



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 11:24 PM UTC

PDB ID : 1FFK / pdb_00001ffk
Title : CRYSTAL STRUCTURE OF THE LARGE RIBOSOMAL SUBUNIT FROM HALOARCUA MARISMORTUI AT 2.4 ANGSTROM RESOLUTION
Authors : Ban, N.; Nissen, P.; Hansen, J.; Moore, P.B.; Steitz, T.A.
Deposited on : 2000-07-25
Resolution : 2.40 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Xtrriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

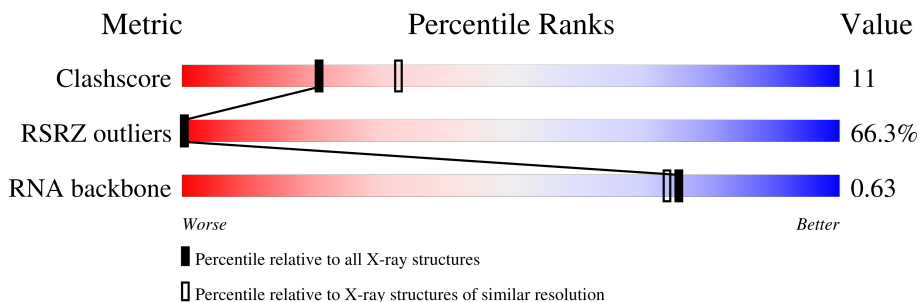
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	190562	5391 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)
RNA backbone	3983	1155 (2.70-2.10)

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 $\leq 5\%$. 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	0	2922	
2	9	122	
3	A	239	
4	B	337	
5	C	246	
6	D	176	
7	E	119	
8	F	157	

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Mol	Chain	Length	Quality of chain
9	G	145	98% 98%
10	H	132	100% 99%
11	I	194	100% 100%
12	J	164	87% 87% 13%
13	K	186	100% 100%
14	L	115	100% 100%
15	M	148	96% 97%
16	N	95	100% 100%
17	O	154	97% 97%
18	P	84	93% 93% 7%
19	Q	119	100% 100%
20	R	66	80% 80% 20%
21	S	70	93% 93% 7%
22	T	154	100% 100%
23	U	91	93% 92% 7%
24	V	143	99% 99%
25	W	73	100% 100%
26	X	56	100% 100%
27	Y	49	63% 63% 37%
28	Z	92	100% 100%
29	1	177	97% 97%

2 Entry composition [i](#)

There are 33 unique types of molecules in this entry. The entry contains 64281 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	0	2706	58012	25885	10685	18737	2705	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
0	560	C	U	conflict	GB 3377779

- Molecule 2 is a RNA chain called 5S RRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	9	122	2600	1160	472	847	121	0	0	0

- Molecule 3 is a protein called RIBOSOMAL PROTEIN L2.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
3	A	237	Total 237	C 237	0	0	237

- Molecule 4 is a protein called RIBOSOMAL PROTEIN L3.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
4	B	337	Total 337	C 337	0	0	337

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	GLU	deletion	UNP P20279
B	311	PHE	-	insertion	UNP P20279

- Molecule 5 is a protein called RIBOSOMAL PROTEIN L4.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
5	C	246	Total C 246 246	0	0	246

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	73	LEU	GLN	conflict	UNP P12735

- Molecule 6 is a protein called RIBOSOMAL PROTEIN L5.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
6	D	140	Total C 140 140	0	0	140

- Molecule 7 is a protein called RIBOSOMAL PROTEIN L7AE.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
7	E	118	Total C 118 118	0	0	118

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	108	LEU	-	insertion	UNP P12743
E	109	GLU	-	insertion	UNP P12743
E	110	GLU	-	insertion	UNP P12743

- Molecule 8 is a protein called RIBOSOMAL PROTEIN L10E.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
8	F	157	Total C 157 157	0	0	157

- Molecule 9 is a protein called RIBOSOMAL PROTEIN L13.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
9	G	142	Total C 142 142	0	0	142

- Molecule 10 is a protein called RIBOSOMAL PROTEIN L14.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
10	H	132	Total C 132 132	0	0	132

- Molecule 11 is a protein called RIBOSOMAL PROTEIN L15E.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
11	I	194	Total C 194 194	0	0	194

- Molecule 12 is a protein called RIBOSOMAL PROTEIN L15.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
12	J	143	Total C 143 143	0	0	143

