



# wwPDB X-ray Structure Validation Summary Report

Feb 27, 2014 – 01:45 PM GMT

PDB ID : 1Q7Q  
Title : Cobalamin-dependent methionine synthase (1-566) from *T. maritima* (Oxidized, Orthorhombic)  
Authors : Evans, J.C.; Huddler, D.P.; Hilgers, M.T.; Romanchuk, G.; Matthews, R.G.; Ludwig, M.L.  
Deposited on : 2003-08-19  
Resolution : 3.10 Å(reported)

This is a wwPDB validation summary 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 <http://wwpdb.org/ValidationPDFNotes.html>

---

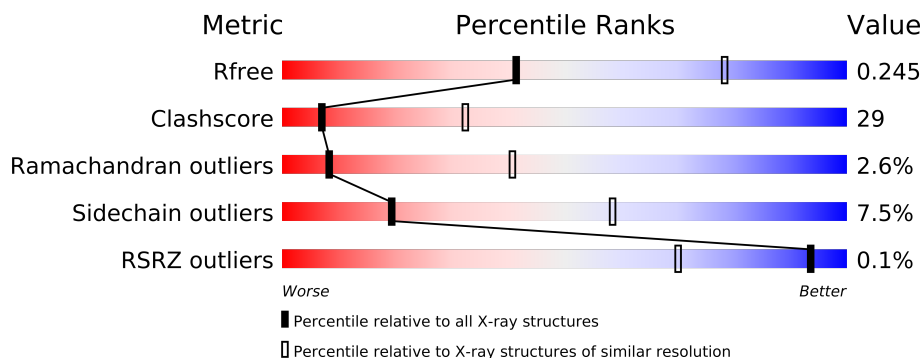
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance



The reported resolution of this entry is 3.10 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 (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	66092	1007 (3.18-3.02)
Clashscore	79885	1078 (3.16-3.04)
Ramachandran outliers	78287	1044 (3.16-3.04)
Sidechain outliers	78261	1044 (3.16-3.04)
RSRZ outliers	66119	1008 (3.18-3.02)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	566	
1	B	566	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9031 atoms, of which 0 are hydrogen and 0 are deuterium.

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 5-methyltetrahydrofolateS-homocysteine methyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	565	Total	C	N	O	S	0	0	0
			4467	2866	747	841	13			
1	B	552	Total	C	N	O	S	0	0	0
			4370	2805	731	821	13			

- Molecule 2 is water.

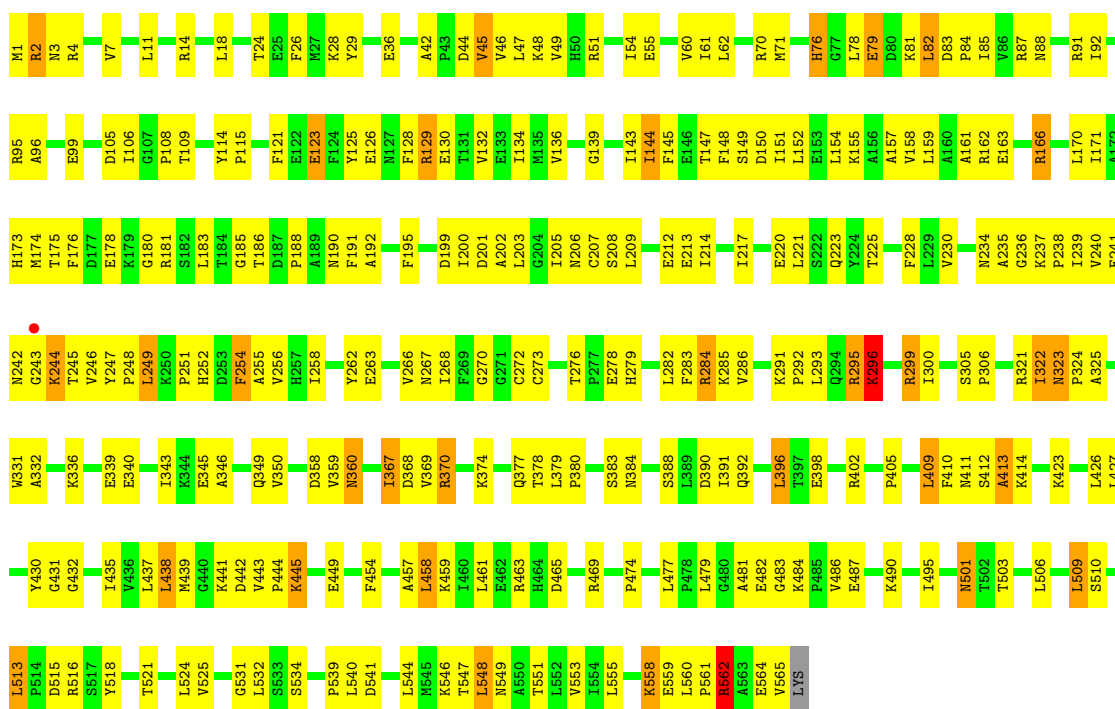
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	103	Total	O	0	0
			103	103		
2	B	91	Total	O	0	0
			91	91		

