wwPDB X-ray Structure Validation Summary Report (i)

Jun 12, 2024 – 02:12 PM EDT

PDB ID	:	3AQM
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 (i) 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 (1)) were used in the production of this report:

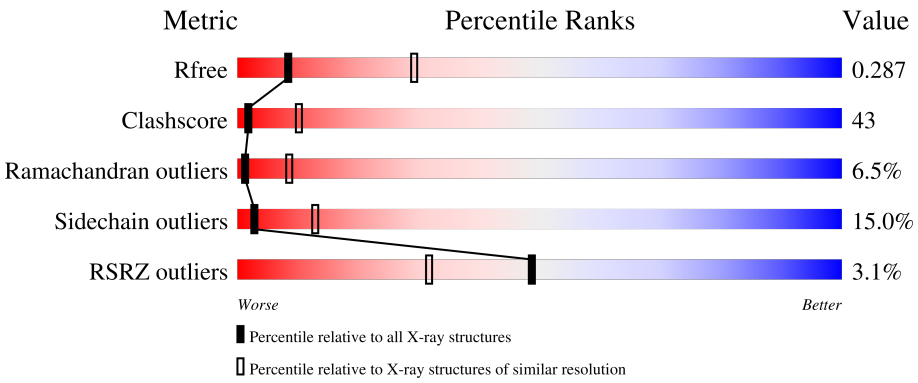
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

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}	130704	1665 (3.20-3.12)
Clashscore	141614	1804 (3.20-3.12)
Ramachandran outliers	138981	1770 (3.20-3.12)
Sidechain outliers	138945	1769 (3.20-3.12)
RSRZ outliers	127900	1616 (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 <=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 (i)

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
			Total	C	N	O	S			
1	A	388	3165	2022	569	560	14	0	0	0
1	B	388	3165	2022	569	560	14	0	0	0

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

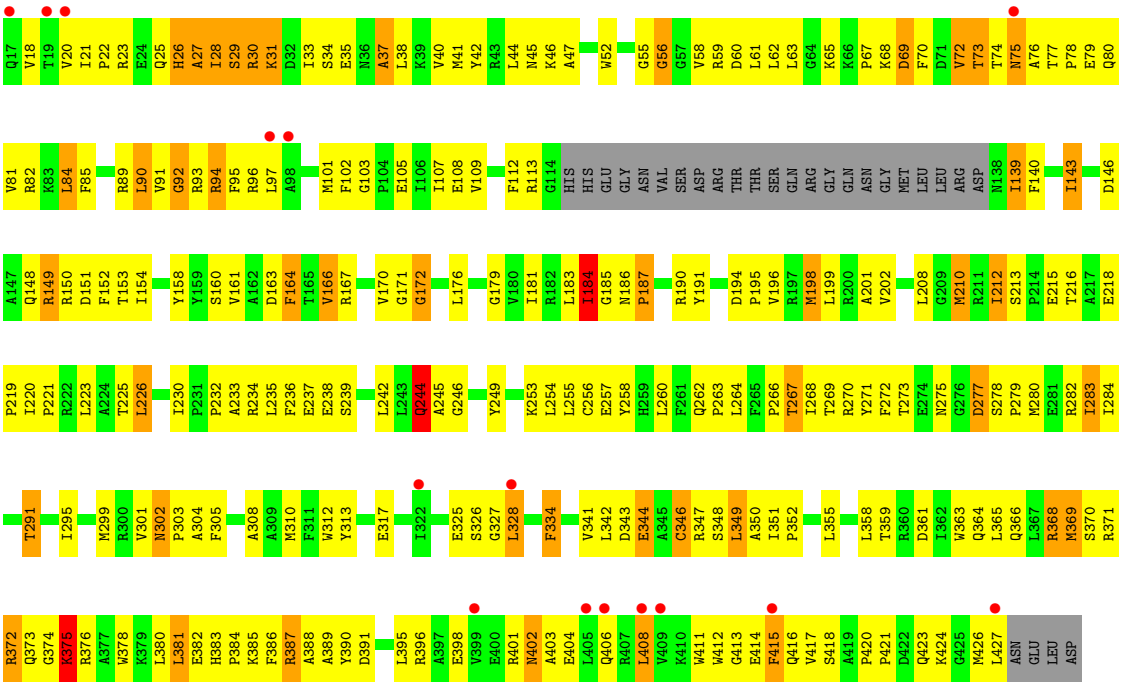
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
2	A	1	1	1	0	0
2	B	1	1	1	0	0

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.

