wwPDB X-ray Structure Validation Summary Report (i)

Jan 31, 2016 – 08:51 PM GMT

PDB ID	:	1MDA
Title	:	CRYSTAL STRUCTURE OF AN ELECTRON-TRANSFER COMPLEX BETWEEN METHYLAMINE DEHYDROGENASE AND AMICYANIN
Authors	:	Chen, L.; Durley, R.; Mathews, F.S.
Deposited on	:	1992-03-02
Resolution	:	2.50 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:

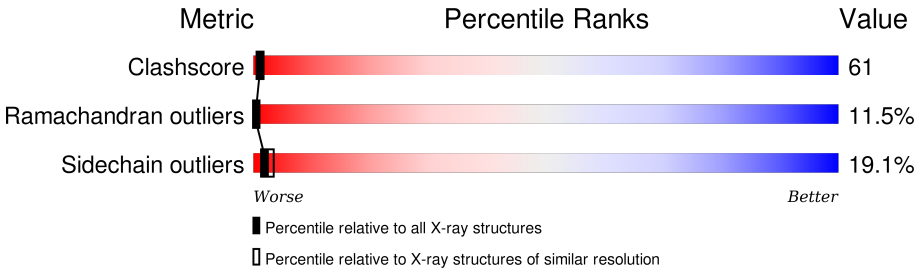
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 2.50 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	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (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. 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	368	39% 42% 15% .
1	J	368	41% 40% 15% .
2	L	121	40% 44% 13% .
2	M	121	31% 50% 13% 5%
3	A	103	9% 36% 38% 17%
3	B	103	16% 38% 33% 14%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	TRQ	M	57	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8567 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
1	H	368	Total	C	N	O	S	0	0	0
			2582	1585	451	532	14			
1	J	368	Total	C	N	O	S	0	0	0
			2583	1585	451	533	14			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	121	Total	C	N	O	S	0	0	0
			910	558	155	184	13			
2	M	121	Total	C	N	O	S	0	0	0
			910	558	155	184	13			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	57	TRQ	TRP	CONFLICT	UNP A44544
M	57	TRQ	TRP	CONFLICT	UNP A44544

- Molecule 3 is a protein called AMICYANIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	103	Total	C	N	O	S	0	0	0
			790	506	130	148	6			
3	B	103	Total	C	N	O	S	0	0	0
			790	506	130	148	6			

- Molecule 4 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Cu	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cu		
4	A	1	1	1	0	0

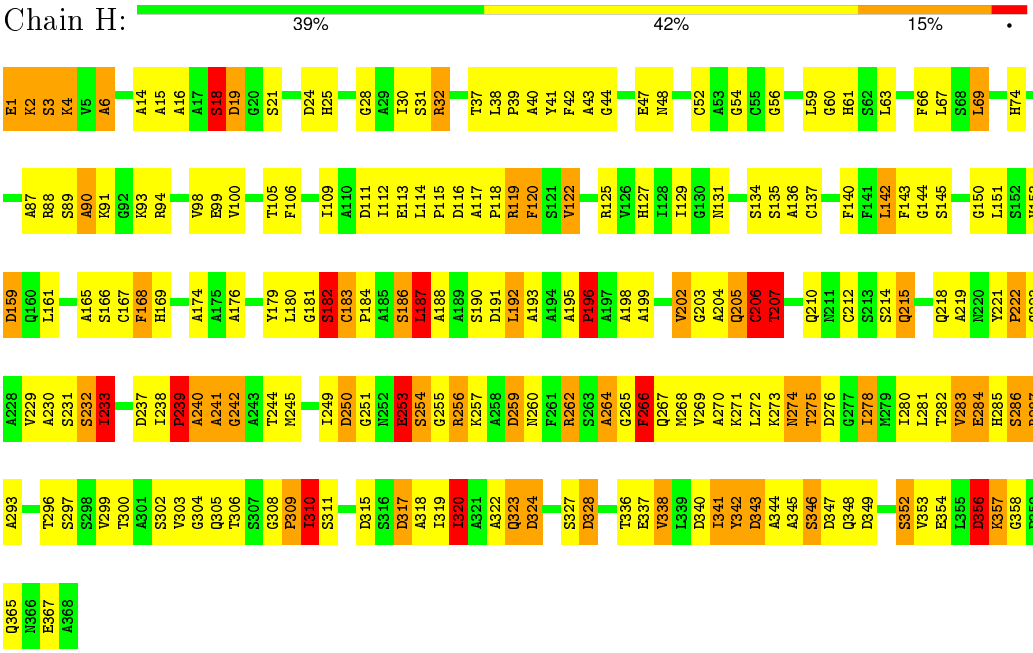
3 Residue-property plots (i)

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.

