



# Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 07:11 am BST

PDB ID : 1TD6  
Title : Crystal structure of the conserved hypothetical protein MP506/MPN330 (gi: 1674200) from *Mycoplasma pneumoniae*  
Authors : Das, D.; Oganessian, N.; Yokota, H.; Jancarik, J.; Kim, R.; Kim, S.H.; Berkeley Structural Genomics Center (BSGC)  
Deposited on : 2004-05-21  
Resolution : 2.50 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

<https://www.wwpdb.org/validation/2017/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
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

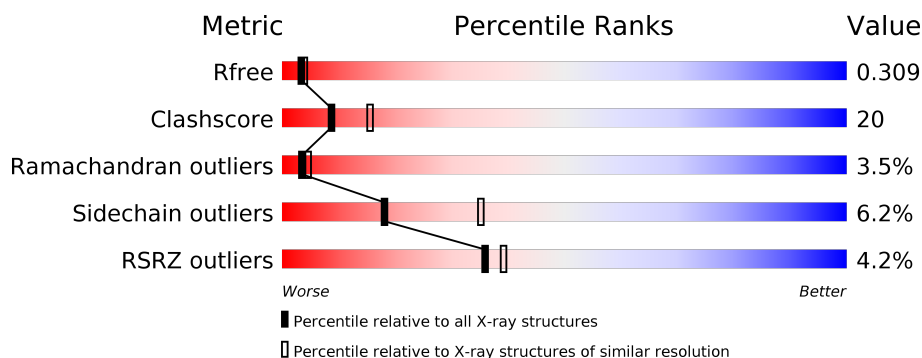
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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 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  $\leq 5\%$ . 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	306	<div> <div>4%</div> <div>62%</div> <div>26%</div> <div>7%</div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2406 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 Hypothetical protein MG237 homolog.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	286	Total	C	N	O	S	0	0	0
			2356	1546	383	424	3			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MET	-	EXPRESSION TAG	UNP P75455
A	-10	HIS	-	EXPRESSION TAG	UNP P75455
A	-9	HIS	-	EXPRESSION TAG	UNP P75455
A	-8	HIS	-	EXPRESSION TAG	UNP P75455
A	-7	HIS	-	EXPRESSION TAG	UNP P75455
A	-6	HIS	-	EXPRESSION TAG	UNP P75455
A	-5	HIS	-	EXPRESSION TAG	UNP P75455
A	-4	GLY	-	EXPRESSION TAG	UNP P75455
A	-3	GLY	-	EXPRESSION TAG	UNP P75455
A	-2	GLY	-	EXPRESSION TAG	UNP P75455
A	-1	GLY	-	EXPRESSION TAG	UNP P75455
A	0	GLY	-	EXPRESSION TAG	UNP P75455

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	50	Total	O	0	0
			50	50		



- Molecule 1: Hypothetical protein MG237 homolog



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 41 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	82.84Å 82.84Å 225.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.40 – 2.50 41.42 – 2.50	Depositor EDS
% Data completeness (in resolution range)	96.7 (41.40-2.50) 98.3 (41.42-2.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.39 (at 2.51Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.244 , 0.298 0.255 , 0.309	Depositor DCC
$R_{free}$ test set	1242 reflections (4.81%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	40.9	Xtriage
Anisotropy	0.027	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 47.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	2406	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.63% 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, 0.333 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	0.41	0/2415	0.63	2/3273 (0.1%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	196	GLU	N-CA-C	-6.61	93.17	111.00
1	A	12	LEU	CA-CB-CG	5.24	127.34	115.30

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	2356	0	2377	97	0
2	A	50	0	0	1	0
All	All	2406	0	2377	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 20.

