



Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 11:30 pm BST

PDB ID : 2INR
Title : Crystal structure of a 59 kDa fragment of topoisomerase IV subunit A (GrlA) from *Staphylococcus aureus*
Authors : Carr, S.B.
Deposited on : 2006-10-09
Resolution : 2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/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	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

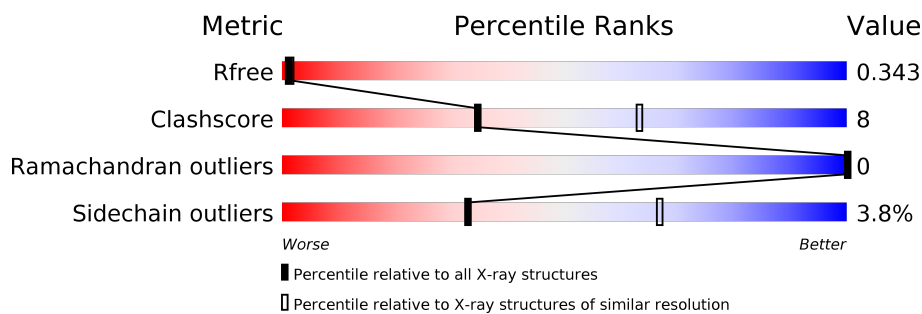
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)

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 respectively. 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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	514	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3591 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
			Total	C	N	O	S			
1	A	442	3528	2227	611	680	10	0	0	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-22	MET	-	EXPRESSION TAG	UNP Q6G9K4
A	-21	GLY	-	EXPRESSION TAG	UNP Q6G9K4
A	-20	SER	-	EXPRESSION TAG	UNP Q6G9K4
A	-19	SER	-	EXPRESSION TAG	UNP Q6G9K4
A	-18	HIS	-	EXPRESSION TAG	UNP Q6G9K4
A	-17	HIS	-	EXPRESSION TAG	UNP Q6G9K4
A	-16	HIS	-	EXPRESSION TAG	UNP Q6G9K4
A	-15	HIS	-	EXPRESSION TAG	UNP Q6G9K4
A	-14	HIS	-	EXPRESSION TAG	UNP Q6G9K4
A	-13	HIS	-	EXPRESSION TAG	UNP Q6G9K4
A	-12	SER	-	EXPRESSION TAG	UNP Q6G9K4
A	-11	SER	-	EXPRESSION TAG	UNP Q6G9K4
A	-10	GLY	-	EXPRESSION TAG	UNP Q6G9K4
A	-9	LEU	-	EXPRESSION TAG	UNP Q6G9K4
A	-8	VAL	-	EXPRESSION TAG	UNP Q6G9K4
A	-7	PRO	-	EXPRESSION TAG	UNP Q6G9K4
A	-6	ARG	-	EXPRESSION TAG	UNP Q6G9K4
A	-5	GLY	-	EXPRESSION TAG	UNP Q6G9K4
A	-4	SER	-	EXPRESSION TAG	UNP Q6G9K4
A	-3	HIS	-	EXPRESSION TAG	UNP Q6G9K4
A	-2	MET	-	EXPRESSION TAG	UNP Q6G9K4
A	-1	LEU	-	EXPRESSION TAG	UNP Q6G9K4
A	0	GLU	-	EXPRESSION TAG	UNP Q6G9K4
A	1	VAL	-	EXPRESSION TAG	UNP Q6G9K4

