



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 07:25 AM GMT

PDB ID : 3AQM  
Title : Structure of bacterial protein (form II)  
Authors : Toh, Y.; Takeshita, D.; Tomita , K.  
Deposited on : 2010-11-09  
Resolution : 3.15 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](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.

---

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

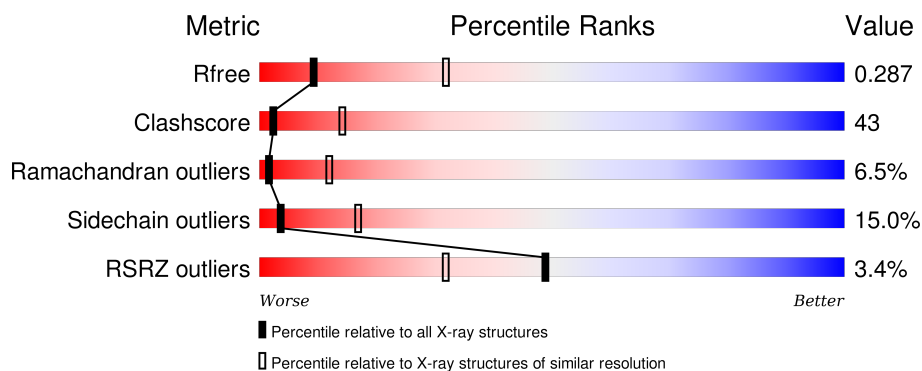
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

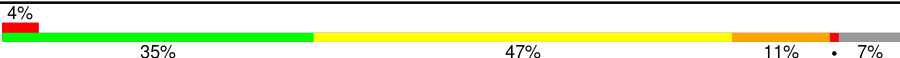
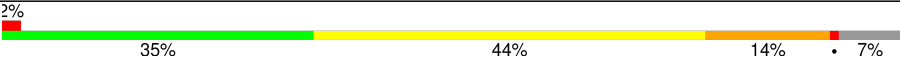
The reported resolution of this entry is 3.15 Å.

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	1112 (3.20-3.12)
Clashscore	102246	1249 (3.20-3.12)
Ramachandran outliers	100387	1222 (3.20-3.12)
Sidechain outliers	100360	1221 (3.20-3.12)
RSRZ outliers	91569	1117 (3.20-3.12)

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	415	 4% 35% 47% 11% • 7%
1	B	415	 2% 35% 44% 14% • 7%

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6332 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 Poly(A) polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	388	Total	C	N	O	S	0	0	0
			3165	2022	569	560	14			
1	B	388	Total	C	N	O	S	0	0	0
			3165	2022	569	560	14			

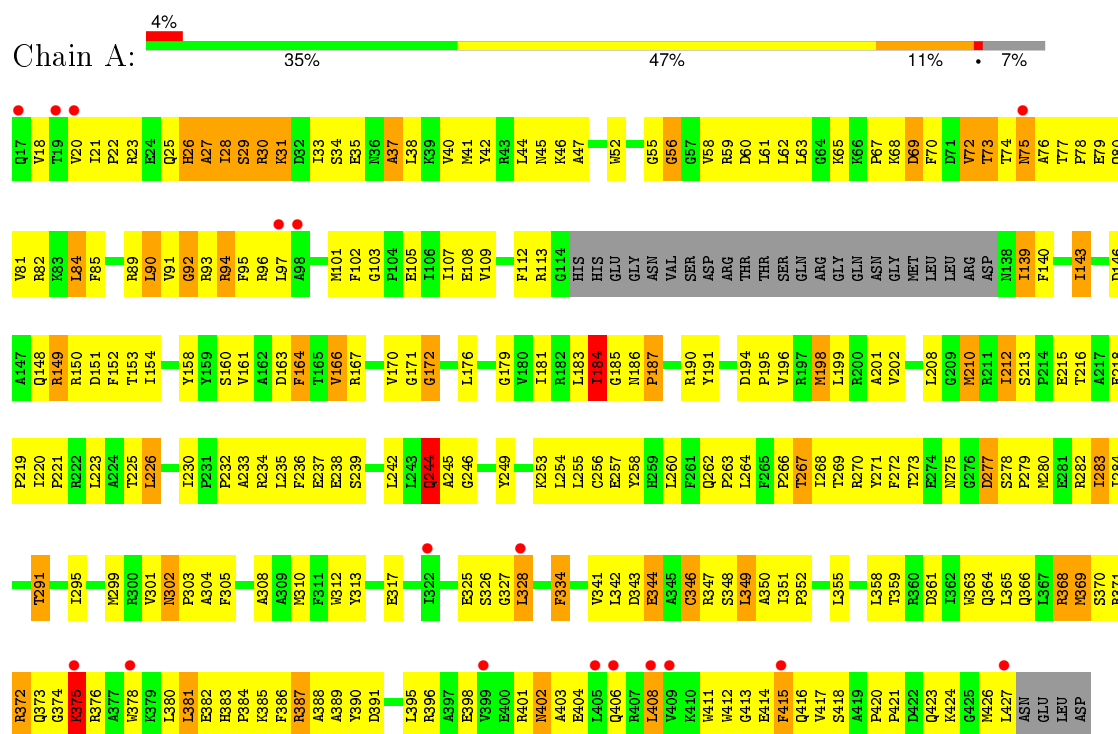
- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mg	0	0
			1	1		
2	A	1	Total	Mg	0	0
			1	1		

