WORLDWIDE wwPDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 21, 2024 – 03:37 PM EDT

PDB ID	:	2R7D
Title	:	Crystal structure of ribonuclease II family protein from Deinococcus radiodurans, triclinic crystal form. NorthEast Structural Genomics target DrR63
Authors	:	Seetharaman, J.; Neely, H.; Forouhar, F.; Wang, D.; Fang, Y.; Cunningham, K.; Ma, L.-C.; Xia, R.; Liu, J.; Baran, M.C.; Acton, T.B.; Rost, B.; Montelione, G.T.; Hunt, J.F.; Tong, L.; Northeast Structural Genomics Consortium (NESG)
Deposited on	:	2007-09-07
Resolution	:	1.80 Å(reported)

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

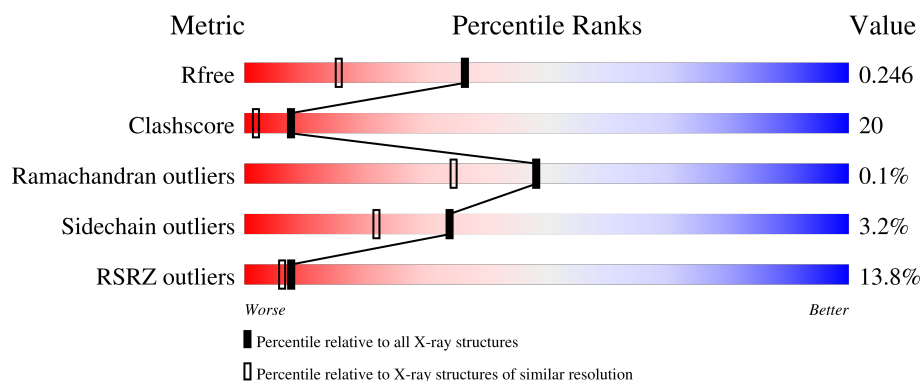|		
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)

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 1.80 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	Percentile Ranks	Value
Rfree		0.246
Clashscore		20
Ramachandran outliers		0.1%
Sidechain outliers		3.2%
RSRZ outliers		13.8%

Worse *Better*

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	164625	7108 (1.80-1.80)
Clashscore	180529	8162 (1.80-1.80)
Ramachandran outliers	177936	8077 (1.80-1.80)
Sidechain outliers	177891	8076 (1.80-1.80)
RSRZ outliers	164620	7108 (1.80-1.80)

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 <=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	469	5% — 71% 26% ••
1	B	469	22% — 64% 32% ••
1	C	469	13% — 70% 26% ••

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 11897 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 II family protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	461	Total	C	N	O	S	Se	0	0	0
			3562	2228	652	671	2	9			
1	B	459	Total	C	N	O	S	Se	0	0	0
			3545	2217	650	667	2	9			
1	C	459	Total	C	N	O	S	Se	0	0	0
			3545	2217	650	667	2	9			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	462	LEU	-	expression tag	UNP Q9RYD0
A	463	GLU	-	expression tag	UNP Q9RYD0
A	464	HIS	-	expression tag	UNP Q9RYD0
A	465	HIS	-	expression tag	UNP Q9RYD0
A	466	HIS	-	expression tag	UNP Q9RYD0
A	467	HIS	-	expression tag	UNP Q9RYD0
A	468	HIS	-	expression tag	UNP Q9RYD0
A	469	HIS	-	expression tag	UNP Q9RYD0
B	462	LEU	-	expression tag	UNP Q9RYD0
B	463	GLU	-	expression tag	UNP Q9RYD0
B	464	HIS	-	expression tag	UNP Q9RYD0
B	465	HIS	-	expression tag	UNP Q9RYD0
B	466	HIS	-	expression tag	UNP Q9RYD0
B	467	HIS	-	expression tag	UNP Q9RYD0
B	468	HIS	-	expression tag	UNP Q9RYD0
B	469	HIS	-	expression tag	UNP Q9RYD0
C	462	LEU	-	expression tag	UNP Q9RYD0
C	463	GLU	-	expression tag	UNP Q9RYD0
C	464	HIS	-	expression tag	UNP Q9RYD0
C	465	HIS	-	expression tag	UNP Q9RYD0
C	466	HIS	-	expression tag	UNP Q9RYD0
C	467	HIS	-	expression tag	UNP Q9RYD0
C	468	HIS	-	expression tag	UNP Q9RYD0