- Molecule 2 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		

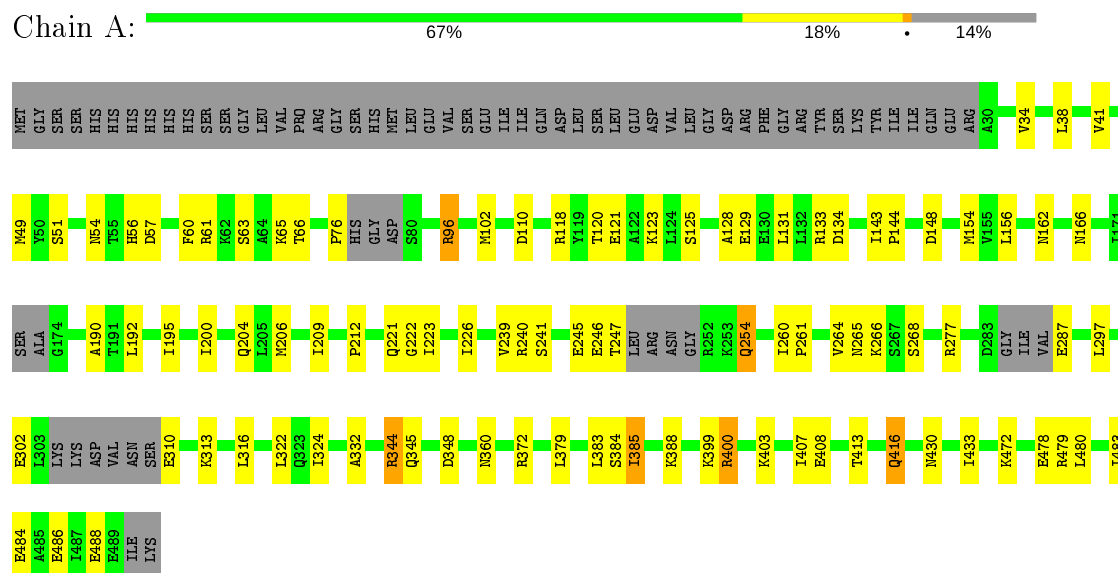
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	43	Total	O	0	0
			43	43		

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 the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	41.46 Å 171.88 Å 87.89 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.64 – 2.80 19.64 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.1 (19.64-2.80) 99.1 (19.64-2.80)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.48 (at 2.79 Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.234 , 0.283 0.310 , 0.343	Depositor DCC
R_{free} test set	802 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	64.8	Xtriage
Anisotropy	0.465	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 20.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	3591	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.73% 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: EDO

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	0.56	4/3575 (0.1%)	0.60	0/4819

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	76	PRO	C-O	12.06	1.47	1.23
1	A	254	GLN	CD-OE1	5.77	1.36	1.24
1	A	246	GLU	CD-OE1	5.22	1.31	1.25
1	A	247	THR	C-O	5.12	1.33	1.23

There are no bond angle outliers.

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	3528	0	3577	59	0
2	A	20	0	30	2	0
3	A	43	0	0	0	0
All	All	3591	0	3607	59	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 8.