### 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 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: Poly(A) polymerase



I295	H296	M297	D298	M299	R300	V301	N302	P303	A304	F305	L306	F307	A308	A309	M310	F311	M312	Y313	P314	L315	L316	E317	I322	A323	Q324	E325	S326	G327	L328	T329	D332	A333	A337	M338	V341	L342	D343	E344	A345	C346	R347	S348	L349	A350	I351	P352	L355	T356	T357	L358	T359	R360	D361	I362
W363	Q364	L365	Q366	L367	R368	M369	S370	R371	R372	Q373	G374	K375	R376	A377	W378	K379	L380	H383	P384	K385	A389	L392	L395	R396	V399	E400	R401	N402	A403	E404	L405	Q406	R407	L408	W411	W412	G413	E414	F415	Q416	V417	S418	A419	P420	Q423	L427	ASN	GLU	LEU	ASP				

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 4 <sub>2</sub> 2 <sub>1</sub> 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	133.25Å 133.25Å 176.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.80 – 3.15 45.52 – 3.16	Depositor EDS
% Data completeness (in resolution range)	99.3 (29.80-3.15) 97.8 (45.52-3.16)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.75 (at 3.19Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, $R_{free}$	0.270 , 0.287 0.289 , 0.287	Depositor DCC
$R_{free}$ test set	1363 reflections (5.02%)	DCC
Wilson B-factor (Å <sup>2</sup> )	91.3	Xtriage
Anisotropy	0.501	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 42.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.37$ , $\langle L^2 \rangle = 0.20$	Xtriage
Outliers	1 of 27191 reflections (0.004%)	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	6332	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	105.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.95% 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](#)

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

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	0.40	0/3234	0.71	3/4370 (0.1%)
1	B	0.41	0/3234	0.70	2/4370 (0.0%)
All	All	0.41	0/6468	0.71	5/8740 (0.1%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	29	SER	N-CA-C	-7.52	90.69	111.00
1	B	103	GLY	N-CA-C	-5.56	99.19	113.10
1	A	349	LEU	CA-CB-CG	5.40	127.73	115.30
1	B	37	ALA	N-CA-C	-5.31	96.67	111.00
1	A	37	ALA	N-CA-C	-5.26	96.79	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	3165	0	3203	286	1
1	B	3165	0	3201	268	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	6332	0	6404	549	1

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 43.

The worst 5 of 549 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:B:183:LEU:HD23	1:B:184:ILE:H	1.07	1.20
1:A:95:PHE:CD1	1:A:96:ARG:HG3	1.78	1.18
1:A:149:ARG:HH11	1:A:149:ARG:HB3	1.22	1.04
1:A:372:ARG:HA	1:A:372:ARG:NH1	1.71	1.03
1:B:233:ALA:HA	1:B:350:ALA:HB3	1.43	0.98

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:ARG:NH1	1:A:361:ASP:OD1[2_545]	1.75	0.45

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	384/415 (92%)	291 (76%)	72 (19%)	21 (6%)	2	17
1	B	384/415 (92%)	298 (78%)	57 (15%)	29 (8%)	1	8
All	All	768/830 (92%)	589 (77%)	129 (17%)	50 (6%)	1	12

5 of 50 Ramachandran outliers are listed below:



Mol	Chain	Res	Type
1	A	28	ILE
1	A	92	GLY
1	A	245	ALA
1	A	372	ARG
1	A	375	LYS

### 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	334/358 (93%)	291 (87%)	43 (13%)	5	24
1	B	334/358 (93%)	277 (83%)	57 (17%)	2	12
All	All	668/716 (93%)	568 (85%)	100 (15%)	3	17

5 of 100 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	26	HIS
1	B	158	TYR
1	B	372	ARG
1	B	30	ARG
1	B	104	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 34 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	364	GLN
1	A	423	GLN
1	B	373	GLN
1	A	406	GLN
1	A	87	ASN

### 5.3.3 RNA ⓘ

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 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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	388/415 (93%)	0.36	17 (4%) 38 22	71, 101, 141, 169	0
1	B	388/415 (93%)	0.31	9 (2%) 64 47	66, 104, 145, 166	0
All	All	776/830 (93%)	0.33	26 (3%) 49 32	66, 103, 143, 169	0

The worst 5 of 26 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	17	GLN	4.0
1	B	100	VAL	3.4
1	A	328	LEU	2.8
1	A	409	VAL	2.8
1	A	405	LEU	2.8

### 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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
2	MG	B	501	1/1	0.84	0.18	-	37,37,37,37	0
2	MG	A	501	1/1	0.88	0.23	-	37,37,37,37	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.