



wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 3AQM / pdb_00003aqm
Title : Structure of bacterial protein (form II)
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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

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
Xtriage (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

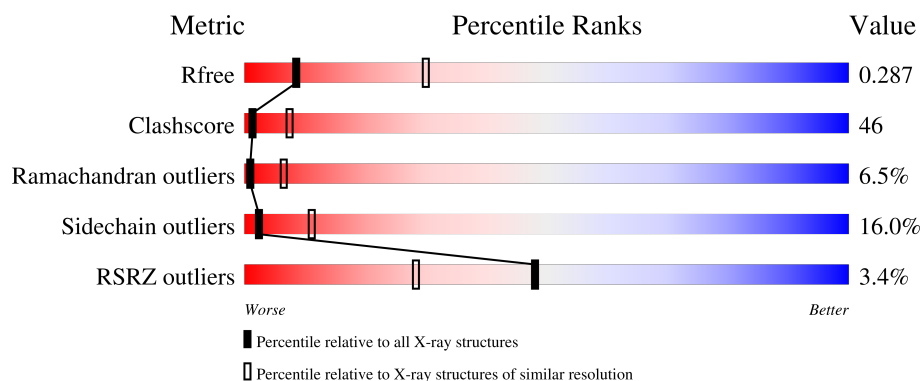
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	2361 (3.20-3.12)
Clashscore	190562	2486 (3.20-3.12)
Ramachandran outliers	187476	2405 (3.20-3.12)
Sidechain outliers	187428	2404 (3.20-3.12)
RSRZ outliers	180081	2361 (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 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	415	
1	B	415	

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			

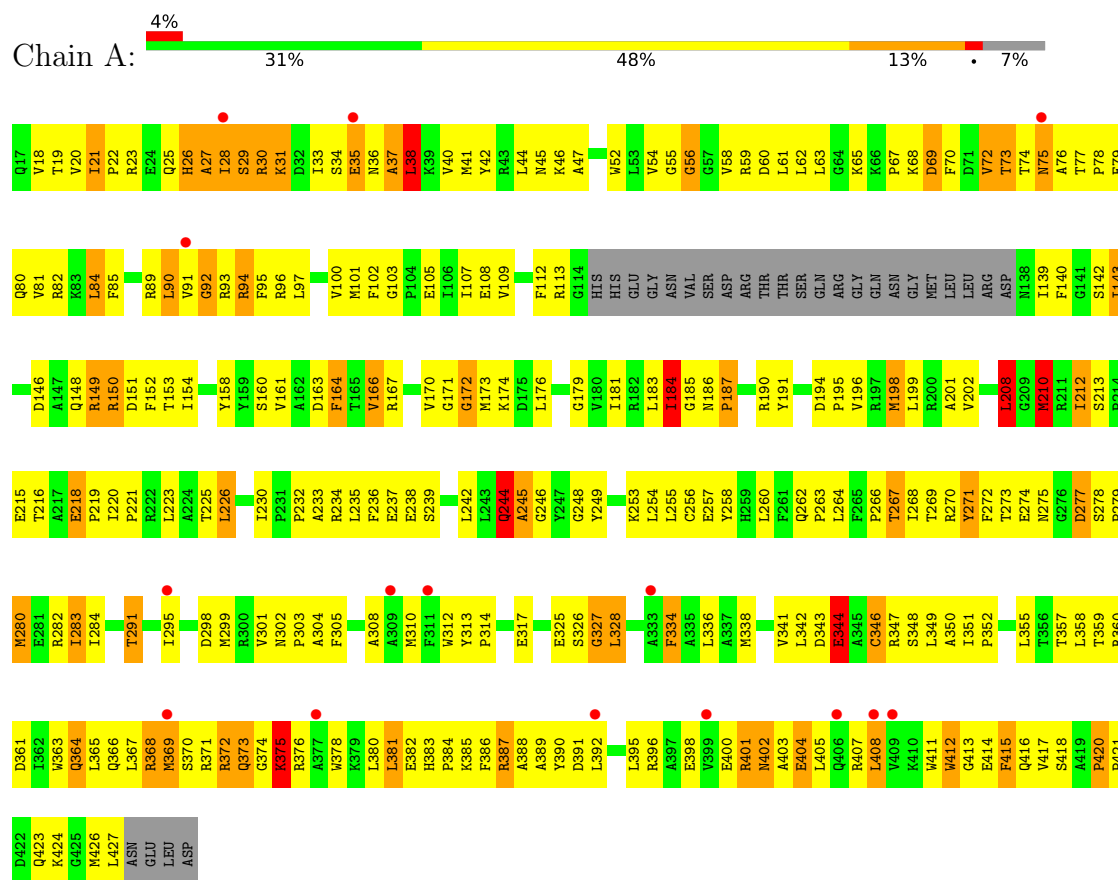
- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