All (59) 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:379:LEU:O	1:A:383:LEU:HD13	1.57	1.01
1:A:316:LEU:HD23	1:A:322:LEU:HD22	1.62	0.80
1:A:277:ARG:HG2	1:A:287:GLU:OE1	1.85	0.76
1:A:399:LYS:HG3	1:A:400:ARG:H	1.53	0.72
1:A:399:LYS:HG3	1:A:400:ARG:N	2.05	0.71
1:A:212:PRO:O	1:A:479:ARG:NH2	2.24	0.69
1:A:96:ARG:HH21	1:A:480:LEU:HG	1.58	0.69
1:A:379:LEU:O	1:A:383:LEU:CD1	2.39	0.67
1:A:110:ASP:OD1	1:A:266:LYS:HB3	1.96	0.64
1:A:125:SER:HB2	1:A:128:ALA:H	1.61	0.64
1:A:61:ARG:HH21	1:A:65:LYS:HG2	1.62	0.64
1:A:385:ILE:HG22	1:A:388:LYS:HB2	1.80	0.63
1:A:60:PHE:HB3	1:A:121:GLU:HB3	1.80	0.63
1:A:430:ASN:HA	1:A:433:ILE:HG22	1.80	0.62
1:A:125:SER:O	1:A:129:GLU:HG3	2.00	0.61
1:A:131:LEU:HD21	1:A:162:ASN:HB2	1.83	0.61
1:A:54:ASN:HB2	1:A:61:ARG:HH11	1.66	0.60
1:A:345:GLN:HB2	2:A:494:EDO:H21	1.84	0.60
1:A:277:ARG:CG	1:A:287:GLU:OE1	2.51	0.58
1:A:261:PRO:HB3	1:A:324:ILE:CG2	2.34	0.57
1:A:413:THR:H	1:A:416:GLN:HG3	1.70	0.56
1:A:316:LEU:CD2	1:A:322:LEU:HD22	2.34	0.56
1:A:63:SER:OG	1:A:120:THR:HG22	2.08	0.54
1:A:379:LEU:C	1:A:383:LEU:HD13	2.27	0.53
1:A:133:ARG:O	1:A:134:ASP:HB2	2.09	0.52
1:A:222:GLY:O	1:A:226:ILE:HG13	2.10	0.51
1:A:49:MET:HG3	1:A:66:THR:HG21	1.91	0.51
1:A:56:HIS:HA	1:A:123:LYS:HD2	1.92	0.51
1:A:400:ARG:HA	1:A:403:LYS:HE3	1.93	0.51
1:A:96:ARG:NH2	1:A:480:LEU:HG	2.26	0.50
1:A:241:SER:OG	1:A:261:PRO:HD3	2.12	0.50
1:A:254:GLN:HG3	1:A:302:GLU:HB2	1.93	0.48
1:A:239:VAL:HB	1:A:324:ILE:HG23	1.95	0.48
1:A:61:ARG:NH2	1:A:65:LYS:HG2	2.27	0.48
1:A:344:ARG:O	1:A:348:ASP:HB2	2.15	0.47
1:A:261:PRO:HB3	1:A:324:ILE:HG21	1.95	0.47
1:A:310:GLU:N	1:A:313:LYS:HZ3	2.13	0.46
1:A:407:ILE:HG13	1:A:408:GLU:N	2.29	0.46
1:A:261:PRO:HB3	1:A:324:ILE:HG22	1.97	0.46
1:A:144:PRO:HB3	1:A:148:ASP:OD1	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:261:PRO:HB2	1:A:264:VAL:HG21	1.98	0.45
1:A:102:MET:SD	1:A:120:THR:HG21	2.56	0.44
1:A:38:LEU:CD1	1:A:156:LEU:HD12	2.47	0.44
1:A:206:MET:HA	1:A:209:ILE:O	2.18	0.43
1:A:34:VAL:CG1	1:A:332:ALA:HB3	2.49	0.43
1:A:192:LEU:HA	1:A:195:ILE:HD12	1.99	0.43
1:A:479:ARG:NH2	1:A:483:ILE:HD11	2.34	0.43
1:A:239:VAL:HB	1:A:324:ILE:CG2	2.49	0.42
1:A:221:GLN:HG2	1:A:484:GLU:HG3	2.02	0.42
1:A:190:ALA:CB	1:A:209:ILE:HG13	2.49	0.42
1:A:200:ILE:HG12	1:A:204:GLN:HB2	2.02	0.42
1:A:260:ILE:HG23	1:A:297:LEU:HD21	2.02	0.41
1:A:265:ASN:HB3	1:A:268:SER:HB3	2.02	0.41
1:A:162:ASN:OD1	1:A:166:ASN:ND2	2.51	0.41
1:A:57:ASP:OD1	1:A:57:ASP:N	2.55	0.40
1:A:34:VAL:HG13	1:A:332:ALA:HB3	2.04	0.40
1:A:360:ASN:ND2	2:A:492:EDO:H11	2.37	0.40
1:A:143:ILE:HD12	1:A:154:MET:SD	2.62	0.40
1:A:240:ARG:NH1	1:A:488:GLU:OE1	2.54	0.40

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	430/514 (84%)	404 (94%)	26 (6%)	0	100	100

There are no Ramachandran outliers to report.

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	390/459 (85%)	375 (96%)	15 (4%)	33 67

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	VAL
1	A	51	SER
1	A	96	ARG
1	A	118	ARG
1	A	223	ILE
1	A	245	GLU
1	A	344	ARG
1	A	372	ARG
1	A	384	SER
1	A	385	ILE
1	A	400	ARG
1	A	416	GLN
1	A	472	LYS
1	A	478	GLU
1	A	486	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	354	GLN
1	A	405	ASN
1	A	457	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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

5 ligands are modelled in this entry.

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	$\# Z > 2$
2	EDO	A	493	-	3,3,3	0.49	0	2,2,2	0.34	0
2	EDO	A	496	-	3,3,3	0.44	0	2,2,2	0.41	0
2	EDO	A	494	-	3,3,3	0.51	0	2,2,2	0.31	0
2	EDO	A	492	-	3,3,3	0.64	0	2,2,2	0.06	0
2	EDO	A	495	-	3,3,3	0.60	0	2,2,2	0.22	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
2	EDO	A	493	-	-	1/1/1/1	-
2	EDO	A	496	-	-	1/1/1/1	-
2	EDO	A	494	-	-	1/1/1/1	-
2	EDO	A	492	-	-	0/1/1/1	-
2	EDO	A	495	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	493	EDO	O1-C1-C2-O2
2	A	494	EDO	O1-C1-C2-O2
2	A	496	EDO	O1-C1-C2-O2
2	A	495	EDO	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	494	EDO	1	0
2	A	492	EDO	1	0

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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.