



wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 3FPP / pdb_00003fpp
Title : Crystal structure of E.coli MacA
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Deposited on : 2009-01-06
Resolution : 2.99 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

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Xtrriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

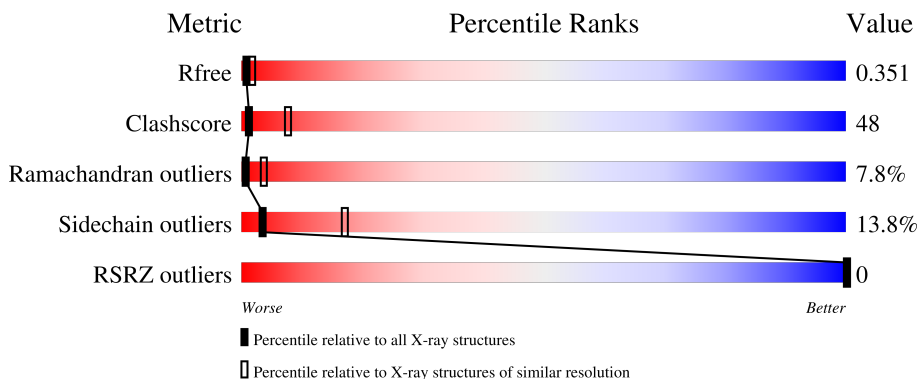
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION



The reported resolution of this entry is 2.99 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}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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 of 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 $\leq 5\%$. 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	341	
1	B	341	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 4097 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 Macrolide-specific efflux protein macA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	266	2043	1274	361	402	6	0	0	0
1	B	267	2054	1280	365	403	6	0	0	0

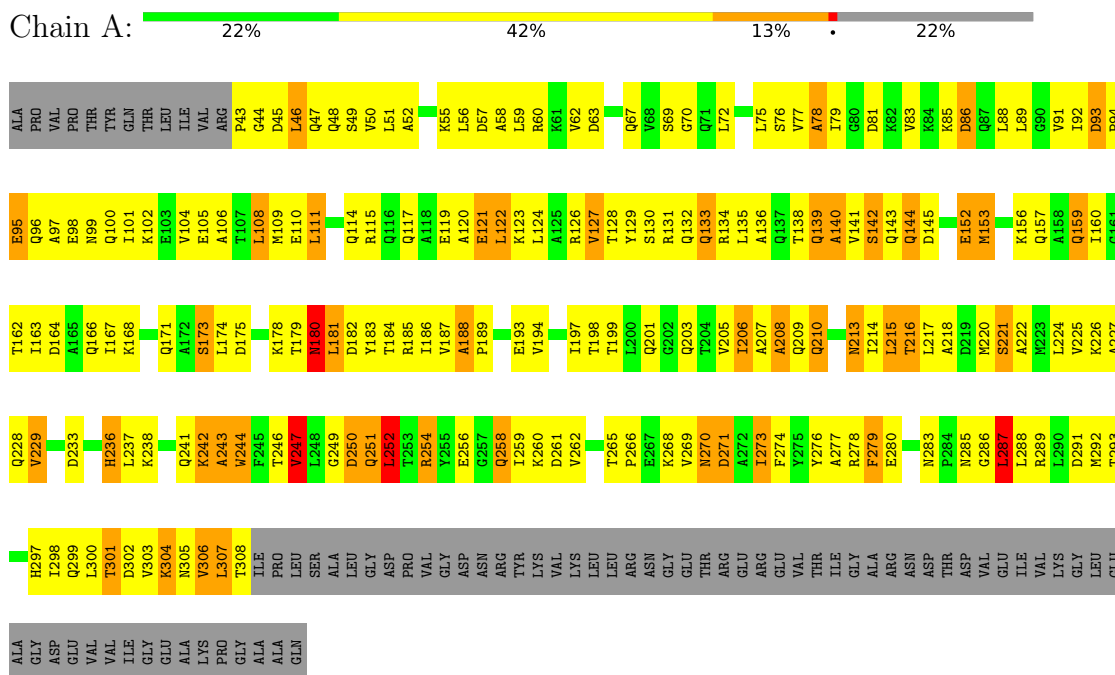
There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	139	GLN	LYS	SEE REMARK 999	UNP P75830
A	148	ASN	THR	SEE REMARK 999	UNP P75830
A	251	GLN	PRO	SEE REMARK 999	UNP P75830
B	139	GLN	LYS	SEE REMARK 999	UNP P75830
B	148	ASN	THR	SEE REMARK 999	UNP P75830
B	251	GLN	PRO	SEE REMARK 999	UNP P75830

