



wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 6, 2017 – 05:22 PM EST

PDB ID : 4JUO
Title : A low-resolution three-gate structure of topoisomerase IV from *Streptococcus pneumoniae* in space group H32
Authors : Laponogov, I.; Veselkov, D.A.; Pan, X.-S.; Crevel, I.; Fisher, L.M.; Sanderson, M.R.
Deposited on : unknown
Resolution : 6.53 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	:	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

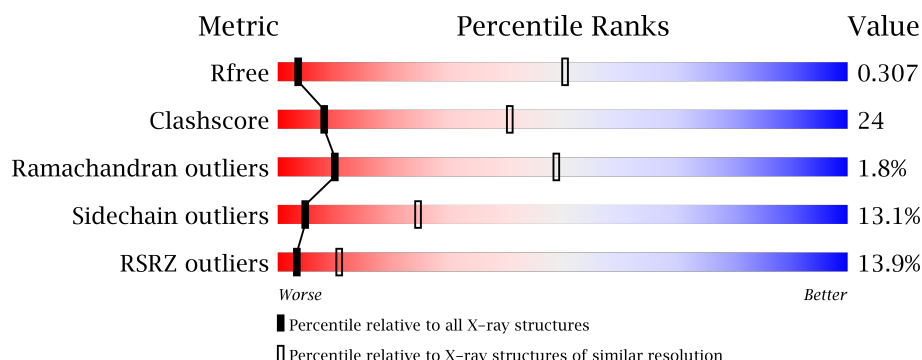
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 6.53 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.



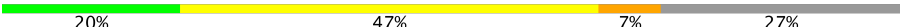
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	1098 (9.00-3.70)
Clashscore	112137	1031 (9.00-3.80)
Ramachandran outliers	110173	1000 (9.00-3.76)
Sidechain outliers	110143	1096 (9.00-3.70)
RSRZ outliers	101464	1000 (9.00-3.72)

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>6%</div> <div>65%</div> <div>28%</div> <div>• •</div> </div>
2	C	670	<div> <div>17%</div> <div>51%</div> <div>23%</div> <div>7%</div> <div>19%</div> </div>
3	E	11	<div> <div>18%</div> <div>36%</div> <div>9%</div> <div>36%</div> </div>
4	F	15	<div> <div>7%</div> <div>20%</div> <div>33%</div> <div>20%</div> <div>27%</div> </div>
5	G	11	<div> <div>36%</div> <div>27%</div> <div>36%</div> </div>

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Mol	Chain	Length	Quality of chain
6	H	15	 <div>20% 47% 7% 27%</div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	MG	C	701	-	-	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 8283 atoms, of which 19 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	479	Total	C	N	O	S	0	1	0
			3720	2357	645	705	13			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	257	THR	ILE	CONFLICT	UNP P72525
A	489	LEU	-	EXPRESSION TAG	UNP P72525
A	490	GLU	-	EXPRESSION TAG	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

- Molecule 2 is a protein called DNA topoisomerase 4 subunit B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	546	Total	C	N	O	S	0	0	0
			3786	2407	653	719	7			

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-22	MET	-	EXPRESSION TAG	UNP Q59961
C	-21	GLY	-	EXPRESSION TAG	UNP Q59961
C	-20	HIS	-	EXPRESSION TAG	UNP Q59961
C	-19	HIS	-	EXPRESSION TAG	UNP Q59961
C	-18	HIS	-	EXPRESSION TAG	UNP Q59961
C	-17	HIS	-	EXPRESSION TAG	UNP Q59961
C	-16	HIS	-	EXPRESSION TAG	UNP Q59961

