



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 09:49 PM GMT

PDB ID : 1QR6  
Title : HUMAN MITOCHONDRIAL NAD(P)-DEPENDENT MALIC ENZYME  
Authors : Xu, Y.; Bhargava, G.; Wu, H.; Loeber, G.; Tong, L.  
Deposited on : 1999-06-18  
Resolution : 2.10 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.

---

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) : **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

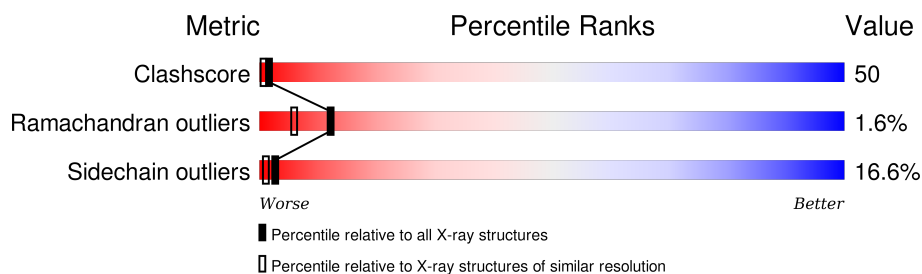
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 Å.

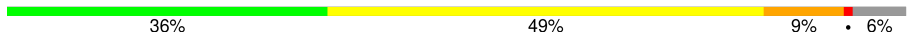
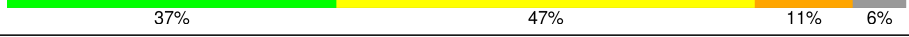
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)

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	584	
1	B	584	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9620 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 MALIC ENZYME 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	551	Total	C	N	O	S	Se	10	0	0
			4342	2779	739	801	9	14			
1	B	551	Total	C	N	O	S	Se	0	0	0
			4342	2779	739	801	9	14			

There are 28 discrepancies between the modelled and reference sequences:

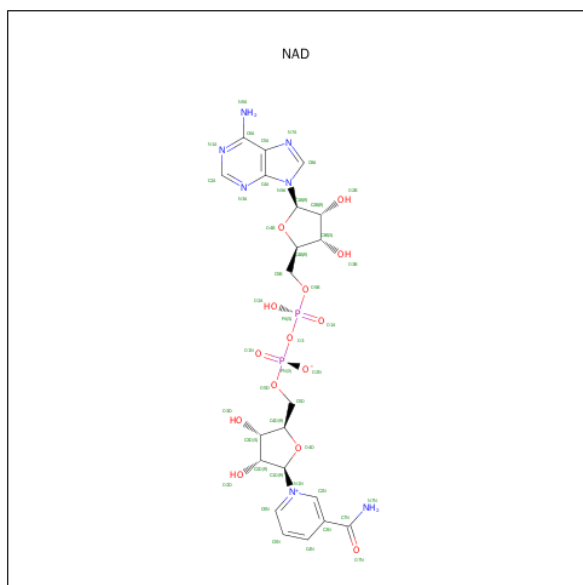
Chain	Residue	Modelled	Actual	Comment	Reference
A	29	MSE	MET	MODIFIED RESIDUE	UNP P23368
A	38	MSE	MET	MODIFIED RESIDUE	UNP P23368
A	47	MSE	MET	MODIFIED RESIDUE	UNP P23368
A	75	MSE	MET	MODIFIED RESIDUE	UNP P23368
A	86	MSE	MET	MODIFIED RESIDUE	UNP P23368
A	108	MSE	MET	MODIFIED RESIDUE	UNP P23368
A	177	MSE	MET	MODIFIED RESIDUE	UNP P23368
A	219	MSE	MET	MODIFIED RESIDUE	UNP P23368
A	239	MSE	MET	MODIFIED RESIDUE	UNP P23368
A	325	MSE	MET	MODIFIED RESIDUE	UNP P23368
A	327	MSE	MET	MODIFIED RESIDUE	UNP P23368
A	343	MSE	MET	MODIFIED RESIDUE	UNP P23368
A	407	MSE	MET	MODIFIED RESIDUE	UNP P23368
A	539	MSE	MET	MODIFIED RESIDUE	UNP P23368
B	1029	MSE	MET	MODIFIED RESIDUE	UNP P23368
B	1038	MSE	MET	MODIFIED RESIDUE	UNP P23368
B	1047	MSE	MET	MODIFIED RESIDUE	UNP P23368
B	1075	MSE	MET	MODIFIED RESIDUE	UNP P23368
B	1086	MSE	MET	MODIFIED RESIDUE	UNP P23368
B	1108	MSE	MET	MODIFIED RESIDUE	UNP P23368
B	1177	MSE	MET	MODIFIED RESIDUE	UNP P23368
B	1219	MSE	MET	MODIFIED RESIDUE	UNP P23368
B	1239	MSE	MET	MODIFIED RESIDUE	UNP P23368
B	1325	MSE	MET	MODIFIED RESIDUE	UNP P23368
B	1327	MSE	MET	MODIFIED RESIDUE	UNP P23368

