



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:19 PM GMT

PDB ID : 1T4O
Title : Crystal structure of rnt1p dsRBD
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Deposited on : 2004-04-30
Resolution : 2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

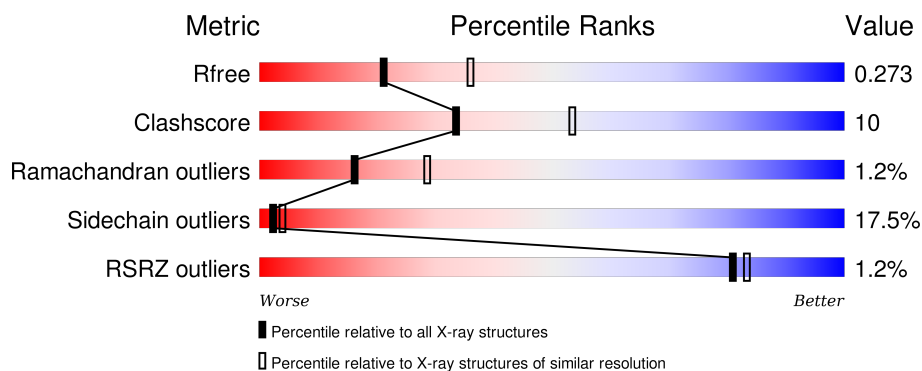
1 Overall quality at a glance

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}	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	 42% 19% 8% 2% 31%
1	B	117	 43% 21% 8% 2% 25%

2 Entry composition [i](#)

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

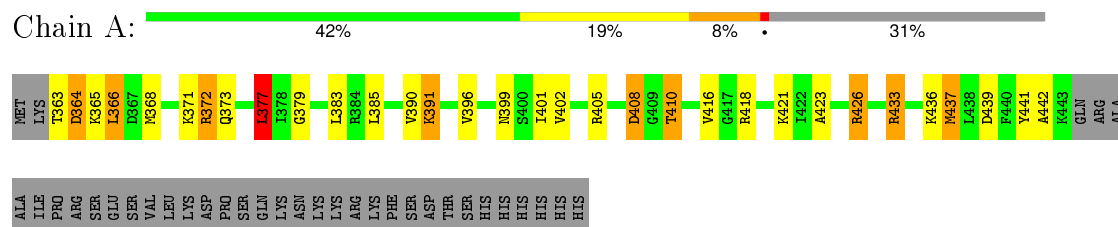
- Molecule 2 is water.

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

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: 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 , 0.273	Depositor DCC
R_{free} test set	779 reflections (10.87%)	DCC
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 , 49.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 7943 reflections (0.013%)	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, 0.375 respectively for untwinned datasets, and 0.333, 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	1.58	6/631 (1.0%)	1.94	12/848 (1.4%)
1	B	3.81	15/684 (2.2%)	4.05	33/916 (3.6%)
All	All	2.96	21/1315 (1.6%)	3.21	45/1764 (2.6%)

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	B	0	5

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	445	ARG	CZ-NH1	-61.37	0.53	1.33
1	B	433	ARG	CZ-NH1	44.97	1.91	1.33
1	B	436	LYS	CE-NZ	-33.60	0.65	1.49
1	B	361	MET	CB-CG	-29.00	0.58	1.51
1	B	363	THR	CB-OG1	-14.93	1.13	1.43
1	A	366	LEU	CG-CD2	-9.84	1.15	1.51
1	B	369	ASN	CG-OD1	-9.41	1.03	1.24
1	B	433	ARG	CZ-NH2	9.20	1.45	1.33
1	B	377	LEU	CG-CD1	-9.01	1.18	1.51
1	A	421	LYS	CE-NZ	8.57	1.70	1.49
1	B	443	LYS	CD-CE	-8.49	1.30	1.51
1	B	435	LYS	CG-CD	8.28	1.80	1.52
1	B	385	LEU	CG-CD2	-8.17	1.21	1.51
1	A	441	TYR	CE1-CZ	-7.18	1.29	1.38
1	B	435	LYS	CB-CG	-6.87	1.34	1.52
1	B	375	TYR	CD2-CE2	6.41	1.49	1.39
1	B	392	LYS	CG-CD	-5.67	1.33	1.52
1	A	437	MET	SD-CE	-5.29	1.48	1.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	433	ARG	CG-CD	5.21	1.65	1.51
1	A	436	LYS	CG-CD	-5.11	1.35	1.52
1	B	385	LEU	C-O	-5.07	1.13	1.23