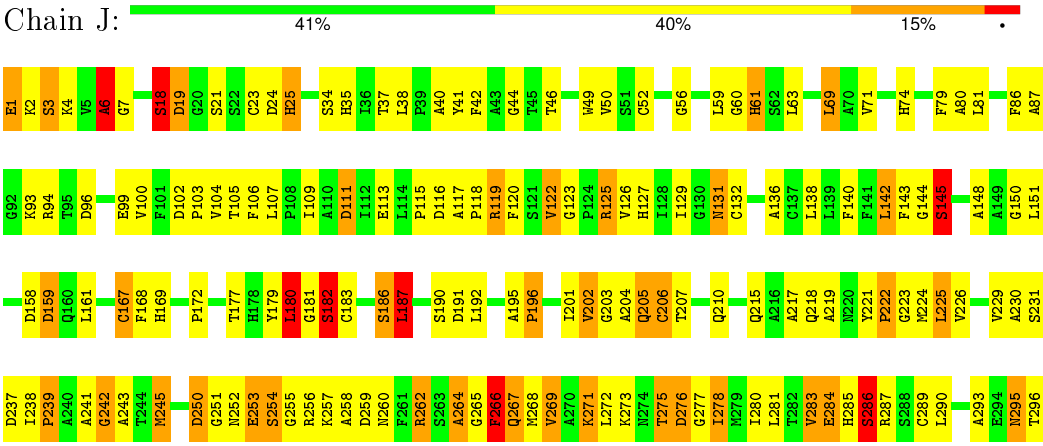
- Molecule 1: METHYLAMINE DEHYDROGENASE (HEAVY SUBUNIT)

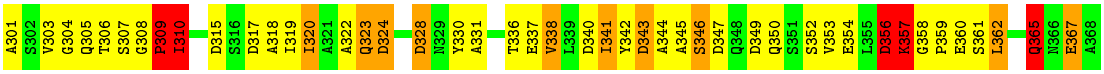
Chain H:



- Molecule 1: METHYLAMINE DEHYDROGENASE (HEAVY SUBUNIT)

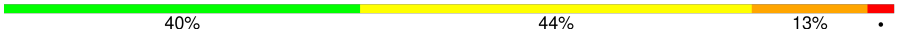
Chain J:

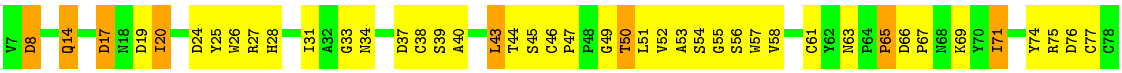




- Molecule 2: METHYLAMINE DEHYDROGENASE (LIGHT SUBUNIT)

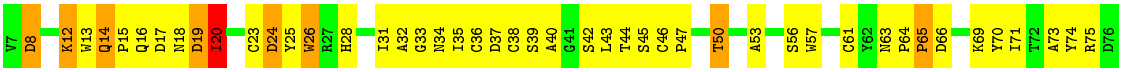
Chain L:

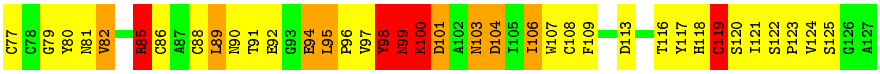




- Molecule 2: METHYLAMINE DEHYDROGENASE (LIGHT SUBUNIT)

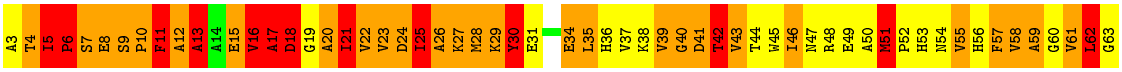
Chain M:

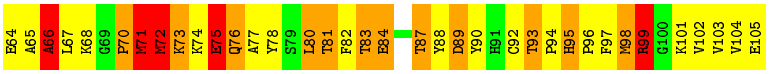




- Molecule 3: AMICYANIN

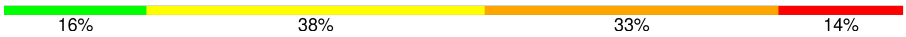
Chain A:





- Molecule 3: AMICYANIN

Chain B:



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 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	124.70Å 124.70Å 247.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.50	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ, TNT	Depositor
R, R_{free}	0.285 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8567	wwPDB-VP
Average B, all atoms (Å^2)	25.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	0.87	9/2629 (0.3%)	1.76	77/3577 (2.2%)
1	J	0.84	7/2630 (0.3%)	1.65	69/3577 (1.9%)
2	L	0.86	2/917 (0.2%)	1.59	21/1250 (1.7%)
2	M	0.84	2/917 (0.2%)	1.59	25/1250 (2.0%)
3	A	1.09	7/811 (0.9%)	1.99	32/1102 (2.9%)
3	B	1.08	4/811 (0.5%)	2.06	29/1102 (2.6%)
All	All	0.90	31/8715 (0.4%)	1.74	253/11858 (2.1%)

