



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 10, 2017 – 02:35 PM EDT

PDB ID : 2NOV
Title : Breakage-reunion domain of S.pneumoniae topo IV: crystal structure of a gram-positive quinolone target
Authors : Laponogov, I.; Veselkov, D.A.; Sohi, M.K.; Pan, X.S.; Achari, A.; Yang, C.; Ferrara, J.D.; Fisher, L.M.; Sanderson, M.R.
Deposited on : unknown
Resolution : 2.67 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
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030345
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)	:	rb-20030345

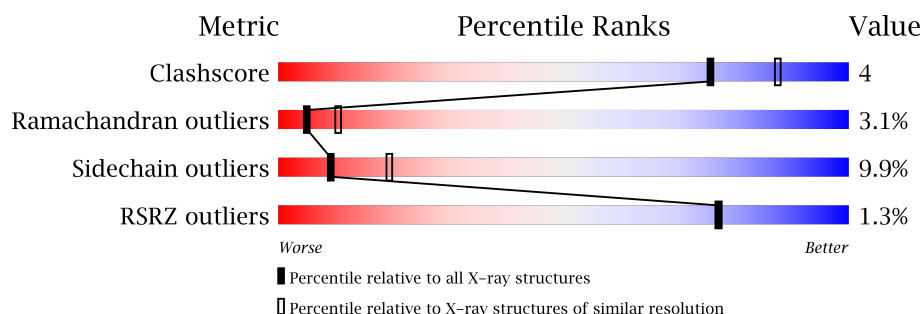
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.67 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))
Clashscore	112137	3418 (2.70-2.66)
Ramachandran outliers	110173	3367 (2.70-2.66)
Sidechain outliers	110143	3367 (2.70-2.66)
RSRZ outliers	101464	3069 (2.70-2.66)

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	496	<div> <div style="width: 73%;"></div> <div style="width: 14%;"></div> <div style="width: 11%;"></div> </div>
1	B	496	<div> <div style="width: 73%;"></div> <div style="width: 15%;"></div> <div style="width: 9%;"></div> </div>
1	C	496	<div> <div style="width: 75%;"></div> <div style="width: 15%;"></div> <div style="width: 9%;"></div> </div>
1	D	496	<div> <div style="width: 73%;"></div> <div style="width: 13%;"></div> <div style="width: 11%;"></div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 13644 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 topoisomerase 4 subunit A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	440	Total	C	N	O	S	0	0	0
			3368	2128	576	652	12			
1	B	451	Total	C	N	O	S	0	0	0
			3458	2179	591	675	13			
1	C	451	Total	C	N	O	S	0	0	0
			3456	2180	592	671	13			
1	D	440	Total	C	N	O	S	0	0	0
			3338	2099	575	652	12			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	257	THR	ILE	CONFLICT	UNP P72525
A	489	LEU	ILE	CONFLICT	UNP P72525
A	491	HIS	-	EXPRESSION TAG	UNP P72525
A	492	HIS	-	EXPRESSION TAG	UNP P72525
A	493	HIS	-	EXPRESSION TAG	UNP P72525
A	494	HIS	-	EXPRESSION TAG	UNP P72525
A	495	HIS	-	EXPRESSION TAG	UNP P72525
A	496	HIS	-	EXPRESSION TAG	UNP P72525
B	257	THR	ILE	CONFLICT	UNP P72525
B	489	LEU	ILE	CONFLICT	UNP P72525
B	491	HIS	-	EXPRESSION TAG	UNP P72525
B	492	HIS	-	EXPRESSION TAG	UNP P72525
B	493	HIS	-	EXPRESSION TAG	UNP P72525
B	494	HIS	-	EXPRESSION TAG	UNP P72525
B	495	HIS	-	EXPRESSION TAG	UNP P72525
B	496	HIS	-	EXPRESSION TAG	UNP P72525
C	257	THR	ILE	CONFLICT	UNP P72525
C	489	LEU	ILE	CONFLICT	UNP P72525
C	491	HIS	-	EXPRESSION TAG	UNP P72525
C	492	HIS	-	EXPRESSION TAG	UNP P72525
C	493	HIS	-	EXPRESSION TAG	UNP P72525

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Chain	Residue	Modelled	Actual	Comment	Reference
C	494	HIS	-	EXPRESSION TAG	UNP P72525
C	495	HIS	-	EXPRESSION TAG	UNP P72525
C	496	HIS	-	EXPRESSION TAG	UNP P72525
D	257	THR	ILE	CONFLICT	UNP P72525
D	489	LEU	ILE	CONFLICT	UNP P72525
D	491	HIS	-	EXPRESSION TAG	UNP P72525
D	492	HIS	-	EXPRESSION TAG	UNP P72525
D	493	HIS	-	EXPRESSION TAG	UNP P72525
D	494	HIS	-	EXPRESSION TAG	UNP P72525
D	495	HIS	-	EXPRESSION TAG	UNP P72525
D	496	HIS	-	EXPRESSION TAG	UNP P72525

