



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2018 – 08:54 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 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
Xtriage (Phenix)	:	1.13
EDS	:	trunk30967
Percentile statistics	:	20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac	:	5.8.0158
CCP4	:	7.0 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk30967

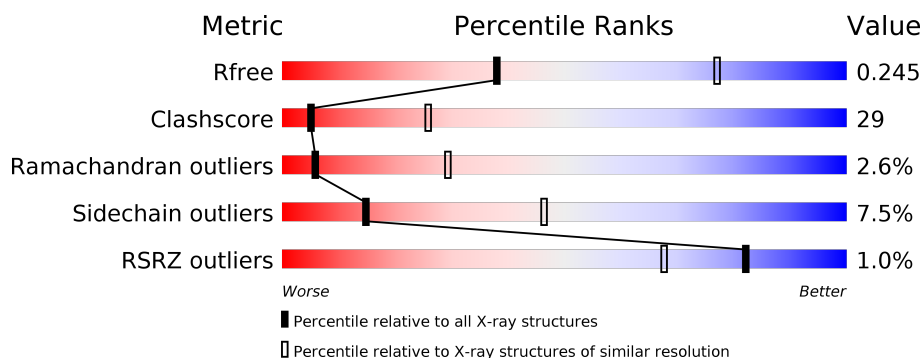
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	111664	1115 (3.12-3.08)
Clashscore	122126	1042 (3.10-3.10)
Ramachandran outliers	120053	1010 (3.10-3.10)
Sidechain outliers	120020	1010 (3.10-3.10)
RSRZ outliers	108989	1089 (3.12-3.08)

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. 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	566	<div> <div>%</div> <div> <div></div> <div>52%</div> <div>42%</div> <div>5%</div> </div> </div>
1	B	566	<div> <div>%</div> <div> <div></div> <div>49%</div> <div>42%</div> <div>6%</div> <div>...</div> </div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9031 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 5-methyltetrahydrofolate S-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			

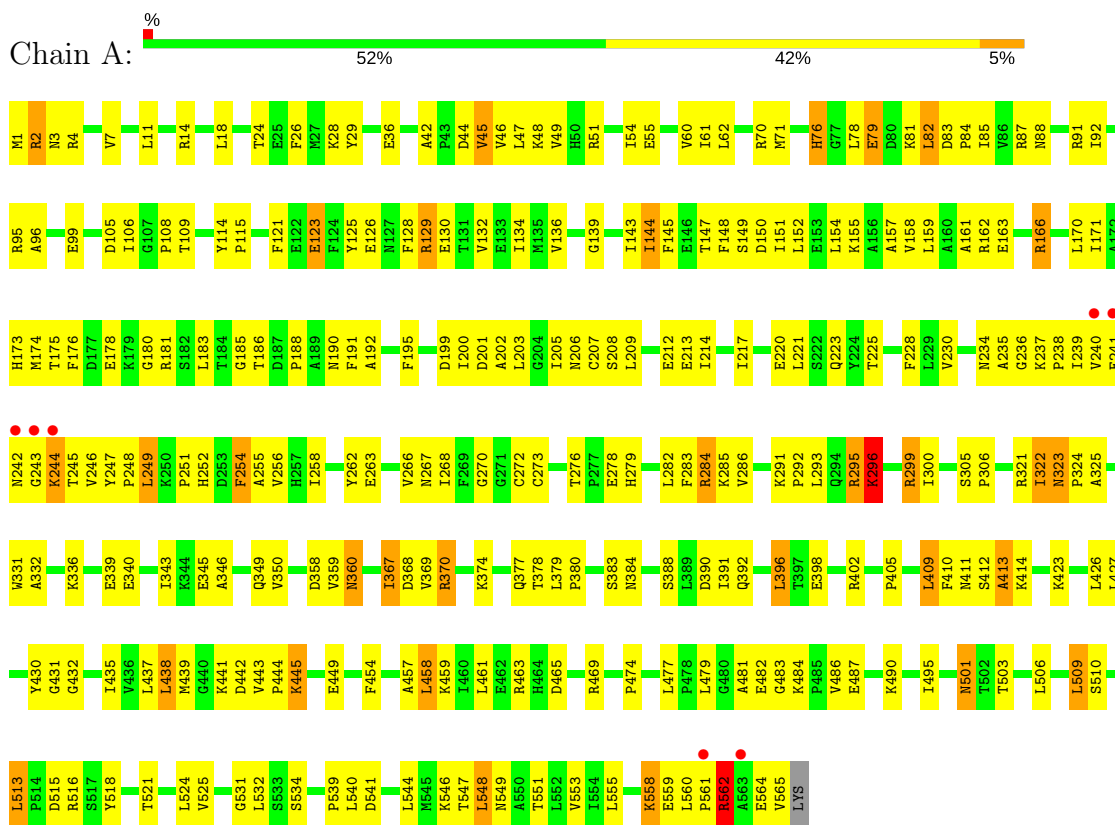
- Molecule 2 is water.

