



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 17, 2026 – 10:55 PM UTC

PDB ID : 8KA2 / pdb_00008ka2
Title : Crystal structure of the RID-dependent transforming NADase domain (RD TND)/calmodulin-binding domain of Rho inactivation domain (RID-CBD) from *Vibrio vulnificus*
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Deposited on : 2023-08-02
Resolution : 3.38 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
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

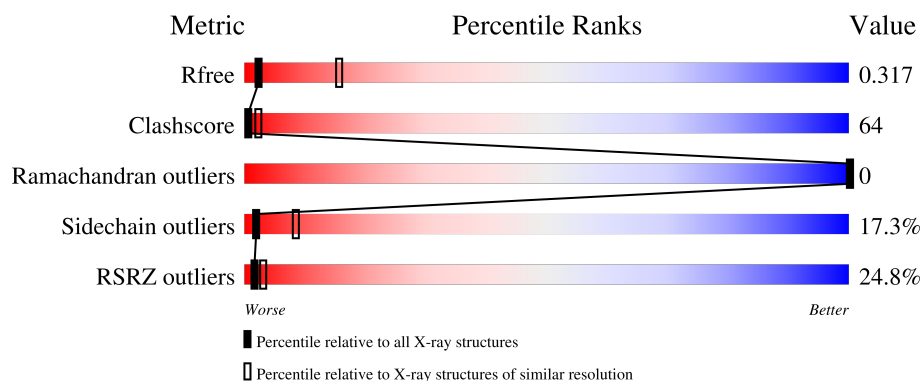
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.38 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))
R_{free}	180053	1047 (3.42-3.34)
Clashscore	190562	1067 (3.42-3.34)
Ramachandran outliers	187476	1056 (3.42-3.34)
Sidechain outliers	187428	1056 (3.42-3.34)
RSRZ outliers	180081	1047 (3.42-3.34)

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 $\leq 5\%$. 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.

Mol	Chain	Length	Quality of chain
1	A	419	15% 35% 45% 12% 8%
1	B	419	27% 28% 46% 8% 18%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 5848 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 RDTND-RID CBD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	387	Total	C	N	O	Se	0	0	0
			3101	1955	530	611	5			
1	B	342	Total	C	N	O	Se	0	0	0
			2747	1738	467	537	5			

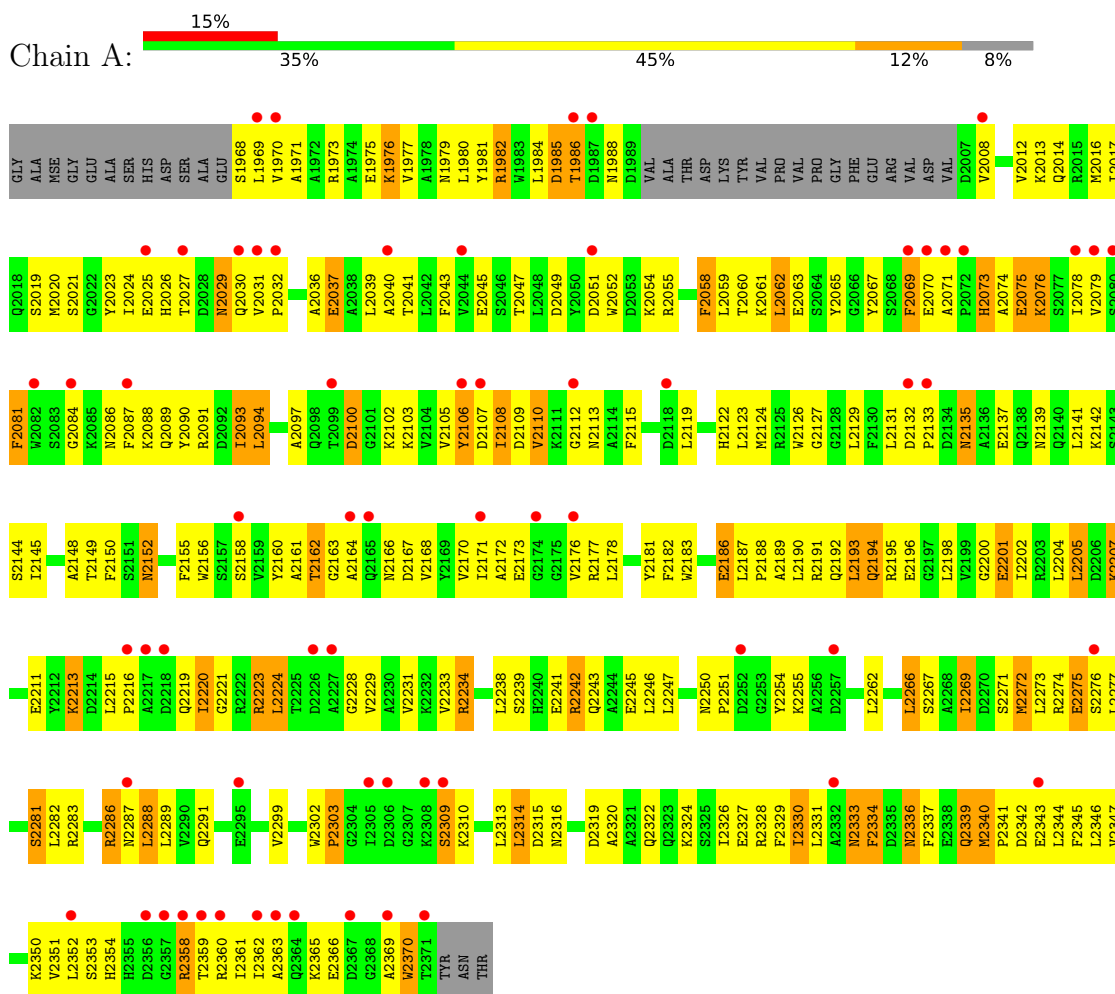
There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1956	GLY	-	cloning artifact	UNP A0A2S3R7M0
A	1957	ALA	-	cloning artifact	UNP A0A2S3R7M0
A	1958	MSE	-	cloning artifact	UNP A0A2S3R7M0
B	1956	GLY	-	cloning artifact	UNP A0A2S3R7M0
B	1957	ALA	-	cloning artifact	UNP A0A2S3R7M0
B	1958	MSE	-	cloning artifact	UNP A0A2S3R7M0

