



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 12:52 am GMT

PDB ID : 5BS3
Title : Crystal Structure of S.A. gyrase in complex with Compound 7
Authors : Lu, J.; Patel, S.; Soisson, S.
Deposited on : 2015-06-01
Resolution : 2.65 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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : recalc28949

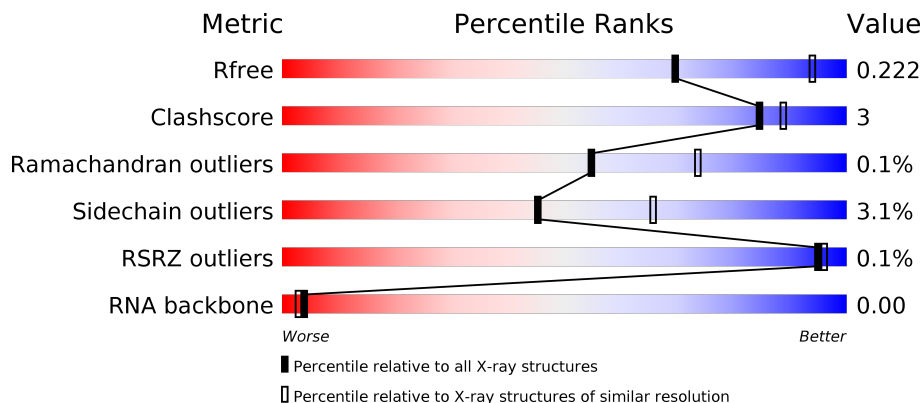
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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}	100719	3491 (2.70-2.62)
Clashscore	112137	1026 (2.68-2.64)
Ramachandran outliers	110173	1010 (2.68-2.64)
Sidechain outliers	110143	1010 (2.68-2.64)
RSRZ outliers	101464	3511 (2.70-2.62)
RNA backbone	2435	1055 (3.02-2.30)

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	B	692	<div> <div>89%</div> <div>8%</div> <div>.</div> </div>
1	D	692	<div> <div>86%</div> <div>10%</div> <div>.</div> </div>
2	E	20	<div> <div>20%</div> <div>70%</div> <div>10%</div> </div>
2	F	20	<div> <div>25%</div> <div>60%</div> <div>10%</div> <div>5%</div> </div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11537 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 and B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	670	Total	C	N	O	S	0	0	0
			5262	3280	948	1009	25			
1	D	670	Total	C	N	O	S	0	2	0
			5284	3292	952	1015	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 2 is a RNA chain called DNA/RNA (5'-R(P*AP*GP*CP*CP*G)-D(P*T)-R(P*A P*GP*GP*GP*CP*CP*C)-D(P*T)-R(P*AP*CP*GP*GP*C)-D(P*T)-3').

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

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

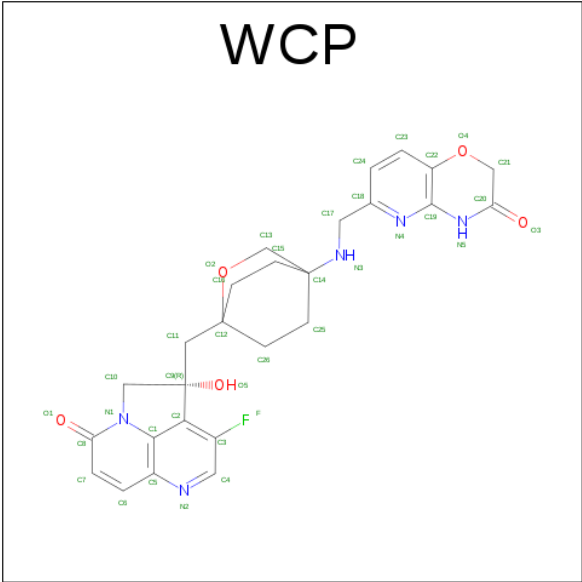
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Mn	0	0
			1	1		
3	D	1	Total	Mn	0	0
			1	1		

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



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

- Molecule 5 is (4R)-3-fluoro-4-hydroxy-4-{[(1r,4R)-4-{[(3-oxo-3,4-dihydro-2H-pyrido[3,2-b][1,4]oxazin-6-yl)methyl]amino}-2-oxabicyclo[2.2.2]oct-1-yl)methyl}-4,5-dihydro-7H-pyrrolo[3,2,1-de][1,5]naphthyridin-7-one (three-letter code: WCP) (formula: C₂₆H₂₆FN₅O₅).

