



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 02:55 PM UTC

PDB ID : 1MZZ / pdb_00001mzz
Title : Crystal Structure of Mutant (M182T)of Nitrite Reductase
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Deposited on : 2002-10-10
Resolution : 2.00 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

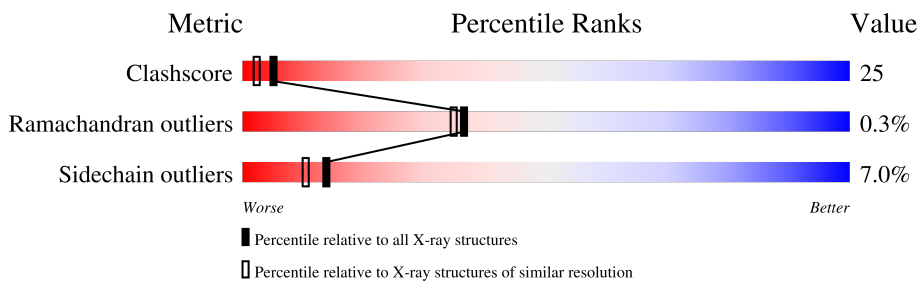
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	334	
1	B	334	
1	C	334	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8561 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 Copper-containing nitrite reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	334	Total	C	N	O	S	0	0	0
			2567	1637	438	480	12			
1	B	334	Total	C	N	O	S	0	0	0
			2567	1637	438	480	12			
1	C	334	Total	C	N	O	S	0	0	0
			2567	1637	438	480	12			

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	182	THR	MET	engineered mutation	UNP Q53239
A	230	ASP	THR	conflict	UNP Q53239
A	281	ASN	LYS	conflict	UNP Q53239
A	351	HIS	SER	conflict	UNP Q53239
A	367	VAL	TRP	conflict	UNP Q53239
A	368	ALA	PRO	conflict	UNP Q53239
A	372	LEU	-	cloning artifact	UNP Q53239
B	1182	THR	MET	engineered mutation	UNP Q53239
B	1230	ASP	THR	conflict	UNP Q53239
B	1281	ASN	LYS	conflict	UNP Q53239
B	1351	HIS	SER	conflict	UNP Q53239
B	1367	VAL	TRP	conflict	UNP Q53239
B	1368	ALA	PRO	conflict	UNP Q53239
B	1372	LEU	-	cloning artifact	UNP Q53239
C	2182	THR	MET	engineered mutation	UNP Q53239
C	2230	ASP	THR	conflict	UNP Q53239
C	2281	ASN	LYS	conflict	UNP Q53239
C	2351	HIS	SER	conflict	UNP Q53239
C	2367	VAL	TRP	conflict	UNP Q53239
C	2368	ALA	PRO	conflict	UNP Q53239
C	2372	LEU	-	cloning artifact	UNP Q53239

- Molecule 2 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total 2	Cu 2	0	0
2	B	2	Total 2	Cu 2	0	0
2	C	2	Total 2	Cu 2	0	0

- Molecule 3 is water.

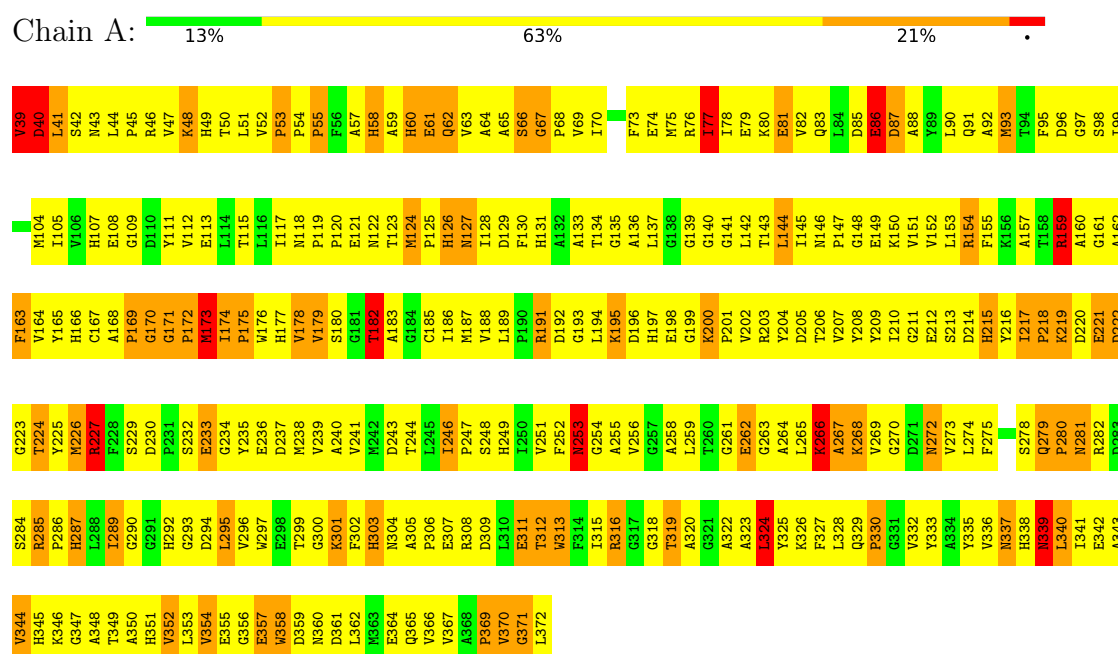
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	289	Total 289	O 289	0	0
3	B	276	Total 276	O 276	0	0
3	C	289	Total 289	O 289	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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: Copper-containing nitrite reductase



