wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 12:40 AM GMT

PDB ID	:	2BBK
Title	:	CRYSTAL STRUCTURE OF THE QUINOPROTEIN METHYLAMINE DEHYDROGENASE FROM PARACOCCUS DENITRIFICANS AT 1.75 ANGSTROMS
Authors	:	Chen, L.; Mathews, F.S.
Deposited on	:	1993-12-17
Resolution	:	1.75 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

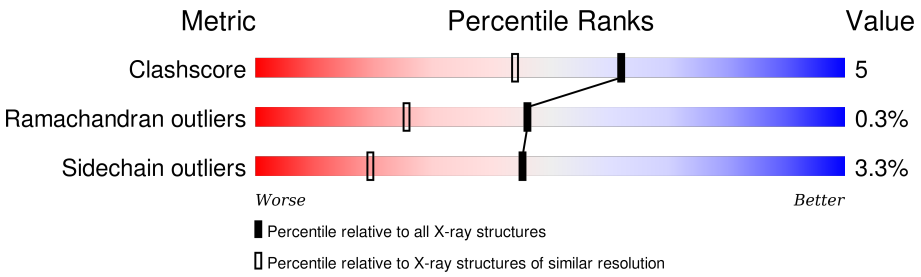
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.75 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	102246	1730 (1.76-1.76)
Ramachandran outliers	100387	1711 (1.76-1.76)
Sidechain outliers	100360	1711 (1.76-1.76)

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 <=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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	H	355	77% 19% • •
1	J	355	79% 18% •
2	L	125	82% 13% 5%
2	M	125	79% 15% 6%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 8038 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 METHYLAMINE DEHYDROGENASE (HEAVY SUBUNIT).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	H	355	2783	1773	474	528	8	0	0	0
1	J	355	2783	1773	474	528	8	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	299	PHE	LEU	CONFLICT	UNP P29894
H	300	VAL	LEU	CONFLICT	UNP P29894
J	299	PHE	LEU	CONFLICT	UNP P29894
J	300	VAL	LEU	CONFLICT	UNP P29894

- Molecule 2 is a protein called METHYLAMINE DEHYDROGENASE (LIGHT SUBUNIT).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	L	125	958	590	161	192	15	0	2	0
2	M	125	958	590	161	192	15	0	2	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	57	TRQ	TRP	CONFLICT	UNP P22619
M	57	TRQ	TRP	CONFLICT	UNP P22619

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	H	199	199	199	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	J	210	210	210	0	0
			Total	O		
3	L	69	69	69	0	0
			Total	O		
3	M	78	78	78	0	0

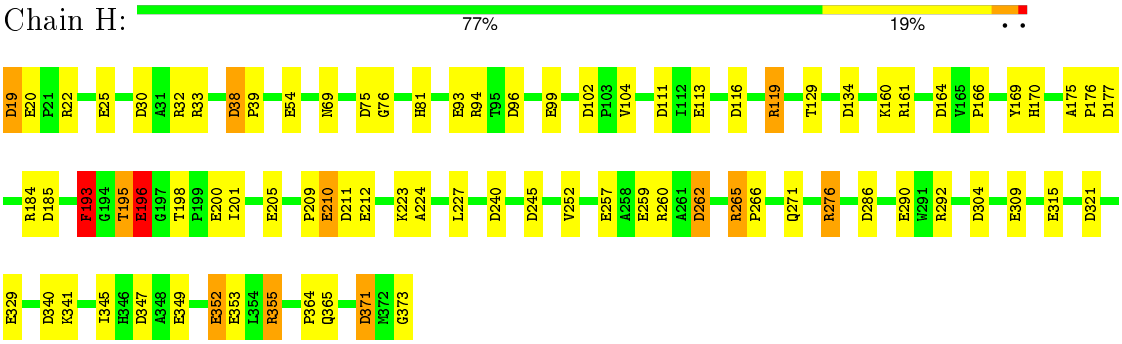
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

Note EDS was not executed.