All (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:282:LEU:HA	1:A:285:GLN:HB2	1.40	1.00
1:A:146:GLN:HE22	1:A:178:GLU:H	0.97	0.92
1:A:146:GLN:NE2	1:A:178:GLU:H	1.70	0.90
1:A:254:LYS:HE3	1:A:271:LYS:HE3	1.54	0.87
1:A:6:ASN:H	1:A:72:ALA:HB2	1.41	0.85
1:A:146:GLN:HE22	1:A:178:GLU:N	1.79	0.80
1:A:78:LYS:HD3	1:A:78:LYS:H	1.49	0.77
1:A:268:VAL:O	1:A:274:LEU:HD12	1.87	0.75
1:A:93:HIS:HB2	1:A:131:PRO:HG3	1.73	0.71
1:A:254:LYS:HG3	1:A:273:GLU:CB	2.23	0.69
1:A:117:GLN:HE21	1:A:117:GLN:CA	2.06	0.69
1:A:117:GLN:HE21	1:A:117:GLN:N	1.92	0.67
1:A:271:LYS:HZ2	1:A:273:GLU:HG2	1.59	0.67
1:A:64:GLN:HE21	1:A:92:ASN:HD21	1.43	0.66
1:A:149:LEU:HD23	1:A:177:VAL:HG11	1.77	0.66
1:A:23:LYS:NZ	1:A:23:LYS:HB2	2.11	0.65
1:A:64:GLN:HE21	1:A:92:ASN:ND2	1.95	0.65
1:A:239:TYR:OH	1:A:280:HIS:HE1	1.79	0.65
1:A:286:LEU:O	1:A:286:LEU:HD12	1.97	0.65
1:A:167:ASN:ND2	1:A:193:GLY:H	1.95	0.64
1:A:271:LYS:NZ	1:A:273:GLU:HG2	2.13	0.63
1:A:6:ASN:CG	1:A:7:GLN:H	2.01	0.63
1:A:43:PHE:O	1:A:46:HIS:HB3	2.00	0.61
1:A:231:ILE:HD13	1:A:277:LEU:HD21	1.83	0.60
1:A:209:GLN:HB3	2:A:341:HOH:O	2.00	0.60
1:A:46:HIS:CE1	1:A:50:LYS:HE2	2.37	0.60
1:A:254:LYS:HG3	1:A:273:GLU:HB3	1.84	0.60
1:A:78:LYS:CD	1:A:78:LYS:H	2.15	0.60
1:A:203:ALA:HB2	1:A:242:LEU:HA	1.84	0.59
1:A:114:LEU:O	1:A:122:LYS:HE2	2.03	0.59
1:A:255:ILE:O	1:A:259:VAL:HG13	2.03	0.57
1:A:236:LEU:O	1:A:240:PHE:HA	2.04	0.57
1:A:240:PHE:CD1	1:A:240:PHE:C	2.77	0.57
1:A:78:LYS:HD3	1:A:78:LYS:N	2.20	0.57
1:A:282:LEU:HA	1:A:285:GLN:CB	2.27	0.56
1:A:120:PRO:HG2	1:A:121:ASN:H	1.71	0.55
1:A:93:HIS:CB	1:A:131:PRO:HG3	2.36	0.55
1:A:164:GLN:HA	1:A:164:GLN:OE1	2.07	0.55
1:A:266:GLU:CD	1:A:266:GLU:H	2.11	0.54
1:A:87:LEU:O	1:A:91:VAL:HG23	2.09	0.52
1:A:236:LEU:C	1:A:236:LEU:HD23	2.29	0.52
1:A:113:GLU:O	1:A:117:GLN:NE2	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:151:ASP:O	1:A:159:ARG:NH2	2.34	0.52
1:A:66:ARG:HE	1:A:66:ARG:HA	1.76	0.51
1:A:214:ILE:C	1:A:214:ILE:HD12	2.31	0.51
1:A:70:GLU:O	1:A:76:LEU:HD12	2.12	0.49
1:A:11:HIS:O	1:A:13:SER:N	2.43	0.49
1:A:23:LYS:HZ2	1:A:23:LYS:HB2	1.76	0.49
1:A:181:ASN:HD22	1:A:241:PRO:HD2	1.77	0.49
1:A:231:ILE:HG21	1:A:277:LEU:HD21	1.94	0.49
1:A:117:GLN:C	1:A:119:TYR:H	2.15	0.48
1:A:16:LYS:NZ	1:A:89:GLN:HE22	2.12	0.48
1:A:280:HIS:O	1:A:282:LEU:N	2.46	0.48
1:A:214:ILE:HG12	1:A:232:ILE:HD11	1.94	0.48
1:A:16:LYS:HZ3	1:A:89:GLN:HE22	1.62	0.48
1:A:273:GLU:O	1:A:277:LEU:HB2	2.15	0.47
1:A:119:TYR:HE1	1:A:148:VAL:HG22	1.79	0.47
1:A:240:PHE:O	1:A:241:PRO:C	2.52	0.47
1:A:6:ASN:CG	1:A:7:GLN:N	2.68	0.47
1:A:264:LEU:O	1:A:265:ASN:HB2	2.13	0.47
1:A:121:ASN:O	1:A:122:LYS:HB2	2.15	0.47
1:A:236:LEU:O	1:A:236:LEU:HD23	2.15	0.46
1:A:26:ARG:O	1:A:30:ASN:ND2	2.48	0.46
1:A:254:LYS:HG3	1:A:273:GLU:HB2	1.96	0.46
1:A:207:PHE:CZ	1:A:236:LEU:HA	2.51	0.45
1:A:243:HIS:HB2	1:A:244:PRO:HD2	1.98	0.45
1:A:281:THR:HG22	1:A:282:LEU:HG	1.99	0.45
1:A:280:HIS:O	1:A:285:GLN:HG2	2.16	0.45
1:A:273:GLU:OE1	1:A:273:GLU:HA	2.16	0.44
1:A:282:LEU:C	1:A:285:GLN:H	2.20	0.44
1:A:134:LYS:HA	1:A:170:PRO:HB2	1.99	0.44
1:A:240:PHE:CG	1:A:241:PRO:N	2.84	0.44
1:A:78:LYS:N	1:A:79:PRO:HD2	2.32	0.44
1:A:167:ASN:HD22	1:A:193:GLY:H	1.64	0.44
1:A:271:LYS:NZ	1:A:273:GLU:CG	2.81	0.44
1:A:9:VAL:HG12	1:A:236:LEU:CD1	2.48	0.43
1:A:120:PRO:HG2	1:A:121:ASN:N	2.32	0.43
1:A:115:VAL:HG22	1:A:125:MET:HB2	2.01	0.43
1:A:16:LYS:NZ	1:A:89:GLN:NE2	2.67	0.43
1:A:146:GLN:NE2	1:A:177:VAL:HG13	2.34	0.43
1:A:117:GLN:C	1:A:119:TYR:N	2.73	0.42
1:A:278:ILE:O	1:A:283:TYR:HD1	2.03	0.42
1:A:117:GLN:HE21	1:A:117:GLN:HA	1.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:ILE:HG22	1:A:197:ILE:O	2.18	0.42
1:A:81:VAL:O	1:A:85:GLN:HG3	2.20	0.42
1:A:167:ASN:HA	1:A:192:LEU:HD22	2.00	0.42
1:A:214:ILE:HG12	1:A:232:ILE:CD1	2.50	0.42
1:A:6:ASN:N	1:A:72:ALA:HB2	2.21	0.41
1:A:117:GLN:CA	1:A:117:GLN:NE2	2.78	0.41
1:A:98:GLN:O	1:A:98:GLN:HG2	2.20	0.41
1:A:209:GLN:HB2	1:A:248:LEU:HD11	2.03	0.41
1:A:251:LEU:O	1:A:255:ILE:HG13	2.21	0.41
1:A:163:PHE:CE1	1:A:192:LEU:HD21	2.56	0.40
1:A:23:LYS:NZ	1:A:23:LYS:CB	2.83	0.40
1:A:118:ASP:O	1:A:120:PRO:HD2	2.21	0.40
1:A:196:GLU:O	1:A:197:ILE:HB	2.21	0.40
1:A:118:ASP:HB3	1:A:121:ASN:HB2	2.02	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	284/306 (93%)	246 (87%)	28 (10%)	10 (4%)	<b>3</b> <b>4</b>