- Molecule 1: Copper-containing nitrite reductase



R1282 D1283 S1284 R1285 P1286 H1287 L1288 L1289 G1290 H1291 H1292 H1293 D1294 L1295 V1296 V1297 E1298 T1299 G1300 G1301 F1302 H1303 H1304 N1305 A1306 E1307 R1308 D1309 L1310 E1311 T1312 W1313 F1314 I1315 R1316 G1317 G1318 T1319 A1320 G1321 A1322 A1323 L1324 Y1325 K1326 F1327 L1328 Q1329 P1330 G1331 V1332 Y1333 A1334 Y1335 V1336 N1337 H1338 N1339 L1340 I1341

E1342 A1343 V1344 S1345 K1346 G1347 A1348 T1349 A1350 H1351 L1352 L1353 V1354 E1355 G1356 E1357 W1358 D1359 G1360 D1361 L1362 M1363 E1364 Q1365 V1366 V1367 A1368 P1369 V1370 L1372

• Molecule 1: Copper-containing nitrite reductase

Chain C: 13% 60% 23% .

V2039 D2040 L2041 S2042 N2043 L2044 P2045 R2046 V2047 K2048 H2049 T2050 L2051 V2052 P2053 P2054 P2055 F2056 A2057 H2058 A2059 H2060 E2061 Q2062 V2063 A2064 A2065 S2066 G2067 P2068 V2069 I2070 N2071 E2072 F2073 E2074 N2075 E2076 I2077 I2078 E2079 K2080 E2081 V2082 Q2083 E2086 D2087 A2088 Y2089 L2090 Q2091 A2092 M2093 T2094 F2095 D2096 G2097 S2098 I2099

P2100 G2101 P2102 L2103 N2104 L2105 V2106 H2107 E2108 G2109 V2112 E2113 L2114 L2115 L2116 L2117 L2118 N2119 P2120 E2121 N2122 L2123 T2124 P2125 H2126 N2127 L2128 D2129 F2130 P2131 H2132 A2133 A2134 A2135 A2136 L2137 G2138 G2139 G2140 G2141 L2142 T2143 L2144 L2145 N2146 P2147 G2148 E2149 K2150 V2151 V2152 L2153 R2154 F2155 K2156 A2157 T2158 P2159 A2160

G2161 A2162 F2163 V2164 Y2165 H2166 C2167 A2168 P2169 G2170 G2171 P2172 H2173 I2174 W2175 W2176 H2177 V2178 N2179 S2180 G2181 T2182 A2183 G2184 C2185 I2186 I2187 V2188 L2189 P2190 R2191 D2192 G2193 L2194 K2195 D2196 H2197 E2198 G2199 R2200 P2201 V2202 R2203 Y2204 D2205 T2206 V2207 Y2208 I2209 I2210 G2211 E2212 S2213 D2214 H2215 Y2216 I2217 P2218 K2219 D2220

E2221 D2222 S2223 T2224 V2225 W2226 R2227 F2228 S2229 D2230 P2231 S2232 E2233 G2234 Y2235 E2236 D2237 N2238 V2239 A2240 M2241 M2242 D2243 T2244 L2245 I2246 F2247 S2248 H2249 L2250 T2251 F2252 N2253 G2254 A2255 V2256 G2257 A2258 L2259 T2260 G2261 E2262 L2265 K2266 A2267 K2268 V2269 G2270 D2271 V2272 V2273 V2274 F2275 V2276 H2277 S2278 Q2279 P2280 N2281