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Chain	Residue	Modelled	Actual	Comment	Reference
C	469	HIS	-	expression tag	UNP Q9RYD0

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total 1	Mg 1	0	0
2	B	1	Total 1	Mg 1	0	0
2	C	1	Total 1	Mg 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	536	Total 536	O 536	0	0
3	B	303	Total 303	O 303	0	0
3	C	403	Total 403	O 403	0	0

3 Residue-property plots ⓘ

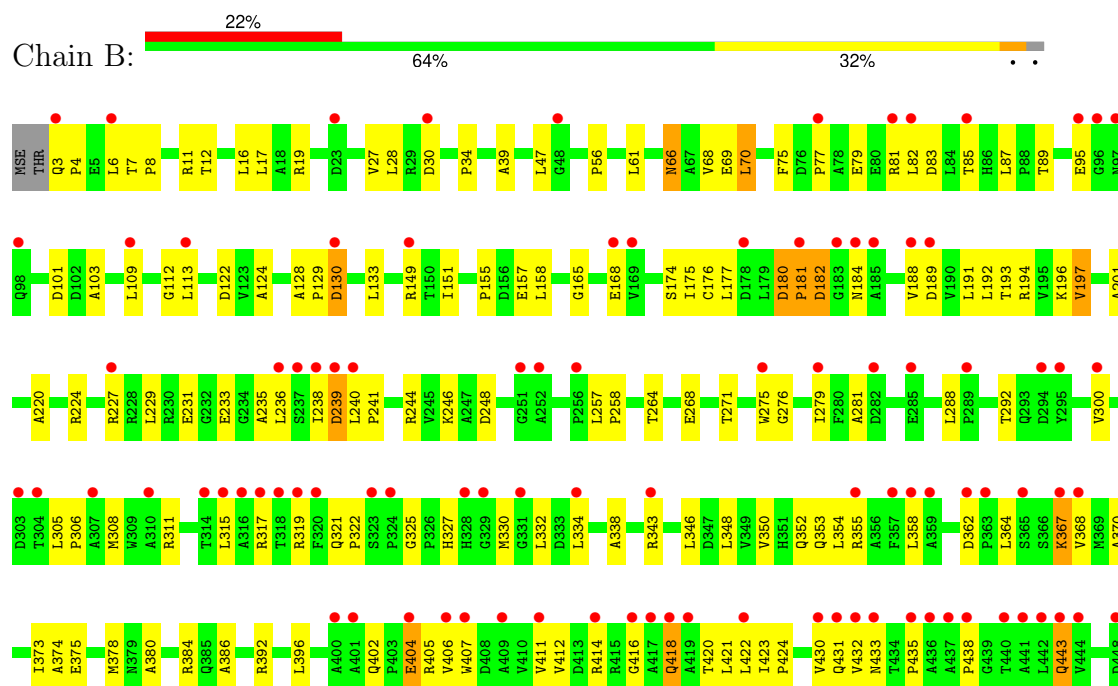These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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.