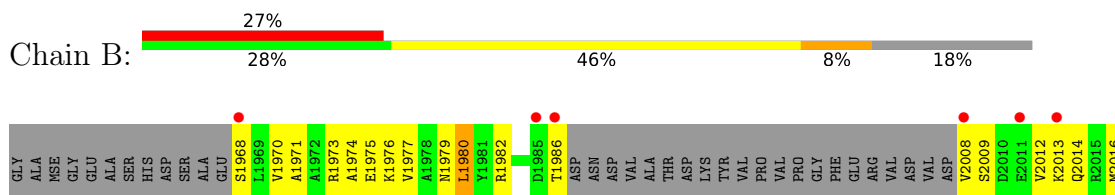
3 Residue-property plots

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 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.

• Molecule 1: RDTND-RID CBD



• Molecule 1: RDTND-RID CBD



A2332	F2333	D2334	D2335	N2336	F2337	E2338	Q2339	M2340	P2341	D2342	E2343	L2344	F2345	L2346	V2347	D2348	M2349	K2350	V2351	L2352	S2353	H2354	H2355	D2356	G2357	R2358	T2359	R2360	I2361	T2362	A2363	Q2364	R2365	E2366	D2367	G2368	A2369	W2370	T2371	TYR	ASN	THR																	
I2269	D2270	S2271	M2272	L2273	R2274	E2275	S2276	L2277	F2278	F2279	Y2280	S2281	L2282	R2283	T2284	E2285	R2286		Y2289	Q2291	E2292	G2293	E2294	E2295		E2298	V2299	R2300	S2301	W2302	P2303	G2304	T2305	D2306	G2307	K2308	S2309	K2310	T2311	I2312	L2313	L2314	D2315	A2316	P2317	E2318	D2319	A2320	A2321	Q2322	Q2323	K2324	S2325	I2326	F2327	R2328	F2329	I2330	L2331
V2209	S2210	E2211	K2213	D2214	L2215	P2216	A2217	D2218	Q2219	L2220	G2221	R2222	R2223	L2224	T2225	D2226	A2227	G2228	V2229	ALA	VAL	LYS	VAL	ARG	PHE	ASP	ALA	LEU	SER	HIS	GLU	ARG	GLN	ALA	GLU	LEU	LEU	ALA	ASP	ASN	PRO	ASP	GLY	TYR	LYS	ALA	ASP	THR	LEU	VAL	GLU	LEU	D2263	V2264	K2265	L2266	S2267	A2268	
N2086	F2087	K2088	Q2089	Y2090	R2091	D2092	L2093	L2094	D2095	N2096	A2097	D2098	THR	ASP	GLY	LYS	V2104	V2105	Y2106	D2107	I2108	D2109	V2110	K2111	G2112	N2113	A2114	F2115	A2116	I2117	D2118	L2119	N2120	K2121	H2122	L2123	N2124	R2125	W2126	G2127	G2128	L2129	F2130	D2131	D2132	P2133	D2134	N2135	A2136	E2137	Q2138	N2139	I2202	Q2140	L2204	K2142	S2143	G2144	I2145
I2017	Q2018	S2019	M2020	S2021		I2024		T2027	D2028	N2029		P2032	K2033	D2034	Q2035	A2036	E2037		T2041	L2042	F2043	V2044	E2045	S2046	T2047	L2048		D2051	W2052	D2053	K2054	R2055	V2056	E2057		K2061	L2062	E2063	S2064	Y2065	G2066	Y2067	S2068	F2069	E2070	A2071		A2074	E2075	K2076	S2077	I2078	V2079	S2080	F2081	W2082	S2083	G2084	K2085

