



wwPDB X-ray Structure Validation Summary Report ⓘ

May 26, 2020 – 09:33 pm BST

PDB ID : 2CHS
Title : CRYSTAL STRUCTURES OF THE MONOFUNCTIONAL CHORISMATE
MUTASE FROM BACILLUS SUBTILIS AND ITS COMPLEX WITH A
TRANSITION STATE ANALOG
Authors : Chook, Y.M.; Ke, H.; Lipscomb, W.N.
Deposited on : 1994-04-08
Resolution : 1.90 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
Xtrriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

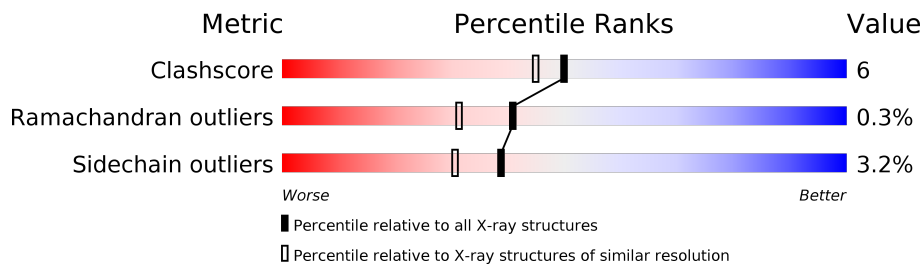
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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))
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)





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 $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	127	
1	B	127	
1	C	127	
1	D	127	
1	E	127	
1	F	127	
1	G	127	
1	H	127	

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Mol	Chain	Length	Quality of chain
1	I	127	 76% 13% • 10%
1	J	127	 72% 15% • 10%
1	K	127	 70% 18% • 10%
1	L	127	 69% 18% • 10%

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 14838 atoms, of which 3456 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 CHORISMATE MUTASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	114	1106	570	201	156	171	8	0	0	0
1	B	114	1106	570	201	156	171	8	0	0	0
1	C	114	1106	570	201	156	171	8	0	0	0
1	D	114	1106	570	201	156	171	8	0	0	0
1	E	114	1106	570	201	156	171	8	0	0	0
1	F	114	1106	570	201	156	171	8	0	0	0
1	G	114	1106	570	201	156	171	8	0	0	0
1	H	114	1106	570	201	156	171	8	0	0	0
1	I	114	1106	570	201	156	171	8	0	0	0
1	J	114	1106	570	201	156	171	8	0	0	0
1	K	114	1106	570	201	156	171	8	0	0	0
1	L	114	1106	570	201	156	171	8	0	0	0

- Molecule 2 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	H	O		
2	A	49	147	98	49	0	0
2	B	35	105	70	35	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	43	Total	H	O	0	0
			129	86	43		
2	D	56	Total	H	O	0	0
			168	112	56		
2	E	55	Total	H	O	0	0
			165	110	55		
2	F	32	Total	H	O	0	0
			96	64	32		
2	G	32	Total	H	O	0	0
			96	64	32		
2	H	10	Total	H	O	0	0
			30	20	10		
2	I	67	Total	H	O	0	0
			201	134	67		
2	J	35	Total	H	O	0	0
			105	70	35		
2	K	43	Total	H	O	0	0
			129	86	43		
2	L	65	Total	H	O	0	0
			195	130	65		

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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. 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. 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.

Note EDS was not executed.

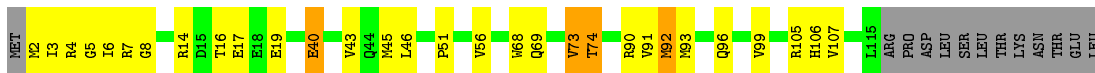
- Molecule 1: CHORISMATE MUTASE

Chain A: 



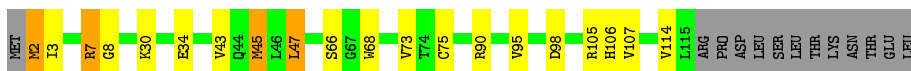
- Molecule 1: CHORISMATE MUTASE

Chain B: 