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-15	HIS	-	EXPRESSION TAG	UNP Q59961
C	-14	HIS	-	EXPRESSION TAG	UNP Q59961
C	-13	HIS	-	EXPRESSION TAG	UNP Q59961
C	-12	HIS	-	EXPRESSION TAG	UNP Q59961
C	-11	HIS	-	EXPRESSION TAG	UNP Q59961
C	-10	SER	-	EXPRESSION TAG	UNP Q59961
C	-9	SER	-	EXPRESSION TAG	UNP Q59961
C	-8	GLY	-	EXPRESSION TAG	UNP Q59961
C	-7	HIS	-	EXPRESSION TAG	UNP Q59961
C	-6	ILE	-	EXPRESSION TAG	UNP Q59961
C	-5	ASP	-	EXPRESSION TAG	UNP Q59961
C	-4	ASP	-	EXPRESSION TAG	UNP Q59961
C	-3	ASP	-	EXPRESSION TAG	UNP Q59961
C	-2	ASP	-	EXPRESSION TAG	UNP Q59961
C	-1	LYS	-	EXPRESSION TAG	UNP Q59961
C	0	HIS	-	EXPRESSION TAG	UNP Q59961
C	217	ASP	ASN	CONFLICT	UNP Q59961
C	460	ILE	VAL	CONFLICT	UNP Q59961
C	644	ALA	THR	CONFLICT	UNP Q59961

- Molecule 3 is a DNA chain called E-site DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	7	Total	C	N	O	P	0	7	0
			140	69	27	38	6			

- Molecule 4 is a DNA chain called E-site DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	11	Total	C	N	O	P	0	11	0
			225	108	39	67	11			

- Molecule 5 is a DNA chain called E-site DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	G	7	Total	C	N	O	P	0	7	0
			139	68	25	40	6			

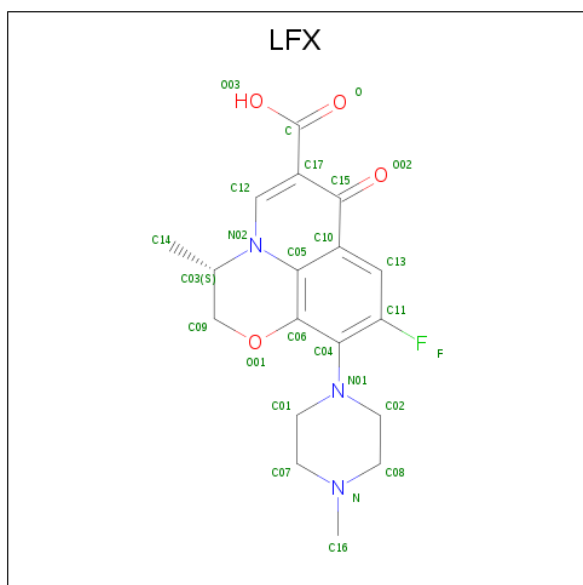
- Molecule 6 is a DNA chain called E-site DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	H	11	Total	C	N	O	P	0	11	0
			226	107	43	65	11			

- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Mg	0	0
			1	1		
7	C	1	Total	Mg	0	0
			1	1		

- Molecule 8 is (3S)-9-fluoro-3-methyl-10-(4-methylpiperazin-1-yl)-7-oxo-2,3-dihydro-7H-[1,4]oxazino[2,3,4-ij]quinoline-6-carboxylic acid (three-letter code: LFX) (formula: C₁₈H₂₀FN₃O₄).





4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	213.58Å 213.58Å 211.83Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.44 – 6.53 53.40 – 6.53	Depositor EDS
% Data completeness (in resolution range)	99.1 (46.44-6.53) 99.3 (53.40-6.53)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.83 (at 6.69Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.247 , 0.298 0.238 , 0.307	Depositor DCC
R_{free} test set	169 reflections (4.57%)	DCC
Wilson B-factor (Å ²)	378.8	Xtriage
Anisotropy	0.474	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 304.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.82	EDS
Total number of atoms	8283	wwPDB-VP
Average B, all atoms (Å ²)	183.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.55% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, LFX

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	0.45	0/3779	0.63	1/5109 (0.0%)
2	C	0.39	0/3845	0.63	2/5251 (0.0%)
3	E	0.88	0/157	1.64	3/241 (1.2%)
4	F	0.83	0/251	1.80	12/385 (3.1%)
5	G	0.76	0/155	1.42	1/238 (0.4%)
6	H	0.75	0/253	1.67	3/388 (0.8%)
All	All	0.47	0/8440	0.81	22/11612 (0.2%)

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
2	C	0	1

There are no bond length outliers.