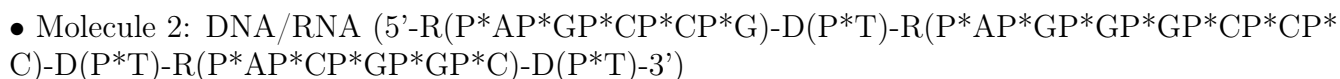
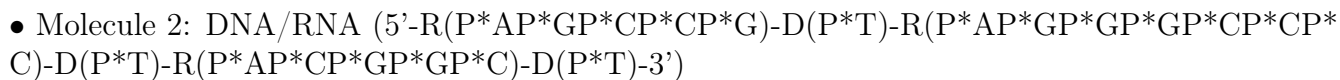


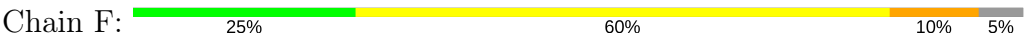
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	F	1	Total	C	F	N	O	0	0
			37	26	1	5	5		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	58	Total	O	0	0
			58	58		
6	D	61	Total	O	0	0
			61	61		
6	E	8	Total	O	0	0
			8	8		
6	F	10	Total	O	0	0
			10	10		

- Molecule 1: DNA gyrase subunit A and B





4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	93.34Å 93.34Å 411.07Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	26.71 – 2.65 26.44 – 2.65	Depositor EDS
% Data completeness (in resolution range)	100.0 (26.71-2.65) 100.0 (26.44-2.65)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.32 (at 2.64Å)	Xtriage
Refinement program	BUSTER 2.9.7	Depositor
R, R_{free}	0.170 , 0.213 0.179 , 0.222	Depositor DCC
R_{free} test set	2952 reflections (5.33%)	DCC
Wilson B-factor (Å ²)	45.7	Xtriage
Anisotropy	0.081	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 19.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.165 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	11537	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.58% 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](#)

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

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	B	0.50	0/5333	0.71	0/7193
1	D	0.51	0/5355	0.72	0/7223
2	E	1.14	0/459	2.10	26/706 (3.7%)
2	F	1.08	0/437	1.97	16/672 (2.4%)
All	All	0.57	0/11584	0.91	42/15794 (0.3%)

There are no bond length outliers.

The worst 5 of 42 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	6	DT	O4'-C1'-N1	8.16	113.71	108.00
2	F	17	G	O4'-C1'-N9	-8.13	101.70	108.20
2	F	14	DT	O4'-C1'-N1	8.11	113.68	108.00
2	F	2	G	O4'-C1'-N9	8.05	114.64	108.20
2	E	1	A	OP1-P-OP2	-7.30	108.64	119.60

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	B	5262	0	5256	24	0
1	D	5284	0	5273	38	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	410	0	224	2	0
2	F	390	0	212	3	0
3	B	1	0	0	0	0
3	D	1	0	0	0	0
4	D	5	0	0	0	0
4	E	5	0	0	0	0
4	F	5	0	0	0	0
5	F	37	0	26	5	0
6	B	58	0	0	0	0
6	D	61	0	0	0	0
6	E	8	0	0	0	0
6	F	10	0	0	0	0
All	All	11537	0	10991	61	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 3.