- Molecule 1: CHORISMATE MUTASE

Chain C: 



- Molecule 1: CHORISMATE MUTASE

Chain D: 



- Molecule 1: CHORISMATE MUTASE

Chain E: 

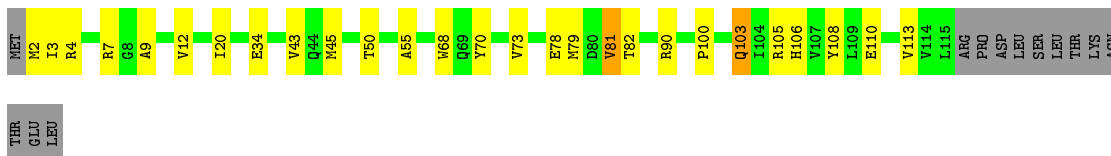


- Molecule 1: CHORISMATE MUTASE

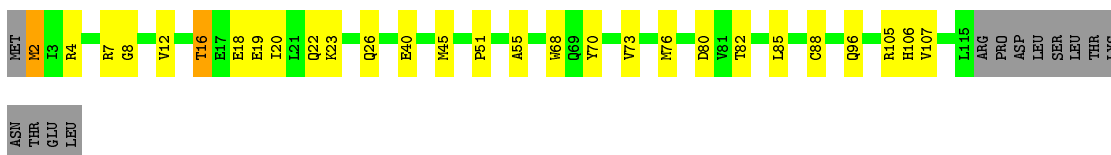
Chain F: 



- Molecule 1: CHORISMATE MUTASE



- Molecule 1: CHORISMATE MUTASE



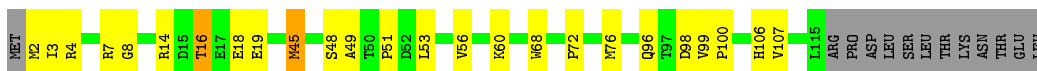
- Molecule 1: CHORISMATE MUTASE



- Molecule 1: CHORISMATE MUTASE



- Molecule 1: CHORISMATE MUTASE



- Molecule 1: CHORISMATE MUTASE



4 Data and refinement statistics

Xtrriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	102.40 Å 68.30 Å 102.80 Å 90.00° 105.60° 90.00°	Depositor
Resolution (Å)	(Not available) – 1.90	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-1.90)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.194 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	14838	wwPDB-VP
Average B, all atoms (Å ²)	10.0	wwPDB-VP

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	0.81	0/917	1.46	10/1240 (0.8%)
1	B	0.81	0/917	1.42	11/1240 (0.9%)
1	C	0.76	0/917	1.42	9/1240 (0.7%)
1	D	0.79	0/917	1.49	12/1240 (1.0%)
1	E	0.77	0/917	1.37	5/1240 (0.4%)
1	F	0.73	0/917	1.39	10/1240 (0.8%)
1	G	0.78	0/917	1.46	8/1240 (0.6%)
1	H	0.76	0/917	1.33	5/1240 (0.4%)
1	I	0.76	0/917	1.48	15/1240 (1.2%)
1	J	0.78	0/917	1.43	14/1240 (1.1%)
1	K	0.78	0/917	1.33	4/1240 (0.3%)
1	L	0.78	0/917	1.49	19/1240 (1.5%)
All	All	0.78	0/11004	1.42	122/14880 (0.8%)

There are no bond length outliers.

