



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 24, 2018 – 02:47 PM EDT

PDB ID : 2D3O
Title : Structure of Ribosome Binding Domain of the Trigger Factor on the 50S ribosomal subunit from *D. radiodurans*
Authors : Schlutzen, F.; Wilson, D.N.; Hansen, H.A.; Tian, P.; Harms, J.M.; McInnes, S.J.; Albrecht, R.; Buerger, J.; Wilbanks, S.M.; Fucini, P.
Deposited on : 2005-09-30
Resolution : 3.35 Å(reported)

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

MolProbity : 4.02b-467
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20031172

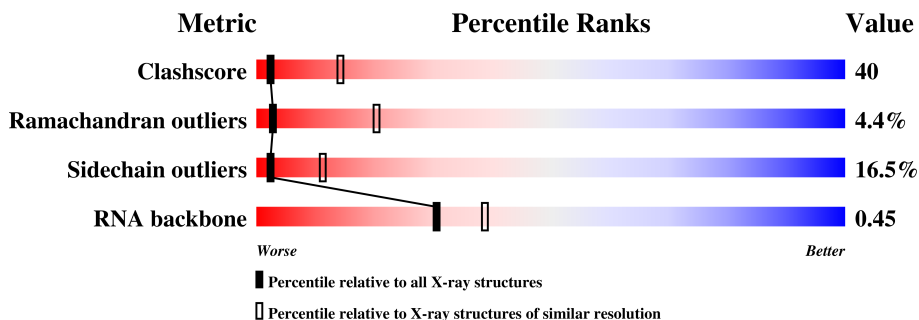
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.35 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))
Clashscore	122126	1380 (3.42-3.30)
Ramachandran outliers	120053	1359 (3.42-3.30)
Sidechain outliers	120020	1358 (3.42-3.30)
RNA backbone	2636	1001 (3.82-2.90)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	0	2880	
2	R	95	
3	S	115	
4	W	67	
5	1	112	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 63004 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 RNA chain called 23S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	0	2802	Total	C	N	O	P	0	0	0
			60132	26824	11089	19418	2801			

- Molecule 2 is a protein called 50S RIBOSOMAL PROTEIN L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	R	93	Total	C	N	O	S	0	0	0
			726	458	136	130	2			

- Molecule 3 is a protein called 50S RIBOSOMAL PROTEIN L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	S	110	Total	C	N	O	S	0	0	0
			825	513	160	151	1			

- Molecule 4 is a protein called 50S RIBOSOMAL PROTEIN L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	W	66	Total	C	N	O	S	0	0	0
			533	327	107	96	3			

- Molecule 5 is a protein called Trigger Factor.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	1	100	Total	C	N	O	0	0	0
			788	494	146	148			

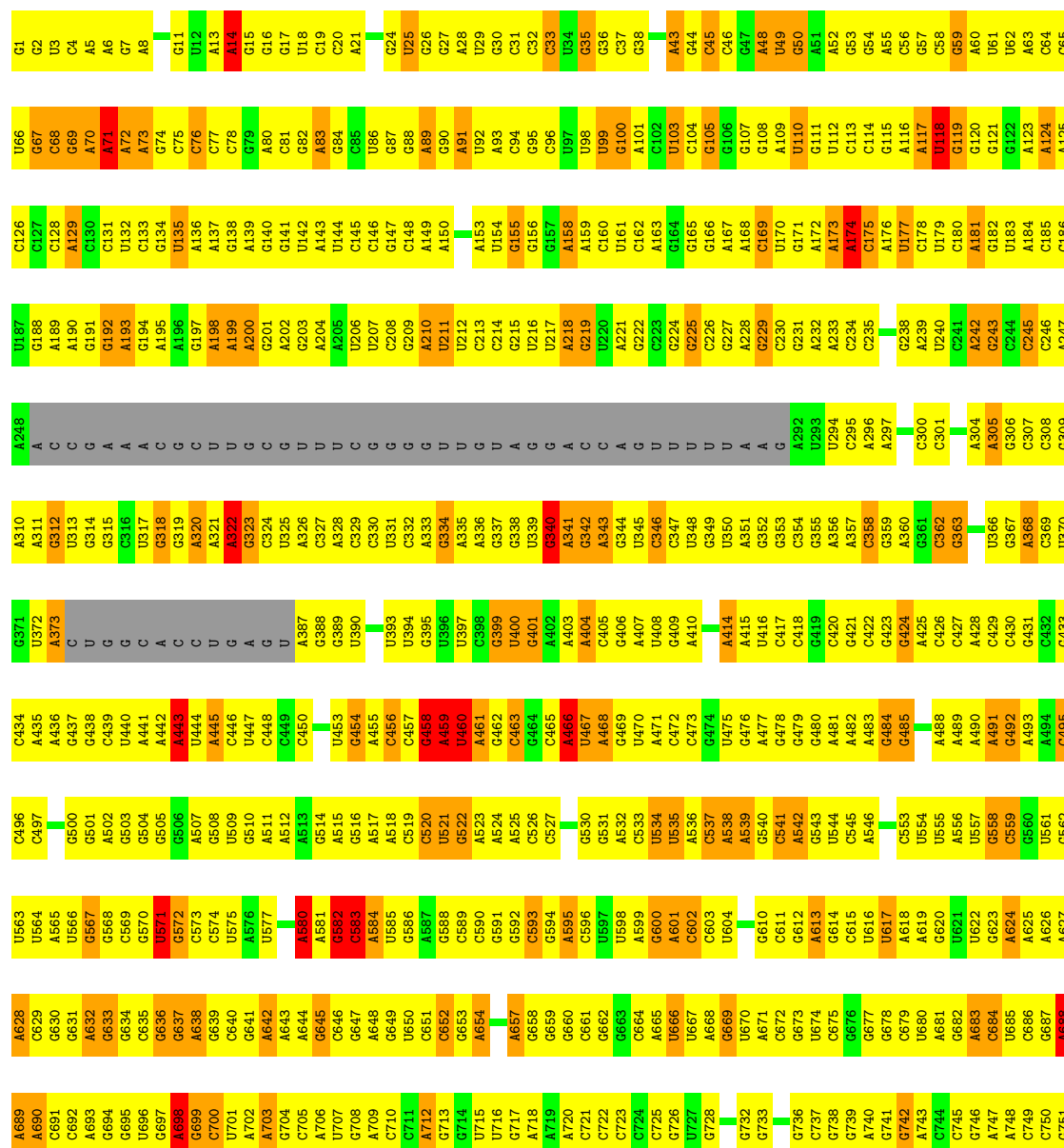
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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. 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. 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.

