



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 07:40 PM GMT

PDB ID : 4PLB
Title : Crystal Structure of S.A. gyrase-AM8191 complex
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Deposited on : 2014-05-16
Resolution : 2.69 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 ⓘ 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

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11503 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 DNA chain called DNA (5'-D(P*AP*GP*CP*CP*GP*TP*AP*GP*GP*GP*CP*CP*CP*TP*AP*CP*GP*GP*CP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	20	Total	C	N	O	P	0	0	0
			410	193	77	120	20			
1	F	19	Total	C	N	O	P	0	0	0
			390	183	75	113	19			

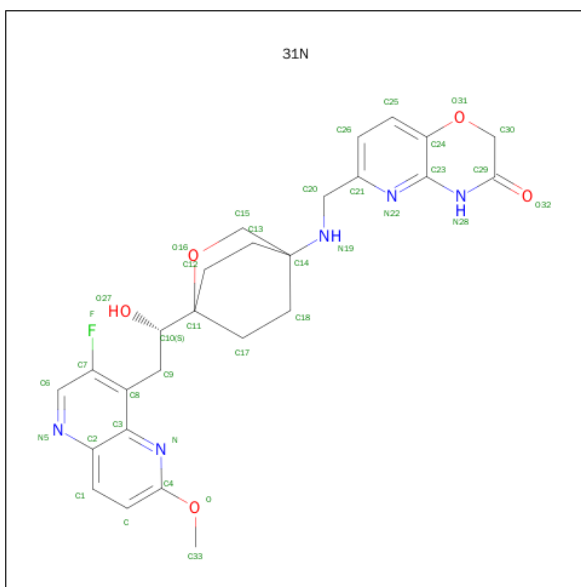
- Molecule 2 is a protein called Chimera protein of DNA gyrase subunits B and A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	672	Total	C	N	O	S	0	1	0
			5279	3288	953	1013	25			
2	D	670	Total	C	N	O	S	0	2	0
			5297	3300	952	1020	25			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	409	PRO	-	expression tag	UNP P0A0K8
B	544	THR	-	linker	UNP P0A0K8
B	545	GLY	-	linker	UNP P0A0K8
B	1123	PHE	TYR	engineered mutation	UNP P20831
B	1457	THR	ALA	engineered mutation	UNP P20831
D	409	PRO	-	expression tag	UNP P0A0K8
D	544	THR	-	linker	UNP P0A0K8
D	545	GLY	-	linker	UNP P0A0K8
D	1123	PHE	TYR	engineered mutation	UNP P20831
D	1457	THR	ALA	engineered mutation	UNP P20831

- Molecule 3 is 6-[(1r,4S)-1-[(1S)-2-(3-fluoro-6-methoxy-1,5-naphthyridin-4-yl)-1-hydroxyethyl]-2-oxabicyclo[2.2.2]oct-4-yl]amino)methyl]-2H-pyrido[3,2-b][1,4]oxazin-3(4H)-one (three-letter code: 31N) (formula: C₂₆H₂₈FN₅O₅).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	F	1	Total	C	F	N	O	0	0
			37	26	1	5	5		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total 1	Mn 1	0	0
5	D	1	Total 1	Mn 1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	E	9	Total 9	O 9	0	0
6	F	5	Total 5	O 5	0	0
6	B	32	Total 32	O 32	0	0
6	D	27	Total 27	O 27	0	0

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.

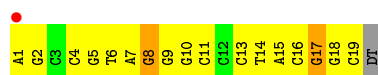
- Molecule 1: DNA (5'-D(P*AP*GP*CP*CP*GP*TP*AP*GP*GP*GP*CP*CP*CP*TP*AP*CP*GP*GP*CP*T)-3')

Chain E: 




