



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:13 AM GMT

PDB ID : 2G5D  
Title : Crystal structure of MltA from Neisseria gonorrhoeae Monoclinic form  
Authors : Davies, C.  
Deposited on : 2006-02-22  
Resolution : 1.95 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](mailto: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.

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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

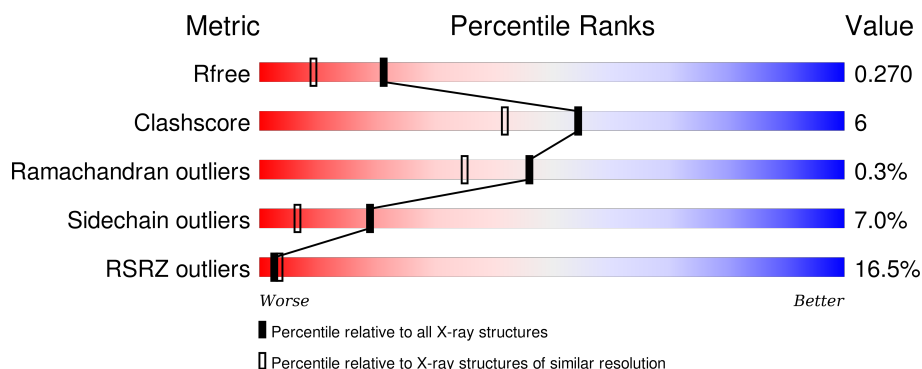
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.95 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))
$R_{free}$	91344	1833 (1.96-1.96)
Clashscore	102246	1953 (1.96-1.96)
Ramachandran outliers	100387	1936 (1.96-1.96)
Sidechain outliers	100360	1936 (1.96-1.96)
RSRZ outliers	91569	1835 (1.96-1.96)

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  $\geq 3$ , 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	422	<div> <div>15%</div> <div> <div></div> <div>76%</div> <div>13%</div> <div>•</div> <div>9%</div> </div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3088 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 GNA33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	382	2977	1901	534	532	10	0	0	0

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	20	GLY	-	CLONING ARTIFACT	UNP Q9L6H1
A	21	SER	-	CLONING ARTIFACT	UNP Q9L6H1
A	109	ILE	VAL	CONFLICT	UNP Q9L6H1
A	342	GLY	ASN	CONFLICT	UNP Q9L6H1
A	343	ASP	GLU	CONFLICT	UNP Q9L6H1

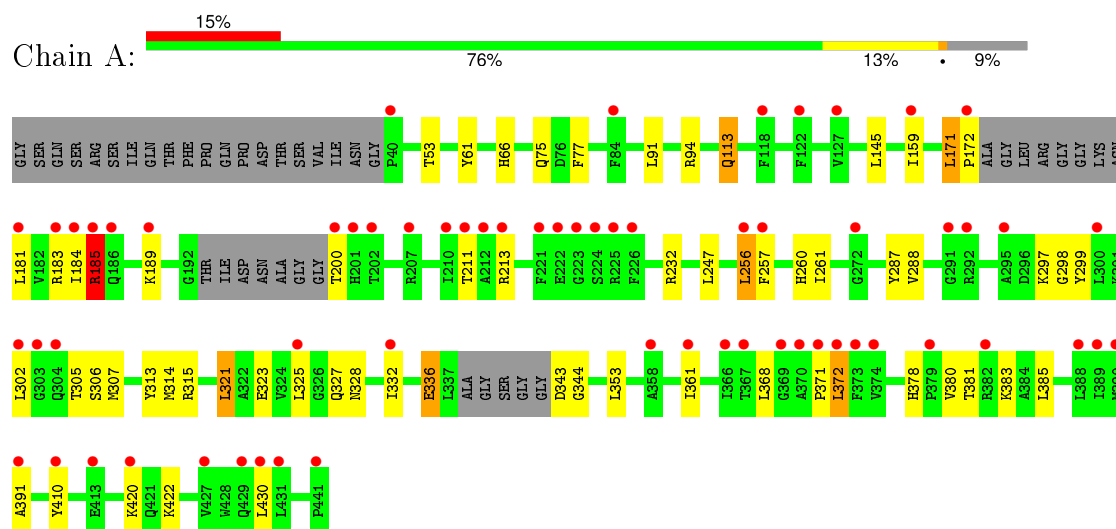
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	111	Total	O	0	0
			111	111		