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	433	ARG	NE-CZ-NH1	-77.17	81.72	120.30
1	B	433	ARG	NE-CZ-NH2	-41.79	99.41	120.30
1	B	361	MET	CA-C-O	-39.85	36.42	120.10
1	B	445	ARG	NE-CZ-NH1	36.03	138.31	120.30
1	B	433	ARG	NH1-CZ-NH2	-31.17	85.11	119.40
1	A	366	LEU	CB-CG-CD2	25.83	154.91	111.00
1	A	437	MET	CG-SD-CE	21.56	134.69	100.20
1	B	377	LEU	CB-CG-CD1	18.18	141.91	111.00
1	B	445	ARG	NH1-CZ-NH2	-15.86	101.96	119.40
1	B	385	LEU	CB-CG-CD2	15.21	136.85	111.00
1	B	436	LYS	CD-CE-NZ	-10.41	87.75	111.70
1	B	384	ARG	NE-CZ-NH2	-10.30	115.15	120.30
1	B	435	LYS	CB-CG-CD	10.03	137.67	111.60
1	B	426	ARG	NE-CZ-NH2	-9.88	115.36	120.30
1	B	444	GLN	OE1-CD-NE2	-9.71	99.57	121.90
1	A	426	ARG	NE-CZ-NH2	-9.57	115.52	120.30
1	A	439	ASP	CB-CG-OD2	9.51	126.86	118.30
1	B	384	ARG	NE-CZ-NH1	9.28	124.94	120.30
1	A	426	ARG	NE-CZ-NH1	9.27	124.94	120.30
1	B	369	ASN	OD1-CG-ND2	-9.05	101.08	121.90
1	B	434	ASP	CB-CG-OD2	8.91	126.32	118.30
1	A	364	ASP	CB-CG-OD2	8.85	126.27	118.30
1	A	366	LEU	CD1-CG-CD2	-8.74	84.27	110.50
1	A	368	MET	CG-SD-CE	8.71	114.14	100.20
1	B	361	MET	CA-C-N	-7.99	99.63	117.20
1	B	426	ARG	NE-CZ-NH1	7.98	124.29	120.30
1	B	445	ARG	NE-CZ-NH2	-6.84	116.88	120.30
1	A	421	LYS	CD-CE-NZ	6.82	127.39	111.70
1	A	408	ASP	CB-CG-OD2	6.75	124.37	118.30
1	B	397	ASP	CB-CG-OD2	6.71	124.34	118.30
1	B	372	ARG	NE-CZ-NH1	6.39	123.50	120.30
1	B	367	ASP	CB-CG-OD2	-6.30	112.63	118.30
1	B	435	LYS	CG-CD-CE	-6.28	93.05	111.90
1	B	420	ILE	CA-CB-CG2	6.18	123.26	110.90
1	B	361	MET	CB-CG-SD	6.10	130.69	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	435	LYS	CA-CB-CG	6.01	126.62	113.40
1	A	377	LEU	CA-CB-CG	5.99	129.07	115.30
1	B	369	ASN	CB-CG-OD1	5.92	133.44	121.60
1	B	364	ASP	CB-CG-OD2	5.79	123.52	118.30
1	B	377	LEU	CA-CB-CG	5.79	128.63	115.30
1	A	372	ARG	NE-CZ-NH1	5.55	123.08	120.30
1	B	385	LEU	CA-CB-CG	5.54	128.03	115.30
1	B	367	ASP	CB-CG-OD1	5.26	123.04	118.30
1	B	444	GLN	CG-CD-NE2	-5.09	104.49	116.70
1	B	392	LYS	CB-CG-CD	5.05	124.74	111.60

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	14	1
2	A	21	0	0	1	0
2	B	12	0	0	4	0
All	All	1335	0	1371	26	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 10.