- Molecule 13 is a protein called RIBOSOMAL PROTEIN L18.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
13	K	186	Total C 186 186	0	0	186

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	186	LEU	-	insertion	UNP P14123

- Molecule 14 is a protein called RIBOSOMAL PROTEIN L18E.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
14	L	115	Total C 115 115	0	0	115

- Molecule 15 is a protein called RIBOSOMAL PROTEIN L19.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
15	M	143	Total C 143 143	0	0	143

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	71	LYS	TYR	conflict	UNP P14119

- Molecule 16 is a protein called RIBOSOMAL PROTEIN L21E.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
16	N	95	Total C 95 95	0	0	95

- Molecule 17 is a protein called RIBOSOMAL PROTEIN L22.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
17	O	150	Total C 150 150	0	0	150

- Molecule 18 is a protein called RIBOSOMAL PROTEIN L23.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
18	P	78	Total C 78 78	0	0	78

- Molecule 19 is a protein called RIBOSOMAL PROTEIN L24.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
19	Q	119	Total C 119 119	0	0	119

- Molecule 20 is a protein called RIBOSOMAL PROTEIN L24E.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
20	R	53	Total C 53 53	0	0	53

- Molecule 21 is a protein called RIBOSOMAL PROTEIN L29.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
21	S	65	Total C 65 65	0	0	65

- Molecule 22 is a protein called RIBOSOMAL PROTEIN L30.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
22	T	154	Total C 154 154	0	0	154

- Molecule 23 is a protein called RIBOSOMAL PROTEIN L31E.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
23	U	85	Total C 85 85	0	0	85

- Molecule 24 is a protein called RIBOSOMAL PROTEIN L32E.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
24	V	143	Total C 143 143	0	0	143

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
V	109	ASN	ALA	conflict	UNP P12736

- Molecule 25 is a protein called RIBOSOMAL PROTEIN L37AE.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
25	W	73	Total C 73 73	0	0	73

- Molecule 26 is a protein called RIBOSOMAL PROTEIN L37E.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
26	X	56	Total C 56 56	0	0	56

- Molecule 27 is a protein called RIBOSOMAL PROTEIN L39E.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
27	Y	31	Total C 31 31	0	0	31

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Y	11	LYS	LEU	conflict	UNP P22452
Y	24	TYR	TRP	conflict	UNP P22452
Y	42	TRP	TYR	conflict	UNP P22452

- Molecule 28 is a protein called RIBOSOMAL PROTEIN L44E.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
28	Z	92	Total C 92 92	0	0	92

- Molecule 29 is a protein called RIBOSOMAL PROTEIN L6.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
29	1	172	Total C 172 172	0	0	172

- Molecule 30 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
30	0	1	Total K 1 1	0	0

- Molecule 31 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
31	0	2	Total Mg 2 2	0	0

- Molecule 32 is CADMIUM ION (CCD ID: CD) (formula: Cd).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	R	1	Total Cd 1 1	0	0
32	W	1	Total Cd 1 1	0	0
32	X	1	Total Cd 1 1	0	0
32	Z	1	Total Cd 1 1	0	0

