



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:09 AM UTC

PDB ID : 7JS4 / pdb\_00007js4  
Title : The structure of the M60 catalytic domain with the CBM51-1 and CBM51-2 domains from *Clostridium perfringens* ZmpB  
Authors : Pluvinage, B.; Boraston, A.B.  
Deposited on : 2020-08-13  
Resolution : 4.60 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](mailto: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>.

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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

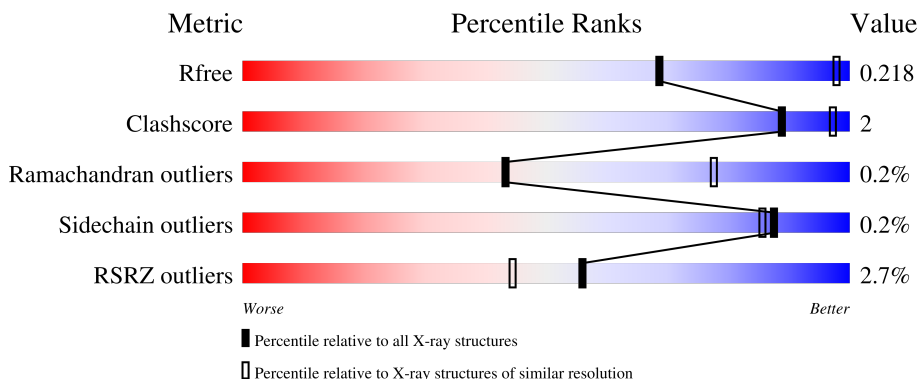
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 4.60 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	1007 (5.28-3.92)
Clashscore	190562	1022 (5.26-3.94)
Ramachandran outliers	187476	1069 (5.30-3.90)
Sidechain outliers	187428	1051 (5.30-3.90)
RSRZ outliers	180081	1002 (5.28-3.92)

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  $\geq 3$ , 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	980	

## 2 Entry composition i

There is only 1 type of molecule in this entry. The entry contains 7510 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 F5/8 type C domain protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	953	7510	4722	1263	1507	18	0	0	0

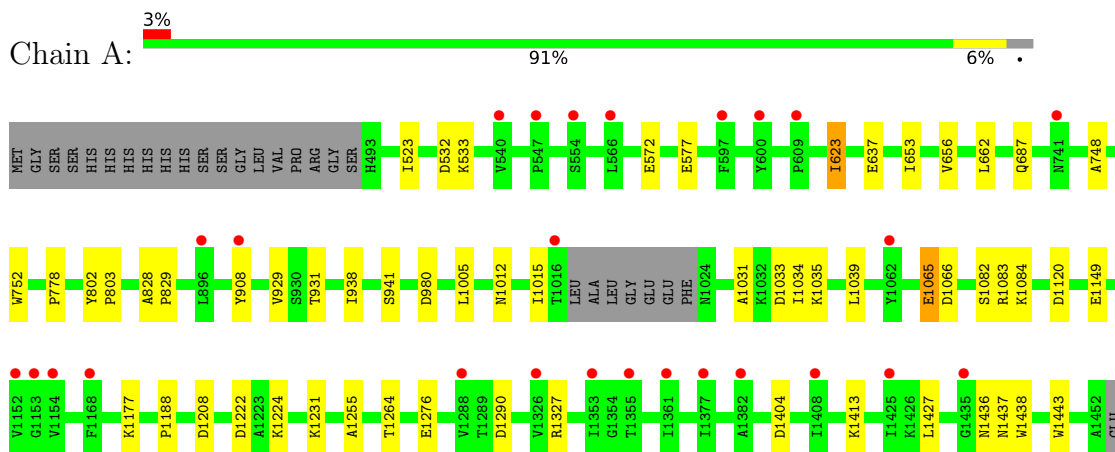
There are 23 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	474	MET	-	expression tag	UNP A0A0H2YN38
A	475	GLY	-	expression tag	UNP A0A0H2YN38
A	476	SER	-	expression tag	UNP A0A0H2YN38
A	477	SER	-	expression tag	UNP A0A0H2YN38
A	478	HIS	-	expression tag	UNP A0A0H2YN38
A	479	HIS	-	expression tag	UNP A0A0H2YN38
A	480	HIS	-	expression tag	UNP A0A0H2YN38
A	481	HIS	-	expression tag	UNP A0A0H2YN38
A	482	HIS	-	expression tag	UNP A0A0H2YN38
A	483	HIS	-	expression tag	UNP A0A0H2YN38
A	484	SER	-	expression tag	UNP A0A0H2YN38
A	485	SER	-	expression tag	UNP A0A0H2YN38
A	486	GLY	-	expression tag	UNP A0A0H2YN38
A	487	LEU	-	expression tag	UNP A0A0H2YN38
A	488	VAL	-	expression tag	UNP A0A0H2YN38
A	489	PRO	-	expression tag	UNP A0A0H2YN38
A	490	ARG	-	expression tag	UNP A0A0H2YN38
A	491	GLY	-	expression tag	UNP A0A0H2YN38
A	492	SER	-	expression tag	UNP A0A0H2YN38
A	493	HIS	-	expression tag	UNP A0A0H2YN38
A	494	MET	-	expression tag	UNP A0A0H2YN38
A	495	ALA	-	expression tag	UNP A0A0H2YN38
A	496	SER	-	expression tag	UNP A0A0H2YN38