All (26) 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	0.83
1:B:397:ASP:HB3	2:B:16:HOH:O	1.78	0.82
1:A:408:ASP:OD1	1:A:410:THR:HG22	1.91	0.70
1:A:379:GLY:O	1:B:384:ARG:NH2	2.26	0.68
1:A:408:ASP:OD1	1:A:408:ASP:C	2.33	0.64
1:B:398:PRO:CD	2:B:20:HOH:O	2.33	0.64
1:B:393:PRO:O	1:B:397:ASP:HB2	2.03	0.58
1:A:385:LEU:C	1:A:385:LEU:HD23	2.25	0.57
1:A:373:GLN:HE21	1:A:377:LEU:HD22	1.72	0.53
1:A:364:ASP:OD1	1:A:426:ARG:NH2	2.40	0.52
1:B:435:LYS:CB	1:B:435:LYS:CD	2.93	0.46
1:B:400:SER:O	1:B:416:VAL:HA	2.16	0.46
1:B:361:MET:HG3	1:B:362:LYS:N	2.31	0.45
1:A:371:LYS:CE	2:A:22:HOH:O	2.64	0.44
1:A:408:ASP:OD1	1:A:410:THR:CG2	2.63	0.44
1:B:402:VAL:HG11	1:B:424:GLY:HA2	2.00	0.44
1:B:374:LEU:O	1:B:375:TYR:C	2.54	0.43
1:B:361:MET:HG3	1:B:362:LYS:H	1.82	0.43
1:A:402:VAL:HG23	1:A:423:ALA:CB	2.49	0.41
1:A:390:VAL:HG11	1:A:405:ARG:HH21	1.84	0.41
1:A:401:ILE:HG12	1:A:416:VAL:HG22	2.02	0.41
1:B:440:PHE:CE2	1:B:444:GLN:CD	2.95	0.40
1:A:363:THR:HG23	1:A:363:THR:O	2.20	0.40

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%)	15	26
1	B	84/117 (72%)	74 (88%)	9 (11%)	1 (1%)	16	29
All	All	163/234 (70%)	148 (91%)	13 (8%)	2 (1%)	16	29

All (2) Ramachandran outliers are listed below:

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

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	66/100 (66%)	55 (83%)	11 (17%)	3	5
1	B	71/100 (71%)	58 (82%)	13 (18%)	2	3
All	All	137/200 (68%)	113 (82%)	24 (18%)	2	4

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	365	LYS
1	A	366	LEU
1	A	372	ARG
1	A	377	LEU
1	A	383	LEU
1	A	391	LYS
1	A	396	VAL
1	A	410	THR
1	A	418	ARG
1	A	433	ARG
1	A	437	MET

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Mol	Chain	Res	Type
1	B	361	MET
1	B	362	LYS
1	B	365	LYS
1	B	372	ARG
1	B	384	ARG
1	B	391	LYS
1	B	397	ASP
1	B	400	SER
1	B	418	ARG
1	B	421	LYS
1	B	432	LEU
1	B	434	ASP
1	B	445	ARG

Some 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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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%)	0.02	0	100 100	33, 48, 62, 71	6 (7%)
1	B	88/117 (75%)	0.26	2 (2%)	64 67	35, 56, 82, 87	14 (15%)
All	All	169/234 (72%)	0.14	2 (1%)	81 83	33, 52, 76, 87	20 (11%)

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	395	ALA	3.1
1	B	394	THR	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 carbohydrates 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.