



wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 5NW5 / pdb_00005nw5
Title : Crystal structure of the Rif1 N-terminal domain (RIF1-NTD) from *Saccharomyces cerevisiae* in complex with DNA
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Deposited on : 2017-05-05
Resolution : 6.50 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
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

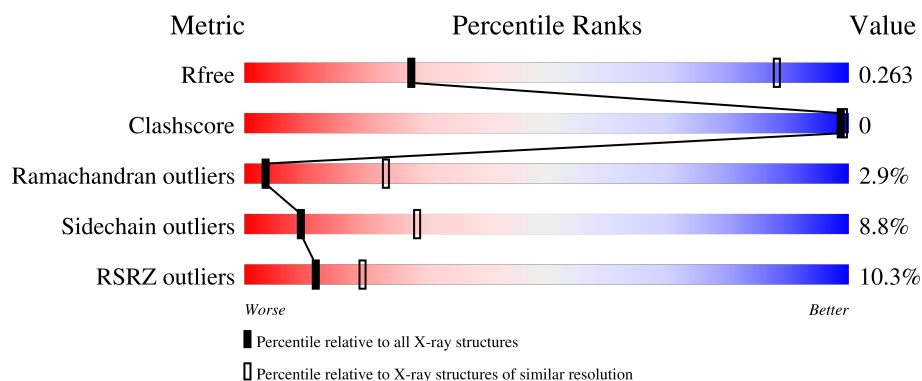
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 6.50 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	1162 (9.00-4.00)
Clashscore	190562	1020 (8.98-4.02)
Ramachandran outliers	187476	1050 (9.00-4.00)
Sidechain outliers	187428	1014 (9.00-4.00)
RSRZ outliers	180081	1155 (9.00-4.00)

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 $\leq 5\%$. 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	1226	10% 76% 11% • 12%
1	B	1226	8% 76% 11% • 12%
2	C	30	7% 67% 30% •
3	D	30	63% 30% 7%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 37748 atoms, of which 18886 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 Telomere length regulator protein RIF1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	1085	Total	C	H	N	O	S	0	0	0
			17916	5717	9096	1455	1614	34			
1	B	1085	Total	C	H	N	O	S	0	0	0
			17914	5717	9096	1453	1614	34			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	96	GLY	-	expression tag	UNP P29539
A	97	GLY	-	expression tag	UNP P29539
A	98	GLY	-	expression tag	UNP P29539
A	99	ARG	-	expression tag	UNP P29539
B	96	GLY	-	expression tag	UNP P29539
B	97	GLY	-	expression tag	UNP P29539
B	98	GLY	-	expression tag	UNP P29539
B	99	ARG	-	expression tag	UNP P29539

- Molecule 2 is a DNA chain called DNA (60-MER).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	C	30	Total	C	H	N	O	P	0	0	0
			959	300	332	150	148	29			

- Molecule 3 is a DNA chain called DNA (30-MER).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	D	30	Total	C	H	N	O	P	0	0	0
			959	300	362	60	208	29			

Chain B: 8% 76% 11% 5%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	92.14Å 169.80Å 390.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.23 – 6.50 43.23 – 6.50	Depositor EDS
% Data completeness (in resolution range)	70.2 (43.23-6.50) 69.9 (43.23-6.50)	Depositor EDS
R_{merge}	0.34	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.59 (at 6.66Å)	Xtriage
Refinement program	PHENIX (dev_2205: AMBER)	Depositor
R, R_{free}	0.253 , 0.277 0.259 , 0.263	Depositor DCC
R_{free} test set	622 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	388.4	Xtriage
Anisotropy	0.395	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 269.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.36$, $\langle L^2 \rangle = 0.19$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.82	EDS
Total number of atoms	37748	wwPDB-VP
Average B, all atoms (Å ²)	327.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.43% 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	0.88	0/8995	1.52	40/12178 (0.3%)
1	B	0.88	0/8993	1.52	51/12175 (0.4%)
2	C	0.73	0/716	1.53	1/1102 (0.1%)
3	D	0.80	0/656	1.62	3/1012 (0.3%)
All	All	0.87	0/19360	1.52	95/26467 (0.4%)

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	8
1	B	0	6
2	C	0	10
3	D	0	11
All	All	0	35

There are no bond length outliers.

The worst 5 of 95 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	455	ASP	CA-CB-CG	8.66	121.26	112.60
1	B	455	ASP	CA-CB-CG	7.81	120.41	112.60
1	A	454	LEU	CA-C-N	7.50	131.08	120.28
1	A	454	LEU	C-N-CA	7.50	131.08	120.28
1	B	454	LEU	CA-C-N	7.00	130.36	120.28

There are no chirality outliers.

5 of 35 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	196	TRP	Peptide
1	A	301	TYR	Sidechain
1	A	394	TYR	Sidechain
1	A	561	HIS	Sidechain
1	A	573	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	8820	9096	9094	13	0
1	B	8818	9096	9094	5	0
2	C	627	332	332	0	0
3	D	597	362	362	0	0
All	All	18862	18886	18882	18	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 0.

The worst 5 of 18 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:1224:ASN:H	1:A:1225:PRO:HD3	1.80	0.47
1:A:703:GLU:OE1	1:A:706:LYS:HE3	2.15	0.47
1:A:1111:PHE:CG	1:A:1139:LYS:HE3	2.50	0.46
1:A:584:SER:OG	1:A:586:LYS:HE2	2.17	0.44
1:A:650:THR:HB	1:A:651:PRO:HD3	2.00	0.44

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	1081/1226 (88%)	930 (86%)	120 (11%)	31 (3%)	3	23
1	B	1081/1226 (88%)	924 (86%)	125 (12%)	32 (3%)	3	22
All	All	2162/2452 (88%)	1854 (86%)	245 (11%)	63 (3%)	3	23

5 of 63 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	227	GLU
1	A	391	ASN
1	A	457	VAL
1	A	806	LYS
1	A	913	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	1020/1148 (89%)	931 (91%)	89 (9%)	9	29
1	B	1020/1148 (89%)	929 (91%)	91 (9%)	9	28
All	All	2040/2296 (89%)	1860 (91%)	180 (9%)	9	28

5 of 180 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	553	ASN
1	B	955	SER
1	B	596	SER
1	B	760	ASP
1	B	1038	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 43 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	716	GLN
1	B	945	ASN
1	B	741	ASN
1	B	817	GLN
1	B	1037	GLN

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	1085/1226 (88%)	0.73	128 (11%) 9 17	316, 316, 316, 316	0
1	B	1085/1226 (88%)	0.70	100 (9%) 14 22	316, 316, 316, 316	0
2	C	30/30 (100%)	0.92	2 (6%) 24 29	547, 547, 547, 547	0
3	D	30/30 (100%)	0.61	0 100 100	547, 547, 547, 547	0
All	All	2230/2512 (88%)	0.72	230 (10%) 12 19	316, 316, 316, 547	0

The worst 5 of 230 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	874	LEU	8.3
1	B	1234	ASN	7.3
1	B	1215	SER	5.6
1	B	212	GLU	5.2
1	B	1205	LEU	5.0

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.