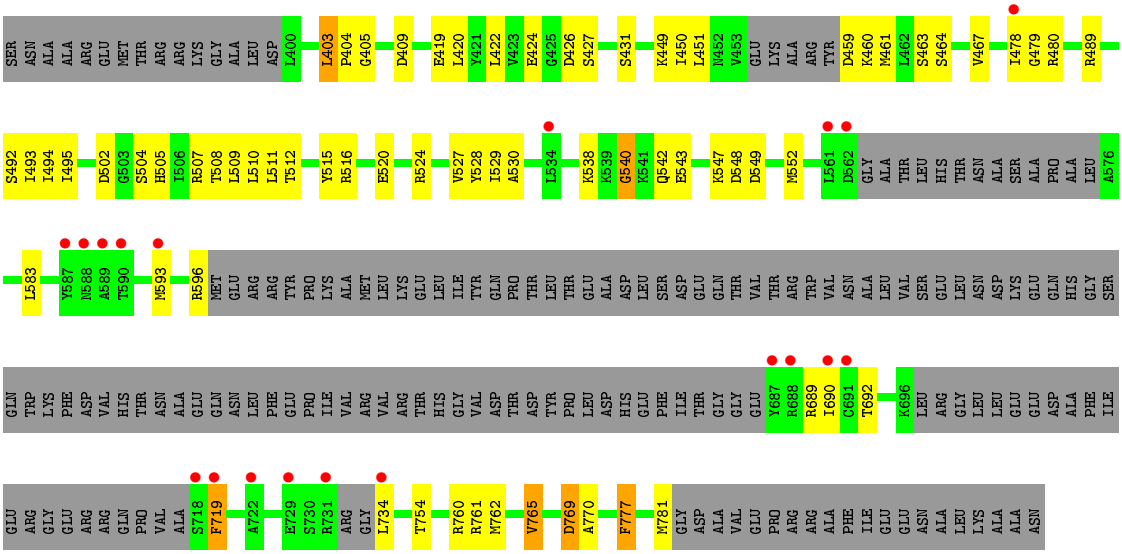
Chain B:



- Molecule 2: DNA gyrase subunit B

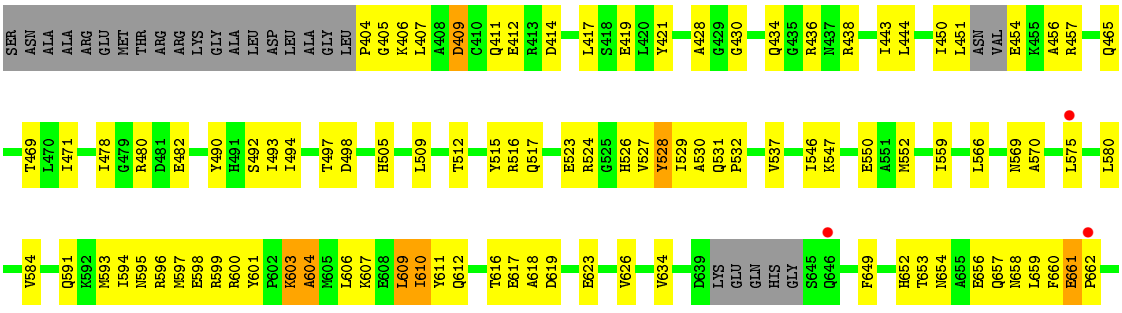
Chain D:

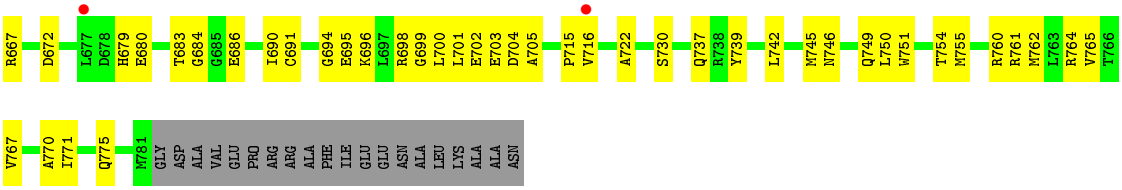




- Molecule 2: DNA gyrase subunit B

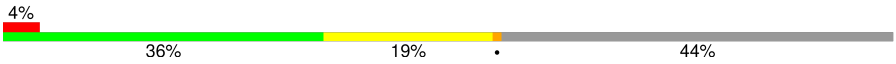
Chain F:

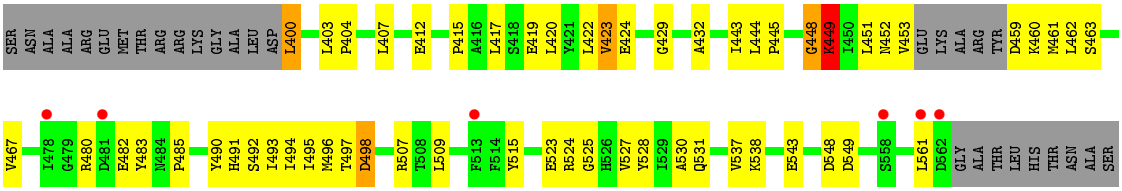


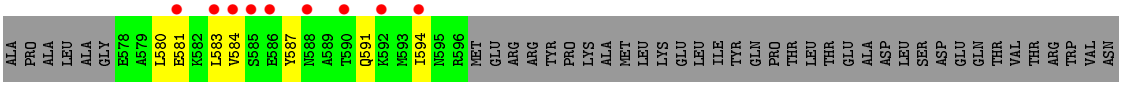


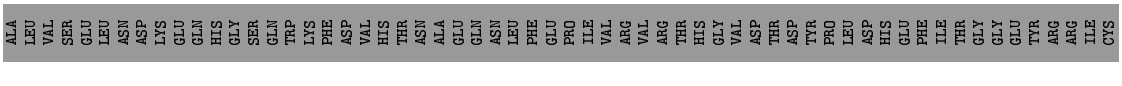
• Molecule 2: DNA gyrase subunit B

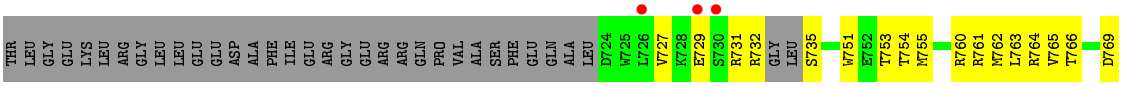
Chain H:





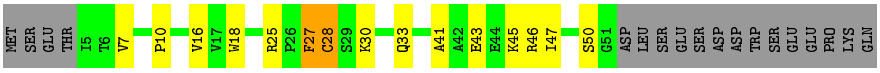






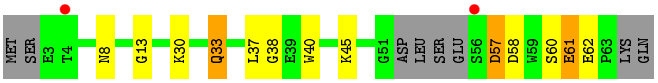
• Molecule 3: DNA gyrase inhibitor YacG

Chain I:



• Molecule 3: DNA gyrase inhibitor YacG

Chain J:

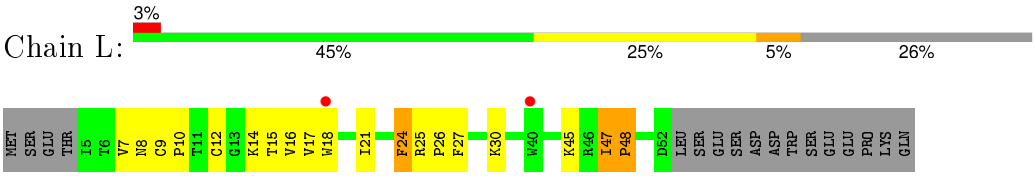


• Molecule 3: DNA gyrase inhibitor YacG

Chain K:

• Molecule 3: DNA gyrase inhibitor YacG

Chain L:


3%
45%
25%
5%
26%
MET SER GLU THR I5 T6 V7 N8 C9 P10 T11 C12 G13 K14 T15 V16 V17 W18 I21 F24 R25 P26 F27 K30 W40 K45 R46 I47 P48 D52 LEU SER GLU SER ASP ASP TRP SER GLU GLU PRO LYS GLN

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	107.21Å 114.46Å 462.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.32 – 3.30 49.32 – 3.30	Depositor EDS
% Data completeness (in resolution range)	77.7 (49.32-3.30) 77.7 (49.32-3.30)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.10 (at 3.33Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.243 , 0.283 0.243 , 0.283	Depositor DCC
R_{free} test set	3398 reflections (5.05%)	DCC
Wilson B-factor (Å^2)	109.9	Xtriage
Anisotropy	0.025	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.24 , 61.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.26$	Xtriage
Outliers	0 of 67314 reflections	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	26792	wwPDB-VP
Average B, all atoms (Å^2)	140.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.20% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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

