



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 16, 2018 – 03:37 am GMT

PDB ID : 1C04
Title : IDENTIFICATION OF KNOWN PROTEIN AND RNA STRUCTURES IN A
5 A MAP OF THE LARGE RIBOSOMAL SUBUNIT FROM HALOARCUA
MARISMORTUI
Authors : Ban, N.; Nissen, P.; Capel, M.; Moore, P.B.; Steitz, T.A.
Deposited on : 1999-07-14
Resolution : 5.00 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 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) : trunk30686

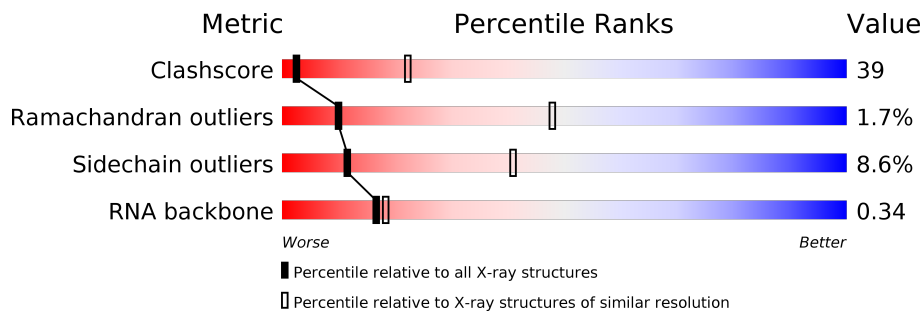
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 5.00 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	122078	1022 (6.20-3.80)
Ramachandran outliers	120005	1002 (6.22-3.76)
Sidechain outliers	119972	1124 (6.30-3.70)
RNA backbone	2633	1000 (7.04-2.92)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	E	58	 22% 50% 26%
2	F	29	 31% 55% 10%
3	A	137	 53% 35% 10%
4	B	177	 71% 20% 7%
5	C	67	 37% 48% 12%
6	D	122	 66% 31%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 5570 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 RRNA FRAGMENT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	58	Total	C	N	O	P	0	0	0
			1243	556	229	400	58			

- Molecule 2 is a RNA chain called 23S RRNA FRAGMENT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	29	Total	C	N	O	P	1	0	0
			621	278	118	197	28			

- Molecule 3 is a protein called RIBOSOMAL PROTEIN L2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	A	135	Total	C	N	O	S	Se	0	0	0
			1024	645	187	188	1	3			

- Molecule 4 is a protein called RIBOSOMAL PROTEIN L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	164	Total	C	N	O	S	0	0	0
			1251	787	225	237	2			

- Molecule 5 is a protein called RIBOSOMAL PROTEIN L11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	C	67	Total	C	N	O	S	0	0	0
			494	304	92	94	4			

- Molecule 6 is a protein called RIBOSOMAL PROTEIN L14.

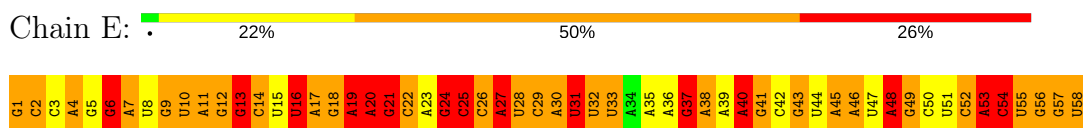
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	D	122	Total	C	N	O	S	0	0	0
			937	585	180	169	3			

3 Residue-property plots [i](#)

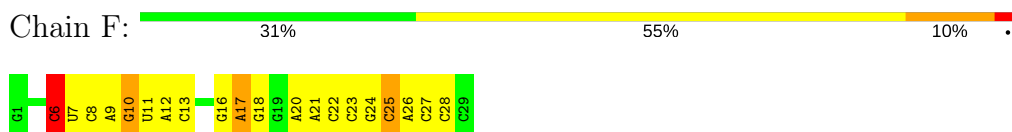
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

Note EDS was not executed.

