



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 19, 2016 – 06:21 PM GMT

PDB ID : 2TMD  
Title : CORRELATION OF X-RAY DEDUCED AND EXPERIMENTAL AMINO ACID SEQUENCES OF TRIMETHYLAMINE DEHYDROGENASE  
Authors : Mathews, F.S.; Lim, L.W.; White, S.  
Deposited on : 1993-10-15  
Resolution : 2.40 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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
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) : rb-20026982

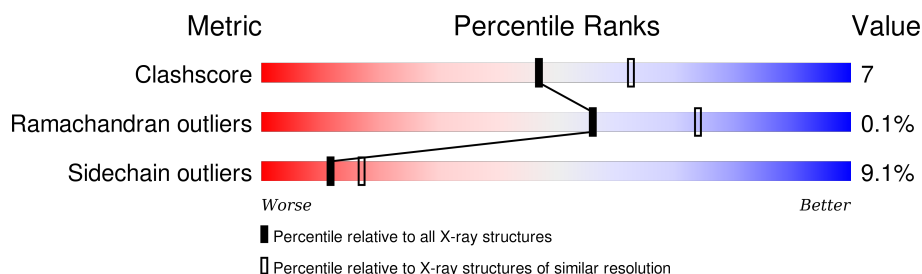
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)

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  $\geq 3$ , 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	729	 76% 20% . .
1	B	729	 80% 16% . .

## 2 Entry composition [i](#)

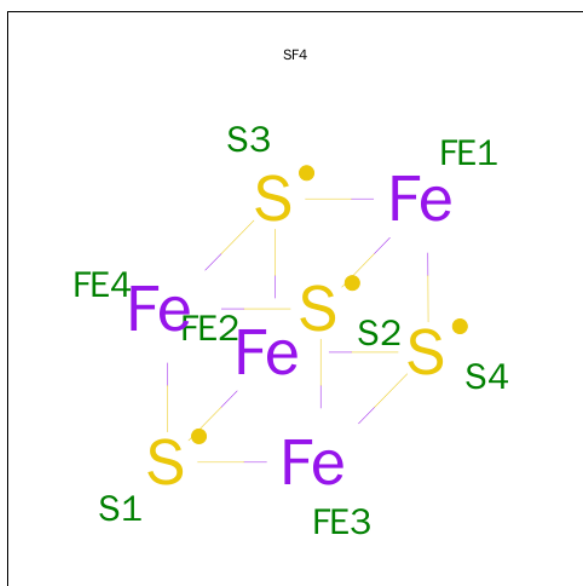
There are 5 unique types of molecules in this entry. The entry contains 12195 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 TRIMETHYLAMINE DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	729	Total	C	N	O	S	0	0	0
			5741	3617	1012	1084	28			
1	B	729	Total	C	N	O	S	0	0	0
			5741	3617	1012	1084	28			

- Molecule 2 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



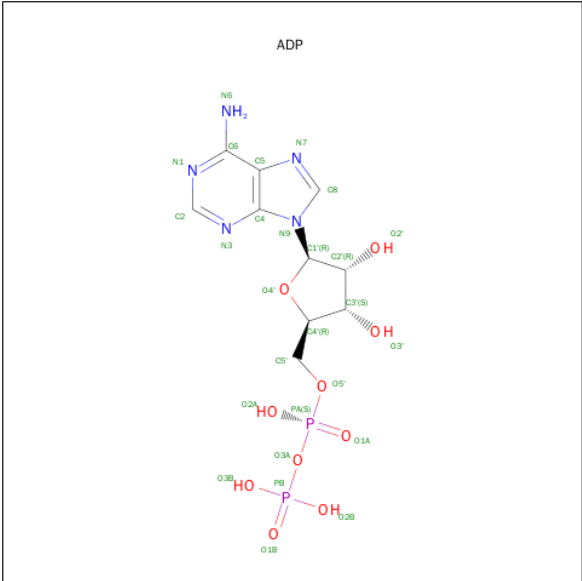
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	Fe	S	0	0
			8	4	4		
2	B	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 3 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: C<sub>17</sub>H<sub>21</sub>N<sub>4</sub>O<sub>9</sub>P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
3	B	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>10</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 5 is water.