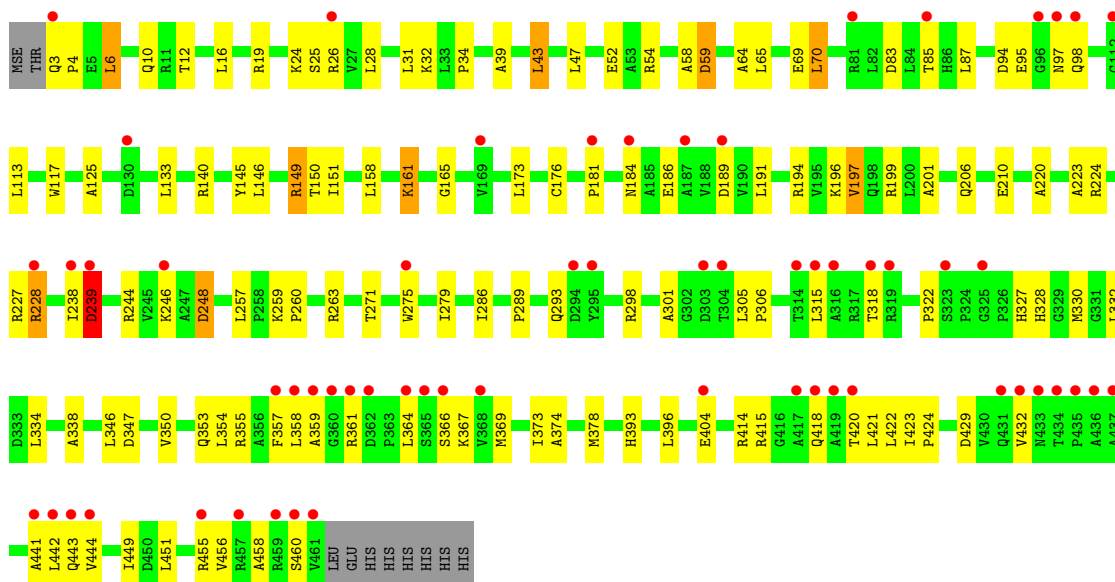- Molecule 1: Ribonuclease II family protein

Chain A:

- Molecule 1: Ribonuclease II family protein

Chain B:

I449 D450 Q453 M454 R455 V456 R457 A458 R459 S460 V461 LEU GLU HIS HIS HIS HIS HIS HIS

● Molecule 1: Ribonuclease II family protein

Chain C:

13%

70% 26%

MSE THR Q3 P4 E5 L6 Q10 R11 T12 L16 R19 K24 S25 R26 V27 L28 L31 K32 L33 P34 A39 L43 L47 E52 A53 R54 A58 D59 A64 L65 E69 L70 R81 L82 D83 L84 T85 H86 L87 D94 E95 G96 N97 Q98 G112

L113 W117 A125 D130 L133 R140 Y145 L146 R149 T150 I151 L158 K161 G165 V169 L173 C176 P181 N184 A185 E186 A187 V188 D189 V190 L191 R194 V195 K196 V197 Q198 R199 L200 A201 Q206 E210 A220 A223 R224

R227 R228 I238 D239 R244 V245 K246 A247 D248 L257 P258 K259 P260 R263 T271 W275 I279 I286 P289 Q293 D294 Y295 R298 A301 G302 D303 T304 L305 P306 T314 L315 A316 R317 T318 R319 P322 S323 P324 G325 P326 H327 H328 G329 M330 G331 L332

D333 L334 A338 L346 D347 V350 Q353 L354 R355 A356 F357 L358 A359 G360 R361 D362 P363 L364 S365 S366 K367 V368 M369 I373 A374 M378 H393 L396 E404 R414 R415 G416 A417 Q418 A419 T420 L421 L422 I423 P424 D429 V430 Q431 V432 N433 T434 P435 A436 A437

A441 L442 Q443 V444 I449 D450 L451 R455 V456 R457 A458 R459 S460 V461 LEU GLU HIS HIS HIS HIS HIS HIS

4   Data and refinement statistics   ⓘ

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	65.76Å 92.20Å 92.34Å 60.08° 89.57° 71.11°	Depositor
Resolution (Å)	36.68 – 1.80 36.68 – 1.80	Depositor EDS
% Data completeness (in resolution range)	80.7 (36.68-1.80) 91.9 (36.68-1.80)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	0.04	Depositor
$<I/\sigma(I)>$ [1]	1.74 (at 1.81Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.221 , 0.243 0.227 , 0.246	Depositor DCC
R_{free} test set	2691 reflections (1.80%)	wwPDB-VP
Wilson B-factor (Å^2)	23.4	Xtriage
Anisotropy	0.161	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 48.1	EDS
L-test for twinning[2]	$<|L|> = 0.49, <L^2> = 0.32$	Xtriage
Estimated twinning fraction	0.014 for h,h-k,-l 0.016 for -h,-k+l,l 0.008 for -h,-h+k-l,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	11897	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.47% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $<|L|>$, $<L^2>$ 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 ⓘ