### 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: GNA33



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	66.78Å 38.46Å 84.59Å 90.00° 106.46° 90.00°	Depositor
Resolution (Å)	25.00 – 1.95 25.12 – 1.95	Depositor EDS
% Data completeness (in resolution range)	99.1 (25.00-1.95) 99.1 (25.12-1.95)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.56 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.226 , 0.273 0.221 , 0.270	Depositor DCC
$R_{free}$ test set	1528 reflections (5.32%)	DCC
Wilson B-factor (Å <sup>2</sup> )	32.0	Xtriage
Anisotropy	0.171	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 41.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 30254 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	3088	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.02% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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](#)

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	0.74	3/3058 (0.1%)	0.68	3/4140 (0.1%)

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
1	A	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	185	ARG	CZ-NH2	19.60	1.58	1.33
1	A	185	ARG	CD-NE	12.86	1.68	1.46
1	A	185	ARG	CG-CD	9.25	1.75	1.51

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	372	LEU	CA-CB-CG	6.17	129.48	115.30
1	A	185	ARG	CG-CD-NE	-5.72	99.78	111.80
1	A	171	LEU	CA-CB-CG	5.18	127.21	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	185	ARG	Sidechain

## 5.2 Too-close contacts ⓘ

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	2977	0	2934	38	0
2	A	111	0	0	1	0
All	All	3088	0	2934	38	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 6.

All (38) 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:185:ARG:CD	1:A:185:ARG:CG	1.75	1.60
1:A:185:ARG:CD	1:A:185:ARG:NE	1.68	1.54
1:A:185:ARG:CD	1:A:185:ARG:CB	2.63	0.76
1:A:185:ARG:CD	1:A:185:ARG:CZ	2.62	0.72
1:A:297:LYS:H	1:A:298:GLY:HA2	1.56	0.70
1:A:247:LEU:HD22	1:A:336:GLU:HG3	1.72	0.70
1:A:336:GLU:H	1:A:336:GLU:CD	1.98	0.66
1:A:378:HIS:CE1	1:A:380:VAL:HG22	2.31	0.65
1:A:297:LYS:N	1:A:298:GLY:HA2	2.11	0.64
1:A:380:VAL:HG12	1:A:420:LYS:HD2	1.79	0.63
1:A:185:ARG:NE	1:A:185:ARG:CG	2.62	0.62
1:A:321:LEU:HD22	1:A:325:LEU:HD22	1.83	0.60
1:A:378:HIS:HE1	1:A:380:VAL:HG22	1.68	0.59
1:A:299:TYR:HB3	1:A:313:TYR:CZ	2.39	0.58
1:A:361:ILE:HG12	1:A:391:ALA:HB1	1.84	0.58
1:A:159:ILE:HG13	1:A:256:LEU:HD21	1.87	0.57
1:A:260:HIS:CD2	1:A:332:ILE:H	2.24	0.55
1:A:260:HIS:HD2	1:A:332:ILE:H	1.55	0.54
1:A:288:VAL:H	1:A:328:ASN:ND2	2.06	0.53
1:A:185:ARG:HG2	1:A:185:ARG:HH11	1.73	0.52
1:A:75:GLN:HB2	1:A:77:PHE:CE1	2.45	0.52
1:A:66:HIS:HD2	2:A:515:HOH:O	1.93	0.51
1:A:113:GLN:H	1:A:113:GLN:HE21	1.60	0.50
1:A:94:ARG:HH22	1:A:368:LEU:HB3	1.76	0.50
1:A:232:ARG:HH22	1:A:260:HIS:CD2	2.31	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:288:VAL:H	1:A:328:ASN:HD22	1.60	0.49
1:A:183:ARG:HD2	1:A:200:THR:N	2.28	0.49
1:A:257:PHE:O	1:A:260:HIS:HB2	2.13	0.48
1:A:344:GLY:HA3	1:A:353:LEU:O	2.13	0.48
1:A:287:TYR:HA	1:A:328:ASN:HD21	1.82	0.45
1:A:257:PHE:CE2	1:A:261:ILE:HD11	2.51	0.44
1:A:171:LEU:HD22	1:A:172:PRO:HD2	1.99	0.44
1:A:381:THR:C	1:A:383:LYS:H	2.20	0.44
1:A:53:THR:HA	1:A:61:TYR:O	2.18	0.44
1:A:257:PHE:HE2	1:A:261:ILE:HD11	1.84	0.41
1:A:113:GLN:H	1:A:113:GLN:NE2	2.18	0.41
1:A:371:PRO:HB2	1:A:430:LEU:HB2	2.01	0.41
1:A:323:GLU:O	1:A:327:GLN:HG2	2.22	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	374/422 (89%)	359 (96%)	14 (4%)	1 (0%)	46	35