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	117	GLN
1	A	119	TYR
1	A	240	PHE
1	A	265	ASN
1	A	281	THR
1	A	11	HIS
1	A	12	LEU

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Mol	Chain	Res	Type
1	A	6	ASN
1	A	264	LEU
1	A	197	ILE

### 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	259/273 (95%)	243 (94%)	16 (6%)	18	35

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	HIS
1	A	12	LEU
1	A	15	LEU
1	A	25	LEU
1	A	29	PHE
1	A	31	ASP
1	A	66	ARG
1	A	87	LEU
1	A	98	GLN
1	A	117	GLN
1	A	149	LEU
1	A	219	LEU
1	A	260	SER
1	A	269	ASN
1	A	276	LYS
1	A	277	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	ASN
1	A	46	HIS

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Mol	Chain	Res	Type
1	A	47	GLN
1	A	89	GLN
1	A	92	ASN
1	A	98	GLN
1	A	117	GLN
1	A	124	ASN
1	A	146	GLN
1	A	167	ASN
1	A	168	GLN
1	A	213	GLN
1	A	216	GLN
1	A	224	ASN
1	A	265	ASN
1	A	280	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](#)

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, 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	286/306 (93%)	0.28	12 (4%) 36 39	26, 41, 67, 78	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	281	THR	9.0
1	A	282	LEU	7.1
1	A	75	TYR	6.1
1	A	9	VAL	3.9
1	A	6	ASN	3.8
1	A	266	GLU	3.1
1	A	35	HIS	2.9
1	A	34	LYS	2.7
1	A	119	TYR	2.5
1	A	280	HIS	2.5
1	A	36	ASN	2.2
1	A	240	PHE	2.2

### 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.