



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 12, 2026 – 10:00 PM UTC

PDB ID : 1T4O / pdb_00001t4o
Title : Crystal structure of rnt1p dsRBD
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Deposited on : 2004-04-30
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
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

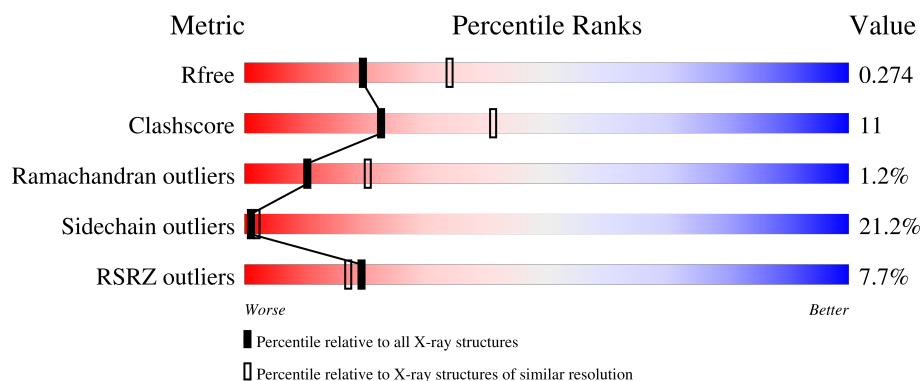
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	A	117	2% 32% 28% 9% 31%
1	B	117	9% 35% 31% 7% 25%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 1335 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 Ribonuclease III.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	81	Total	C	N	O	S	12	0	0
			624	393	114	114	3			
1	B	88	Total	C	N	O	S	23	0	0
			678	427	125	122	4			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	361	MET	-	initiating methionine	UNP Q02555
A	472	HIS	-	expression tag	UNP Q02555
A	473	HIS	-	expression tag	UNP Q02555
A	474	HIS	-	expression tag	UNP Q02555
A	475	HIS	-	expression tag	UNP Q02555
A	476	HIS	-	expression tag	UNP Q02555
A	477	HIS	-	expression tag	UNP Q02555
B	361	MET	-	initiating methionine	UNP Q02555
B	472	HIS	-	expression tag	UNP Q02555
B	473	HIS	-	expression tag	UNP Q02555
B	474	HIS	-	expression tag	UNP Q02555
B	475	HIS	-	expression tag	UNP Q02555
B	476	HIS	-	expression tag	UNP Q02555
B	477	HIS	-	expression tag	UNP Q02555

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	21	Total	O	0	0
			21	21		
2	B	12	Total	O	0	0
			12	12		

- Molecule 1: Ribonuclease III



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	73.81Å 68.31Å 57.18Å 90.00° 121.91° 90.00°	Depositor
Resolution (Å)	48.80 – 2.50 48.54 – 2.50	Depositor EDS
% Data completeness (in resolution range)	94.3 (48.80-2.50) 94.3 (48.54-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.99 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.198 , 0.276 0.209 , 0.274	Depositor DCC
R_{free} test set	779 reflections (9.81%)	wwPDB-VP
Wilson B-factor (Å ²)	45.9	Xtriage
Anisotropy	0.024	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 47.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	1335	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.17% 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	2.02	16/631 (2.5%)	1.82	10/848 (1.2%)
1	B	3.85	23/684 (3.4%)	3.22	23/916 (2.5%)
All	All	3.11	39/1315 (3.0%)	2.64	33/1764 (1.9%)

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	B	0	5

The worst 5 of 39 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	445	ARG	CZ-NH1	-56.77	0.53	1.32
1	B	433	ARG	CZ-NH1	41.97	1.91	1.32
1	B	361	MET	CB-CG	-31.30	0.58	1.52
1	B	436	LYS	CE-NZ	-28.10	0.65	1.49
1	B	363	THR	CB-OG1	-18.98	1.13	1.43

The worst 5 of 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	361	MET	CA-C-O	-49.63	36.42	120.80
1	B	433	ARG	NE-CZ-NH1	-39.78	81.72	121.50
1	B	433	ARG	NH1-CZ-NH2	-26.30	85.11	119.30
1	B	444	GLN	OE1-CD-NE2	-23.03	99.57	122.60
1	B	433	ARG	NE-CZ-NH2	-21.99	99.41	119.20

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	361	MET	Mainchain,Peptide
1	B	369	ASN	Sidechain
1	B	433	ARG	Sidechain
1	B	444	GLN	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	624	0	655	13	1
1	B	678	0	716	15	1
2	A	21	0	0	1	0
2	B	12	0	0	4	0
All	All	1335	0	1371	27	1

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 11.

The worst 5 of 27 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:384:ARG:HD3	2:B:12:HOH:O	1.54	1.08
1:B:398:PRO:HD2	2:B:20:HOH:O	1.63	0.96
1:A:391:LYS:NZ	1:A:399:ASN:O	2.02	0.92
1:B:406:VAL:C	1:B:407:GLY:CA	2.47	0.88
1:B:397:ASP:HB3	2:B:16:HOH:O	1.78	0.82

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:373:GLN:OE1	1:B:361:MET:N[4_546]	1.20	1.00

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	79/117 (68%)	74 (94%)	4 (5%)	1 (1%)	9	18
1	B	84/117 (72%)	74 (88%)	9 (11%)	1 (1%)	10	20
All	All	163/234 (70%)	148 (91%)	13 (8%)	2 (1%)	10	20

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	447	ALA
1	A	442	ALA

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	66/100 (66%)	53 (80%)	13 (20%)	1	2
1	B	71/100 (71%)	55 (78%)	16 (22%)	1	1
All	All	137/200 (68%)	108 (79%)	29 (21%)	1	2

5 of 29 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	362	LYS
1	B	445	ARG
1	B	384	ARG
1	B	421	LYS

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Mol	Chain	Res	Type
1	B	372	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	369	ASN
1	A	373	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	81/117 (69%)	0.15	2 (2%) 58 54	32, 47, 62, 71	6 (7%)
1	B	88/117 (75%)	0.75	11 (12%) 8 6	35, 52, 82, 87	14 (15%)
All	All	169/234 (72%)	0.46	13 (7%) 19 17	32, 50, 76, 87	20 (11%)

The worst 5 of 13 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	448	ILE	5.8
1	B	395	ALA	4.3
1	B	394	THR	4.1
1	B	396	VAL	2.9
1	B	435	LYS	2.7

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.