



wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 3AZY / pdb_00003azy
Title : Crystal structure of the laminarinase catalytic domain from *Thermotoga maritima* MSB8
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Deposited on : 2011-06-03
Resolution : 1.65 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

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<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>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
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

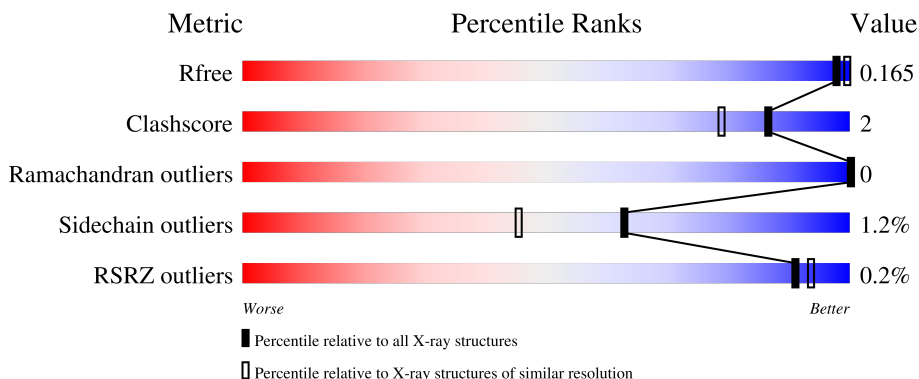
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.65 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	2563 (1.66-1.66)
Clashscore	190562	2662 (1.66-1.66)
Ramachandran outliers	187476	2621 (1.66-1.66)
Sidechain outliers	187428	2621 (1.66-1.66)
RSRZ outliers	180081	2564 (1.66-1.66)

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 $\leq 5\%$. 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	272	86% 6% • 8%
1	B	272	90% • 8%
1	C	272	88% 5% 8%
1	D	272	90% • 8%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9049 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 Laminarinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	251	Total	C	N	O	S	0	7	0
			2070	1336	327	399	8			
1	B	251	Total	C	N	O	S	0	0	0
			2033	1313	320	392	8			
1	C	251	Total	C	N	O	S	0	1	0
			2040	1318	322	392	8			
1	D	251	Total	C	N	O	S	0	0	0
			2033	1313	320	392	8			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	expression tag	UNP Q9WXN1
A	265	VAL	-	expression tag	UNP Q9WXN1
A	266	GLU	-	expression tag	UNP Q9WXN1
A	267	HIS	-	expression tag	UNP Q9WXN1
A	268	HIS	-	expression tag	UNP Q9WXN1
A	269	HIS	-	expression tag	UNP Q9WXN1
A	270	HIS	-	expression tag	UNP Q9WXN1
A	271	HIS	-	expression tag	UNP Q9WXN1
A	272	HIS	-	expression tag	UNP Q9WXN1
B	1	MET	-	expression tag	UNP Q9WXN1
B	265	VAL	-	expression tag	UNP Q9WXN1
B	266	GLU	-	expression tag	UNP Q9WXN1
B	267	HIS	-	expression tag	UNP Q9WXN1
B	268	HIS	-	expression tag	UNP Q9WXN1
B	269	HIS	-	expression tag	UNP Q9WXN1
B	270	HIS	-	expression tag	UNP Q9WXN1
B	271	HIS	-	expression tag	UNP Q9WXN1
B	272	HIS	-	expression tag	UNP Q9WXN1
C	1	MET	-	expression tag	UNP Q9WXN1
C	265	VAL	-	expression tag	UNP Q9WXN1
C	266	GLU	-	expression tag	UNP Q9WXN1