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	3	0
1	J	1	1
2	M	1	1
3	B	0	1
All	All	5	3

The worst 5 of 31 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	253	GLU	CD-OE1	6.93	1.33	1.25
2	L	94	GLU	CD-OE1	6.83	1.33	1.25
1	J	113	GLU	CD-OE1	6.74	1.33	1.25
1	H	284	GLU	CD-OE2	6.46	1.32	1.25
1	H	47	GLU	CD-OE1	6.40	1.32	1.25

The worst 5 of 253 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	5	ILE	C-N-CD	-19.12	78.54	120.60
3	B	5	ILE	C-N-CD	-18.21	80.53	120.60
1	H	240	ALA	N-CA-CB	-14.04	90.45	110.10
3	B	9	SER	C-N-CD	-11.45	95.41	120.60
1	J	182	SER	N-CA-CB	10.74	126.61	110.50

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	H	232	SER	CA
1	H	310	ILE	CA
1	H	320	ILE	CA
1	J	232	SER	CA
2	M	94	GLU	CA

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	B	11	PHE	Mainchain
1	J	180	LEU	Mainchain
2	M	98	TYR	Mainchain

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	2582	0	2472	219	0
1	J	2583	0	2472	237	0
2	L	910	0	808	85	0
2	M	910	0	809	108	0
3	A	790	0	774	226	0
3	B	790	0	774	206	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
All	All	8567	0	8109	1009	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 61.

The worst 5 of 1009 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)
3:B:6:PRO:HB3	3:B:83:THR:HG23	1.22	1.19
1:H:222:PRO:HG3	1:H:273:LYS:HD2	1.21	1.15
2:M:121:ILE:HG23	2:M:123:PRO:HD3	1.22	1.15
2:L:121:ILE:HG23	2:L:123:PRO:HD3	1.27	1.12
3:A:52:PRO:HD3	3:A:73:LYS:HE3	1.29	1.10

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	366/368 (100%)	290 (79%)	45 (12%)	31 (8%)	1	1
1	J	366/368 (100%)	291 (80%)	42 (12%)	33 (9%)	1	1
2	L	118/121 (98%)	98 (83%)	12 (10%)	8 (7%)	1	1
2	M	118/121 (98%)	94 (80%)	14 (12%)	10 (8%)	1	1
3	A	101/103 (98%)	49 (48%)	23 (23%)	29 (29%)	0	0
3	B	101/103 (98%)	60 (59%)	18 (18%)	23 (23%)	0	0
All	All	1170/1184 (99%)	882 (75%)	154 (13%)	134 (12%)	0	0

5 of 134 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	182	SER
1	H	186	SER
1	H	206	CYS
1	H	222	PRO
1	H	223	GLY

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	H	264/264 (100%)	219 (83%)	45 (17%)	2	4
1	J	264/264 (100%)	225 (85%)	39 (15%)	4	7
2	L	99/99 (100%)	83 (84%)	16 (16%)	3	5
2	M	99/99 (100%)	85 (86%)	14 (14%)	4	7
3	A	83/83 (100%)	54 (65%)	29 (35%)	0	0
3	B	83/83 (100%)	56 (68%)	27 (32%)	0	0
All	All	892/892 (100%)	722 (81%)	170 (19%)	2	3

5 of 170 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	J	192	LEU
1	J	341	ILE
3	B	51	MET
1	J	205	GLN
1	J	278	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 31 such sidechains are listed below:

Mol	Chain	Res	Type
1	J	48	ASN
1	J	205	GLN
2	M	103	ASN
1	J	131	ASN
1	J	210	GLN

5.3.3 RNA

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	3.09	4 (28%)	8,24,26	2.24	3 (37%)
2	TRQ	M	57	2	14,17,18	2.83	4 (28%)	8,24,26	1.86	2 (25%)

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 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	57	TRQ	CE2-CZ2	-9.63	1.38	1.49
2	M	57	TRQ	CE2-CZ2	-8.42	1.39	1.49
2	M	57	TRQ	CZ3-CH2	-3.37	1.36	1.45
2	L	57	TRQ	CZ3-CH2	-2.55	1.38	1.45
2	L	57	TRQ	CD2-CE3	-2.25	1.39	1.44

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	L	57	TRQ	O7-CZ2-CE2	-3.97	117.69	122.10
2	M	57	TRQ	CB-CG-CD1	-2.76	124.55	127.97
2	L	57	TRQ	CB-CG-CD1	-2.59	124.77	127.97
2	L	57	TRQ	CB-CG-CD2	2.23	129.64	124.40
2	M	57	TRQ	CE3-CZ3-CH2	2.40	123.07	121.12

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	L	57	TRQ	2	0
2	M	57	TRQ	7	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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

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

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

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

6.3 Carbohydrates

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

6.4 Ligands

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

6.5 Other polymers

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