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
B	1343	MSE	MET	MODIFIED RESIDUE	UNP P23368
B	1407	MSE	MET	MODIFIED RESIDUE	UNP P23368
B	1539	MSE	MET	MODIFIED RESIDUE	UNP P23368

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: C<sub>21</sub>H<sub>27</sub>N<sub>7</sub>O<sub>14</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	374	Total	O	0	0
			374	374		
3	B	386	Total	O	0	0
			386	386		



Y1562	W490	I1410	Y1347	L1266	A1191	G1124	D1062
L1565	F1491	M1411	G1348	R1267	G1192	H1125	I1063
L1566	E1492	E1413	L1349	R1270	R1193	I1126	Q1064
E1571	A1494	P1414	V1351	F1276	P1195	F1127	A1065
H1572	A1495	V1415	K1352	M1277	R1196	R1128	L1066
P1573	K1496	I1416	G1353	D1278	R1197	F1068	F1068
GLU	A1497	F1417	R1354	D1279	C1198	G1132	H1069
SER	L1498	A1418	K1355	I1280	L1199	L1133	R1070
SER	Q1501	L1419	A1356	I1281	C1202	S1136	M1071
SER	L1502	S1420	K1357	G1282	V1205	I1137	L1072
PRO	E1505	T1423	D1359	V1286	G1206	R1140	K1073
PRO	E1506	A1424	S1360	A1287	T1207	V1143	K1074
VAL	L1507	Q1425	Y1361	L1288	I1210	S1077	M1075
ILE	A1508	E1427	A1362	A1289	L1213	R1144	P1078
THR	Q1509	C1428	E1363	P1364	L1214	S1145	L1079
GLU	G1510	T1429	H1367	L1292	K1224	I1146	E1080
	R1511	E1432	S1368	A1293	R1225	V1147	K1081
	L1512	A1433	A1369	K1295	D1226	D1148	I1082
	Y1513	E1437	L1372	K1296	R1227	M1149	I1083
	P1514	L1436	I1373	V1297	Y1218	W1150	Y1084
	P1515	T1437	S1372	I1298	E1151	P1151	I1085
	L1516	R1440	I1374	S1299	M1152	M1086	M1086
	A1517	C1441	D1375	K1300	H1153	G1087	G1087
	M1518	L1442	T1376	P1301	H1154	I1088	I1088
	I1519	L1445	F1377	S1302	V1155	Q1089	Q1089
	Q1520	S1446	E1378	S1303	K1156	E1090	E1090
	E1521	G1445	D1379	E1304	Y1160	R1091	R1091
	V1522	T1446	A1380	H1305	T1161	M1092	M1092
	S1523	K1453	V1381	K1306	I1162	E1093	E1093
	I1524	L1454	M1382	I1307	G1163	K1094	K1094
	M1525	T1455	I1383	L1308	E1164	L1095	L1095
	I1526	D1456	L1384	F1309	R1165	M1107	S1106
	A1527	G1457	K1385	L1310	M1239	V1174	L1107
	I1528	R1458	P1386	A1315	K1240	Y1175	M1108
	K1529	V1459	S1387	A1316	A1241	G1176	P1109
	V1530	F1460	T1388	L1317	I1242	M1177	I1110
	T1531	T1461	I1389	G1318	T1243	G1178	V1111
	E1532	P1462	I1390	I1319	D1244	I1179	Y1112
	Y1533	G1463	G1391	A1320	R1245	P1180	T1113
	K1538	Q1464	V1392	M1321	Y1246	V1181	P1114
	R1542	G1465	A1393	L1322	R1248	G1182	T1115
	Y1543	M1466	L1397	V1324	T1250	K1183	G1117
	P1544	N1467	R1398	M1325	Q1253	C1185	L1118
	E1545	V1468	F1399	V1328	F1254	I1186	A1119
	P1546	Y1469	T1400	L1332	E1255	Y1187	C1120
	E1547	P1472	P1401	L1332	G1258	T1188	S1121
	K1551	V1478	D1402	K1340	L1184	A1189	Q1122
	E1554	N1482	I1404	M1343	M1259	R1264	Y1123
	E1555	T1483	R1405	F1344	H1260		
	W1558	R1484	M1406	D1345	N1261		
	R1559	S1489	M1407	K1346	R1265		

