



wwPDB X-ray Structure Validation Summary Report i

Feb 28, 2014 – 04:30 AM GMT

PDB ID : 2D0V
Title : Crystal structure of methanol dehydrogenase from *Hyphomicrobium denitrificans*
Authors : Nojiri, M.; Hira, D.; Yamaguchi, K.; Suzuki, S.
Deposited on : 2005-08-09
Resolution : 2.49 Å (reported)

This is a wwPDB validation summary 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/ValidationPDFNotes.html>

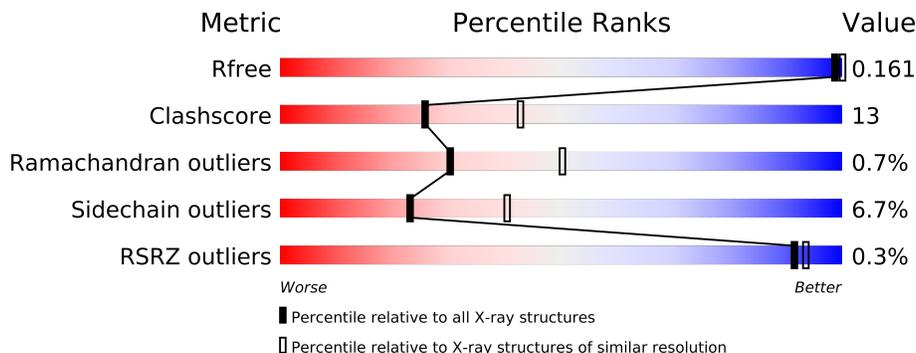
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.49 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	2784 (2.50-2.50)
Clashscore	79885	3562 (2.50-2.50)
Ramachandran outliers	78287	3480 (2.50-2.50)
Sidechain outliers	78261	3482 (2.50-2.50)
RSRZ outliers	66119	2785 (2.50-2.50)

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. 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	597	
1	D	597	
1	I	597	
2	B	72	
2	E	72	
2	J	72	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	CA	A	775	-	X
4	PQQ	A	601	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
4	PQQ	D	601	-	X
4	PQQ	I	601	-	X

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 16491 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 methanol dehydrogenase large subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	597	4668	2962	797	889	20	0	0	0
1	D	597	4668	2962	797	889	20	0	0	0
1	I	595	4655	2954	794	887	20	0	0	0

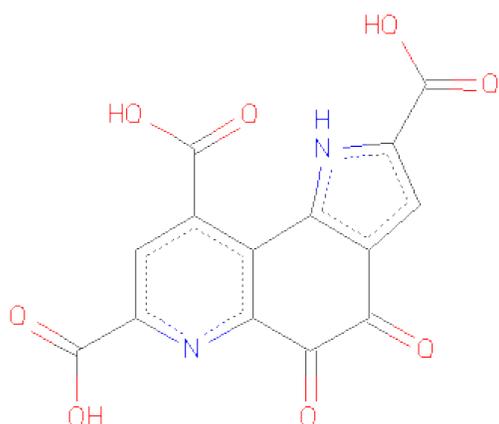
- Molecule 2 is a protein called methanol dehydrogenase small subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	70	572	359	105	106	2	0	0	0
2	E	68	554	347	101	104	2	0	0	0
2	J	70	572	359	105	106	2	0	0	0

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	I	1	Total	Ca	0	0
			1	1		
3	A	1	Total	Ca	0	0
			1	1		
3	D	1	Total	Ca	0	0
			1	1		

- Molecule 4 is PYRROLOQUINOLINE QUINONE (three-letter code: PQQ) (formula: C₁₄H₆N₂O₈).