The worst 5 of 61 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:1058:MET:HG2	1:B:1065:LYS:HG3	1.74	0.68
5:F:101:WCP:H19	5:F:101:WCP:C10	2.25	0.66
1:D:1058:MET:HG2	1:D:1065:LYS:HG3	1.77	0.66
1:B:1403:THR:HG22	1:D:1436:LEU:HD22	1.78	0.64
5:F:101:WCP:H27	5:F:101:WCP:H19	1.83	0.61

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	
1	B	664/692 (96%)	642 (97%)	22 (3%)	0	100	100
1	D	666/692 (96%)	643 (96%)	22 (3%)	1 (0%)	51	69
All	All	1330/1384 (96%)	1285 (97%)	44 (3%)	1 (0%)	55	73

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	490	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	B	561/591 (95%)	541 (96%)	20 (4%)	40	59
1	D	564/591 (95%)	549 (97%)	15 (3%)	50	71
All	All	1125/1182 (95%)	1090 (97%)	35 (3%)	45	66

5 of 35 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1327	LEU
1	B	1448	LEU
1	D	1413	GLN
1	B	1344	LYS
1	B	1396	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	1010	ASN
1	B	1153	ASN
1	D	605	GLN
1	B	631	GLN
1	D	590	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	E	0/20	-	-
2	F	0/20	-	-
All	All	0/40	-	-

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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	D	1502	-	4,4,4	0.23	0	6,6,6	0.06	0
4	SO4	E	101	-	4,4,4	0.42	0	6,6,6	0.19	0
5	WCP	F	101	-	39,43,43	2.49	11 (28%)	29,68,68	1.69	6 (20%)
4	SO4	F	102	-	4,4,4	0.38	0	6,6,6	0.14	0

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	D	1502	-	-	0/0/0/0	0/0/0/0
4	SO4	E	101	-	-	0/0/0/0	0/0/0/0
5	WCP	F	101	-	-	1/12/53/53	0/4/7/7
4	SO4	F	102	-	-	0/0/0/0	0/0/0/0

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	101	WCP	C25-C14	2.06	1.56	1.53
5	F	101	WCP	C22-C19	2.58	1.44	1.41
5	F	101	WCP	C8-N1	2.59	1.42	1.38
5	F	101	WCP	C6-C5	3.24	1.47	1.41
5	F	101	WCP	C15-C14	3.27	1.57	1.53

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	101	WCP	C19-N5-C20	-3.62	121.33	124.48
5	F	101	WCP	C1-C5-N2	-3.36	118.93	122.55
5	F	101	WCP	O5-C9-C2	-3.25	103.78	111.89
5	F	101	WCP	N5-C19-N4	2.48	119.50	116.33
5	F	101	WCP	C9-C2-C3	3.28	135.99	131.17

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	F	101	WCP	C2-C9-C11-C12

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	F	101	WCP	5	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1
1	D	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	545:GLY	C	580:TYR	N	3.23
1	B	545:GLY	C	580:TYR	N	3.08

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	B	670/692 (96%)	-0.16	1 (0%) 95 96	28, 46, 62, 76	0
1	D	670/692 (96%)	-0.15	1 (0%) 95 96	30, 45, 65, 81	0
2	E	20/20 (100%)	-0.74	0 100 100	30, 39, 51, 57	0
2	F	19/20 (95%)	-0.57	0 100 100	33, 39, 60, 85	0
All	All	1379/1424 (96%)	-0.17	2 (0%) 95 96	28, 45, 64, 85	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1433	LEU	2.1
1	D	490	GLY	2.1

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
5	WCP	F	101	37/37	0.90	0.20	1.60	42,50,65,67	0
4	SO4	E	101	5/5	0.91	0.15	1.43	101,106,106,107	0
3	MN	B	1501	1/1	1.00	0.17	0.98	45,45,45,45	0
4	SO4	F	102	5/5	0.92	0.14	0.44	93,97,98,98	0
3	MN	D	1501	1/1	0.98	0.16	0.03	44,44,44,44	0
4	SO4	D	1502	5/5	0.96	0.15	-	128,132,133,134	0

6.5 Other polymers [i](#)

There are no such residues in this entry.