



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 29, 2026 – 11:22 am BST

PDB ID : 9RQU / pdb_00009rqu
Title : The C-terminal domain of remorin from *Nicotiana benthamiana*
Authors : Chen, L.; Isupov, M.N.; Wu, Y.
Deposited on : 2025-06-26
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

<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 : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.015 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

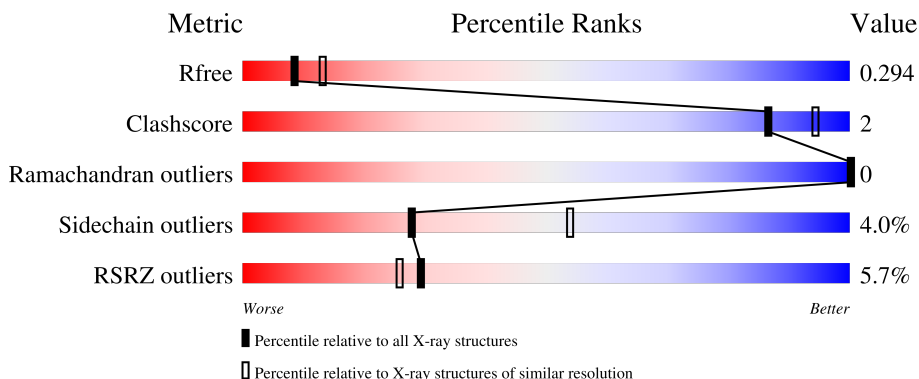
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

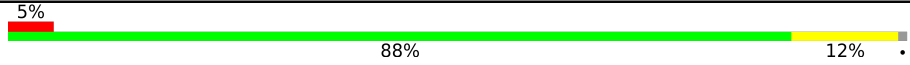
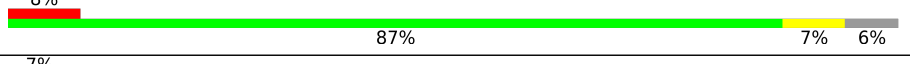

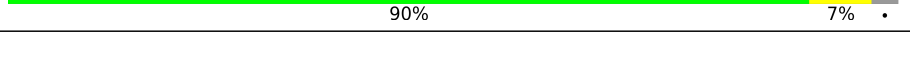
The reported resolution of this entry is 2.50 Å.

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))
R_{free}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (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 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	AAA	121	 5% 88% 12% .
1	BBB	121	 8% 87% 7% 6%
1	CCC	121	 7% 86% 12% ..
1	DDD	121	 2% 90% 7% .

2 Entry composition [i](#)

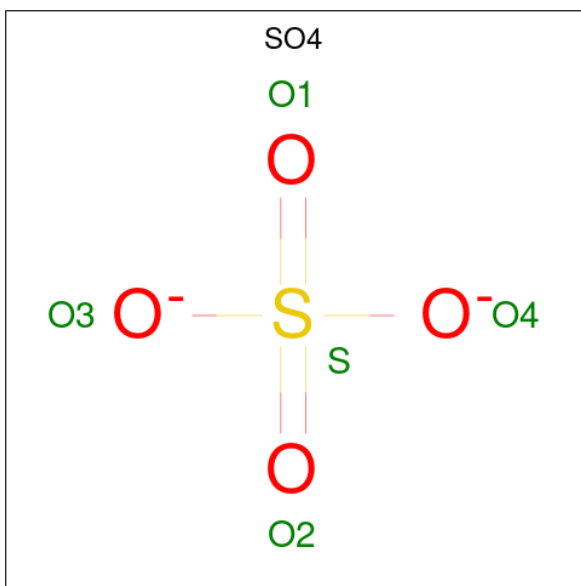
There are 4 unique types of molecules in this entry. The entry contains 3802 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 REM1.1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	N	O	S				Se
1	AAA	120	Total 951	C 595	N 166	O 185	S 1	Se 4	0	1	0
1	BBB	114	Total 900	C 561	N 160	O 175	S 4	Se	0	0	0
1	CCC	119	Total 938	C 587	N 165	O 181	S 1	Se 4	0	0	0
1	DDD	117	Total 919	C 573	N 163	O 179	S 4	Se	0	0	0

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
2	AAA	1	Total 5	O 4	S 1	0	0

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	BBB	1	Total C O 4 2 2	0	0
3	BBB	1	Total C O 4 2 2	0	0
3	CCC	1	Total C O 4 2 2	0	0

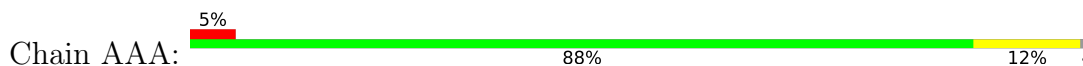
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	AAA	18	Total O 18 18	0	0
4	BBB	14	Total O 14 14	0	0
4	CCC	20	Total O 20 20	0	0
4	DDD	25	Total O 25 25	0	0

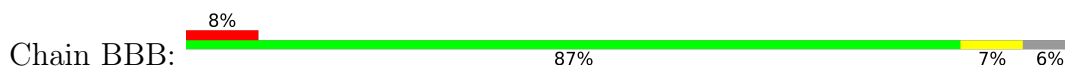
3 Residue-property plots [i](#)

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.