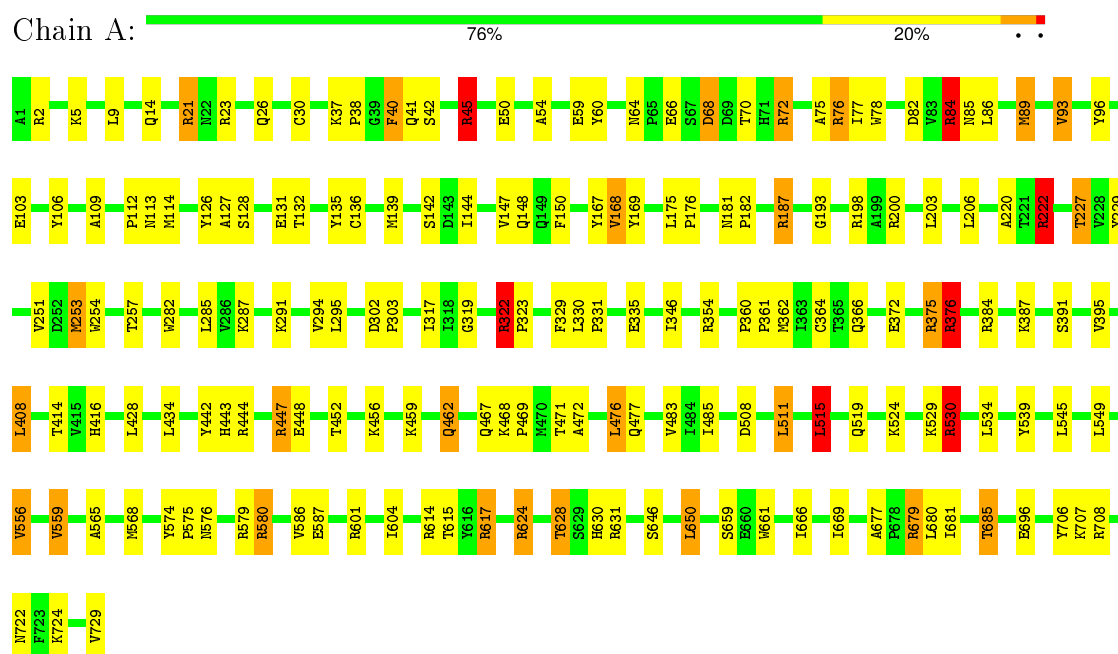
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	287	Total	O	0	0
			287	287		
5	B	294	Total	O	0	0
			294	294		

### 3 Residue-property plots

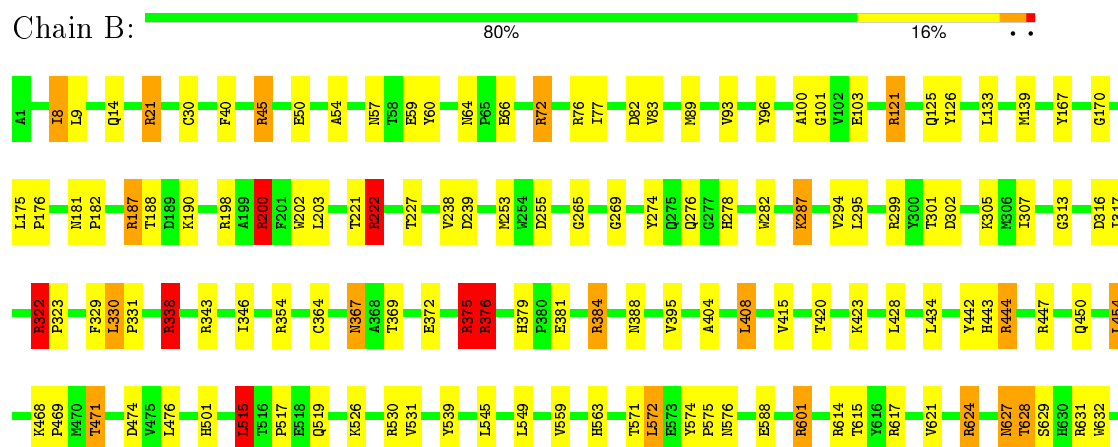
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

Note EDS was not executed.

#### • Molecule 1: TRIMETHYLAMINE DEHYDROGENASE



#### • Molecule 1: TRIMETHYLAMINE DEHYDROGENASE



L638	L639	L640	C648	T648	L650	T651	T652	L672	S679	L680	T681	Y691	Y706	K707	K708	K724	Y729
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## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	147.75Å 71.95Å 83.82Å 90.00° 97.69° 90.00°	Depositor
Resolution (Å)	10.00 – 2.40	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-2.40)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, $R_{free}$	0.154 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	12195	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	17.0	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: FMN, SF4, ADP

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	0.38	0/5885	0.58	2/7980 (0.0%)
1	B	0.37	0/5885	0.59	4/7980 (0.1%)
All	All	0.38	0/11770	0.58	6/15960 (0.0%)

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	0	18
1	B	0	16
All	All	0	34

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	708	ARG	NE-CZ-NH2	-6.96	116.82	120.30
1	B	515	LEU	CA-CB-CG	5.85	128.76	115.30
1	A	515	LEU	CA-CB-CG	5.60	128.19	115.30
1	A	322	ARG	NE-CZ-NH2	-5.37	117.61	120.30
1	B	72	ARG	NE-CZ-NH2	-5.12	117.74	120.30

There are no chirality outliers.