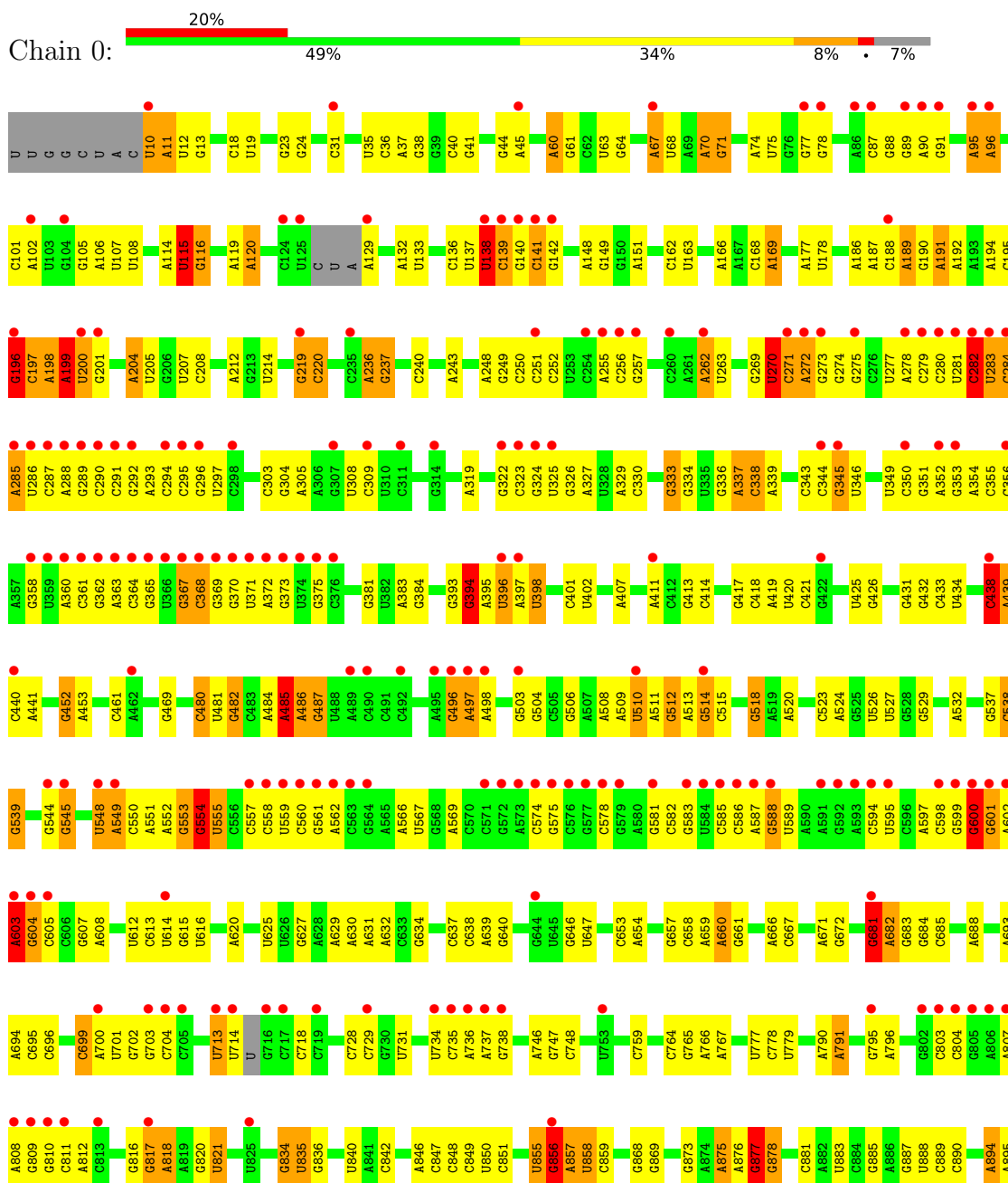
- Molecule 33 is water.