The worst 5 of 122 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	90	ARG	NE-CZ-NH1	15.71	128.15	120.30
1	A	4	ARG	NE-CZ-NH2	-12.20	114.20	120.30
1	A	4	ARG	NE-CZ-NH1	11.61	126.11	120.30
1	L	14	ARG	NE-CZ-NH1	10.67	125.64	120.30
1	D	2	MET	CA-CB-CG	-10.34	95.71	113.30

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	905	201	936	11	0
1	B	905	201	936	11	0
1	C	905	201	936	13	0
1	D	905	201	936	13	0
1	E	905	201	936	12	0
1	F	905	201	936	16	0
1	G	905	201	936	12	1
1	H	905	201	936	16	1
1	I	905	201	936	7	0
1	J	905	201	936	12	0
1	K	905	201	936	11	0
1	L	905	201	936	11	0
2	A	49	98	0	0	0
2	B	35	70	0	0	0
2	C	43	86	0	0	0
2	D	56	112	0	0	0
2	E	55	110	0	0	0
2	F	32	64	0	0	0
2	G	32	64	0	0	0
2	H	10	20	0	0	0
2	I	67	134	0	0	1
2	J	35	70	0	0	0
2	K	43	86	0	0	1
2	L	65	130	0	0	0
All	All	11382	3456	11232	129	2

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 6.

The worst 5 of 129 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:D:3:ILE:HD13	1:E:3:ILE:HD11	1.58	0.85
1:A:45:MET:HB3	1:A:73:VAL:HG12	1.61	0.82
1:G:45:MET:HB3	1:G:73:VAL:HG12	1.64	0.79
1:C:45:MET:HB3	1:C:73:VAL:HG12	1.63	0.79
1:G:7:ARG:H	1:G:106:HIS:HD2	1.31	0.78

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:82:THR:OG1	2:K:153:HOH:H1[2_657]	1.55	0.05
1:G:12:VAL:O	2:I:183:HOH:H1[2_657]	1.57	0.03

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	112/127 (88%)	108 (96%)	3 (3%)	1 (1%)	17	7
1	B	112/127 (88%)	108 (96%)	3 (3%)	1 (1%)	17	7
1	C	112/127 (88%)	103 (92%)	8 (7%)	1 (1%)	17	7
1	D	112/127 (88%)	106 (95%)	6 (5%)	0	100	100
1	E	112/127 (88%)	111 (99%)	1 (1%)	0	100	100
1	F	112/127 (88%)	106 (95%)	6 (5%)	0	100	100
1	G	112/127 (88%)	108 (96%)	4 (4%)	0	100	100
1	H	112/127 (88%)	107 (96%)	5 (4%)	0	100	100
1	I	112/127 (88%)	110 (98%)	2 (2%)	0	100	100
1	J	112/127 (88%)	110 (98%)	2 (2%)	0	100	100
1	K	112/127 (88%)	107 (96%)	4 (4%)	1 (1%)	17	7
1	L	112/127 (88%)	109 (97%)	3 (3%)	0	100	100
All	All	1344/1524 (88%)	1293 (96%)	47 (4%)	4 (0%)	41	31

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	114	VAL
1	B	51	PRO
1	K	51	PRO
1	C	114	VAL

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	103/116 (89%)	100 (97%)	3 (3%)	42	35
1	B	103/116 (89%)	98 (95%)	5 (5%)	25	15
1	C	103/116 (89%)	100 (97%)	3 (3%)	42	35
1	D	103/116 (89%)	101 (98%)	2 (2%)	57	53
1	E	103/116 (89%)	99 (96%)	4 (4%)	32	23
1	F	103/116 (89%)	101 (98%)	2 (2%)	57	53
1	G	103/116 (89%)	101 (98%)	2 (2%)	57	53
1	H	103/116 (89%)	97 (94%)	6 (6%)	20	10
1	I	103/116 (89%)	102 (99%)	1 (1%)	76	76
1	J	103/116 (89%)	101 (98%)	2 (2%)	57	53
1	K	103/116 (89%)	98 (95%)	5 (5%)	25	15
1	L	103/116 (89%)	99 (96%)	4 (4%)	32	23
All	All	1236/1392 (89%)	1197 (97%)	39 (3%)	39	30

5 of 39 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	16	THR
1	H	2	MET
1	L	19	GLU
1	F	69	GLN
1	G	2	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 34 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	26	GLN
1	H	44	GLN
1	L	26	GLN
1	G	77	GLN

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Mol	Chain	Res	Type
1	C	44	GLN

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 carbohydrates 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

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.