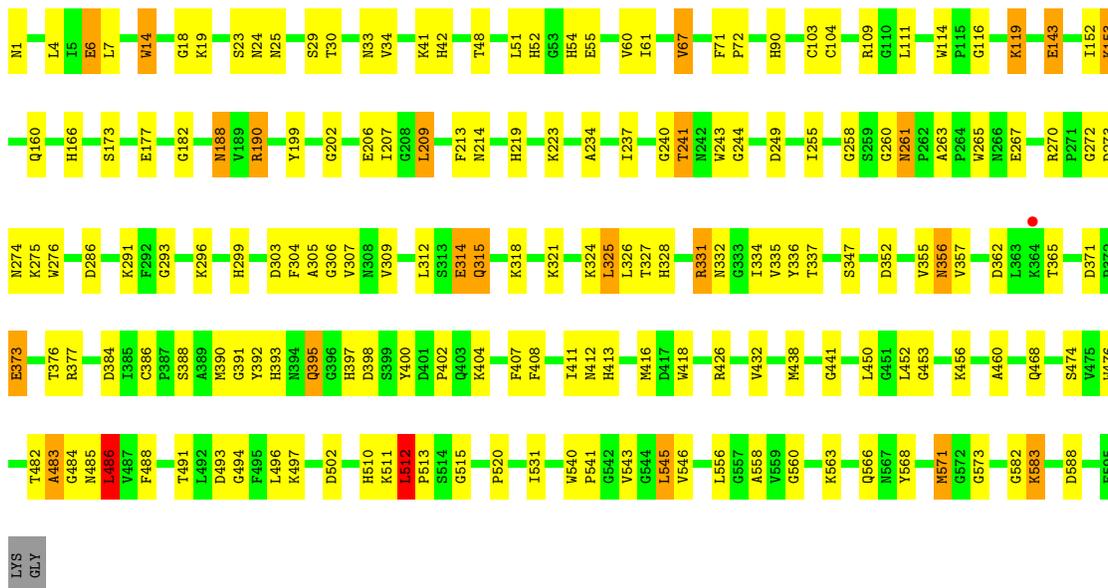
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			24	14	2	8		
4	D	1	Total	C	N	O	0	0
			24	14	2	8		
4	I	1	Total	C	N	O	0	0
			24	14	2	8		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	278	Total	O	0	0
			278	278		
5	B	31	Total	O	0	0
			31	31		
5	D	188	Total	O	0	0
			188	188		
5	E	31	Total	O	0	0
			31	31		
5	I	171	Total	O	0	0
			171	171		
5	J	28	Total	O	0	0
			28	28		

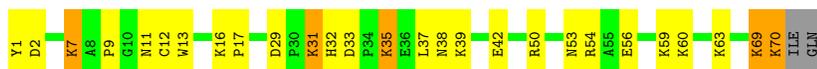
- Molecule 1: methanol dehydrogenase large subunit

Chain I:



- Molecule 2: methanol dehydrogenase small subunit

Chain B:



- Molecule 2: methanol dehydrogenase small subunit

Chain E:



- Molecule 2: methanol dehydrogenase small subunit

Chain J:



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	291.32Å 64.00Å 109.94Å 90.00° 105.74° 90.00°	Depositor
Resolution (Å)	44.60 – 2.49 44.60 – 2.49	Depositor EDS
% Data completeness (in resolution range)	99.6 (44.60-2.49) 95.4 (44.60-2.49)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.64 (at 2.48Å)	Xtrriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.149 , 0.247 0.162 , 0.161	Depositor DCC
R_{free} test set	6603 reflections (11.23%)	DCC
Wilson B-factor (Å ²)	31.6	Xtrriage
Anisotropy	0.561	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 16.1	EDS
Estimated twinning fraction	No twinning to report.	Xtrriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Outliers	1 of 65421 reflections (0.002%)	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	16491	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.32% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality i

5.1 Standard geometry i

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

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	1.30	12/4803 (0.2%)	1.17	21/6534 (0.3%)
1	D	1.28	12/4803 (0.2%)	1.16	22/6534 (0.3%)
1	I	1.26	10/4790 (0.2%)	1.14	20/6518 (0.3%)
2	B	1.36	4/589 (0.7%)	1.18	6/789 (0.8%)
2	E	1.26	1/571 (0.2%)	1.10	1/767 (0.1%)
2	J	1.33	2/589 (0.3%)	1.06	1/789 (0.1%)
All	All	1.28	41/16145 (0.3%)	1.15	71/21931 (0.3%)

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	1	1

The worst 5 of 41 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	143	GLU	CG-CD	8.78	1.65	1.51
1	I	314	GLU	CG-CD	8.68	1.65	1.51
2	J	42	GLU	CG-CD	8.17	1.64	1.51
1	D	39	GLN	CG-CD	7.89	1.69	1.51
1	I	143	GLU	CD-OE2	6.88	1.33	1.25

The worst 5 of 71 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	190	ARG	NE-CZ-NH2	-13.46	113.57	120.30
1	A	190	ARG	NE-CZ-NH1	11.79	126.20	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	446	ARG	NE-CZ-NH1	-9.81	115.39	120.30
1	D	167	ASP	CB-CG-OD1	9.02	126.42	118.30
1	A	275	LYS	C-N-CA	8.58	143.15	121.70

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	276	TRP	CA

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	190	ARG	Sidechain

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	4668	0	4426	112	0
1	D	4668	0	4426	107	0
1	I	4655	0	4410	140	0
2	B	572	0	553	19	0
2	E	554	0	527	23	0
2	J	572	0	553	24	0
3	A	1	0	0	0	0
3	D	1	0	0	0	0
3	I	1	0	0	0	0
4	A	24	0	3	5	0
4	D	24	0	3	5	0
4	I	24	0	3	4	0
5	A	278	0	0	15	0
5	B	31	0	0	2	0
5	D	188	0	0	10	0
5	E	31	0	0	3	0
5	I	171	0	0	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	J	28	0	0	1	0
All	All	16491	0	14904	413	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 13.