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

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	0.33	0/3624	0.62	3/4927 (0.1%)
1	B	0.27	0/3607	0.58	6/4904 (0.1%)
1	C	0.30	0/3607	0.59	2/4904 (0.0%)
All	All	0.30	0/10838	0.60	11/14735 (0.1%)

There are no bond length outliers.

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	239	ASP	CB-CG-OD2	5.27	123.04	118.30
1	B	130	ASP	CB-CG-OD2	5.27	123.04	118.30
1	B	180	ASP	CB-CG-OD2	5.27	123.04	118.30
1	B	362	ASP	CB-CG-OD2	5.25	123.02	118.30
1	B	182	ASP	CB-CG-OD2	5.24	123.01	118.30

There are no chirality outliers.

There are no planarity outliers.

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	3562	0	3564	134	0
1	B	3545	0	3547	159	0
1	C	3545	0	3547	127	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
3	A	536	0	0	34	0
3	B	303	0	0	24	0
3	C	403	0	0	26	0
All	All	11897	0	10658	420	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 20.

The worst 5 of 420 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:C:328:HIS:HB3	3:C:3394:HOH:O	1.60	1.01
1:B:180:ASP:HB2	1:B:181:PRO:HD2	1.41	0.98
1:A:353:GLN:HE22	1:A:364:LEU:H	1.00	0.96
1:B:239:ASP:O	1:B:308:MSE:SE	2.39	0.91
1:A:375:GLU:HA	1:A:378:MSE:HE2	1.53	0.90

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	459/469 (98%)	450 (98%)	9 (2%)	0	100	100
1	B	457/469 (97%)	441 (96%)	15 (3%)	1 (0%)	44	31
1	C	457/469 (97%)	450 (98%)	6 (1%)	1 (0%)	44	31
All	All	1373/1407 (98%)	1341 (98%)	30 (2%)	2 (0%)	48	34

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	239	ASP
1	B	181	PRO

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	371/369 (100%)	357 (96%)	14 (4%)	28	16
1	B	369/369 (100%)	359 (97%)	10 (3%)	40	28
1	C	369/369 (100%)	357 (97%)	12 (3%)	33	21
All	All	1109/1107 (100%)	1073 (97%)	36 (3%)	34	22

5 of 36 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	149	ARG
1	C	404	GLU
1	C	161	LYS
1	C	239	ASP
1	A	404	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	66	ASN
1	C	184	ASN
1	C	443	GLN
1	C	353	GLN
1	C	98	GLN

5.3.3   RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	452/469 (96%)	0.25	23 (5%)	34	31	10, 24, 41, 58	0
1	B	450/469 (95%)	1.20	103 (22%)	2	2	15, 37, 59, 66	0
1	C	450/469 (95%)	0.70	61 (13%)	8	6	15, 30, 50, 59	0
All	All	1352/1407 (96%)	0.71	187 (13%)	8	6	10, 30, 53, 66	0

The worst 5 of 187 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	189	ASP	6.2
1	C	97	ASN	5.7
1	A	97	ASN	5.3
1	B	97	ASN	5.1
1	A	189	ASP	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 monosaccharides 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(Å^2)	Q<0.9
2	MG	B	2000	1/1	0.96	0.07	19,19,19,19	0
2	MG	C	3000	1/1	0.96	0.05	20,20,20,20	0
2	MG	A	1000	1/1	0.97	0.05	20,20,20,20	0

6.5 Other polymers (i)

There are no such residues in this entry.