

Full wwPDB X-ray Structure Validation Report (i)

Oct 31, 2021 – 07:48 PM EDT

PDB ID : 3BBZ

Title : Structure of the nucleocapsid-binding domain from the mumps virus phospho-

protein

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Deposited on : 2007-11-11

Resolution : 2.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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 following versions of software and data (see references (1)) were used in the production of this report:

MolProbity : 4.02b-467

Mogul: 1.8.5 (274361), CSD as541be (2020)

Xtriage (Phenix) : 1.13 EDS : 2.23.2

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)

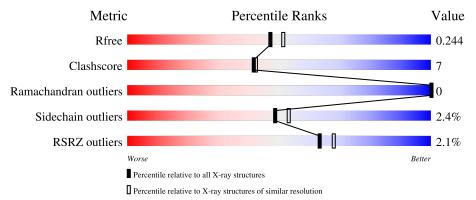
Validation Pipeline (wwPDB-VP) : 2.23.2

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 2.10 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	Similar resolution
Metric	$(\# ext{Entries})$	$(\# ext{Entries}, ext{ resolution range}(ext{Å}))$
R_{free}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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	49	88%	10%	•			
1	В	49	84%	12%				

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:



Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	FMT	В	2	_	-	X	-



2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 823 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 P protein.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	Λ	48	Total C N O S	S	0	0	0			
1	A	40	373	230	68	72	3	0	U	U
1	B	48	Total	С	N	О	S	0	9	0
1	ъ	40	378	233	69	73	3		<u> </u>	0

There are 2 discrepancies between the modelled and reference sequences:

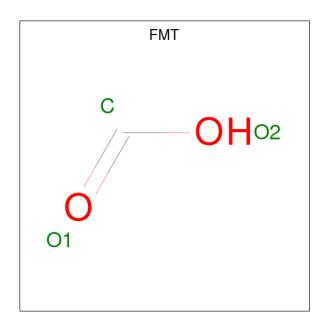
	Chain	Residue	Modelled	Actual	Comment	Reference
	A	356	SER	CYS	engineered mutation	UNP Q9J4L6
ĺ	В	356	SER	CYS	engineered mutation	UNP Q9J4L6

• Molecule 2 is BROMIDE ION (three-letter code: BR) (formula: Br).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Br 1 1	0	0
2	В	1	Total Br 1 1	0	0

• Molecule 3 is FORMIC ACID (three-letter code: FMT) (formula: CH₂O₂).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 3 1 2	0	0
3	A	1	Total C O 3 1 2	0	0
3	A	1	Total C O 3 1 2	0	0
3	В	1	Total C O 3 1 2	0	0
3	В	1	Total C O 3 1 2	0	0
3	В	1	Total C O 3 1 2	0	0

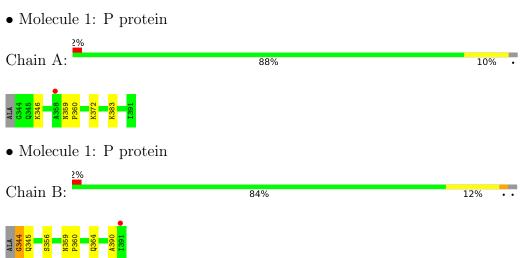
• Molecule 4 is water.

Mo	d (Chain	Residues	Atoms	ZeroOcc	AltConf
4		A	35	Total O 35 35	0	0
4		В	17	Total O 17 17	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.





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	23.99Å 55.48Å 60.02Å	Donositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.74 - 2.10	Depositor
rtesolution (A)	40.74 - 2.10	EDS
% Data completeness	97.1 (40.74-2.10)	Depositor
(in resolution range)	97.1 (40.74-2.10)	EDS
R_{merge}	0.14	Depositor
R_{sym}	0.14	Depositor
$< I/\sigma(I) > 1$	7.11 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
D D.	0.190 , 0.241	Depositor
R, R_{free}	0.190 , 0.244	DCC
R_{free} test set	238 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å ²)	10.6	Xtriage
Anisotropy	0.730	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.32, 45.8	EDS
L-test for twinning ²	$ < L >=0.56, < L^2>=0.41$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	823	wwPDB-VP
Average B, all atoms (Å ²)	10.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The analyses of the Patterson function reveals a significant off-origin peak that is 43.85 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.6609e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.

²Theoretical 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.



¹Intensities estimated from amplitudes.

