



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:50 PM GMT

PDB ID : 1VE2
Title : Crystal structure of uroporphyrin-III-C-methyltransferase from thermus thermophilus
Authors : Jeyakanthan, J.; Tahirov, T.H.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on : 2004-03-26
Resolution : 1.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

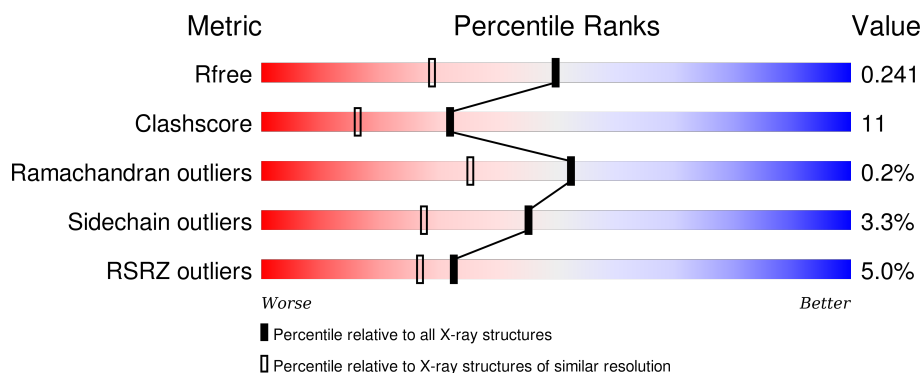
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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}	91344	4533 (1.80-1.80)
Clashscore	102246	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (1.80-1.80)
RSRZ outliers	91569	4547 (1.80-1.80)

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	235	
1	B	235	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3695 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 Uroporphyrin-III C-methyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	222	Total	C	N	O	S	0	0	0
			1637	1055	297	282	3			
1	B	220	Total	C	N	O	S	0	0	0
			1617	1046	292	277	2			

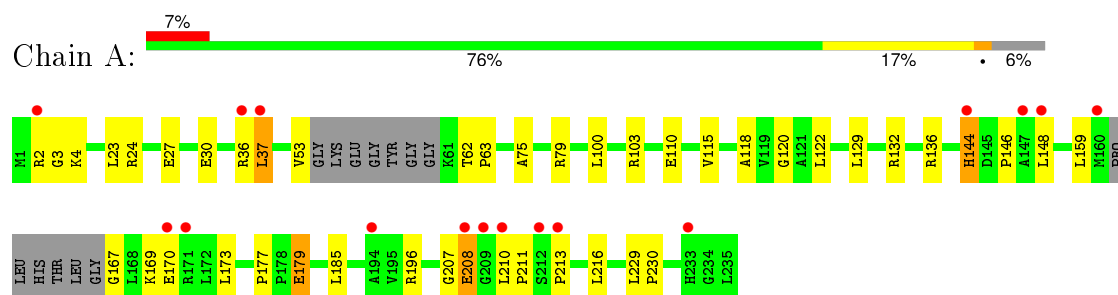
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	249	Total	O	0	0
			249	249		
2	B	192	Total	O	0	0
			192	192		

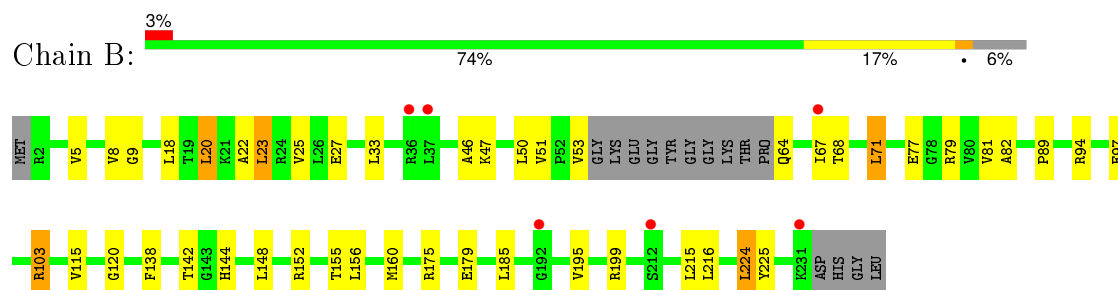
3 Residue-property plots

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: Uroporphyrin-III C-methyltransferase



