



wwPDB X-ray Structure Validation Summary Report ⓘ

May 29, 2020 – 07:28 am BST

PDB ID : 5KDJ
Title : ZmpB metallopeptidase from Clostridium perfringens
Authors : Noach, I.; Ficko-Blean, E.; Stuart, C.; Boraston, A.B.
Deposited on : 2016-06-08
Resolution : 2.15 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 following versions of software and data (see [references ⓘ](#)) 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	:	2.11
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)	:	2.11

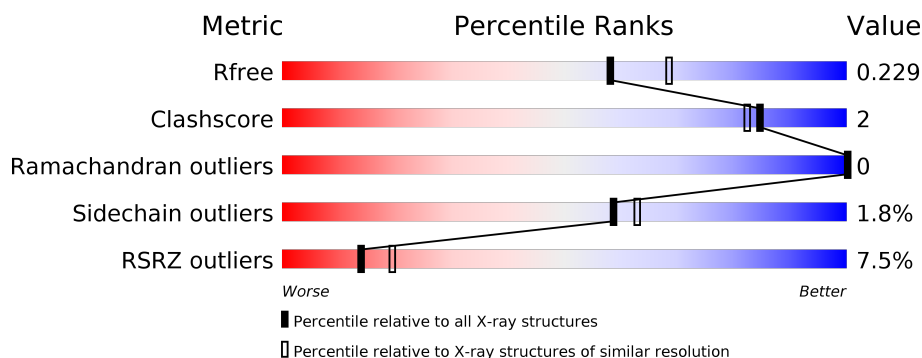
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

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 on 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	674	<div> <div>10%</div> <div> <div></div> <div>69%</div> <div>5%</div> <div>26%</div> </div> </div>
1	B	674	<div> <div>%</div> <div> <div></div> <div>69%</div> <div>•</div> <div>26%</div> </div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8827 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
1	B	501	Total	C	N	O	S	0	0	0
			4019	2552	675	782	10			
1	A	498	Total	C	N	O	S	0	3	0
			4019	2555	672	782	10			

There are 46 discrepancies between the modelled and reference sequences:

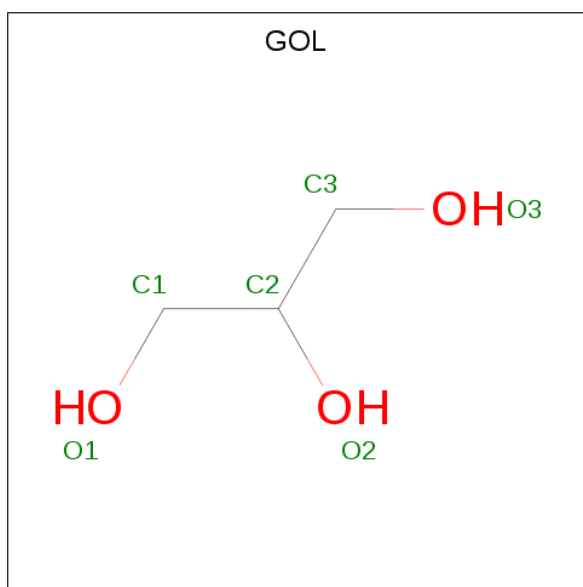
Chain	Residue	Modelled	Actual	Comment	Reference
B	411	MET	-	initiating methionine	UNP A0A0H2YN38
B	412	GLY	-	expression tag	UNP A0A0H2YN38
B	413	SER	-	expression tag	UNP A0A0H2YN38
B	414	SER	-	expression tag	UNP A0A0H2YN38
B	415	HIS	-	expression tag	UNP A0A0H2YN38
B	416	HIS	-	expression tag	UNP A0A0H2YN38
B	417	HIS	-	expression tag	UNP A0A0H2YN38
B	418	HIS	-	expression tag	UNP A0A0H2YN38
B	419	HIS	-	expression tag	UNP A0A0H2YN38
B	420	HIS	-	expression tag	UNP A0A0H2YN38
B	421	SER	-	expression tag	UNP A0A0H2YN38
B	422	SER	-	expression tag	UNP A0A0H2YN38
B	423	GLY	-	expression tag	UNP A0A0H2YN38
B	424	LEU	-	expression tag	UNP A0A0H2YN38
B	425	VAL	-	expression tag	UNP A0A0H2YN38
B	426	PRO	-	expression tag	UNP A0A0H2YN38
B	427	ARG	-	expression tag	UNP A0A0H2YN38
B	428	GLY	-	expression tag	UNP A0A0H2YN38
B	429	SER	-	expression tag	UNP A0A0H2YN38
B	430	HIS	-	expression tag	UNP A0A0H2YN38
B	431	MET	-	expression tag	UNP A0A0H2YN38
B	432	ALA	-	expression tag	UNP A0A0H2YN38
B	433	SER	-	expression tag	UNP A0A0H2YN38
A	411	MET	-	initiating methionine	UNP A0A0H2YN38
A	412	GLY	-	expression tag	UNP A0A0H2YN38