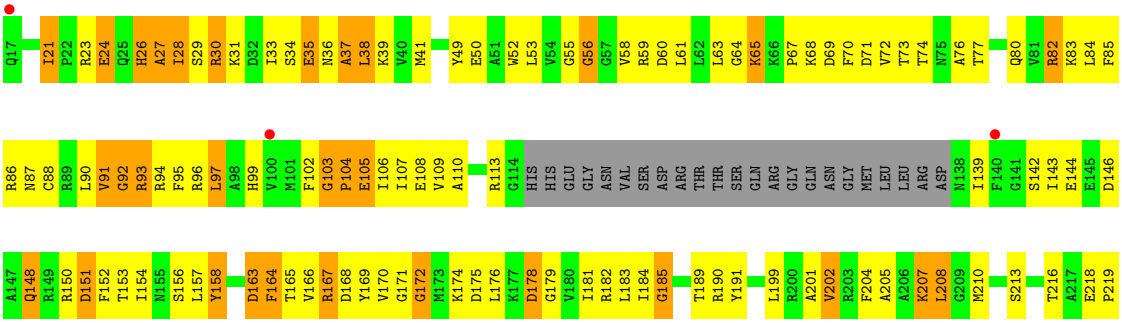
- Molecule 1: Poly(A) polymerase

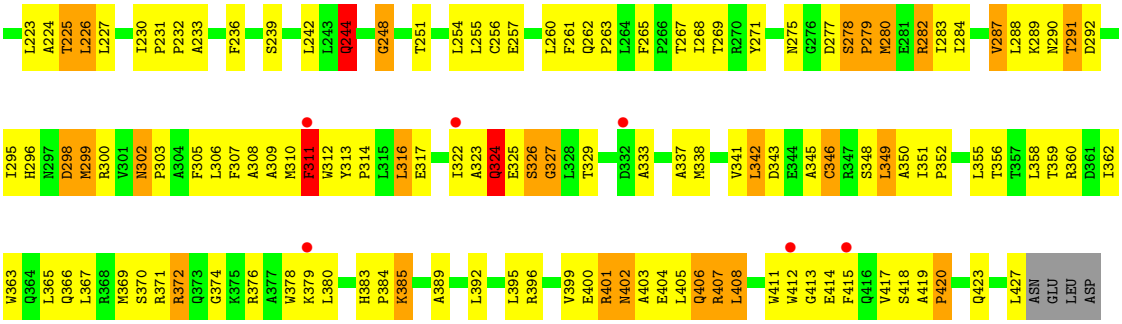
Chain A:



- Molecule 1: Poly(A) polymerase

Chain B:




L223 A224 T225 L226 L227 I230 P231 P232 A233 F236 S239 L242 L243 Q244 G248 T251 L254 L255 C256 E257 L260 F261 Q262 P263 L264 F265 P266 T267 I268 T269 R270 Y271 N275 G276 D277 S278 P279 M280 E281 R282 I283 I284 V287 L288 K289 N290 T291 D292
I295 H296 N297 D298 M299 R300 V301 N302 P303 A304 F305 L306 F307 A308 A309 M310 F311 W312 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 (i)

Property	Value	Source
Space group	P 42 21 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 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
$< I/\sigma(I) >$ [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 , 42.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.37$, $< L^2 > = 0.20$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	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.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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)

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(^{o})	Ideal(^{o})
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

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

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%)	291 (87%)	43 (13%)	4 18
1	B	334/358 (93%)	277 (83%)	57 (17%)	2 9
All	All	668/716 (93%)	568 (85%)	100 (15%)	3 13

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

Mol	Chain	Res	Type
1	B	164	PHE
1	B	277	ASP
1	B	420	PRO
1	B	178	ASP
1	B	239	SER

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

Mol	Chain	Res	Type
1	B	275	ASN
1	B	290	ASN
1	B	402	ASN
1	A	286	GLN
1	A	275	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 monosaccharides 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%)	0.33	15 (3%)	39	24	71, 101, 141, 169	0
1	B	388/415 (93%)	0.28	9 (2%)	60	46	66, 104, 145, 166	0
All	All	776/830 (93%)	0.30	24 (3%)	49	32	66, 103, 143, 169	0

The worst 5 of 24 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	17	GLN	3.9
1	B	100	VAL	3.3
1	A	328	LEU	2.7
1	A	409	VAL	2.7
1	A	405	LEU	2.7

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 monosaccharides 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(Å^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.