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Chain	Residue	Modelled	Actual	Comment	Reference
C	267	HIS	-	expression tag	UNP Q9WXN1
C	268	HIS	-	expression tag	UNP Q9WXN1
C	269	HIS	-	expression tag	UNP Q9WXN1
C	270	HIS	-	expression tag	UNP Q9WXN1
C	271	HIS	-	expression tag	UNP Q9WXN1
C	272	HIS	-	expression tag	UNP Q9WXN1
D	1	MET	-	expression tag	UNP Q9WXN1
D	265	VAL	-	expression tag	UNP Q9WXN1
D	266	GLU	-	expression tag	UNP Q9WXN1
D	267	HIS	-	expression tag	UNP Q9WXN1
D	268	HIS	-	expression tag	UNP Q9WXN1
D	269	HIS	-	expression tag	UNP Q9WXN1
D	270	HIS	-	expression tag	UNP Q9WXN1
D	271	HIS	-	expression tag	UNP Q9WXN1
D	272	HIS	-	expression tag	UNP Q9WXN1

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Ca 1 1	0	0
2	B	1	Total Ca 1 1	0	0
2	C	1	Total Ca 1 1	0	0
2	D	1	Total Ca 1 1	0	0

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	203	Total 203	O 203	0	0
4	B	162	Total 162	O 162	0	0
4	C	187	Total 187	O 187	0	0
4	D	257	Total 257	O 257	0	0

i

- Molecule 1: Laminarinase

[illegible]

MET
GLU
ASP
LYS
VAL
E8
D20
G21
N34
G35
H36
H200
E238
N258
PRO
GLU
THR
ILE
THR
GLY
VAL
GLU
HIS
HIS
HIS
HIS
HIS
HIS

[illegible]

MET	GLU	ASP	GLU	ASP	LYS	VAL	E8	G21	N34	G42	E100	H179	N258	PRO	GLU	THR	ILE	THR	GLY	VAL	GLU	HIS	HIS	HIS	HIS	HIS	HIS
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4 Data and refinement statistics

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α , β , γ	120.42Å 120.42Å 107.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.60 – 1.65 24.60 – 1.65	Depositor EDS
% Data completeness (in resolution range)	99.8 (24.60-1.65) 99.8 (24.60-1.65)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.84 (at 1.65Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.163 , 0.192 0.158 , 0.165	Depositor DCC
R_{free} test set	9202 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	23.6	Xtriage
Anisotropy	0.195	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 35.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.165 for h,-k,-l	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	9049	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 3.03% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, SO4

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	0.42	0/2144	0.84	1/2919 (0.0%)
1	B	0.39	0/2100	0.81	0/2860
1	C	0.41	0/2111	0.83	1/2875 (0.0%)
1	D	0.47	0/2100	0.84	1/2860 (0.0%)
All	All	0.42	0/8455	0.83	3/11514 (0.0%)

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	A	0	1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	158	GLY	N-CA-C	-9.02	104.39	114.40
1	D	21	GLY	N-CA-C	6.53	124.03	115.47
1	A	257	MET	CB-CA-C	5.10	118.23	111.14

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	257	MET	Peptide

5.2 Too-close contacts ⓘ

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	2070	0	1904	15	0
1	B	2033	0	1866	5	0
1	C	2040	0	1873	8	0
1	D	2033	0	1866	4	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	10	0	0	0	0
3	B	15	0	0	1	0
3	C	20	0	0	0	0
3	D	15	0	0	1	0
4	A	203	0	0	3	0
4	B	162	0	0	1	0
4	C	187	0	0	2	0
4	D	257	0	0	3	0
All	All	9049	0	7509	33	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 33 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:C:20:ASP:CG	1:C:21:GLY:H	1.82	0.86
1:B:20:ASP:CG	1:B:21:GLY:H	1.92	0.77
1:A:107:LYS:NZ	4:A:1036:HOH:O	2.15	0.72
1:D:100:GLU:OE1	4:D:936:HOH:O	2.08	0.71
1:A:20:ASP:OD2	1:A:20:ASP:C	2.36	0.67

