

wwPDB X-ray Structure Validation Summary Report (i)

Oct 15, 2023 – 01:42 AM EDT

PDB ID	:	7TJE
Title	:	Bacteriophage Q beta capsid protein A38K
Authors	:	Jin, X.
Deposited on	:	2022-01-16
Resolution	:	2.80 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:

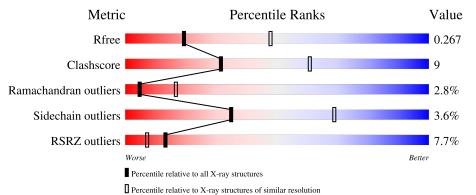
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 2.80 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	$\begin{array}{c} \textbf{Whole archive} \\ \textbf{(\#Entries)} \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$		
R_{free}	130704	3140(2.80-2.80)		
Clashscore	141614	3569(2.80-2.80)		
Ramachandran outliers	138981	3498 (2.80-2.80)		
Sidechain outliers	138945	3500 (2.80-2.80)		
RSRZ outliers	127900	3078 (2.80-2.80)		

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		190	6%		
1	A	132	68% 	28%	•
1	В	132	80%	16%	•••
1	С	132	7%	27%	
	0		10%	27,0	-
1	D	132	77%	23%	
1		100	7%		
	E	132	86%	12%	•



2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 5146 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	А	132	Total	С	Ν	0	S	0	0	0
	A	132	997	619	178	198	2	0	0	0
1	В	132	Total	С	Ν	0	S	0	0	0
	D	132	997	619	178	198	2	0	0	
1	С	132	Total	С	Ν	0	S	0	0	0
		132	997	619	178	198	2	0		0
1	р	132	Total	С	Ν	0	S	0	0	0
		132	997	619	178	198	2	0	0	0
1	1 E	132	Total	С	Ν	Ο	S	0	0	0
		132	997	619	178	198	2		0	0

• Molecule 1 is a protein called Minor capsid protein A1.

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	38	LYS	ALA	engineered mutation	UNP Q8LTE1
В	38	LYS	ALA	engineered mutation	UNP Q8LTE1
С	38	LYS	ALA	engineered mutation	UNP Q8LTE1
D	38	LYS	ALA	engineered mutation	UNP Q8LTE1
Е	38	LYS	ALA	engineered mutation	UNP Q8LTE1

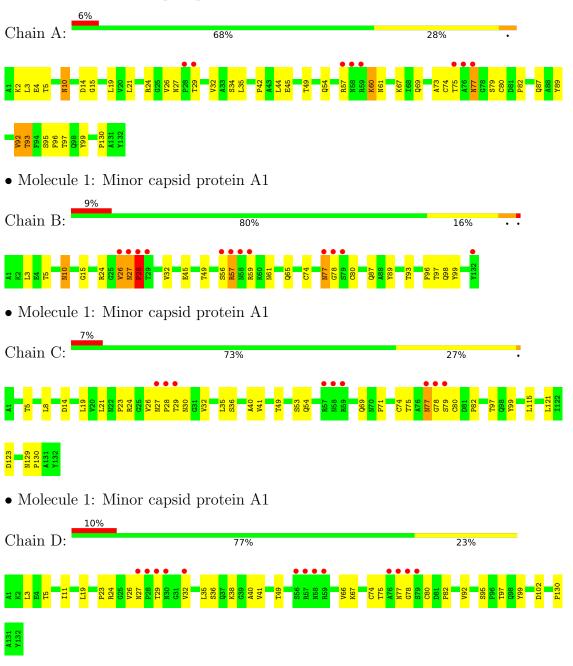
• Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	33	Total O 33 33	0	0
2	В	40	Total O 40 40	0	0
2	С	23	TotalO2323	0	0
2	D	35	Total O 35 35	0	0
2	Е	30	Total O 30 30	0	0



3 Residue-property plots (i)

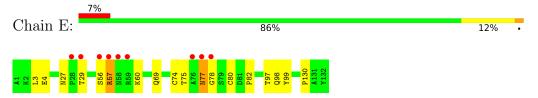
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Minor capsid protein A1



• Molecule 1: Minor capsid protein A1





4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 3	Depositor
Cell constants	194.14Å 194.14Å 194.14Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.76 - 2.80	Depositor
Resolution (A)	45.76 - 2.80	EDS
% Data completeness	97.9 (45.76-2.80)	Depositor
(in resolution range)	97.9(45.76-2.80)	EDS
R _{merge}	(Not available)	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$2.06 (at 2.81 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
P. P.	0.219 , 0.268	Depositor
R, R_{free}	0.220 , 0.267	DCC
R_{free} test set	1501 reflections (5.10%)	wwPDB-VP
Wilson B-factor $(Å^2)$	58.5	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.31 , 40.5	EDS
L-test for twinning ²	$< L > = 0.51, < L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.021 for -l,-k,-h	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	5146	wwPDB-VP
Average B, all atoms $(Å^2)$	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 2.36% of the height of the origin peak. No significant pseudotranslation is detected.

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.



¹Intensities estimated from amplitudes.