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	0.60	2/4044 (0.0%)	0.71	12/5466 (0.2%)
1	C	0.44	0/3785	0.61	4/5111 (0.1%)
1	E	0.47	0/3896	0.57	2/5258 (0.0%)
1	G	0.40	0/3855	0.51	1/5209 (0.0%)
2	B	0.47	1/3046 (0.0%)	0.73	8/4111 (0.2%)
2	D	0.37	0/2015	0.57	0/2705
2	F	0.40	0/3021	0.66	7/4074 (0.2%)
2	H	0.43	0/1887	0.66	4/2534 (0.2%)
3	I	0.65	0/372	0.92	4/504 (0.8%)
3	J	0.35	0/457	0.67	2/620 (0.3%)
3	K	0.81	1/441 (0.2%)	0.63	1/598 (0.2%)
3	L	0.73	2/380 (0.5%)	0.73	1/515 (0.2%)
All	All	0.47	6/27199 (0.0%)	0.64	46/36705 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1
2	D	0	1
2	H	0	1
All	All	0	3

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	K	63	PRO	N-CD	-15.54	1.26	1.47
3	L	26	PRO	N-CD	9.27	1.60	1.47
3	L	48	PRO	N-CD	5.42	1.55	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	502	ASP	CA-C	5.37	1.67	1.52
1	A	218	PRO	N-CD	5.17	1.55	1.47

The worst 5 of 46 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	I	28	CYS	O-C-N	-9.19	107.99	122.70
2	B	475	GLY	N-CA-C	8.69	134.84	113.10
1	A	419	ASN	N-CA-C	8.50	133.96	111.00
2	F	603	LYS	N-CA-C	8.06	132.76	111.00
3	I	47	ILE	CB-CA-C	-7.48	96.64	111.60

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	251	ASP	Peptide
2	D	540	GLY	Peptide
2	H	449	LYS	Peptide

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	3983	0	4040	184	1
1	C	3733	0	3810	152	1
1	E	3841	0	3910	120	14
1	G	3800	0	3867	106	0
2	B	2995	0	2972	159	1
2	D	1990	0	2013	83	0
2	F	2971	0	2959	128	14
2	H	1863	0	1887	69	1
3	I	363	0	357	17	0
3	J	446	0	416	11	0
3	K	430	0	404	38	0
3	L	371	0	362	18	0
4	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	1	0	0	0	0
4	I	1	0	0	0	0
4	J	1	0	0	0	0
4	K	1	0	0	0	0
4	L	1	0	0	0	0
All	All	26792	0	26997	1011	16

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 19.

The worst 5 of 1011 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)
2:D:760:ARG:HD3	2:D:762:MET:CE	1.40	1.52
1:G:257:GLU:OE2	1:G:313:GLY:N	1.61	1.31
2:D:760:ARG:CD	2:D:762:MET:CE	2.09	1.30
2:D:760:ARG:CD	2:D:762:MET:HE2	1.63	1.28
1:G:255:GLY:O	1:G:309:ARG:HD3	1.17	1.27

The worst 5 of 16 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:476:ASP:OD2	2:F:596:ARG:CZ[3_757]	1.27	0.93
1:E:476:ASP:OD2	2:F:596:ARG:NE[3_757]	1.27	0.93
1:E:476:ASP:CG	2:F:596:ARG:NE[3_757]	1.32	0.88
1:E:476:ASP:CG	2:F:596:ARG:CZ[3_757]	1.33	0.87
1:E:476:ASP:CG	2:F:596:ARG:NH2[3_757]	1.39	0.81