5 of 34 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	126	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	A	23	ARG	Sidechain
1	A	45	ARG	Sidechain
1	A	72	ARG	Sidechain
1	A	84	ARG	Sidechain

## 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	5741	0	5574	99	0
1	B	5741	0	5574	86	0
2	A	8	0	0	1	0
2	B	8	0	0	1	0
3	A	31	0	18	1	0
3	B	31	0	18	3	0
4	A	27	0	12	0	0
4	B	27	0	12	0	0
5	A	287	0	0	6	0
5	B	294	0	0	10	0
All	All	12195	0	11208	171	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 7.

The worst 5 of 171 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:646:SER:H	1:B:125:GLN:HE22	1.12	0.90
1:B:276:GLN:HE22	1:B:302:ASP:H	1.24	0.81
1:B:379:HIS:HD2	1:B:381:GLU:H	1.33	0.74
1:A:646:SER:H	1:B:125:GLN:NE2	1.89	0.69
1:B:627:ASN:HD22	1:B:628:THR:N	1.89	0.69

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	727/729 (100%)	698 (96%)	29 (4%)	0	100	100
1	B	727/729 (100%)	704 (97%)	22 (3%)	1 (0%)	56	74
All	All	1454/1458 (100%)	1402 (96%)	51 (4%)	1 (0%)	56	74

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	238	VAL

### 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	602/602 (100%)	545 (90%)	57 (10%)	11	15
1	B	602/602 (100%)	549 (91%)	53 (9%)	12	18
All	All	1204/1204 (100%)	1094 (91%)	110 (9%)	12	17

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

Mol	Chain	Res	Type
1	A	617	ARG
1	B	40	PHE
1	B	615	THR
1	A	631	ARG
1	A	685	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	241	GLN
1	B	288	GLN
1	B	652	ASN
1	B	276	GLN
1	B	278	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](#)

6 ligands 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	SF4	A	801	1	0,12,12	0.00	-	0,24,24	0.00	-
3	FMN	A	802	-	32,33,33	2.38	6 (18%)	34,50,50	3.49	11 (32%)
4	ADP	A	803	-	24,29,29	1.22	3 (12%)	23,45,45	1.50	4 (17%)
2	SF4	B	801	1	0,12,12	0.00	-	0,24,24	0.00	-
3	FMN	B	802	-	32,33,33	2.20	5 (15%)	34,50,50	3.56	11 (32%)
4	ADP	B	803	-	24,29,29	1.32	2 (8%)	23,45,45	1.25	2 (8%)

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	SF4	A	801	1	-	0/0/48/48	0/6/5/5
3	FMN	A	802	-	-	0/18/18/18	0/3/3/3
4	ADP	A	803	-	-	0/12/32/32	0/3/3/3
2	SF4	B	801	1	-	0/0/48/48	0/6/5/5
3	FMN	B	802	-	-	0/18/18/18	0/3/3/3
4	ADP	B	803	-	-	0/12/32/32	0/3/3/3

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	802	FMN	C1'-N10	-10.58	1.37	1.48
3	B	802	FMN	C1'-N10	-9.67	1.38	1.48
3	B	802	FMN	C10-N10	-3.92	1.34	1.39
4	B	803	ADP	C2'-C1'	-3.70	1.47	1.53
4	A	803	ADP	PB-O2B	-2.45	1.46	1.54

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	802	FMN	C4A-C4-N3	-7.95	113.12	123.52
3	A	802	FMN	C4A-C4-N3	-7.59	113.60	123.52
3	A	802	FMN	N3-C2-N1	-7.13	115.68	127.69
3	B	802	FMN	N3-C2-N1	-6.60	116.58	127.69
4	A	803	ADP	C4'-O4'-C1'	-4.43	104.95	109.64

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	SF4	1	0
3	A	802	FMN	1	0
2	B	801	SF4	1	0
3	B	802	FMN	3	0

## 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.