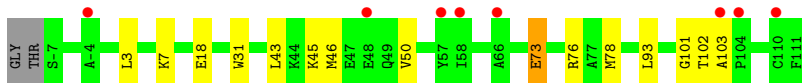
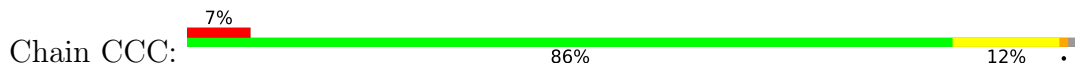
- Molecule 1: REM1.1



- Molecule 1: REM1.1



- Molecule 1: REM1.1



- Molecule 1: REM1.1



4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	26.55Å 99.13Å 128.70Å 90.00° 95.79° 90.00°	Depositor
Resolution (Å)	78.51 – 2.50 78.51 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.8 (78.51-2.50) 99.8 (78.51-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.49 (at 2.51Å)	Xtrriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.246 , 0.291 0.250 , 0.294	Depositor DCC
R_{free} test set	1102 reflections (2.46%)	wwPDB-VP
Wilson B-factor (Å ²)	49.5	Xtrriage
Anisotropy	0.984	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 42.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.086 for h,-k,-h-l	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3802	wwPDB-VP
Average B, all atoms (Å ²)	81.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.30% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: EDO, SO4

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	AAA	0.48	0/958	1.17	2/1262 (0.2%)
1	BBB	0.49	0/903	1.19	2/1189 (0.2%)
1	CCC	0.51	0/942	1.19	1/1240 (0.1%)
1	DDD	0.50	0/922	1.17	0/1215
All	All	0.50	0/3725	1.18	5/4906 (0.1%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	CCC	78	MSE	CG-SE-CE	5.78	111.64	98.92
1	AAA	46	MSE	CG-SE-CE	5.27	110.51	98.92
1	BBB	-5	MSE	CG-SE-CE	5.20	110.35	98.92
1	AAA	-5	MSE	CG-SE-CE	5.11	110.16	98.92
1	BBB	78	MSE	CG-SE-CE	5.08	110.10	98.92

There are no chirality outliers.

There are no planarity outliers.

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	AAA	951	0	1002	6	0
1	BBB	900	0	950	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	CCC	938	0	989	8	0
1	DDD	919	0	971	6	0
2	AAA	5	0	0	0	0
3	BBB	8	0	12	0	0
3	CCC	4	0	6	0	0
4	AAA	18	0	0	0	0
4	BBB	14	0	0	0	0
4	CCC	20	0	0	1	0
4	DDD	25	0	0	0	0
All	All	3802	0	3930	16	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 2.

The worst 5 of 16 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:AAA:18:GLU:OE1	1:BBB:83:ARG:NH2	2.32	0.62
1:CCC:46:MSE:HE2	1:CCC:50:VAL:HG11	1.82	0.60
1:CCC:101:GLY:HA2	1:DDD:2:ARG:CZ	2.34	0.57
1:BBB:43:LEU:O	1:BBB:47:GLU:HG2	2.10	0.52
1:CCC:103:ALA:HB2	1:DDD:2:ARG:HG3	1.92	0.52

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	AAA	119/121 (98%)	115 (97%)	4 (3%)	0	100 100
1	BBB	112/121 (93%)	111 (99%)	1 (1%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	CCC	117/121 (97%)	117 (100%)	0	0	100	100
1	DDD	115/121 (95%)	114 (99%)	1 (1%)	0	100	100
All	All	463/484 (96%)	457 (99%)	6 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	AAA	98/93 (105%)	94 (96%)	4 (4%)	27	53
1	BBB	92/93 (99%)	90 (98%)	2 (2%)	45	73
1	CCC	96/93 (103%)	90 (94%)	6 (6%)	16	34
1	DDD	94/93 (101%)	91 (97%)	3 (3%)	34	62
All	All	380/372 (102%)	365 (96%)	15 (4%)	28	55

5 of 15 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	CCC	7	LYS
1	DDD	44	LYS
1	CCC	45	LYS
1	DDD	82	LYS
1	CCC	102	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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](#)

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	$\# Z > 2$
3	EDO	BBB	201	-	3,3,3	0.10	0	2,2,2	0.34	0
2	SO4	AAA	201	-	4,4,4	0.37	0	6,6,6	0.09	0
3	EDO	BBB	202	-	3,3,3	0.09	0	2,2,2	0.28	0
3	EDO	CCC	201	-	3,3,3	0.09	0	2,2,2	0.29	0

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
3	EDO	BBB	201	-	-	1/1/1/1	-
3	EDO	BBB	202	-	-	1/1/1/1	-
3	EDO	CCC	201	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	BBB	202	EDO	O1-C1-C2-O2
3	CCC	201	EDO	O1-C1-C2-O2
3	BBB	201	EDO	O1-C1-C2-O2

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 [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	AAA	116/121 (95%)	0.57	6 (5%) 33 29	27, 74, 140, 152	1 (0%)
1	BBB	110/121 (90%)	0.60	10 (9%) 15 13	37, 73, 126, 152	0
1	CCC	115/121 (95%)	0.49	8 (6%) 22 20	39, 74, 133, 149	0
1	DDD	113/121 (93%)	0.34	2 (1%) 67 64	45, 73, 122, 141	0
All	All	454/484 (93%)	0.50	26 (5%) 29 26	27, 74, 133, 152	1 (0%)

The worst 5 of 26 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	DDD	107	LEU	6.8
1	CCC	104	PRO	5.8
1	CCC	110	CYS	5.0
1	CCC	103	ALA	3.2
1	BBB	17	ALA	3.0

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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	EDO	CCC	201	4/4	0.83	0.14	95,101,109,118	0
3	EDO	BBB	201	4/4	0.88	0.15	59,73,73,77	0
2	SO4	AAA	201	5/5	0.90	0.14	68,74,78,80	1
3	EDO	BBB	202	4/4	0.91	0.09	74,76,76,80	0

6.5 Other polymers [i](#)

There are no such residues in this entry.