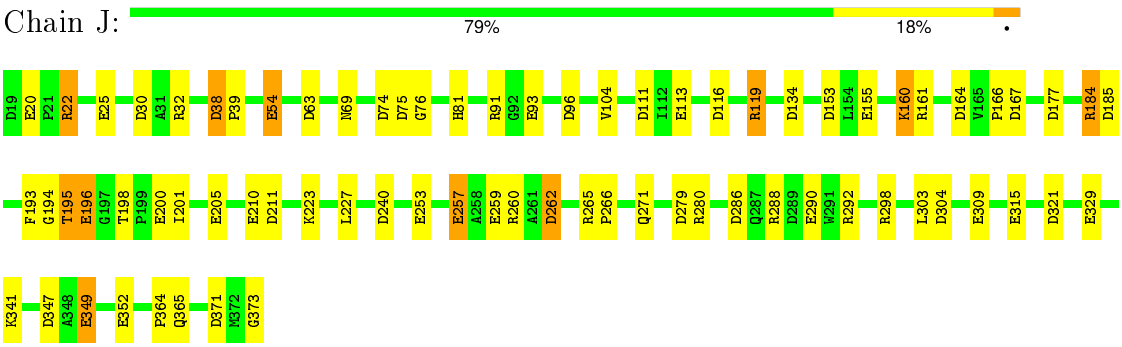
- Molecule 1: METHYLAMINE DEHYDROGENASE (HEAVY SUBUNIT)

Chain H:



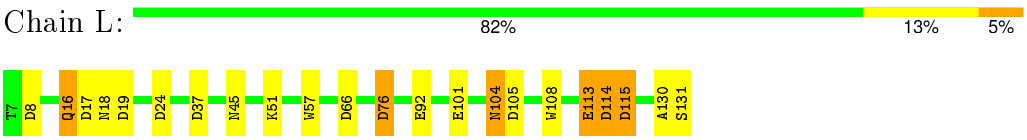
- Molecule 1: METHYLAMINE DEHYDROGENASE (HEAVY SUBUNIT)

Chain J:



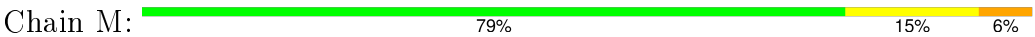
- Molecule 2: METHYLAMINE DEHYDROGENASE (LIGHT SUBUNIT)

Chain L:



- Molecule 2: METHYLAMINE DEHYDROGENASE (LIGHT SUBUNIT)

Chain M:



T7
D8
P9
R10
Q16
D17
N18
D19
D24
Y25
H28
N45
K51
W57
Q68
D76
Y80
E92
G93
E94
E101
N104
D105
W108
E113
D114
D115
S131

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	152.07Å 135.92Å 55.26Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	11.00 – 1.75	Depositor
% Data completeness (in resolution range)	(Not available) (11.00-1.75)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT	Depositor
R, R_{free}	0.167 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8038	wwPDB-VP
Average B, all atoms ($Å^2$)	19.0	wwPDB-VP

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: TRQ

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	H	0.90	18/2860 (0.6%)	1.31	47/3898 (1.2%)
1	J	0.84	18/2860 (0.6%)	1.31	42/3898 (1.1%)
2	L	0.74	3/976 (0.3%)	1.24	12/1331 (0.9%)
2	M	0.73	4/976 (0.4%)	1.36	17/1331 (1.3%)
All	All	0.84	43/7672 (0.6%)	1.31	118/10458 (1.1%)

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	H	0	1

The worst 5 of 43 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	193	PHE	C-N	-17.34	1.01	1.33
1	H	352	GLU	CD-OE1	6.59	1.32	1.25
1	H	290	GLU	CD-OE1	6.41	1.32	1.25
1	H	329	GLU	CD-OE2	6.30	1.32	1.25
1	J	257	GLU	CD-OE1	6.30	1.32	1.25