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: BR, FMT

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	Bon	nd lengths	Bond angles		
IVIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z >5	
1	A	0.83	0/374	0.79	0/499	
1	В	0.93	1/389 (0.3%)	0.77	0/518	
All	All	0.88	1/763 (0.1%)	0.78	0/1017	

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\operatorname{Observed}(\text{\AA})$	$\operatorname{Ideal}(ext{\AA})$
1	В	344	GLY	N-CA	5.28	1.53	1.46

There are no bond angle outliers.

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	373	0	393	6	0
1	В	378	0	399	5	0
2	A	1	0	0	0	0
2	В	1	0	0	0	0
3	A	9	0	3	0	0
3	В	9	0	3	5	0
4	A	35	0	0	1	0
4	В	17	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	823	0	798	11	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 7.

All (11) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	Clash overlap (Å)
1:A:346:LYS:NZ	3:B:2:FMT:H	1.94	0.83
1:A:346:LYS:HZ1	3:B:2:FMT:H	1.58	0.68
1:A:346:LYS:CE	3:B:2:FMT:H	2.25	0.66
1:B:344:GLY:HA2	3:B:2:FMT:O2	2.09	0.53
1:A:346:LYS:HE3	3:B:2:FMT:H	1.97	0.45
1:B:359:ASN:HA	1:B:360:PRO:HD3	1.91	0.44
1:A:359:ASN:HA	1:A:360:PRO:HD3	1.78	0.44
1:B:360:PRO:O	1:B:364:GLN:HG3	2.17	0.44
1:A:383:LYS:NZ	4:A:415:HOH:O	2.51	0.44
1:B:356[B]:SER:OG	1:B:390:ALA:HB2	2.21	0.41
1:B:364:GLN:HB3	4:B:408:HOH:O	2.20	0.40

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	Perce	ntiles
1	A	46/49 (94%)	45 (98%)	1 (2%)	0	100	100
1	В	48/49 (98%)	48 (100%)	0	0	100	100
All	All	94/98 (96%)	93 (99%)	1 (1%)	0	100	100

There are no Ramachandran outliers to report.



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	41/41 (100%)	40 (98%)	1 (2%)	49 53		
1	В	43/41 (105%)	42 (98%)	1 (2%)	50 55		
All	All	84/82 (102%)	82 (98%)	2 (2%)	49 53		

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	372	LYS
1	В	345	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The



Link column lists molecule types, if any, to which the group is linked. 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| > 2 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
MIOI			nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2
3	FMT	В	2	-	0,2,2	-	-	0,1,1	-	-
3	FMT	A	1	-	0,2,2	-	-	0,1,1	-	-
3	FMT	В	7	-	0,2,2	-	-	0,1,1	-	-
3	FMT	A	4	-	0,2,2	-	-	0,1,1	-	-
3	FMT	A	8	-	0,2,2	-	-	0,1,1	-	-
3	FMT	В	3	-	0,2,2	-	-	0,1,1	-	-

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.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	В	2	FMT	5	0

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^{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 $>$	$\#\mathrm{RSRZ}{>}2$	$OWAB(A^2)$	Q<0.9
1	A	48/49 (97%)	-0.33	1 (2%) 63 68	2, 8, 23, 29	3 (6%)
1	В	48/49 (97%)	-0.27	1 (2%) 63 68	2, 8, 20, 30	1 (2%)
All	All	$96/98 \; (97\%)$	-0.30	2 (2%) 63 68	2, 8, 23, 30	4 (4%)

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	В	391	ILE	2.5
1	A	358	ALA	2.0

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, 95^{th} 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	$\operatorname{B-factors}(\mathrm{\AA}^2)$	Q<0.9
3	FMT	A	4	3/3	0.86	0.16	36,36,36,36	0
3	FMT	A	8	3/3	0.91	0.19	7,7,9,10	3
3	FMT	В	7	3/3	0.93	0.17	7,7,8,8	3

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q < 0.9
3	FMT	В	3	3/3	0.94	0.14	23,23,24,26	0
3	FMT	В	2	3/3	0.95	0.14	6,6,6,10	0
3	FMT	A	1	3/3	0.97	0.12	9,9,10,14	0
2	BR	A	65	1/1	0.99	0.04	17,17,17,17	1
2	BR	В	64	1/1	0.99	0.04	16,16,16,16	1

6.5 Other polymers (i)

There are no such residues in this entry.