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		Boi	nd lengths	Bond angles		
	Moi Cham		# Z > 5	RMSZ	# Z > 5	
1	А	0.69	2/1011~(0.2%)	0.88	5/1375~(0.4%)	
1	В	0.46	0/1011	0.72	1/1375~(0.1%)	
1	С	0.47	0/1011	0.65	0/1375	
1	D	0.46	0/1011	0.65	0/1375	
1	Ε	0.44	0/1011	0.66	0/1375	
All	All	0.51	2/5055~(0.0%)	0.72	6/6875~(0.1%)	

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	А	0	3
1	В	0	2
1	С	0	1
1	D	0	1
1	Е	0	1
All	All	0	8

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\mathrm{Ideal}(\mathrm{\AA})$
1	А	92	VAL	C-N	-12.30	1.05	1.34
1	А	93	THR	C-N	-8.07	1.15	1.34

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	А	93	THR	O-C-N	-14.59	99.36	122.70
1	В	28	PRO	CA-N-CD	-10.72	96.49	111.50
1	А	92	VAL	O-C-N	-10.27	106.27	122.70
1	А	92	VAL	C-N-CA	9.46	145.35	121.70

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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	А	93	THR	CA-C-N	7.03	132.67	117.20

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	А	77	ASN	Peptide
1	А	92	VAL	Mainchain
1	А	93	THR	Mainchain
1	В	28	PRO	Peptide
1	В	77	ASN	Peptide

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	А	997	0	1012	25	0
1	В	997	0	1014	21	1
1	С	997	0	1014	22	0
1	D	997	0	1014	19	0
1	Ε	997	0	1014	13	0
2	А	33	0	0	2	1
2	В	40	0	0	4	1
2	С	23	0	0	0	0
2	D	35	0	0	1	0
2	Ε	30	0	0	1	1
All	All	5146	0	5068	90	3

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 9.

The worst 5 of 90 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:26:VAL:HG23	2:B:236:HOH:O	1.49	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:97:THR:HG22	1:D:99:TYR:H	1.30	0.97
1:B:26:VAL:CG2	2:B:236:HOH:O	2.10	0.96
1:B:97:THR:HG22	1:B:99:TYR:H	1.33	0.93
1:E:97:THR:HG22	1:E:99:TYR:H	1.30	0.92

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All (3) 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:B:27:ASN:ND2	1:B:27:ASN:ND2[5_564]	1.26	0.94
2:E:203:HOH:O	2:E:203:HOH:O[3_555]	2.02	0.18
2:A:222:HOH:O	2:B:224:HOH:O[5_564]	2.16	0.04

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	Perce	ntiles
1	А	130/132~(98%)	114 (88%)	11 (8%)	5(4%)	3	10
1	В	130/132~(98%)	116 (89%)	10 (8%)	4(3%)	4	14
1	С	130/132~(98%)	119 (92%)	8~(6%)	3~(2%)	6	21
1	D	130/132~(98%)	117 (90%)	10 (8%)	3~(2%)	6	21
1	Ε	130/132~(98%)	116 (89%)	11 (8%)	3~(2%)	6	21
All	All	650/660~(98%)	582 (90%)	$50 \ (8\%)$	18 (3%)	5	17

5 of 18 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	В	27	ASN
1	В	28	PRO
1	Е	29	THR

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Mol	Chain	Res	Type
1	А	3	LEU
1	А	29	THR

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain 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 side chain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Perce	entiles
1	А	111/111~(100%)	106~(96%)	5(4%)	27	60
1	В	111/111 (100%)	107~(96%)	4 (4%)	35	69
1	С	111/111 (100%)	106~(96%)	5(4%)	27	60
1	D	111/111 (100%)	108~(97%)	3~(3%)	44	78
1	Ε	111/111 (100%)	108~(97%)	3~(3%)	44	78
All	All	555/555~(100%)	535~(96%)	20~(4%)	35	69

5 of 20 residues with a non-rotameric side chain are listed below:

Mol	Chain	Res	Type
1	D	38	LYS
1	Е	4	GLU
1	Ε	57	ARG
1	Е	27	ASN
1	В	28	PRO

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such side chains are listed below:

Mol	Chain	Res	Type
1	Ε	27	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)

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)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	А	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	А	93:THR	С	94:PHE	Ν	1.15
1	А	92:VAL	С	93:THR	N	1.05



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^{th} 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	$OWAB(A^2)$	$\mathbf{Q}{<}0.9$
1	А	132/132~(100%)	0.07	8 (6%) 21 13	34, 55, 102, 119	0
1	В	132/132~(100%)	0.31	12 (9%) 9 5	33, 53, 107, 131	0
1	С	132/132~(100%)	0.14	9 (6%) 17 10	32, 56, 107, 127	0
1	D	132/132~(100%)	0.29	13 (9%) 7 4	33, 53, 108, 127	0
1	Ε	132/132~(100%)	0.28	9 (6%) 17 10	37, 56, 104, 127	0
All	All	660/660~(100%)	0.22	51 (7%) 13 7	32, 55, 107, 131	0

The worst 5 of 51 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	58	ASN	11.0
1	В	57	ARG	9.6
1	В	58	ASN	8.6
1	Е	57	ARG	7.0
1	Е	58	ASN	6.8

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 monosaccharides 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.