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	302	LEU

### 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	301/328 (92%)	280 (93%)	21 (7%)	19 6

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	91	LEU
1	A	113	GLN
1	A	145	LEU
1	A	181	LEU
1	A	184	ILE
1	A	189	LYS
1	A	211	THR
1	A	213	ARG
1	A	256	LEU
1	A	305	THR
1	A	306	SER
1	A	307	MET
1	A	314	MET
1	A	315	ARG
1	A	321	LEU
1	A	336	GLU
1	A	343	ASP
1	A	372	LEU
1	A	385	LEU
1	A	410	TYR
1	A	422	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	66	HIS
1	A	106	GLN
1	A	113	GLN
1	A	236	ASN
1	A	260	HIS
1	A	328	ASN

### 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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	382/422 (90%)	0.85	63 (16%) 2 3	23, 31, 39, 49	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	372	LEU	6.7
1	A	181	LEU	6.3
1	A	371	PRO	6.1
1	A	213	ARG	5.5
1	A	304	GLN	5.2
1	A	370	ALA	4.8
1	A	388	LEU	4.5
1	A	212	ALA	4.3
1	A	186	GLN	4.3
1	A	430	LEU	4.1
1	A	122	PHE	4.0
1	A	211	THR	4.0
1	A	172	PRO	3.9
1	A	223	GLY	3.9
1	A	390	MET	3.8
1	A	221	PHE	3.7
1	A	222	GLU	3.7
1	A	389	ILE	3.7
1	A	431	LEU	3.7
1	A	189	LYS	3.6
1	A	224	SER	3.6
1	A	200	THR	3.5
1	A	358	ALA	3.4
1	A	303	GLY	3.4
1	A	210	ILE	3.3
1	A	272	GLY	3.3
1	A	183	ARG	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	302	LEU	3.2
1	A	420	LYS	3.2
1	A	84	PHE	3.2
1	A	366	ILE	3.1
1	A	373	PHE	3.0
1	A	256	LEU	3.0
1	A	374	VAL	2.9
1	A	295	ALA	2.9
1	A	391	ALA	2.9
1	A	427	VAL	2.9
1	A	40	PRO	2.8
1	A	332	ILE	2.8
1	A	202	THR	2.6
1	A	382	ARG	2.6
1	A	300	LEU	2.6
1	A	184	ILE	2.5
1	A	127	VAL	2.5
1	A	413	GLU	2.5
1	A	429	GLN	2.5
1	A	207	ARG	2.4
1	A	201	HIS	2.4
1	A	226	PHE	2.4
1	A	410	TYR	2.4
1	A	225	ARG	2.4
1	A	291	GLY	2.3
1	A	118	PHE	2.2
1	A	185	ARG	2.1
1	A	369	GLY	2.1
1	A	257	PHE	2.1
1	A	159	ILE	2.1
1	A	325	LEU	2.1
1	A	367	THR	2.1
1	A	441	PRO	2.1
1	A	379	PRO	2.1
1	A	361	ILE	2.0
1	A	292	ARG	2.0

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

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 [i](#)

There are no such residues in this entry.