wwPDB X-ray Structure Validation Summary Report (i)

Oct 20, 2024 – 11:04 AM EDT

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

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	Percentile Ranks	Value
Clashscore		39
Ramachandran outliers		1.7%
Sidechain outliers		8.6%
RNA backbone		0.34

Worse   *Better*

■ Percentile relative to all X-ray structures

❚ Percentile relative to X-ray structures of similar resolution
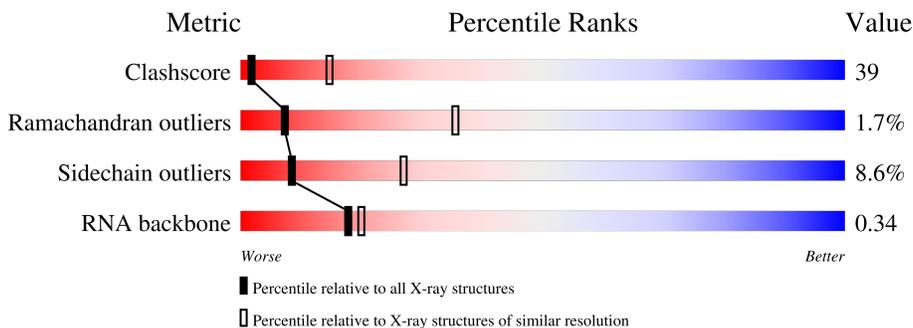
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	180529	1031 (6.04-3.96)
Ramachandran outliers	177936	1102 (6.10-3.90)
Sidechain outliers	177891	1081 (6.10-3.90)
RNA backbone	3690	1166 (7.00-3.00)

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%

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 ⓘ

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 1243	C 556	N 229	O 400	P 58	0	0	0

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

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

- Molecule 3 is a protein called RIBOSOMAL PROTEIN L2.

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

- Molecule 4 is a protein called RIBOSOMAL PROTEIN L6.

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

- Molecule 5 is a protein called RIBOSOMAL PROTEIN L11.

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

- Molecule 6 is a protein called RIBOSOMAL PROTEIN L14.

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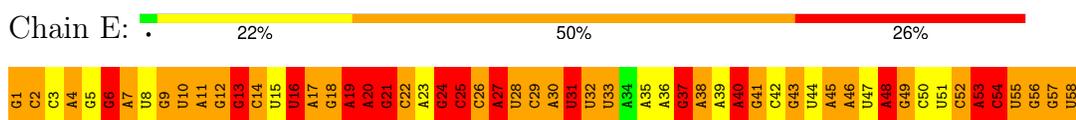
Chain E:

- Molecule 2: 23S RRNA FRAGMENT
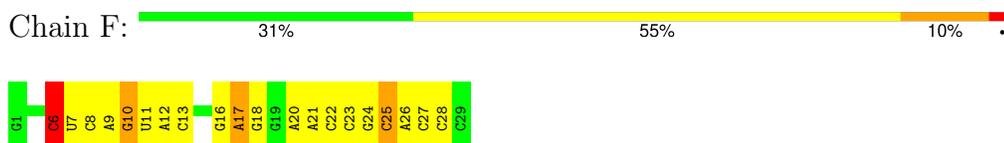
Chain F:

- Molecule 3: RIBOSOMAL PROTEIN L2
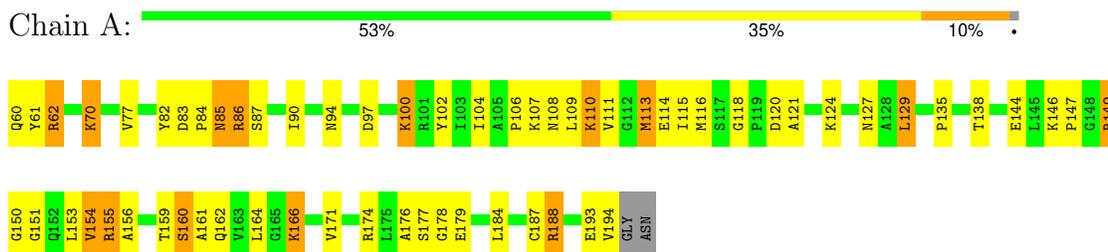
Chain A:

- Molecule 4: RIBOSOMAL PROTEIN L6
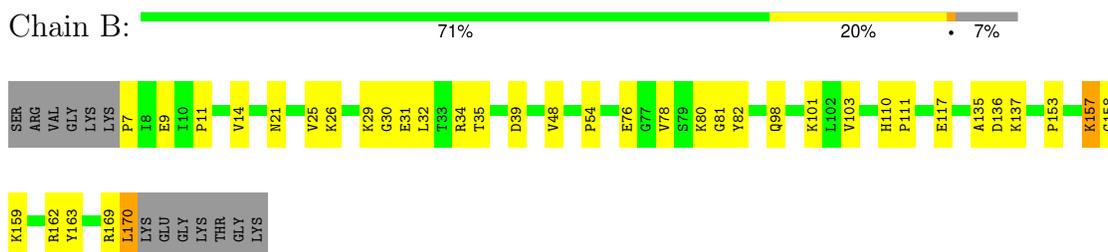
Chain B:

- Molecule 5: RIBOSOMAL PROTEIN L11

Chain C:

K6 T7 P8 P9 A10 A11 V12 L13 L14 K15 A18 G19 I20 E21 S22 G23 S24 G25 E26 P27 N28 R29 N30 K31 V32 I35 K36 R37 D38 K39 V40 R41 E42 I43 A44 E45 L46 K47 D50 L51 N52 A53 A54 S55 I56 E57 M60 R61 M62 I63 E64 S69 M70 G71 I72

• **Molecule 6: RIBOSOMAL PROTEIN L14**

Chain D:

66% 31% • •

M1 A11 D12 N13 S14 G15 I22 I35 G36 T42 T47 P48 G49 G50 V51 V52 K53 V61 V62 V63 R64 R67 G68 V69 R70 Y76 F79 V85 I86 I87 R88 R94 G95 T96 R97 I98 P101 V102 A103 R104 E105 L106 R107 D108 K109 D110 F111

I114 A118 P119 I122
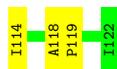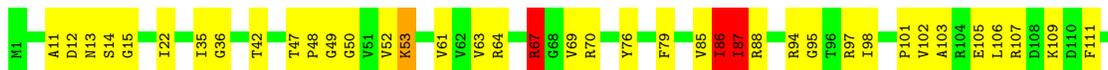
4 Data and refinement statistics (i)

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 ⓘ

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	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 ⓘ

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	
3	A	133/137 (97%)	124 (93%)	7 (5%)	2 (2%)	8	39
4	B	159/177 (90%)	156 (98%)	3 (2%)	0	100	100
5	C	65/67 (97%)	49 (75%)	12 (18%)	4 (6%)	1	13
6	D	120/122 (98%)	114 (95%)	4 (3%)	2 (2%)	7	35
All	All	477/503 (95%)	443 (93%)	26 (6%)	8 (2%)	7	35

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 ⓘ

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	7
4	B	137/147 (93%)	132 (96%)	5 (4%)	30	51
5	C	51/51 (100%)	44 (86%)	7 (14%)	3	14
6	D	101/101 (100%)	99 (98%)	2 (2%)	50	68
All	All	396/404 (98%)	362 (91%)	34 (9%)	8	27

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

Mol	Chain	Res	Type
5	C	32	VAL
5	C	38	ASP
6	D	53	LYS
3	A	127	ASN
3	A	124	LYS

Sometimes 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	127	ASN
4	B	146	ASN
6	D	56	GLN
3	A	94	ASN
3	A	85	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 ⓘ

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 ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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.