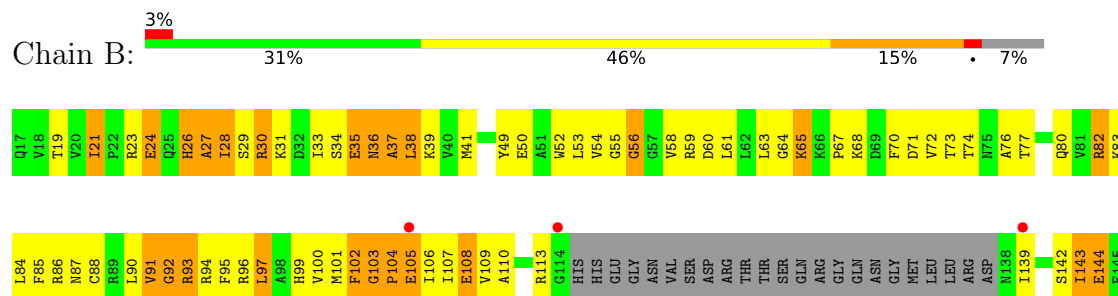
3 Residue-property plots

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: Poly(A) polymerase



• Molecule 1: Poly(A) polymerase



Q423	T356	K289	T216	D146
N426	T357	N290	A217	A147
L427	T358	T291	E218	Q148
ASN	T359	D292	P219	R149
GLU	R360		I220	R150
LEU	D361	I295	L223	D151
ASP	T362	H296	A224	F152
	W363	N297	T225	T153
	Q364	D298	L226	I154
	L365	M299	L227	N155
	Q366	R300		S156
	L367	V301		L157
	R368	N302	I230	L158
	R369	P303	P231	
	S370	A304	P232	D163
	R371	F305	A233	F164
	R372	L306	R234	T165
	Q373	F307	L235	V166
	G374	A308	F236	R167
	K375	A309		D168
	R376	M310	L242	Y169
	A377	F311	L243	V170
	W378	W312	Q244	G171
	K379	Y313		M172
	L380	P314	Y247	W173
		L315	G248	K174
	H383	L316		D175
	P384	E317	T251	L176
	K385		L254	K177
		I322	L255	D178
		A323	C256	G179
		Q324	E257	W180
		E325		I181
		S326	L260	R182
		G327	F261	L183
		L328	Q262	I184
		T329	P263	I185
			L264	
		A333	F265	T189
		F334	P266	R190
		A335	T267	Y191
		L336	L268	
		A337	T269	D194
		M338	R270	
			Y271	L199
		V341		R200
		L342	N275	A201
		D343	G276	V202
		F344	D277	R203
		A345	S278	F204
		C346	P279	A205
		R347	M280	A206
		S348	E281	K207
		L349	R282	L208
		A350	I283	G209
		I351	L284	M210
		P352		
		R353	V287	S213
		R354	L288	P214
		L355		E215

4 Data and refinement statistics

Property	Value	Source
Space group	P 4 ₂ 2 ₁ 2	Depositor
Cell constants a, b, c, α , β , γ	133.25Å 133.25Å 176.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.80 – 3.15 29.80 – 3.17	Depositor EDS
% Data completeness (in resolution range)	99.3 (29.80-3.15) 97.7 (29.80-3.17)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.75 (at 3.19Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, R_{free}	0.270 , 0.287 0.290 , 0.287	Depositor DCC
R_{free} test set	1364 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	91.3	Xtriage
Anisotropy	0.501	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 47.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.37$, $\langle L^2 \rangle = 0.20$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	6332	wwPDB-VP
Average B, all atoms (Å ²)	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.*

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

5.1 Standard geometry

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	0.51	0/3234	1.10	23/4370 (0.5%)
1	B	0.51	0/3234	1.13	32/4370 (0.7%)
All	All	0.51	0/6468	1.11	55/8740 (0.6%)

There are no bond length outliers.

The worst 5 of 55 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	37	ALA	N-CA-C	-13.61	96.67	113.28
1	A	37	ALA	N-CA-C	-12.47	96.79	112.88
1	A	29	SER	N-CA-C	-10.27	90.69	108.56
1	B	420	PRO	N-CA-C	9.54	122.34	110.70
1	B	376	ARG	N-CA-C	-9.51	101.44	113.23

There are no chirality outliers.

There are no planarity outliers.

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	3165	0	3203	304	1
1	B	3165	0	3201	286	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	6332	0	6404	585	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 46.

The worst 5 of 585 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:NH1	1:A:372:ARG:HA	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 [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	384/415 (92%)	291 (76%)	72 (19%)	21 (6%)	1	9
1	B	384/415 (92%)	298 (78%)	57 (15%)	29 (8%)	1	4
All	All	768/830 (92%)	589 (77%)	129 (17%)	50 (6%)	1	6

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 [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	334/358 (93%)	284 (85%)	50 (15%)	3	13
1	B	334/358 (93%)	277 (83%)	57 (17%)	2	9
All	All	668/716 (93%)	561 (84%)	107 (16%)	2	11

5 of 107 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	104	PRO
1	B	226	LEU
1	B	372	ARG
1	B	108	GLU
1	B	202	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 32 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	364	GLN
1	B	373	GLN
1	A	290	ASN
1	A	275	ASN
1	B	402	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 oligosaccharides 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, 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	388/415 (93%)	0.32	15 (3%)	43 25	71, 101, 141, 169	0
1	B	388/415 (93%)	0.25	11 (2%)	55 34	66, 104, 145, 166	0
All	All	776/830 (93%)	0.29	26 (3%)	48 28	66, 103, 143, 169	0

The worst 5 of 26 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	295	ILE	3.8
1	A	409	VAL	3.8
1	A	399	VAL	3.0
1	A	377	ALA	2.9
1	A	392	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 oligosaccharides 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. The B-factors column lists the minimum, median, 95th 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	B-factors($\text{\AA}^2$)	Q<0.9
2	MG	A	501	1/1	0.87	0.20	37,37,37,37	0
2	MG	B	501	1/1	0.92	0.12	37,37,37,37	0

6.5 Other polymers [i](#)

There are no such residues in this entry.