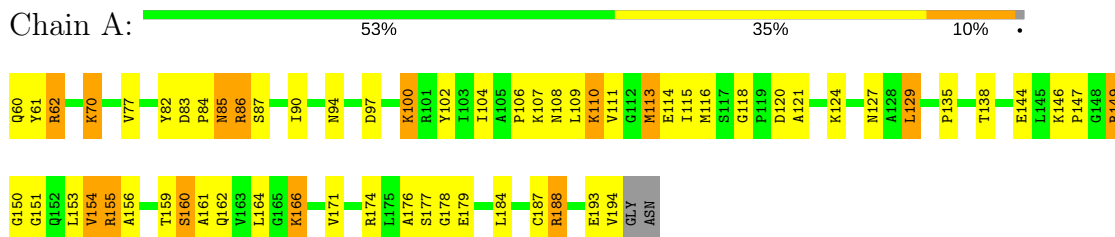
• Molecule 1: 23S RRNA FRAGMENT



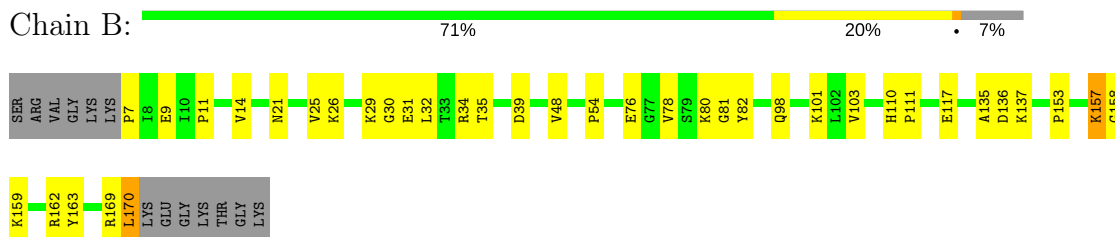
• Molecule 2: 23S RRNA FRAGMENT



• Molecule 3: RIBOSOMAL PROTEIN L2



• Molecule 4: RIBOSOMAL PROTEIN L6

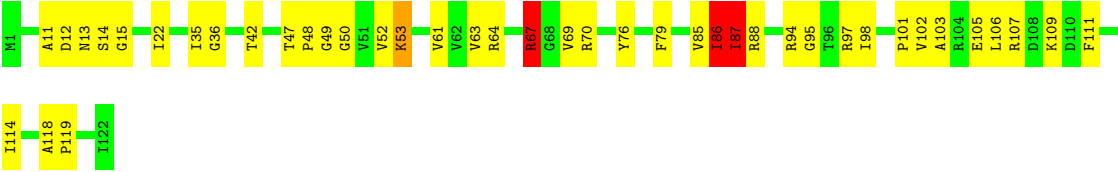


• Molecule 5: RIBOSOMAL PROTEIN L11





● Molecule 6: RIBOSOMAL PROTEIN L14



4 Data and refinement statistics

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

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	212.00Å 301.40Å 576.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	60.00 – 5.00	Depositor
% Data completeness (in resolution range)	(Not available) (60.00-5.00)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	(Not available) , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5570	wwPDB-VP
Average B, all atoms (Å ²)	38.0	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	E	2.12	42/1392 (3.0%)	2.79	125/2168 (5.8%)
2	F	0.81	0/695	0.91	3/1083 (0.3%)
3	A	0.48	0/1034	0.65	0/1388
4	B	0.63	0/1270	0.76	0/1715
5	C	0.56	0/497	0.86	2/663 (0.3%)
6	D	0.86	2/946 (0.2%)	1.18	7/1269 (0.6%)
All	All	1.19	44/5834 (0.8%)	1.61	137/8286 (1.7%)