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	256/272 (94%)	248 (97%)	8 (3%)	0	100	100
1	B	249/272 (92%)	241 (97%)	8 (3%)	0	100	100
1	C	250/272 (92%)	239 (96%)	11 (4%)	0	100	100
1	D	249/272 (92%)	242 (97%)	7 (3%)	0	100	100
All	All	1004/1088 (92%)	970 (97%)	34 (3%)	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	214/230 (93%)	210 (98%)	4 (2%)	50	28
1	B	210/230 (91%)	209 (100%)	1 (0%)	81	72
1	C	211/230 (92%)	207 (98%)	4 (2%)	50	28
1	D	210/230 (91%)	209 (100%)	1 (0%)	81	72
All	All	845/920 (92%)	835 (99%)	10 (1%)	63	45

5 of 10 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	94	ILE
1	C	257	MET
1	D	258	ASN

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Mol	Chain	Res	Type
1	A	151	HIS
1	B	238	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	11	GLN
1	D	29	ASN
1	D	241	GLN
1	D	34	ASN
1	C	26	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 4 are monoatomic - leaving 12 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	$\# Z > 2$
3	SO4	D	303	-	4,4,4	0.22	0	6,6,6	0.31	0
3	SO4	A	303	-	4,4,4	0.23	0	6,6,6	0.22	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	SO4	C	305	-	4,4,4	0.26	0	6,6,6	0.24	0
3	SO4	C	303	-	4,4,4	0.26	0	6,6,6	0.25	0
3	SO4	C	304	-	4,4,4	0.24	0	6,6,6	0.40	0
3	SO4	C	302	-	4,4,4	0.23	0	6,6,6	0.09	0
3	SO4	D	305	-	4,4,4	0.25	0	6,6,6	0.21	0
3	SO4	A	302	-	4,4,4	0.24	0	6,6,6	0.09	0
3	SO4	B	303	-	4,4,4	0.25	0	6,6,6	0.29	0
3	SO4	B	302	-	4,4,4	0.25	0	6,6,6	0.12	0
3	SO4	D	302	-	4,4,4	0.24	0	6,6,6	0.12	0
3	SO4	B	304	-	4,4,4	0.21	0	6,6,6	0.26	0

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.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	303	SO4	1	0
3	B	304	SO4	1	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	251/272 (92%)	-1.22	1 (0%) 88 92	11, 19, 30, 43	7 (2%)
1	B	251/272 (92%)	-1.12	0 100 100	15, 21, 34, 46	0
1	C	251/272 (92%)	-1.18	1 (0%) 88 92	11, 19, 33, 43	1 (0%)
1	D	251/272 (92%)	-1.30	0 100 100	13, 17, 30, 42	0
All	All	1004/1088 (92%)	-1.20	2 (0%) 91 93	11, 19, 32, 46	8 (0%)

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	159[A]	ALA	2.5
1	C	162	GLY	2.3

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](#)

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($\text{\AA}^2$)	Q<0.9
3	SO4	A	302	5/5	0.96	0.09	89,89,89,89	0
3	SO4	C	302	5/5	0.96	0.10	79,79,79,79	0
3	SO4	B	303	5/5	0.97	0.06	58,58,59,59	0
3	SO4	B	304	5/5	0.97	0.13	66,67,67,68	0
3	SO4	D	302	5/5	0.97	0.07	78,78,78,79	0
3	SO4	D	303	5/5	0.97	0.07	59,59,60,60	0
3	SO4	C	303	5/5	0.98	0.07	58,58,59,60	0
3	SO4	C	305	5/5	0.98	0.04	50,50,52,52	0
3	SO4	A	303	5/5	0.98	0.06	58,59,60,60	0
3	SO4	B	302	5/5	0.98	0.05	79,79,79,79	0
3	SO4	C	304	5/5	0.99	0.06	50,51,52,52	0
3	SO4	D	305	5/5	0.99	0.04	59,59,60,60	0
2	CA	A	301	1/1	1.00	0.04	22,22,22,22	0
2	CA	B	301	1/1	1.00	0.02	20,20,20,20	0
2	CA	C	301	1/1	1.00	0.02	18,18,18,18	0
2	CA	D	301	1/1	1.00	0.04	20,20,20,20	0

6.5 Other polymers ⓘ

There are no such residues in this entry.