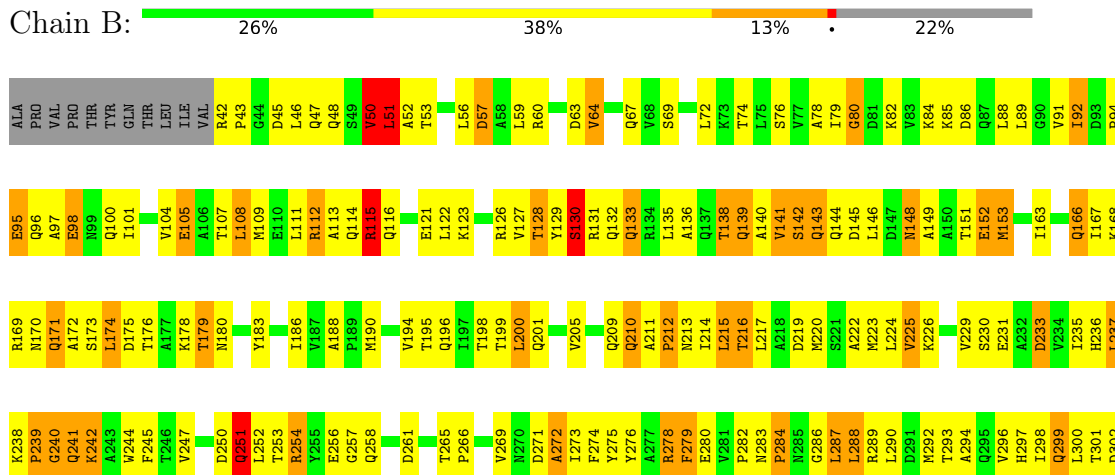
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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 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: Macrolide-specific efflux protein macA



- Molecule 1: Macrolide-specific efflux protein macA



V303
K304
N305
V306
L307
T308
ILE
PRO
LEU
SER
ALA
LEU
GLY
ASP
PRO
VAL
GLY
ASP
ASN
ARG
TYR
LYS
VAL
VAL
LYS
LEU
LEU
ARG
ASN
GLY
GLY
THR
ARG
GLU
ARG
GLU
VAL
THR
ILE
ILE
GLY
ALA
ARG
ASN
ASN
THR
ASP
ASP
VAL
GLU
ILE
ILE
VAL
VAL
LYS
GLY
LEU
GLU
ALA
GLY
ASP
GLU
VAL
VAL
ILE

GLY
GLU
ALA
LYS
PRO
GLY
ALA
ALA
GLN

4 Data and refinement statistics i

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants a, b, c, α , β , γ	128.52Å 128.52Å 110.31Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.69 – 2.99 49.69 – 3.00	Depositor EDS
% Data completeness (in resolution range)	92.0 (49.69-2.99) 92.1 (49.69-3.00)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.84 (at 3.01Å)	Xtrriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.283 , 0.349 0.284 , 0.351	Depositor DCC
R_{free} test set	1950 reflections (9.81%)	wwPDB-VP
Wilson B-factor (Å ²)	37.7	Xtrriage
Anisotropy	0.126	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 12.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.22$	Xtrriage
Estimated twinning fraction	0.447 for -h,-k,l	Xtrriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	4097	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.11% 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](#)

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	0.58	0/2063	1.19	24/2797 (0.9%)
1	B	0.58	0/2074	1.14	20/2812 (0.7%)
All	All	0.58	0/4137	1.16	44/5609 (0.8%)

There are no bond length outliers.

The worst 5 of 44 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	76	SER	N-CA-C	10.00	125.30	113.20
1	A	152	GLU	N-CA-C	-9.28	101.11	111.14
1	A	127	VAL	N-CA-C	-9.04	103.04	111.45
1	B	278	ARG	N-CA-C	8.78	121.86	110.53
1	B	143	GLN	N-CA-C	-8.03	104.08	114.04

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	2043	0	2104	212	0
1	B	2054	0	2116	198	0
All	All	4097	0	4220	396	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 48.

The worst 5 of 396 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:159:GLN:HE21	1:A:159:GLN:HA	1.15	1.10
1:B:135:LEU:HD22	1:B:140:ALA:HB2	1.35	1.06
1:B:205:VAL:HG21	1:B:212:PRO:HG3	1.32	1.05
1:B:226:LYS:HZ2	1:B:278:ARG:HD3	1.23	1.04
1:A:285:ASN:ND2	1:A:286:GLY:H	1.55	1.03

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	264/341 (77%)	207 (78%)	39 (15%)	18 (7%)	1	5
1	B	265/341 (78%)	203 (77%)	39 (15%)	23 (9%)	0	3
All	All	529/682 (78%)	410 (78%)	78 (15%)	41 (8%)	1	4

5 of 41 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	140	ALA
1	A	221	SER
1	A	242	LYS
1	A	247	VAL
1	A	252	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	221/281 (79%)	190 (86%)	31 (14%)	3	16
1	B	222/281 (79%)	192 (86%)	30 (14%)	4	18
All	All	443/562 (79%)	382 (86%)	61 (14%)	3	17

5 of 61 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	293	THR
1	B	251	GLN
1	B	92	ILE
1	B	241	GLN
1	B	299	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	114	GLN
1	B	305	ASN
1	B	143	GLN
1	B	241	GLN
1	B	133	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 oligosaccharides 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, 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	266/341 (78%)	-1.63	0 100 100	10, 28, 60, 75	0
1	B	267/341 (78%)	-1.61	0 100 100	9, 28, 51, 69	0
All	All	533/682 (78%)	-1.62	0 100 100	9, 28, 57, 75	0

There are no RSRZ outliers to report.

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 oligosaccharides 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.