The worst 5 of 413 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:447:GLN:HG3	5:A:903:HOH:O	1.63	0.97
1:I:314:GLU:HG2	5:I:942:HOH:O	1.74	0.87
1:D:211:ASP:HB3	5:D:793:HOH:O	1.74	0.86
1:I:540:TRP:CZ3	4:I:601:PQQ:O4	2.32	0.83
1:A:51:LEU:O	1:A:52:HIS:HB2	1.78	0.83

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	595/597 (100%)	561 (94%)	32 (5%)	2 (0%)	50 73
1	D	595/597 (100%)	537 (90%)	53 (9%)	5 (1%)	27 46
1	I	593/597 (99%)	546 (92%)	43 (7%)	4 (1%)	30 50
2	B	68/72 (94%)	63 (93%)	5 (7%)	0	100 100
2	E	66/72 (92%)	60 (91%)	5 (8%)	1 (2%)	15 25
2	J	68/72 (94%)	60 (88%)	6 (9%)	2 (3%)	7 9
All	All	1985/2007 (99%)	1827 (92%)	144 (7%)	14 (1%)	30 50

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	266	ASN

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Mol	Chain	Res	Type
2	E	67	ASP
1	I	261	ASN
1	I	331	ARG
1	D	587	ASP

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	487/487 (100%)	457 (94%)	30 (6%)	26	45
1	D	487/487 (100%)	461 (95%)	26 (5%)	32	54
1	I	486/487 (100%)	457 (94%)	29 (6%)	27	47
2	B	60/62 (97%)	50 (83%)	10 (17%)	3	6
2	E	58/62 (94%)	53 (91%)	5 (9%)	15	27
2	J	60/62 (97%)	50 (83%)	10 (17%)	3	6
All	All	1638/1647 (100%)	1528 (93%)	110 (7%)	23	40

5 of 110 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	322	LYS
1	D	496	LEU
2	J	31	LYS
1	D	364	LYS
1	D	418	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 60 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	194	GLN
1	D	299	HIS
1	I	395	GLN
1	D	219	HIS
1	D	356	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 ⓘ

Of 6 ligands modelled in this entry, 3 are monoatomic - leaving 3 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
4	PQQ	A	601	3	26,26,26	3.87	11 (42%)	39,40,40	3.49	21 (53%)
4	PQQ	D	601	3	26,26,26	4.08	12 (46%)	39,40,40	2.93	14 (35%)
4	PQQ	I	601	3	26,26,26	3.39	11 (42%)	39,40,40	2.78	15 (38%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PQQ	A	601	3	-	0/10/28/28	0/0/3/3
4	PQQ	D	601	3	-	0/10/28/28	0/0/3/3
4	PQQ	I	601	3	-	0/10/28/28	0/0/3/3

The worst 5 of 34 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	601	PQQ	C9A-C6A	13.25	1.54	1.40
4	D	601	PQQ	C9A-C6A	12.72	1.53	1.40
4	I	601	PQQ	C9A-C6A	11.11	1.52	1.40
4	D	601	PQQ	C9-C9A	10.96	1.54	1.40
4	A	601	PQQ	C9-C9A	10.46	1.53	1.40

The worst 5 of 50 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	601	PQQ	C2X-C2-N1	13.33	127.14	116.85
4	D	601	PQQ	C2X-C2-N1	11.32	125.58	116.85
4	I	601	PQQ	C2X-C2-N1	9.46	124.15	116.85
4	A	601	PQQ	C9-C9A-C1A	8.19	129.95	122.52
4	D	601	PQQ	C6A-N6-C7	5.47	126.55	117.97

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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 (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	597/597 (100%)	-0.60	0 100 100	17, 28, 39, 55	0
1	D	597/597 (100%)	-0.40	3 (0%) 88 90	18, 32, 45, 61	0
1	I	595/597 (99%)	-0.33	1 (0%) 93 94	20, 34, 48, 57	0
2	B	70/72 (97%)	-0.35	0 100 100	26, 36, 48, 54	0
2	E	68/72 (94%)	0.06	1 (1%) 70 72	35, 49, 58, 68	0
2	J	70/72 (97%)	0.07	0 100 100	34, 47, 59, 68	0
All	All	1997/2007 (99%)	-0.40	5 (0%) 91 93	17, 32, 49, 68	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	68	VAL	4.3
1	D	307	VAL	2.3
1	D	421	PHE	2.2
1	D	305	ALA	2.2
1	I	364	LYS	2.2

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

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	PQQ	A	601	24/24	0.34	4.41	59,68,69,69	0
4	PQQ	D	601	24/24	0.36	4.19	69,77,78,78	0
4	PQQ	I	601	24/24	0.31	2.99	67,75,75,76	0
3	CA	A	775	1/1	0.18	2.59	55,55,55,55	1
3	CA	D	775	1/1	0.13	-0.92	49,49,49,49	1
3	CA	I	775	1/1	0.11	-1.27	49,49,49,49	1

6.5 Other polymers

There are no such residues in this entry.