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

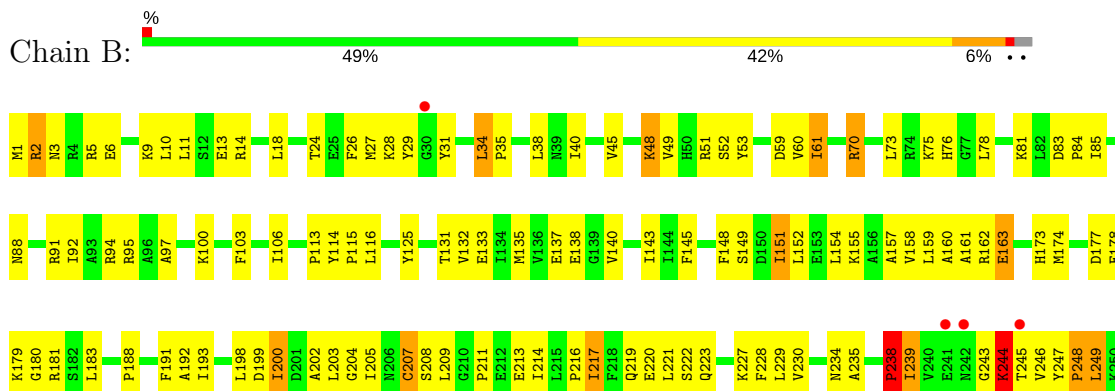
3 Residue-property plots

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



- Molecule 1: 5-methyltetrahydrofolate S-homocysteine methyltransferase



E493	E494	T503	L506	S507	N508	L509	SER	PHE	GLY	LEU	PRO	ASP	R516	S517	Y518	T521	A522	F523	L524	V525	I528	S529	K530	G531	L532	I536	M537	N538	P539	L540	E541	E542	L548	T551	I554	L555	K558	GLU	LEU	PRO	ARG	ALA	GLU	VAL	LYS				
L420	E421	K422	I424	N425	L426	L427	Y430	L434	I435	M439	G440	K441	D442	V443	P444	K445	E448	E449	R450	K451	E452	Y453	F454	E455	L458	K459	I460	L461	E462	R463	H464	S467	V470	I471	P474	L479	G480	A481	E482	G483	K484	P485	V486	V487	V488	L489	K490	T491	I492
E340	I341	V342	I343	K344	E345	A346	K347	T348	Q349	V350	E351	L357	N360	F361	G362	I363	E364	V369	R370	Y371	V372	I375	L379	P380	P386	L387	S388	Q392	N393	L396	T397	E398	R399	A400	L401	R402	A403	Y404	P405	S408	L409	F410	N411	S412	A413	D416	E417	N418	E419
P251	H252	D253	F254	A255	V256	I257	I258	D259	S260	V261	Y262	E263	V266	N267	I268	F269	G270	G271	C272	C273	G274	T275	E278	H279	V280	I281	L282	K285	V286	R290	L293	D294	R295	K296	I300	P306	E320	R321	I322	N323	P324	K329	L330	W331	A332	F333	W334	N338	E339

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	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 (10.04%)	wwPDB-VP
Wilson B-factor (Å ²)	61.3	Xtriage
Anisotropy	0.340	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 73.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.031 for -h,l,k	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	9031	wwPDB-VP
Average B, all atoms (Å ²)	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.*

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

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 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	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

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 29.

The worst 5 of 510 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:B:259:ASP:O	1:B:263:GLU:HG2	1.64	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (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 [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	563/566 (100%)	490 (87%)	61 (11%)	12 (2%)	8	34
1	B	548/566 (97%)	462 (84%)	69 (13%)	17 (3%)	4	25
All	All	1111/1132 (98%)	952 (86%)	130 (12%)	29 (3%)	6	29

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 [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	492/494 (100%)	456 (93%)	36 (7%)	15	47
1	B	482/494 (98%)	445 (92%)	37 (8%)	14	45
All	All	974/988 (99%)	901 (92%)	73 (8%)	15	46

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 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 ⓘ

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 [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	565/566 (99%)	-0.42	7 (1%) 79 61	30, 51, 85, 100	0
1	B	552/566 (97%)	-0.40	4 (0%) 87 75	29, 49, 81, 100	0
All	All	1117/1132 (98%)	-0.41	11 (0%) 82 67	29, 50, 82, 100	0

The worst 5 of 11 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	243	GLY	4.7
1	A	241	GLU	2.9
1	A	561	PRO	2.9
1	A	242	ASN	2.7
1	B	242	ASN	2.6

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.