Note EDS was not executed.

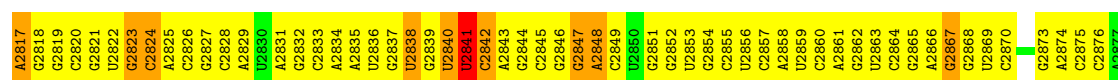
• Molecule 1: 23S RIBOSOMAL RNA

Chain 0: 

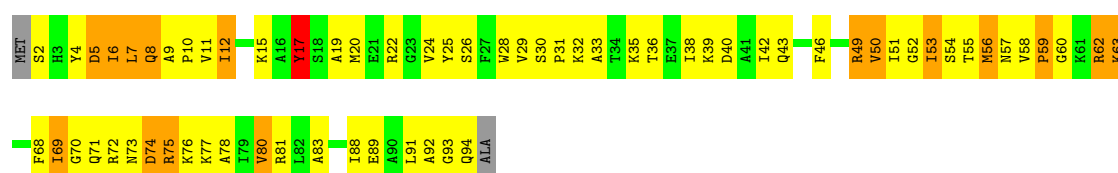


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C1653	A1583	C1517	C1456	A1395	G1331	A1259	C1198	G1136	G1070	C1003	G938	U816	C755
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C1724	A1586	C1520	U1459	G1398	A1334	U1262	G1201	A1139	G1073	C1006	U941	C819	G758
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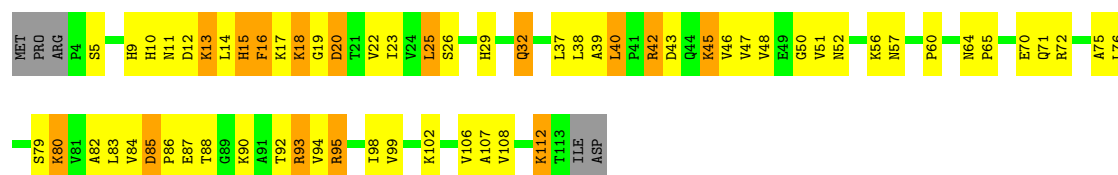
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G2810	U2749	G2687	G2619	G2555	G2494	C2431	A2371	A2306	C2179		A2097	A2031	G1968	C1835	
G2811	G2750	G2688	G2620	A2556	G2495	A2432	A2372	A2307	U2241		G2098	G2032	G1969	C1836	
G2812	C2751	G2689	G2621	G2557	A2496	C2433	C2373	A2308	C2242		A2181	C2033	G1970	A1910	
G2813	C2752	A2690	C2622	C2558	U2488	G2434	C2374	G2309			G2099	A2034	C1971	G1837	
G2814	G2753	C2691	A2623	G2559	U2489	G2435	C2375	G2310	A2245		A2100	G2035	G1972	G1838	
G2815	C2754	A2692	G2624	G2560	C2499	U2436	G2376	U2311	A2246			G2036	C1973	A1839	
C2816	A2755	U2693	U2625	G2561	U2501	G2437	U2377	G2313	A2247		U2105	C2037	U1974	A1840	
											G2106	C2038	G1975	G1841	