• Molecule 1: Uroporphyrin-III C-methyltransferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	54.61Å 87.92Å 91.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.98 – 1.80 28.84 – 1.80	Depositor EDS
% Data completeness (in resolution range)	95.1 (19.98-1.80) 95.1 (28.84-1.80)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.22 (at 1.80Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.207 , 0.241 0.207 , 0.241	Depositor DCC
R_{free} test set	1971 reflections (4.98%)	DCC
Wilson B-factor (Å ²)	21.2	Xtriage
Anisotropy	0.375	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 51.7	EDS
Estimated twinning fraction	0.012 for -h,l,k	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 41129 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3695	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.92% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.30	0/1668	0.61	0/2265
1	B	0.33	0/1649	0.67	0/2244
All	All	0.32	0/3317	0.64	0/4509

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	1637	0	1739	35	0
1	B	1617	0	1722	41	0
2	A	249	0	0	4	0
2	B	192	0	0	2	0
All	All	3695	0	3461	71	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 11.

All (71) 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:23:LEU:HD11	1:B:20:LEU:HG	1.53	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:156:LEU:HB2	2:B:419:HOH:O	1.83	0.78
1:A:118:ALA:HB2	1:A:159:LEU:HD21	1.68	0.76
1:B:142:THR:HB	1:B:144:HIS:HD2	1.52	0.72
1:A:177:PRO:HB2	1:A:179:GLU:OE2	1.89	0.72
1:B:185:LEU:HD23	1:B:215:LEU:CD1	2.29	0.63
1:A:23:LEU:O	1:A:27:GLU:HG3	1.99	0.63
1:A:167:GLY:HA2	1:A:170:GLU:HG2	1.79	0.62
1:B:67:ILE:O	1:B:71:LEU:HD22	2.00	0.61
1:B:185:LEU:CD1	1:B:195:VAL:HG13	2.32	0.60
1:B:142:THR:HB	1:B:144:HIS:CD2	2.36	0.59
1:B:9:GLY:N	1:B:89:PRO:HG3	2.18	0.58
1:B:185:LEU:HD23	1:B:215:LEU:HD11	1.84	0.58
1:A:169:LYS:O	1:A:173:LEU:HG	2.04	0.57
1:A:36:ARG:HG2	1:A:53:VAL:O	2.05	0.56
1:B:53:VAL:HG11	1:B:67:ILE:HG12	1.86	0.56
1:B:185:LEU:HD12	1:B:195:VAL:HG22	1.87	0.55
1:A:179:GLU:HG2	2:A:337:HOH:O	2.05	0.55
1:A:122:LEU:HD13	1:A:129:LEU:HD21	1.90	0.54
1:B:8:VAL:HG21	1:B:25:VAL:HG11	1.88	0.54
1:B:23:LEU:O	1:B:27:GLU:HG3	2.08	0.53
1:A:185:LEU:HD12	1:A:185:LEU:N	2.24	0.52
1:A:167:GLY:CA	1:A:170:GLU:HG2	2.42	0.50
1:A:4:LYS:NZ	1:A:110:GLU:OE1	2.43	0.49
1:A:144:HIS:C	1:A:146:PRO:HD3	2.33	0.48
1:B:179:GLU:O	1:B:199:ARG:NH1	2.42	0.48
1:A:122:LEU:CD1	1:A:129:LEU:HD21	2.44	0.48
1:B:33:LEU:HD23	1:B:51:VAL:HB	1.94	0.48
1:A:132:ARG:HD2	1:B:97:GLU:OE1	2.13	0.48
1:A:148:LEU:N	1:A:148:LEU:HD12	2.30	0.47
1:B:152:ARG:NH1	1:B:175:ARG:HD3	2.29	0.47
1:A:216:LEU:HD23	1:A:216:LEU:C	2.35	0.47
1:B:64:GLN:HG2	1:B:94:ARG:HD3	1.96	0.47
1:B:185:LEU:HD13	1:B:195:VAL:HG13	1.97	0.47
1:A:115:VAL:HG12	1:A:120:GLY:HA3	1.96	0.47
1:A:37:LEU:HD11	1:A:213:PRO:HD3	1.96	0.47
1:A:169:LYS:HB3	1:A:169:LYS:NZ	2.30	0.46
1:A:27:GLU:CD	2:A:479:HOH:O	2.53	0.46
1:B:185:LEU:N	1:B:185:LEU:HD22	2.30	0.46
1:A:3:GLY:HA3	1:A:75:ALA:O	2.16	0.46
1:B:215:LEU:C	1:B:215:LEU:HD12	2.36	0.45
1:A:118:ALA:HB3	2:A:301:HOH:O	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:VAL:CG1	1:A:120:GLY:HA3	2.47	0.45
1:B:47:LYS:NZ	1:B:47:LYS:HB3	2.31	0.45
1:B:115:VAL:HG12	1:B:120:GLY:HA3	1.98	0.45
1:B:5:VAL:HG22	1:B:81:VAL:CG1	2.47	0.45
1:B:115:VAL:CG1	1:B:120:GLY:HA3	2.47	0.45
1:B:18:LEU:HD22	1:B:22:ALA:HB3	2.00	0.44
1:B:185:LEU:HD23	1:B:215:LEU:HD12	1.99	0.44
1:B:81:VAL:HG22	1:B:82:ALA:N	2.33	0.44
1:B:152:ARG:NH2	2:B:266:HOH:O	2.36	0.43
1:A:30:GLU:OE1	1:A:79:ARG:NH1	2.51	0.43
1:B:8:VAL:C	1:B:89:PRO:HG3	2.37	0.43
1:A:207:GLY:O	1:A:208:GLU:C	2.56	0.43
1:A:24:ARG:HD3	2:A:471:HOH:O	2.17	0.43
1:A:210:LEU:HD23	1:A:211:PRO:HD2	2.00	0.43
1:B:64:GLN:HG2	1:B:94:ARG:CD	2.49	0.43
1:A:196:ARG:NE	1:A:210:LEU:HG	2.33	0.42
1:A:136:ARG:NE	1:B:148:LEU:HD23	2.34	0.42
1:A:100:LEU:HD11	1:B:224:LEU:HG	2.00	0.42
1:B:46:ALA:HB3	1:B:50:LEU:HD21	2.01	0.42
1:B:77:GLU:OE2	1:B:79:ARG:NH1	2.52	0.42
1:A:62:THR:HA	1:A:63:PRO:HD3	1.96	0.41
1:B:138:PHE:HA	1:B:155:THR:O	2.21	0.41
1:B:68:THR:HA	1:B:71:LEU:HD23	2.03	0.41
1:A:230:PRO:O	1:B:103:ARG:NH1	2.38	0.41
1:B:79:ARG:HG3	1:B:79:ARG:HH11	1.86	0.41
1:B:216:LEU:HD23	1:B:216:LEU:C	2.41	0.41
1:A:170:GLU:O	1:A:173:LEU:HB2	2.21	0.40
1:A:229:LEU:HB3	1:A:230:PRO:HD3	2.04	0.40
1:B:225:TYR:N	1:B:225:TYR:CD1	2.88	0.40