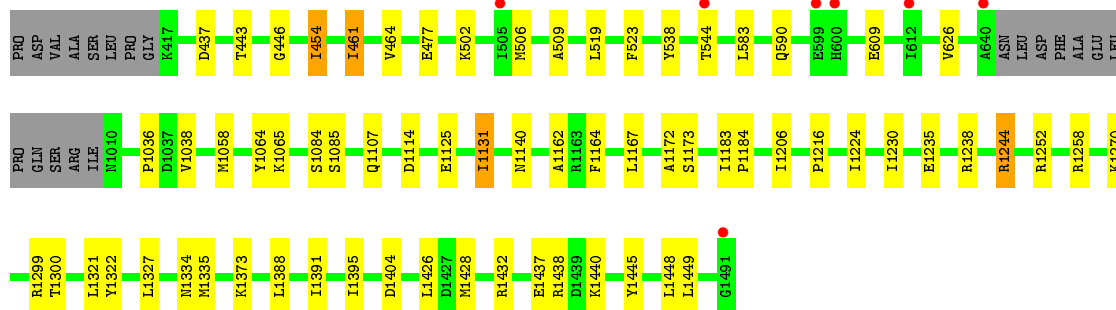
- Molecule 1: DNA (5'-D(P*AP*GP*CP*CP*GP*TP*AP*GP*GP*GP*CP*CP*CP*TP*AP*CP*GP*GP*CP*T)-3')

Chain F: 




- Molecule 2: Chimera protein of DNA gyrase subunits B and A

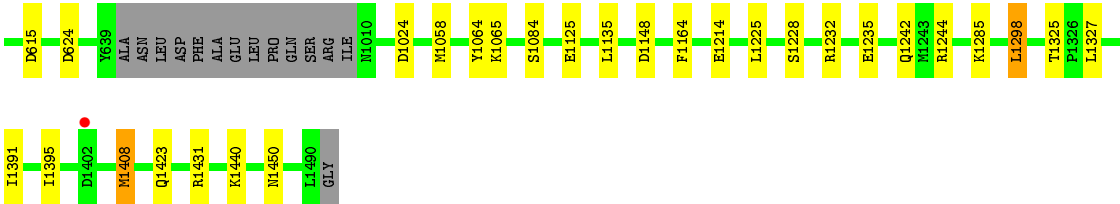
Chain B: 



- Molecule 2: Chimera protein of DNA gyrase subunits B and A

Chain D: 





4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	93.31Å 93.31Å 410.20Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	27.12 – 2.69 27.08 – 2.69	Depositor EDS
% Data completeness (in resolution range)	99.6 (27.12-2.69) 100.0 (27.08-2.69)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.49 (at 2.68Å)	Xtriage
Refinement program	BUSTER 2.9.7	Depositor
R, R_{free}	0.176 , 0.220 0.179 , 0.218	Depositor DCC
R_{free} test set	2812 reflections (5.34%)	DCC
Wilson B-factor (Å ²)	49.3	Xtriage
Anisotropy	0.181	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 40.0	EDS
Estimated twinning fraction	0.064 for h,-h-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 55447 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	11503	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.22% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MN, SO4, 31N

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	E	1.17	0/459	2.13	26/706 (3.7%)
1	F	1.16	0/437	2.13	28/672 (4.2%)
2	B	0.53	0/5351	0.72	0/7218
2	D	0.52	0/5369	0.73	0/7241
All	All	0.60	0/11616	0.93	54/15837 (0.3%)

There are no bond length outliers.

The worst 5 of 54 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	10	DG	P-O3'-C3'	10.03	131.73	119.70
1	E	6	DT	O4'-C1'-N1	9.96	114.97	108.00
1	F	16	DC	O4'-C4'-C3'	-9.75	100.15	106.00
1	E	13	DC	O4'-C1'-N1	8.99	114.29	108.00
1	E	9	DG	O4'-C4'-C3'	-8.89	100.67	106.00

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	E	410	0	224	1	0
1	F	390	0	212	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	5279	0	5266	31	0
2	D	5297	0	5293	19	0
3	F	37	0	28	0	0
4	B	5	0	0	0	0
4	D	10	0	0	0	0
5	B	1	0	0	0	0
5	D	1	0	0	0	0
6	B	32	0	0	0	0
6	D	27	0	0	0	0
6	E	9	0	0	0	0
6	F	5	0	0	0	0
All	All	11503	0	11023	48	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.