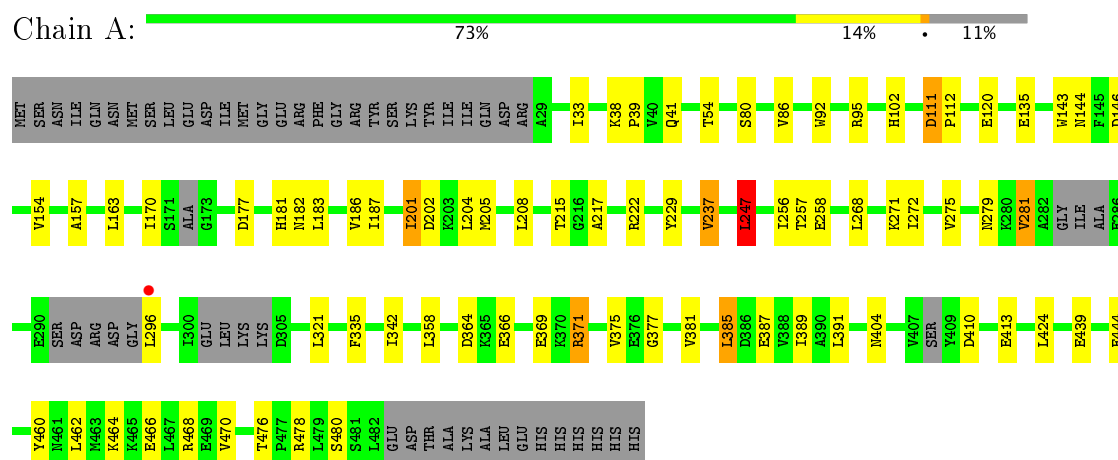
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	6	Total O 6 6	0	0
2	B	7	Total O 7 7	0	0
2	C	8	Total O 8 8	0	0
2	D	3	Total O 3 3	0	0

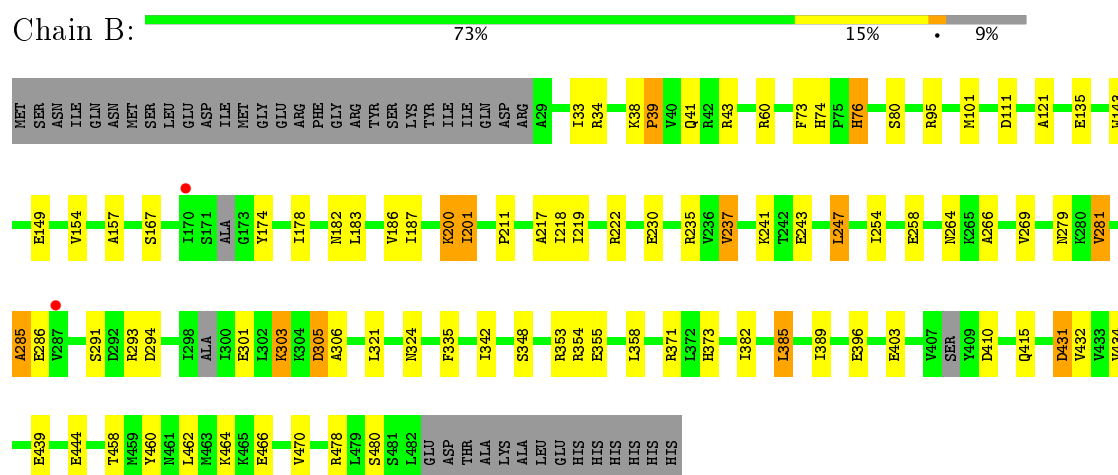
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

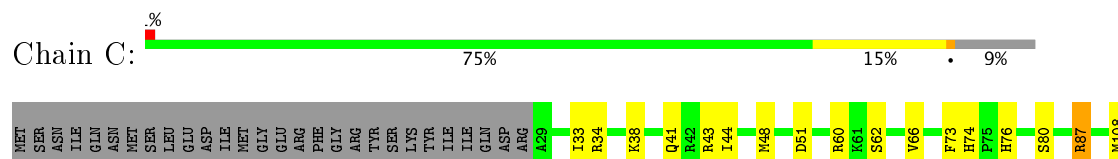
• Molecule 1: DNA topoisomerase 4 subunit A