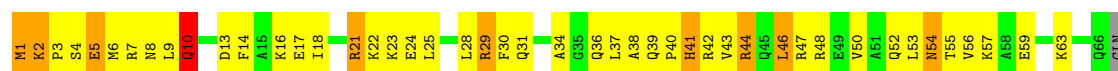
• Molecule 2: 50S RIBOSOMAL PROTEIN L23



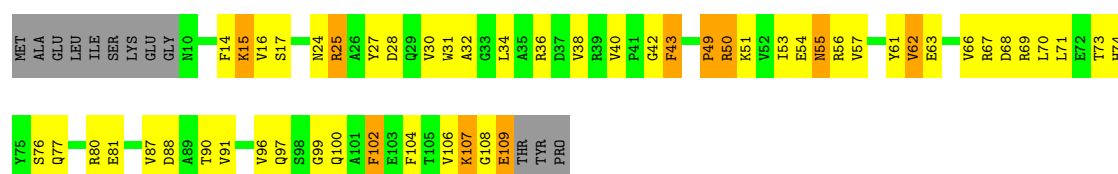
• Molecule 3: 50S RIBOSOMAL PROTEIN L24



• Molecule 4: 50S RIBOSOMAL PROTEIN L29



• Molecule 5: Trigger Factor



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	169.50Å 410.50Å 695.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.84 – 3.35	Depositor
% Data completeness (in resolution range)	(Not available) (29.84-3.35)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.299 , 0.322	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	63004	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0	0.67	3/67338 (0.0%)	0.82	72/105044 (0.1%)
2	R	0.48	0/737	0.80	0/988
3	S	0.42	0/835	0.73	1/1121 (0.1%)
4	W	0.44	0/537	0.58	0/714
5	1	0.48	0/802	0.68	0/1084
All	All	0.66	3/70249 (0.0%)	0.82	73/108951 (0.1%)

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	0	0	169
2	R	0	1
All	All	0	170

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	0	2776	U	C1'-N1	6.38	1.58	1.48
1	0	2775	U	C1'-N1	6.21	1.58	1.48
1	0	567	G	C5-C6	-5.13	1.37	1.42

The worst 5 of 73 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	2034	A	N9-C1'-C2'	10.22	127.28	114.00
1	0	1342	U	N1-C1'-C2'	9.78	126.71	114.00
1	0	1467	U	N1-C1'-C2'	8.63	125.23	114.00
1	0	2775	U	C2-N1-C1'	-8.26	107.78	117.70
1	0	1631	C	N1-C1'-C2'	8.21	124.68	114.00

There are no chirality outliers.

5 of 170 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	118	U	Sidechain
1	0	14	A	Sidechain
1	0	25	U	Sidechain
1	0	43	A	Sidechain
1	0	71	A	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	0	60132	0	30298	3519	0
2	R	726	0	753	126	0
3	S	825	0	881	117	0
4	W	533	0	558	81	0
5	1	788	0	784	74	0
All	All	63004	0	33274	3848	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 40.

The worst 5 of 3848 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)
2:R:69:ILE:CG2	2:R:70:GLY:H	1.26	1.38
1:0:1325:U:H1'	1:0:1619:A:N1	1.50	1.25
2:R:69:ILE:HG22	2:R:70:GLY:N	1.30	1.19
3:S:92:THR:HB	3:S:95:ARG:HH22	1.05	1.18
1:0:67:G:H21	1:0:72:A:H2'	1.09	1.16

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	
2	R	91/95 (96%)	70 (77%)	16 (18%)	5 (6%)	2	15
3	S	108/115 (94%)	79 (73%)	24 (22%)	5 (5%)	2	19
4	W	64/67 (96%)	54 (84%)	8 (12%)	2 (3%)	4	29
5	1	98/112 (88%)	81 (83%)	13 (13%)	4 (4%)	3	22
All	All	361/389 (93%)	284 (79%)	61 (17%)	16 (4%)	3	20

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	S	42	ARG
3	S	65	PRO
4	W	2	LYS
5	1	49	PRO
2	R	69	ILE

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	
2	R	75/76 (99%)	61 (81%)	14 (19%)	1	7
3	S	91/96 (95%)	77 (85%)	14 (15%)	3	13
4	W	54/55 (98%)	43 (80%)	11 (20%)	1	5
5	1	83/93 (89%)	72 (87%)	11 (13%)	4	18
All	All	303/320 (95%)	253 (84%)	50 (16%)	2	11

5 of 50 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	S	40	LEU
3	S	112	LYS
5	1	88	ASP
3	S	43	ASP
3	S	80	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
3	S	64	ASN
3	S	71	GLN
5	1	55	ASN
3	S	57	ASN
5	1	24	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2798/2880 (97%)	580 (20%)	88 (3%)

5 of 580 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	0	14	A
1	0	25	U
1	0	33	C
1	0	35	G
1	0	45	C

5 of 88 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	1342	U
1	0	1664	G
1	0	2660	C
1	0	1355	A
1	0	1626	A

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 [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

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.