The worst 5 of 48 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:B:461:ILE:HD11	2:B:477:GLU:HB3	1.73	0.71
2:B:1058:MET:HG2	2:B:1065:LYS:HG3	1.72	0.69
2:B:461:ILE:HG22	2:B:519:LEU:HB3	1.78	0.66
2:B:1238[B]:ARG:HE	2:B:1334:ASN:ND2	1.99	0.60
2:B:443:THR:HG22	2:B:454:ILE:HG12	1.87	0.56

There are no symmetry-related clashes.

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
2	B	669/692 (97%)	648 (97%)	20 (3%)	1 (0%)	56 83

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	668/692 (96%)	650 (97%)	18 (3%)	0	100	100
All	All	1337/1384 (97%)	1298 (97%)	38 (3%)	1 (0%)	56	83

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	1162	ALA

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	
2	B	561/591 (95%)	546 (97%)	15 (3%)	52	82
2	D	567/591 (96%)	548 (97%)	19 (3%)	44	75
All	All	1128/1182 (95%)	1094 (97%)	34 (3%)	48	79

5 of 34 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	442	SER
2	D	615	ASP
2	D	1408	MET
2	D	476	ASN
2	B	1131	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	1334	ASN
2	D	590	GLN
2	D	1242	GLN
2	B	1324	GLN
2	D	605	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 ⓘ

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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	$\# Z > 2$
4	SO4	B	1501	-	4,4,4	0.40	0	6,6,6	0.12	0
4	SO4	D	1501	-	4,4,4	0.51	0	6,6,6	0.17	0
4	SO4	D	1502	-	4,4,4	0.80	0	6,6,6	0.28	0
3	31N	F	101	-	38,42,42	1.23	5 (13%)	37,63,63	1.79	11 (29%)

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
4	SO4	B	1501	-	-	0/0/0/0	0/0/0/0
4	SO4	D	1501	-	-	0/0/0/0	0/0/0/0
4	SO4	D	1502	-	-	0/0/0/0	0/0/0/0
3	31N	F	101	-	-	0/16/48/48	0/4/6/6

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	101	31N	C3-C2	-2.48	1.39	1.42
3	F	101	31N	C9-C8	-2.27	1.48	1.51
3	F	101	31N	C1-C2	-2.02	1.38	1.41
3	F	101	31N	C4-N	2.49	1.34	1.30
3	F	101	31N	O-C4	3.11	1.40	1.35

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	101	31N	C33-O-C4	-4.24	111.62	117.38
3	F	101	31N	C6-C7-C8	-2.80	118.06	123.45
3	F	101	31N	C1-C2-C3	-2.53	116.85	119.48
3	F	101	31N	C-C4-N	-2.40	122.62	125.39
3	F	101	31N	O27-C10-C9	-2.26	103.68	109.19

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 [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	E	20/20 (100%)	-0.76	0 100 100	31, 43, 52, 61	0
1	F	19/20 (95%)	-0.37	1 (5%) 30 28	33, 41, 67, 93	0
2	B	672/692 (97%)	-0.21	7 (1%) 84 85	32, 48, 67, 87	0
2	D	670/692 (96%)	-0.22	7 (1%) 84 85	33, 49, 68, 83	0
All	All	1381/1424 (96%)	-0.22	15 (1%) 82 83	31, 48, 67, 93	0

The worst 5 of 15 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	1491	GLY	3.9
2	D	491	GLY	3.2
2	B	612	ILE	3.0
2	B	640	ALA	3.0
2	D	518	THR	2.8

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](#)

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	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	31N	F	101	37/37	0.91	0.18	1.39	42,57,66,66	0
4	SO4	D	1502	5/5	0.91	0.31	1.04	107,111,112,113	0
5	MN	B	1502	1/1	0.99	0.14	-0.27	50,50,50,50	0
5	MN	D	1503	1/1	0.99	0.10	-0.97	47,47,47,47	0
4	SO4	D	1501	5/5	0.94	0.12	-	88,93,93,94	0
4	SO4	B	1501	5/5	0.89	0.18	-	107,111,112,112	0

6.5 Other polymers [i](#)

There are no such residues in this entry.