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: 5-methyltetrahydrofolateS-homocysteine methyltransferase

Chain A: 



T503	M422	V342
R516	K423	L343
S517	I424	K344
Y518	N425	E345
T521	L426	A346
A522	L427	K347
F523	Y430	T348
L524	SER	Q349
L525	PHE	V350
I528	GLY	E351
S529	LEU	L357
K530	PRO	N360
G531	ASP	F361
L532	R516	K362
I536	S517	T363
M537	Y518	E364
N538	T521	V369
P539	A522	R370
L540	F523	Y371
D541	L524	V372
E542	L525	I375
L548	I528	L379
T551	S529	P380
I554	K530	P386
L555	G531	L387
K558	L532	S388
GLU	I536	Q392
LEU	M537	N393
PRO	N538	L396
ARG	P539	T397
GLA	L540	E398
GLU	D541	R399
VAL	E542	A400
LYS	L548	L401
	T551	R402
	I554	A403
	L555	Y404
	K558	P405
	GLU	S408
	LEU	L409
	PRO	F410
	ARG	N411
	GLA	S412
	GLU	A413
	VAL	D416
	LYS	E417
		E418
		F419
		L420
		E421

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	92.58Å 169.02Å 174.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.10 46.39 – 3.10	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-3.10) 90.6 (46.39-3.10)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.62 (at 3.12Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.221 , 0.265 0.204 , 0.245	Depositor DCC
$R_{free}$ test set	4583 reflections (10.08%)	DCC
Wilson B-factor (Å <sup>2</sup> )	61.3	Xtriage
Anisotropy	0.340	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 35.3	EDS
Estimated twinning fraction	0.031 for -h,l,k	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	1 of 45652 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	9031	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.83% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality

### 5.1 Standard geometry

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	0.39	0/4550	0.66	0/6145
1	B	0.41	0/4449	0.66	0/6005
All	All	0.40	0/8999	0.66	0/12150

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4467	0	4553	254	0
1	B	4370	0	4467	257	0
2	A	103	0	0	26	0
2	B	91	0	0	7	0
All	All	9031	0	9020	510	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 29.

The worst 5 of 510 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:259:ASP:O	1:B:263:GLU:HG2	1.64	0.97

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:166:ARG:HH21	1:A:166:ARG:HB2	1.29	0.93
1:A:296:LYS:NZ	1:A:296:LYS:HA	1.89	0.87
1:B:271:GLY:HA3	1:B:275:THR:HG21	1.57	0.86
1:A:54:ILE:HD11	1:A:61:ILE:HD13	1.57	0.86

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

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	563/566 (100%)	490 (87%)	61 (11%)	12 (2%)	11	48
1	B	548/566 (97%)	462 (84%)	69 (13%)	17 (3%)	7	36
All	All	1111/1132 (98%)	952 (86%)	130 (12%)	29 (3%)	8	41

5 of 29 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	244	LYS
1	A	413	ALA
1	B	238	PRO
1	B	244	LYS
1	B	248	PRO

### 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	492/494 (100%)	456 (93%)	36 (7%)	20	59

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	482/494 (98%)	445 (92%)	37 (8%)	18	57
All	All	974/988 (99%)	901 (92%)	73 (8%)	19	58

5 of 73 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	548	LEU
1	B	70	ARG
1	B	471	ILE
1	B	34	LEU
1	B	151	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	338	ASN
1	B	508	ASN
1	B	393	ASN
1	A	335	GLN
1	B	425	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

There are no ligands in this entry.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	565/566 (99%)	-0.30	1 (0%) 93 61	30, 51, 85, 100	0
1	B	552/566 (97%)	-0.30	0 100 100	29, 49, 81, 100	0
All	All	1117/1132 (98%)	-0.30	1 (0%) 93 70	29, 50, 82, 100	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	243	GLY	2.5

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

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

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 6.4 Ligands ⓘ

There are no ligands in this entry.

### 6.5 Other polymers ⓘ

There are no such residues in this entry.