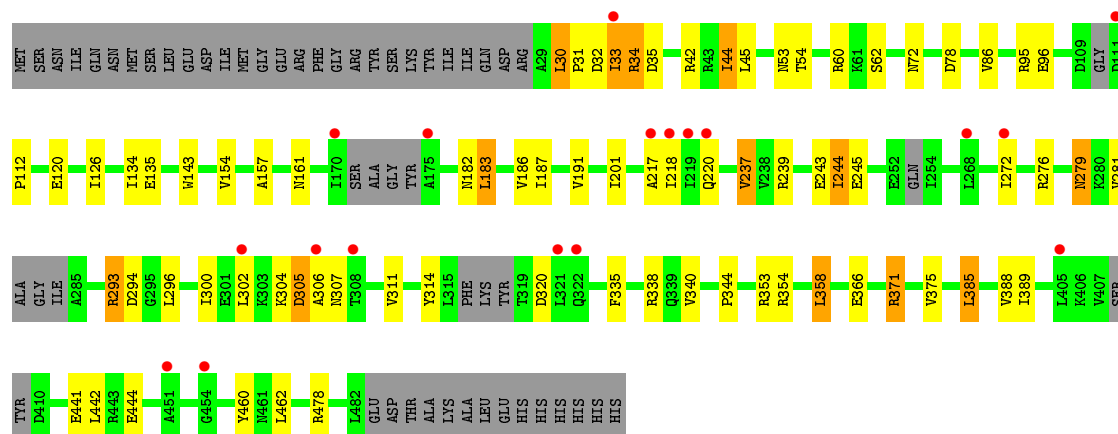


• Molecule 1: DNA topoisomerase 4 subunit A



• Molecule 1: DNA topoisomerase 4 subunit A





4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	136.92Å 137.85Å 326.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	500.00 – 2.67 19.53 – 2.68	Depositor EDS
% Data completeness (in resolution range)	97.2 (500.00-2.67) 97.3 (19.53-2.68)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.26 (at 2.67Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.224 , 0.276 (Not available) , (Not available)	Depositor DCC
R_{free} test set	NotAvailable	DCC
Wilson B-factor (Å ²)	61.1	Xtriage
Anisotropy	0.257	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	(Not available) , (Not available)	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.307 for k,h,-l	Xtriage
Reported twinning fraction	0.323 for k,-h,l	Depositor
Outliers	3 of 85700 reflections (0.004%)	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	13644	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.37% 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](#)

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	0.65	0/3418	0.79	1/4621 (0.0%)
1	B	0.64	0/3510	0.80	1/4744 (0.0%)
1	C	0.65	0/3509	0.80	2/4747 (0.0%)
1	D	0.64	0/3385	0.78	0/4583
All	All	0.64	0/13822	0.79	4/18695 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	247	LEU	CA-CB-CG	6.73	130.77	115.30
1	B	247	LEU	CA-CB-CG	6.21	129.58	115.30
1	C	462	LEU	CA-CB-CG	5.71	128.43	115.30
1	C	236	VAL	N-CA-C	5.43	125.67	111.00

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	A	3368	0	3260	25	0
1	B	3458	0	3349	23	0
1	C	3456	0	3358	28	0
1	D	3338	0	3184	21	0
2	A	6	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	7	0	0	0	0
2	C	8	0	0	0	0
2	D	3	0	0	0	0
All	All	13644	0	13151	97	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 4.

The worst 5 of 97 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:A:38:LYS:H	1:A:41:GLN:HE21	1.05	0.98
1:C:33:ILE:HD11	1:C:333:ASP:HB3	1.68	0.76
1:C:38:LYS:H	1:C:41:GLN:HE21	1.30	0.76
1:A:38:LYS:H	1:A:41:GLN:NE2	1.85	0.74
1:B:264:ASN:HD22	1:B:266:ALA:HB3	1.52	0.74

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	A	428/496 (86%)	386 (90%)	31 (7%)	11 (3%)	6	14
1	B	443/496 (89%)	400 (90%)	26 (6%)	17 (4%)	4	7
1	C	445/496 (90%)	392 (88%)	43 (10%)	10 (2%)	8	18
1	D	426/496 (86%)	357 (84%)	53 (12%)	16 (4%)	4	7
All	All	1742/1984 (88%)	1535 (88%)	153 (9%)	54 (3%)	5	10

5 of 54 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	157	ALA
1	A	279	ASN
1	A	335	PHE
1	B	76	HIS
1	B	174	TYR

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	346/431 (80%)	312 (90%)	34 (10%)	9	20
1	B	357/431 (83%)	316 (88%)	41 (12%)	6	14
1	C	358/431 (83%)	331 (92%)	27 (8%)	16	34
1	D	337/431 (78%)	301 (89%)	36 (11%)	8	16
All	All	1398/1724 (81%)	1260 (90%)	138 (10%)	9	19

5 of 138 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	355	GLU
1	C	87	ARG
1	D	358	LEU
1	B	371	ARG
1	B	439	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	326	ASN
1	C	72	ASN
1	D	72	ASN
1	B	423	GLN
1	C	41	GLN

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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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	A	440/496 (88%)	-0.15	1 (0%) 94 96	33, 60, 88, 105	0
1	B	451/496 (90%)	-0.12	2 (0%) 92 93	30, 60, 93, 104	0
1	C	451/496 (90%)	-0.16	3 (0%) 87 88	21, 52, 83, 97	0
1	D	440/496 (88%)	0.22	18 (4%) 38 36	54, 81, 109, 123	0
All	All	1782/1984 (89%)	-0.05	24 (1%) 77 77	21, 65, 96, 123	0

The worst 5 of 24 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	302	LEU	4.5
1	D	272	ILE	3.8
1	D	308	THR	3.6
1	D	306	ALA	3.3
1	D	218	ILE	3.2

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](#)

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.