R2282 D2283 S2284 R2285 P2286 H2287 L2288 I2289 G2290 G2291 H2292 D2293 G2294 L2295 E2298 T2299 G2300 K2301 P2302 H2303 A2304 Q2305 P2306 E2307 R2308 D2309 L2310 E2311 T2312 W2313 F2314 L2315 R2316 G2317 G2318 T2319 A2320 G2321 A2322 A2323 L2324 Y2325 K2326 F2327 L2328 Q2329 P2330 G2331 V2332 Y2333 A2334 Y2335 V2336 N2337 H2338 N2339 L2340 I2341 E2342

A2343 V2344 H2345 K2346 G2347 A2348 T2349 A2350 H2351 L2352 L2353 V2354 E2355 G2356 E2357 W2358 D2359 N2360 D2361 L2362 M2363 E2364 Q2365 V2366 V2367 A2368 F2369 V2370 G2371 L2372

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	92.50Å 123.73Å 130.17Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.00	Depositor
% Data completeness (in resolution range)	91.4 (30.00-2.00)	Depositor
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.170 , 0.218	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8561	wwPDB-VP
Average B, all atoms (Å ²)	23.0	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:
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	A	4.08	478/2640 (18.1%)	2.77	226/3599 (6.3%)
1	B	4.00	509/2640 (19.3%)	2.69	242/3599 (6.7%)
1	C	4.01	462/2640 (17.5%)	2.74	242/3599 (6.7%)
All	All	4.03	1449/7920 (18.3%)	2.73	710/10797 (6.6%)

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	5
1	B	0	8
1	C	0	7
All	All	0	20

The worst 5 of 1449 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	191	ARG	CZ-NH1	41.64	1.91	1.32
1	C	2226	MET	SD-CE	-27.78	1.10	1.79
1	C	2065	ALA	CA-CB	22.89	1.87	1.53
1	B	1040	ASP	C-O	19.77	1.48	1.24
1	A	226	MET	SD-CE	19.32	2.27	1.79

The worst 5 of 710 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	191	ARG	NE-CZ-NH2	-22.35	99.08	119.20
1	A	124	MET	CG-SD-CE	-21.90	52.72	100.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1124	MET	CG-SD-CE	-18.11	61.06	100.90
1	C	2227	ARG	NE-CZ-NH2	-17.71	103.26	119.20
1	A	203	ARG	NE-CZ-NH2	-17.46	103.48	119.20

There are no chirality outliers.

5 of 20 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	108	GLU	Mainchain
1	A	159	ARG	Sidechain
1	A	173	MET	Mainchain
1	A	272	ASN	Mainchain
1	A	352	VAL	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	A	2567	0	2477	139	0
1	B	2567	0	2477	118	0
1	C	2567	0	2477	143	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
3	A	289	0	0	11	0
3	B	276	0	0	7	0
3	C	289	0	0	10	0
All	All	8561	0	7431	375	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 25.

The worst 5 of 375 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:C:2178:VAL:CB	1:C:2178:VAL:CG1	1.74	1.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:173:MET:CB	1:A:173:MET:CA	1.74	1.64
1:B:1086:GLU:CB	1:B:1086:GLU:CG	1.75	1.63
1:C:2295:LEU:CG	1:C:2295:LEU:CD1	1.75	1.62
1:A:289:ILE:CB	1:A:289:ILE:CG2	1.75	1.62

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	332/334 (99%)	321 (97%)	10 (3%)	1 (0%)	36	35
1	B	332/334 (99%)	319 (96%)	12 (4%)	1 (0%)	36	35
1	C	332/334 (99%)	316 (95%)	15 (4%)	1 (0%)	36	35
All	All	996/1002 (99%)	956 (96%)	37 (4%)	3 (0%)	36	35

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	40	ASP
1	B	1040	ASP
1	C	2040	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	270/270 (100%)	250 (93%)	20 (7%)	13	9
1	B	270/270 (100%)	251 (93%)	19 (7%)	14	10
1	C	270/270 (100%)	252 (93%)	18 (7%)	15	11
All	All	810/810 (100%)	753 (93%)	57 (7%)	14	10

5 of 57 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1182	THR
1	C	2357	GLU
1	B	1313	TRP
1	C	2339	ASN
1	C	2253	ASN

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

Mol	Chain	Res	Type
1	C	2058	HIS
1	C	2215	HIS
1	C	2146	ASN
1	C	2253	ASN
1	A	339	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](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 6 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 is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.