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	H	10[B]	DC	O4'-C4'-C3'	-11.97	98.82	106.00
4	F	1[A]	DA	O4'-C1'-N9	10.86	115.60	108.00
3	E	10[A]	DA	O4'-C1'-N9	8.04	113.63	108.00
6	H	1[B]	DG	O4'-C1'-N9	7.95	113.56	108.00
4	F	3[A]	DT	O4'-C4'-C3'	-7.89	101.26	106.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	102	LEU	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	3720	0	3629	179	0
2	C	3786	0	3303	181	0
3	E	140	0	71	3	0
4	F	225	0	116	5	0
5	G	139	0	71	1	0
6	H	226	0	115	8	0
7	A	1	0	0	0	0
7	C	1	0	0	0	0
8	F	26	19	19	1	0
All	All	8264	19	7324	368	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 24.

The worst 5 of 368 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:C:583:LEU:HB3	2:C:586:MET:CE	1.24	1.67
2:C:583:LEU:CB	2:C:586:MET:CE	1.75	1.56
2:C:583:LEU:CB	2:C:586:MET:HE3	1.28	1.53
2:C:583:LEU:HD22	2:C:586:MET:CE	1.56	1.35
2:C:583:LEU:CD2	2:C:586:MET:CE	2.06	1.32

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	468/496 (94%)	443 (95%)	20 (4%)	5 (1%)	17	60
2	C	524/670 (78%)	455 (87%)	56 (11%)	13 (2%)	6	41
All	All	992/1166 (85%)	898 (90%)	76 (8%)	18 (2%)	10	49

5 of 18 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	305	THR
2	C	373	GLU
1	A	145	PHE
1	A	329	MET
2	C	105	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	377/431 (88%)	348 (92%)	29 (8%)	15	47
2	C	313/558 (56%)	252 (80%)	61 (20%)	1	10
All	All	690/989 (70%)	600 (87%)	90 (13%)	5	25

5 of 90 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	100	THR
2	C	208	THR
2	C	509	THR
2	C	102	LEU
2	C	148	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	328	ASN
2	C	477	ASN
2	C	51	ASN
1	A	267	ASN
1	A	423	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](#)

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 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	$\# Z > 2$
8	LFX	F	101	7	21,29,29	1.70	2 (9%)	27,44,44	1.84	9 (33%)

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
8	LFX	F	101	7	-	0/4/27/27	0/3/4/4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	F	101	LFX	O02-C15	3.57	1.29	1.23
8	F	101	LFX	C15-C10	6.40	1.50	1.41

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	F	101	LFX	C17-C15-C10	-5.32	112.63	122.09
8	F	101	LFX	F-C11-C04	-2.30	114.99	118.30
8	F	101	LFX	C14-C03-C09	-2.27	105.16	112.50
8	F	101	LFX	O01-C06-C04	-2.22	115.37	117.87
8	F	101	LFX	C06-C04-C11	-2.17	113.89	116.01

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	F	101	LFX	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	2
2	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	585:GLU	C	586:MET	N	3.85
1	A	384:ILE	C	385:LEU	N	2.39
1	A	455:ASP	C	456:GLU	N	2.09

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	479/496 (96%)	0.34	31 (6%) 20 24	37, 120, 215, 273	0
2	C	546/670 (81%)	0.95	116 (21%) 1 7	62, 212, 491, 533	0
3	E	7/11 (63%)	0.61	0 100 100	54, 61, 129, 144	7 (100%)
4	F	11/15 (73%)	0.81	1 (9%) 10 16	55, 92, 113, 136	11 (100%)
5	G	7/11 (63%)	0.60	0 100 100	53, 59, 129, 144	7 (100%)
6	H	11/15 (73%)	0.78	0 100 100	56, 95, 113, 134	11 (100%)
All	All	1061/1218 (87%)	0.67	148 (13%) 3 11	37, 161, 464, 533	36 (3%)

The worst 5 of 148 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	100	THR	16.7
2	C	101	ILE	12.3
2	C	99	PHE	10.7
2	C	164	THR	8.7
2	C	125	SER	8.1

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(Å ²)	Q<0.9
7	MG	C	701	1/1	0.85	0.75	1.98	71,71,71,71	0
8	LFX	F	101	26/26	0.94	0.35	-0.84	63,89,142,148	0
7	MG	A	501	1/1	0.95	0.29	-1.30	64,64,64,64	0

6.5 Other polymers [i](#)

There are no such residues in this entry.