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	216/235 (92%)	206 (95%)	9 (4%)	1 (0%)	34	17
1	B	216/235 (92%)	213 (99%)	3 (1%)	0	100	100
All	All	432/470 (92%)	419 (97%)	12 (3%)	1 (0%)	52	35

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	208	GLU

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	166/175 (95%)	161 (97%)	5 (3%)	48	31
1	B	164/175 (94%)	158 (96%)	6 (4%)	41	23
All	All	330/350 (94%)	319 (97%)	11 (3%)	45	27

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ARG
1	A	37	LEU
1	A	103	ARG
1	A	144	HIS
1	A	179	GLU
1	B	20	LEU
1	B	23	LEU
1	B	71	LEU
1	B	103	ARG
1	B	160	MET
1	B	224	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	131	HIS

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 ⓘ

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	222/235 (94%)	0.29	16 (7%) 18 14	14, 27, 54, 67	0
1	B	220/235 (93%)	0.10	6 (2%) 58 53	11, 24, 49, 64	0
All	All	442/470 (94%)	0.20	22 (4%) 32 27	11, 26, 52, 67	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	37	LEU	8.3
1	A	208	GLU	5.4
1	B	37	LEU	4.8
1	A	210	LEU	4.0
1	A	148	LEU	3.9
1	A	144	HIS	3.7
1	A	2	ARG	3.4
1	A	36	ARG	3.4
1	A	171	ARG	3.1
1	B	231	LYS	3.1
1	A	213	PRO	3.0
1	B	36	ARG	2.9
1	A	209	GLY	2.9
1	B	67	ILE	2.8
1	A	160	MET	2.6
1	A	233	HIS	2.6
1	A	212	SER	2.6
1	A	194	ALA	2.5
1	A	147	ALA	2.4
1	B	212	SER	2.3
1	A	170	GLU	2.2
1	B	192	GLY	2.1

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.