### 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: F5/8 type C domain protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	70.91Å 119.32Å 129.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.69 – 4.60 29.69 – 4.60	Depositor EDS
% Data completeness (in resolution range)	98.5 (29.69-4.60) 98.6 (29.69-4.60)	Depositor EDS
$R_{merge}$	0.20	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.82 (at 4.61Å)	Xtrriage
Refinement program	REFMAC 5.8.0258	Depositor
R, $R_{free}$	0.191 , 0.258 0.193 , 0.218	Depositor DCC
$R_{free}$ test set	250 reflections (3.85%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	70.5	Xtrriage
Anisotropy	0.049	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.24 , 57.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.85	EDS
Total number of atoms	7510	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	84.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.36% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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	0.55	0/7653	1.12	11/10341 (0.1%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1222	ASP	CA-CB-CG	6.73	119.33	112.60
1	A	1065	GLU	CB-CG-CD	6.56	123.76	112.60
1	A	577	GLU	CB-CG-CD	6.55	123.73	112.60
1	A	1208	ASP	CA-CB-CG	6.16	118.76	112.60
1	A	532	ASP	CA-CB-CG	6.11	118.70	112.60
1	A	1188	PRO	CA-C-N	6.05	129.70	121.05
1	A	1188	PRO	C-N-CA	6.05	129.70	121.05
1	A	637	GLU	CB-CG-CD	6.04	122.86	112.60
1	A	1120	ASP	CA-CB-CG	5.16	117.76	112.60
1	A	1177	LYS	N-CA-C	-5.15	107.54	113.88
1	A	1276	GLU	N-CA-CB	5.04	117.37	109.97

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	7510	0	7326	28	0
All	All	7510	0	7326	28	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 2.

All (28) 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:980:ASP:OD1	1:A:1035:LYS:NZ	2.34	0.60
1:A:1031:ALA:O	1:A:1039:LEU:HB2	2.02	0.59
1:A:1065:GLU:HG2	1:A:1066:ASP:N	2.20	0.55
1:A:1231:LYS:O	1:A:1231:LYS:HG3	2.07	0.53
1:A:1082:SER:OG	1:A:1083:ARG:N	2.42	0.53
1:A:1015:ILE:HG21	1:A:1224:LYS:CD	2.39	0.52
1:A:687:GLN:HB3	1:A:748:ALA:HB3	1.92	0.51
1:A:1290:ASP:OD1	1:A:1290:ASP:C	2.55	0.50
1:A:653:ILE:HG13	1:A:653:ILE:O	2.12	0.49
1:A:1033:ASP:CG	1:A:1034:ILE:N	2.72	0.48
1:A:1255:ALA:H	1:A:1264:THR:HG22	1.82	0.45
1:A:1015:ILE:O	1:A:1015:ILE:HG23	2.16	0.45
1:A:931:THR:HG23	1:A:938:ILE:HG23	1.99	0.45
1:A:1437:ASN:O	1:A:1438:TRP:HB2	2.17	0.45
1:A:752:TRP:CE3	1:A:778:PRO:HB2	2.53	0.44
1:A:1327:ARG:HH11	1:A:1327:ARG:HG2	1.81	0.44
1:A:1224:LYS:HB2	1:A:1224:LYS:HE2	1.75	0.43
1:A:931:THR:HG21	1:A:1005:LEU:H	1.84	0.42
1:A:523:ILE:CG2	1:A:623:ILE:HD11	2.50	0.42
1:A:1427:LEU:HB3	1:A:1443:TRP:CZ2	2.55	0.42
1:A:929:VAL:HA	1:A:941:SER:O	2.20	0.42
1:A:1404:ASP:OD1	1:A:1413:LYS:NZ	2.52	0.41
1:A:802:TYR:HB2	1:A:803:PRO:HD3	2.03	0.41
1:A:1149:GLU:OE1	1:A:1224:LYS:HE3	2.21	0.41
1:A:533:LYS:CE	1:A:572:GLU:OE1	2.69	0.41
1:A:828:ALA:N	1:A:829:PRO:CD	2.84	0.41
1:A:656:VAL:O	1:A:662:LEU:HA	2.22	0.40
1:A:908:TYR:HD1	1:A:908:TYR:HA	1.68	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	Percentiles
1	A	949/980 (97%)	921 (97%)	26 (3%)	2 (0%)	43 77

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1084	LYS
1	A	1436	ASN

### 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	828/850 (97%)	826 (100%)	2 (0%)	87 85

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

Mol	Chain	Res	Type
1	A	623	ILE
1	A	1012	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	732	ASN
1	A	1440	HIS

### 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

### 6.1 Protein, DNA and RNA chains

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	953/980 (97%)	0.29	26 (2%) 56 44	32, 80, 134, 259	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1382	ALA	4.0
1	A	1377	ILE	3.7
1	A	1435	GLY	3.5
1	A	1408	ILE	3.3
1	A	540	VAL	3.2
1	A	566	LEU	3.2
1	A	554	SER	2.9
1	A	1326	VAL	2.8
1	A	1288	VAL	2.8
1	A	1154	VAL	2.7
1	A	1153	GLY	2.7
1	A	609	PRO	2.6
1	A	547	PRO	2.6
1	A	741	ASN	2.6
1	A	1353	ILE	2.6
1	A	896	LEU	2.5
1	A	1062	TYR	2.4
1	A	908	TYR	2.2
1	A	1361	ILE	2.2
1	A	1016	THR	2.2
1	A	1168	PHE	2.1
1	A	1355	THR	2.1
1	A	600	TYR	2.1
1	A	1425	ILE	2.1
1	A	597	PHE	2.1
1	A	1152	VAL	2.1

## 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.