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	497/525 (95%)	473 (95%)	22 (4%)	2 (0%)	39	76
1	C	469/525 (89%)	438 (93%)	30 (6%)	1 (0%)	52	85
1	E	477/525 (91%)	454 (95%)	22 (5%)	1 (0%)	52	85
1	G	475/525 (90%)	443 (93%)	31 (6%)	1 (0%)	52	85
2	B	370/417 (89%)	341 (92%)	28 (8%)	1 (0%)	46	81
2	D	239/417 (57%)	225 (94%)	13 (5%)	1 (0%)	39	76
2	F	365/417 (88%)	347 (95%)	18 (5%)	0	100	100
2	H	224/417 (54%)	206 (92%)	17 (8%)	1 (0%)	39	76
3	I	45/65 (69%)	42 (93%)	3 (7%)	0	100	100
3	J	53/65 (82%)	50 (94%)	3 (6%)	0	100	100
3	K	51/65 (78%)	47 (92%)	4 (8%)	0	100	100
3	L	46/65 (71%)	46 (100%)	0	0	100	100
All	All	3311/4028 (82%)	3112 (94%)	191 (6%)	8 (0%)	52	85

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	220	ALA
1	E	401	PRO
2	B	696	LYS
1	A	136	ALA
1	G	439	PRO

5.3.2 Protein sidechains (i)

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	422/440 (96%)	406 (96%)	16 (4%)	40	75
1	C	397/440 (90%)	387 (98%)	10 (2%)	55	82
1	E	407/440 (92%)	397 (98%)	10 (2%)	55	82
1	G	403/440 (92%)	387 (96%)	16 (4%)	38	74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	322/352 (92%)	306 (95%)	16 (5%)	30	68
2	D	214/352 (61%)	207 (97%)	7 (3%)	45	78
2	F	319/352 (91%)	311 (98%)	8 (2%)	55	82
2	H	202/352 (57%)	196 (97%)	6 (3%)	48	79
3	I	41/59 (70%)	40 (98%)	1 (2%)	57	83
3	J	51/59 (86%)	48 (94%)	3 (6%)	24	63
3	K	49/59 (83%)	47 (96%)	2 (4%)	37	74
3	L	42/59 (71%)	41 (98%)	1 (2%)	57	83
All	All	2869/3404 (84%)	2773 (97%)	96 (3%)	45	78

5 of 96 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	463	SER
1	E	272[B]	ARG
2	H	587	TYR
2	D	719	PHE
2	D	777	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 42 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	775	GLN
1	E	512	GLN
2	H	749	GLN
1	E	45	HIS
1	E	471	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

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 6 ligands modelled in this entry, 6 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

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, 95^{th} 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	505/525 (96%)	-0.00	14 (2%) 56 50	67, 110, 249, 473	0
1	C	475/525 (90%)	0.13	26 (5%) 29 23	75, 145, 252, 431	0
1	E	486/525 (92%)	0.01	16 (3%) 50 43	65, 104, 254, 314	0
1	G	483/525 (92%)	0.04	16 (3%) 50 43	59, 139, 235, 370	0
2	B	374/417 (89%)	-0.09	4 (1%) 82 78	69, 132, 176, 208	0
2	D	251/417 (60%)	0.30	19 (7%) 17 14	86, 145, 270, 299	0
2	F	371/417 (88%)	0.01	5 (1%) 79 74	59, 121, 200, 247	0
2	H	233/417 (55%)	0.23	18 (7%) 16 13	79, 132, 263, 362	0
3	I	47/65 (72%)	-0.33	0 100 100	65, 106, 140, 149	0
3	J	57/65 (87%)	-0.07	2 (3%) 48 40	66, 108, 144, 153	0
3	K	55/65 (84%)	0.50	6 (10%) 7 6	136, 176, 205, 211	0
3	L	48/65 (73%)	0.13	2 (4%) 40 33	166, 194, 227, 283	0
All	All	3385/4028 (84%)	0.06	128 (3%) 44 37	59, 130, 246, 473	0

The worst 5 of 128 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	386	ALA	8.4
2	D	719	PHE	8.1
1	A	385	VAL	7.6
1	A	17	LEU	6.4
3	K	51	GLY	5.8

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)

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, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
4	ZN	E	601	1/1	0.76	0.27	1.12	346,346,346,346	0
4	ZN	I	101	1/1	0.97	0.16	0.32	95,95,95,95	0
4	ZN	L	101	1/1	0.80	0.14	-0.99	225,225,225,225	0
4	ZN	K	101	1/1	0.71	0.11	-1.17	202,202,202,202	0
4	ZN	J	101	1/1	0.99	0.10	-1.36	137,137,137,137	0
4	ZN	B	1001	1/1	0.83	0.54	-	346,346,346,346	0

6.5 Other polymers (i)

There are no such residues in this entry.