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Chain	Residue	Modelled	Actual	Comment	Reference
A	413	SER	-	expression tag	UNP A0A0H2YN38
A	414	SER	-	expression tag	UNP A0A0H2YN38
A	415	HIS	-	expression tag	UNP A0A0H2YN38
A	416	HIS	-	expression tag	UNP A0A0H2YN38
A	417	HIS	-	expression tag	UNP A0A0H2YN38
A	418	HIS	-	expression tag	UNP A0A0H2YN38
A	419	HIS	-	expression tag	UNP A0A0H2YN38
A	420	HIS	-	expression tag	UNP A0A0H2YN38
A	421	SER	-	expression tag	UNP A0A0H2YN38
A	422	SER	-	expression tag	UNP A0A0H2YN38
A	423	GLY	-	expression tag	UNP A0A0H2YN38
A	424	LEU	-	expression tag	UNP A0A0H2YN38
A	425	VAL	-	expression tag	UNP A0A0H2YN38
A	426	PRO	-	expression tag	UNP A0A0H2YN38
A	427	ARG	-	expression tag	UNP A0A0H2YN38
A	428	GLY	-	expression tag	UNP A0A0H2YN38
A	429	SER	-	expression tag	UNP A0A0H2YN38
A	430	HIS	-	expression tag	UNP A0A0H2YN38
A	431	MET	-	expression tag	UNP A0A0H2YN38
A	432	ALA	-	expression tag	UNP A0A0H2YN38
A	433	SER	-	expression tag	UNP A0A0H2YN38

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Na	0	0
			1	1		

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Zn	0	0
			1	1		
4	A	1	Total	Zn	0	0
			1	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	472	Total	O	0	2
			474	474		
5	A	300	Total	O	0	0
			300	300		

GLU VAL LEU TYR SER LEU GLU ASP SER LYS GLY ASN GLU TYR THR LYS THR SER LYS VAL ASN VAL VAL SER ARG LYS

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	65.62Å 95.80Å 187.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.82 – 2.15 29.82 – 2.15	Depositor EDS
% Data completeness (in resolution range)	96.2 (29.82-2.15) 96.2 (29.82-2.15)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.61 (at 2.16Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.191 , 0.229 0.191 , 0.229	Depositor DCC
R_{free} test set	3170 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	18.1	Xtriage
Anisotropy	0.380	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 43.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8827	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.87% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, ZN, NA

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	0.63	3/4118 (0.1%)	0.73	4/5568 (0.1%)
1	B	0.65	1/4109 (0.0%)	0.73	4/5554 (0.1%)
All	All	0.64	4/8227 (0.0%)	0.73	8/11122 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	673	TRP	CD2-CE2	5.87	1.48	1.41
1	A	752	TRP	CD2-CE2	5.51	1.48	1.41
1	B	797	TRP	CD2-CE2	5.41	1.47	1.41
1	A	699	TRP	CD2-CE2	5.02	1.47	1.41

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	689[A]	ASP	CB-CG-OD1	10.22	127.50	118.30
1	A	689[B]	ASP	CB-CG-OD1	10.22	127.50	118.30
1	B	529	ARG	NE-CZ-NH1	7.88	124.24	120.30
1	B	594	ASP	CB-CG-OD1	6.14	123.83	118.30
1	A	594	ASP	CB-CG-OD1	6.11	123.80	118.30

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	4019	0	3901	20	0
1	B	4019	0	3895	16	0
2	A	6	0	8	3	0
2	B	6	0	8	0	0
3	B	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	300	0	0	3	0
5	B	474	0	0	5	0
All	All	8827	0	7812	36	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.

The worst 5 of 36 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:666:GLN:HE22	2:A:1101:GOL:H31	1.32	0.93
1:A:826:GLN:HE22	1:A:858:ARG:HH11	1.32	0.75
1:A:756:HIS:HD1	1:A:775:ASN:HD21	1.33	0.74
1:B:756:HIS:HD1	1:B:775:ASN:HD21	1.37	0.72
1:B:496:ASP:N	5:B:1201:HOH:O	2.23	0.71

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	495/674 (73%)	482 (97%)	13 (3%)	0	100	100
1	B	495/674 (73%)	482 (97%)	13 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	990/1348 (73%)	964 (97%)	26 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	435/591 (74%)	428 (98%)	7 (2%)	62	67
1	B	433/591 (73%)	424 (98%)	9 (2%)	53	57
All	All	868/1182 (73%)	852 (98%)	16 (2%)	59	63

5 of 16 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	984	VAL
1	B	1003	ASN
1	A	699	TRP
1	B	946	ASP
1	A	767	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	775	ASN
1	A	924	ASN
1	A	795	ASN
1	B	924	ASN
1	A	826	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 5 ligands modelled in this entry, 3 are monoatomic - leaving 2 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		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	GOL	B	1101	-	5,5,5	0.16	0	5,5,5	1.07	0
2	GOL	A	1101	-	5,5,5	0.29	0	5,5,5	0.51	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	B	1101	-	-	4/4/4/4	-
2	GOL	A	1101	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1101	GOL	O1-C1-C2-C3
2	B	1101	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
2	B	1101	GOL	O2-C2-C3-O3
2	B	1101	GOL	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1101	GOL	3	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, 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	498/674 (73%)	0.62	66 (13%) 3 4	8, 23, 59, 72	0
1	B	501/674 (74%)	0.01	9 (1%) 68 75	8, 15, 32, 49	0
All	All	999/1348 (74%)	0.31	75 (7%) 14 19	8, 18, 51, 72	0

The worst 5 of 75 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	724	GLY	9.4
1	A	725	GLY	8.4
1	B	724	GLY	7.8
1	A	961	GLY	6.3
1	A	1004	ALA	5.9

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 carbohydrates 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(\AA^2)	Q<0.9
2	GOL	B	1101	6/6	0.87	0.18	34,38,41,45	0
2	GOL	A	1101	6/6	0.96	0.14	35,36,37,38	0
3	NA	B	1102	1/1	0.97	0.29	27,27,27,27	0
4	ZN	A	1102	1/1	0.98	0.07	39,39,39,39	0
4	ZN	B	1103	1/1	0.99	0.04	27,27,27,27	0

6.5 Other polymers [i](#)

There are no such residues in this entry.