The worst 5 of 118 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	119	ARG	NE-CZ-NH2	-9.46	115.57	120.30
1	H	119	ARG	NE-CZ-NH1	9.37	124.98	120.30
1	J	262	ASP	CB-CG-OD1	-8.40	110.74	118.30
1	J	119	ARG	NE-CZ-NH1	8.05	124.33	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	L	105	ASP	CB-CG-OD2	-7.89	111.20	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	H	193	PHE	Peptide

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	H	2783	0	2679	33	0
1	J	2783	0	2680	19	0
2	L	958	0	857	17	0
2	M	958	0	857	13	0
3	H	199	0	0	3	0
3	J	210	0	0	5	0
3	L	69	0	0	1	0
3	M	78	0	0	2	0
All	All	8038	0	7073	78	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 5.

The worst 5 of 78 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)
2:L:16:GLN:NE2	2:L:18:ASN:H	1.65	0.93
2:L:45:ASN:HD22	1:J:22:ARG:H	1.20	0.88
1:H:177:ASP:HB2	1:H:193:PHE:O	1.76	0.85
1:H:195:THR:HG22	1:H:195:THR:O	1.78	0.80
2:M:16:GLN:HE22	2:M:19:ASP:H	1.32	0.78

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	H	353/355 (99%)	338 (96%)	13 (4%)	2 (1%)	30	12
1	J	353/355 (99%)	338 (96%)	14 (4%)	1 (0%)	46	25
2	L	124/125 (99%)	121 (98%)	3 (2%)	0	100	100
2	M	124/125 (99%)	120 (97%)	4 (3%)	0	100	100
All	All	954/960 (99%)	917 (96%)	34 (4%)	3 (0%)	46	25

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	196	GLU
1	J	196	GLU
1	H	195	THR

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	H	294/294 (100%)	284 (97%)	10 (3%)	44	18
1	J	294/294 (100%)	284 (97%)	10 (3%)	44	18
2	L	106/104 (102%)	104 (98%)	2 (2%)	65	43
2	M	106/104 (102%)	102 (96%)	4 (4%)	40	15
All	All	800/796 (100%)	774 (97%)	26 (3%)	45	19

5 of 26 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	L	104	ASN
1	J	104	VAL
2	M	104	ASN
1	J	22	ARG
1	J	81	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
2	L	104	ASN
1	J	69	ASN
2	M	34	ASN
2	L	45	ASN
2	M	45	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\#\|Z\| > 2$
2	TRQ	L	57	2	14,17,18	2.79	3 (21%)	8,24,26	2.17	4 (50%)
2	TRQ	M	57	2	14,17,18	3.04	3 (21%)	8,24,26	2.19	5 (62%)

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
2	TRQ	L	57	2	-	0/3/19/21	0/2/2/2
2	TRQ	M	57	2	-	0/3/19/21	0/2/2/2

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	M	57	TRQ	CE2-CZ2	-9.43	1.38	1.49
2	L	57	TRQ	CE2-CZ2	-8.61	1.39	1.49
2	L	57	TRQ	CZ3-CE3	2.93	1.39	1.34
2	M	57	TRQ	CZ3-CE3	3.57	1.40	1.34
2	L	57	TRQ	CD2-CG	4.03	1.45	1.40

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	M	57	TRQ	CB-CG-CD1	-3.70	123.40	127.97
2	L	57	TRQ	CB-CG-CD1	-3.70	123.40	127.97
2	L	57	TRQ	O7-CZ2-CE2	-3.05	118.70	122.10
2	M	57	TRQ	CD2-CE3-CZ3	-2.50	118.36	121.16
2	M	57	TRQ	O7-CZ2-CE2	-2.46	119.37	122.10

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	L	57	TRQ	2	0
2	M	57	TRQ	2	0

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 (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates (i)

EDS was not executed - this section will therefore be empty.

6.4 Ligands (i)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers (i)

EDS was not executed - this section will therefore be empty.