## 4 Data and refinement statistics

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

Property	Value	Source
Space group	B 1 1 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	204.40 Å   107.00 Å   59.20 Å 90.00°   90.00°   101.90°	Depositor
Resolution (Å)	20.00 – 2.10	Depositor
% Data completeness (in resolution range)	87.0 (20.00-2.10)	Depositor
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR 3.843	Depositor
R, $R_{free}$	0.228 , 0.287	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9620	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	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: NAD

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	0.37	0/4422	0.64	2/5967 (0.0%)
1	B	0.37	0/4422	0.63	3/5967 (0.1%)
All	All	0.37	0/8844	0.63	5/11934 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1543	TYR	N-CA-C	7.24	130.53	111.00
1	A	543	TYR	N-CA-C	6.19	127.71	111.00
1	A	542	ARG	N-CA-C	-5.91	95.03	111.00
1	B	1542	ARG	N-CA-C	-5.62	95.81	111.00
1	B	1543	TYR	C-N-CD	5.00	138.90	128.40

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	4342	0	4366	455	0
1	B	4342	0	4366	441	0
2	A	88	0	52	2	0
2	B	88	0	52	4	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	374	0	0	145	0
3	B	386	0	0	155	0
All	All	9620	0	8836	884	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 50.

The worst 5 of 884 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:B:1107:LEU:HD12	3:B:2496:HOH:O	1.42	1.19
1:A:218:TYR:HB2	3:A:2698:HOH:O	1.44	1.18
1:B:1472:PRO:HB2	3:B:2252:HOH:O	1.48	1.11
1:A:215:ASP:HB3	3:A:2698:HOH:O	1.51	1.10
1:B:1243:THR:HB	1:B:1248:ARG:HE	1.20	1.06

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	549/584 (94%)	505 (92%)	35 (6%)	9 (2%)	12	6
1	B	549/584 (94%)	502 (91%)	38 (7%)	9 (2%)	12	6
All	All	1098/1168 (94%)	1007 (92%)	73 (7%)	18 (2%)	12	6

5 of 18 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	113	THR
1	B	1113	THR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	1299	SER
1	B	1571	GLU
1	A	259	ASN

### 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	465/484 (96%)	390 (84%)	75 (16%)	3	1
1	B	465/484 (96%)	386 (83%)	79 (17%)	2	1
All	All	930/968 (96%)	776 (83%)	154 (17%)	3	1

5 of 154 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	520	GLN
1	B	1104	ILE
1	B	1509	GLN
1	A	543	TYR
1	B	1048	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 34 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	509	GLN
1	B	1046	GLN
1	B	1501	GLN
1	B	1031	ASN
1	A	261	ASN

### 5.3.3 RNA ⓘ

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](#)

4 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	NAD	A	601	-	38,48,48	1.59	8 (21%)	47,73,73	1.97	4 (8%)
2	NAD	A	602	-	38,48,48	1.83	8 (21%)	47,73,73	1.97	4 (8%)
2	NAD	B	1601	-	38,48,48	1.59	9 (23%)	47,73,73	1.99	6 (12%)
2	NAD	B	1602	-	38,48,48	1.80	7 (18%)	47,73,73	1.97	4 (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	NAD	A	601	-	-	0/22/62/62	0/5/5/5
2	NAD	A	602	-	-	0/22/62/62	0/5/5/5
2	NAD	B	1601	-	-	0/22/62/62	0/5/5/5
2	NAD	B	1602	-	-	0/22/62/62	0/5/5/5

The worst 5 of 32 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1602	NAD	C5A-C4A	-3.15	1.33	1.40
2	A	602	NAD	C5A-C4A	-3.05	1.33	1.40

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	NAD	C5A-C4A	-2.82	1.34	1.40
2	B	1601	NAD	C5A-C4A	-2.79	1.34	1.40
2	A	601	NAD	C5A-N7A	-2.43	1.31	1.39

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	602	NAD	N3A-C2A-N1A	-11.06	120.42	128.89
2	B	1602	NAD	N3A-C2A-N1A	-11.05	120.44	128.89
2	A	601	NAD	N3A-C2A-N1A	-10.50	120.85	128.89
2	B	1601	NAD	N3A-C2A-N1A	-10.47	120.88	128.89
2	B	1601	NAD	C4D-O4D-C1D	-2.52	106.95	109.72

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	NAD	1	0
2	A	602	NAD	1	0
2	B	1601	NAD	4	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.