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	E	0	4
6	D	0	1
All	All	0	5

The worst 5 of 44 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	86	ILE	C-N	-16.95	0.95	1.34
6	D	87	ILE	C-N	14.60	1.67	1.34
1	E	46	A	C5-C6	-8.99	1.32	1.41
1	E	29	C	C2-N3	-8.27	1.29	1.35
1	E	50	C	C4'-C3'	-8.06	1.44	1.53

The worst 5 of 137 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	53	A	O5'-P-OP2	-38.72	64.23	110.70
1	E	58	U	O5'-P-OP2	-26.48	78.93	110.70
1	E	20	A	N9-C1'-C2'	-19.63	88.48	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	86	ILE	O-C-N	-15.55	97.81	122.70
1	E	47	U	C4'-C3'-C2'	-15.18	87.42	102.60

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	D	86	ILE	Mainchain
1	E	19	A	Sidechain
1	E	37	G	Sidechain
1	E	45	A	Sidechain
1	E	48	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	E	1243	0	625	127	0
2	F	621	0	318	32	0
3	A	1024	0	1073	47	0
4	B	1251	0	1294	55	0
5	C	494	0	524	126	0
6	D	937	0	995	114	31
All	All	5570	0	4829	404	31

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 39.

The worst 5 of 404 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)
6:D:79:PHE:CZ	6:D:103:ALA:HB2	1.33	1.58
6:D:79:PHE:CZ	6:D:103:ALA:CB	1.87	1.57
6:D:63:VAL:CB	6:D:106:LEU:HD21	1.34	1.55
6:D:63:VAL:HG12	6:D:106:LEU:CD2	1.38	1.51
1:E:31:U:C5'	5:C:53:ALA:HA	1.23	1.49

The worst 5 of 31 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)
6:D:15:GLY:CA	6:D:48:PRO:CG[3_655]	0.17	2.03
6:D:49:GLY:CA	6:D:52:VAL:O[3_655]	0.35	1.85
6:D:47:THR:CB	6:D:47:THR:CB[3_655]	0.69	1.51
6:D:47:THR:CA	6:D:47:THR:OG1[3_655]	0.70	1.50
6:D:47:THR:CA	6:D:47:THR:CB[3_655]	0.96	1.24

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	
3	A	133/137 (97%)	124 (93%)	7 (5%)	2 (2%)	11	50
4	B	159/177 (90%)	156 (98%)	3 (2%)	0	100	100
5	C	65/67 (97%)	49 (75%)	12 (18%)	4 (6%)	1	21
6	D	120/122 (98%)	114 (95%)	4 (3%)	2 (2%)	10	48
All	All	477/503 (95%)	443 (93%)	26 (6%)	8 (2%)	10	48

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	C	26	GLU
6	D	87	ILE
5	C	24	SER
5	C	32	VAL
6	D	86	ILE

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	
3	A	107/105 (102%)	87 (81%)	20 (19%)	1	11
4	B	137/147 (93%)	132 (96%)	5 (4%)	38	66
5	C	51/51 (100%)	44 (86%)	7 (14%)	4	22
6	D	101/101 (100%)	99 (98%)	2 (2%)	58	79
All	All	396/404 (98%)	362 (91%)	34 (9%)	11	41

5 of 34 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	155	ARG
3	A	188	ARG
5	C	61	ARG
3	A	166	LYS
3	A	110	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
3	A	108	ASN
6	D	56	GLN
3	A	127	ASN
3	A	94	ASN
4	B	146	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	E	57/58 (98%)	18 (31%)	2 (3%)
2	F	28/29 (96%)	5 (17%)	0
All	All	85/87 (97%)	23 (27%)	2 (2%)

5 of 23 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	E	6	G
1	E	7	A
1	E	13	G

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Mol	Chain	Res	Type
1	E	16	U
1	E	19	A

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	E	20	A
1	E	53	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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
4	B	2
6	D	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	81:GLY	C	82:TYR	N	2.53
1	B	80:LYS	C	81:GLY	N	2.18

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	87:ILE	C	88:ARG	N	1.67
1	D	86:ILE	C	87:ILE	N	0.95

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.