4 Data and refinement statistics

Property	Value	Source
Space group	P 6	Depositor
Cell constants a, b, c, α , β , γ	207.73Å 207.73Å 54.65Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.42 – 3.38 40.42 – 3.38	Depositor EDS
% Data completeness (in resolution range)	82.8 (40.42-3.38) 82.8 (40.42-3.38)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.95 (at 3.40Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.286 , 0.322 0.284 , 0.317	Depositor DCC
R_{free} test set	830 reflections (4.31%)	wwPDB-VP
Wilson B-factor (Å ²)	40.3	Xtriage
Anisotropy	0.383	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 35.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.029 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.82	EDS
Total number of atoms	5848	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.08% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	1.01	2/3157 (0.1%)	1.47	7/4265 (0.2%)
1	B	1.02	2/2796 (0.1%)	1.44	5/3772 (0.1%)
All	All	1.02	4/5953 (0.1%)	1.46	12/8037 (0.1%)

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	A	2	2
1	B	2	0
All	All	4	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2333	ASN	CA-C	6.70	1.55	1.52
1	A	2250	ASN	N-CA	5.94	1.50	1.46
1	B	2266	LEU	N-CA	5.08	1.52	1.46
1	B	2361	ILE	N-CA	5.01	1.50	1.46

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	2356	ASP	N-CA-C	-6.03	107.75	114.62
1	A	2176	VAL	CB-CA-C	5.97	121.09	111.29
1	A	2303	PRO	N-CA-C	-5.93	101.19	110.50
1	A	2272	MSE	CG-SE-CE	5.83	111.75	98.92
1	B	2086	ASN	N-CA-C	-5.73	101.82	110.70

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	2020	MSE	CA
1	A	2124	MSE	CA
1	B	2020	MSE	CA
1	B	2124	MSE	CA

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	2081	PHE	Mainchain
1	A	2370	TRP	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	3101	0	2997	394	0
1	B	2747	0	2649	351	0
All	All	5848	0	5646	732	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 64.

The worst 5 of 732 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:2020:MSE:SE	1:A:2119:LEU:HD12	1.69	1.43
1:B:2329:PHE:CE2	1:B:2362:ILE:HD13	1.61	1.35
1:A:2024:ILE:CG2	1:A:2031:VAL:HG11	1.56	1.34
1:A:2334:PHE:CE2	1:A:2341:PRO:HD3	1.63	1.32
1:A:2020:MSE:SE	1:A:2119:LEU:CD1	2.40	1.20

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	383/419 (91%)	354 (92%)	29 (8%)	0	100	100
1	B	332/419 (79%)	311 (94%)	21 (6%)	0	100	100
All	All	715/838 (85%)	665 (93%)	50 (7%)	0	100	100

There are no Ramachandran outliers to report.

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	332/351 (95%)	266 (80%)	66 (20%)	1	5
1	B	294/351 (84%)	252 (86%)	42 (14%)	3	13
All	All	626/702 (89%)	518 (83%)	108 (17%)	2	8

5 of 108 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2314	LEU
1	B	2062	LEU
1	B	2312	ILE
1	A	2334	PHE
1	A	2360	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	2113	ASN
1	B	2364	GLN
1	B	2152	ASN
1	A	2287	ASN
1	B	2086	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](#)

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](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	382/419 (91%)	1.09	64 (16%) 4 5	8, 46, 95, 112	0
1	B	337/419 (80%)	1.55	114 (33%) 1 1	6, 73, 127, 148	0
All	All	719/838 (85%)	1.31	178 (24%) 2 3	6, 55, 121, 148	0

The worst 5 of 178 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	2219	GLN	6.7
1	B	2228	GLY	6.6
1	B	2220	ILE	5.9
1	A	2358	ARG	5.7
1	B	2080	SER	5.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.