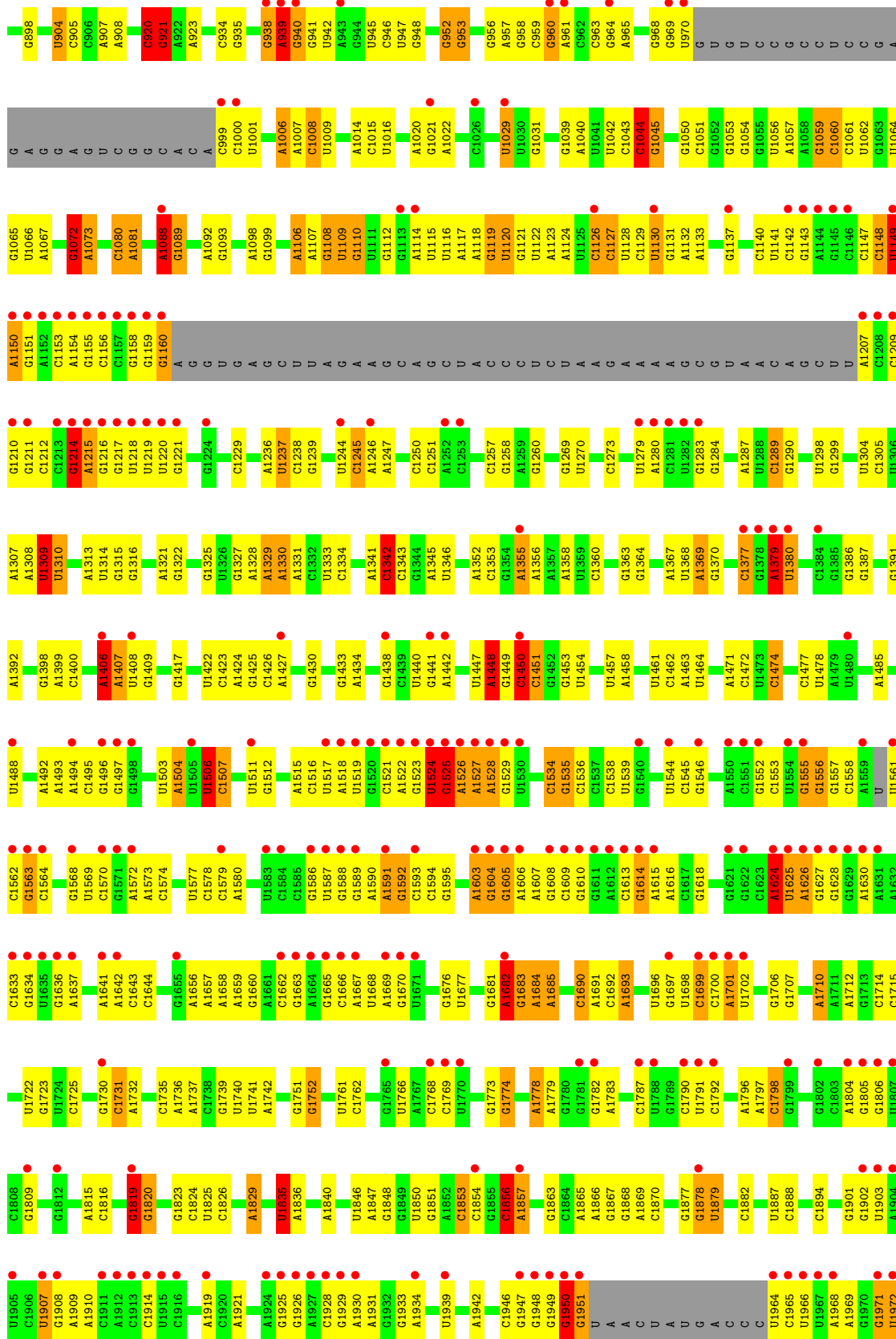
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	0	6	Total O 6 6	0	0

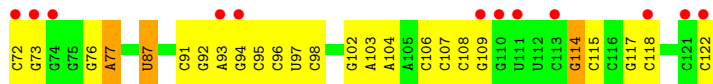
3 Residue-property plots

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.

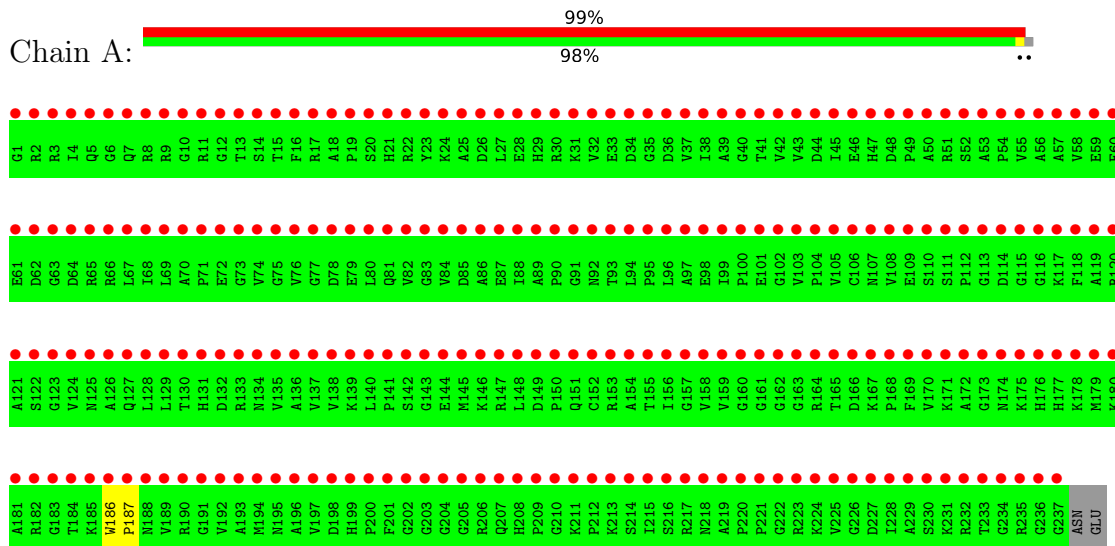
• Molecule 1: 23S RRNA



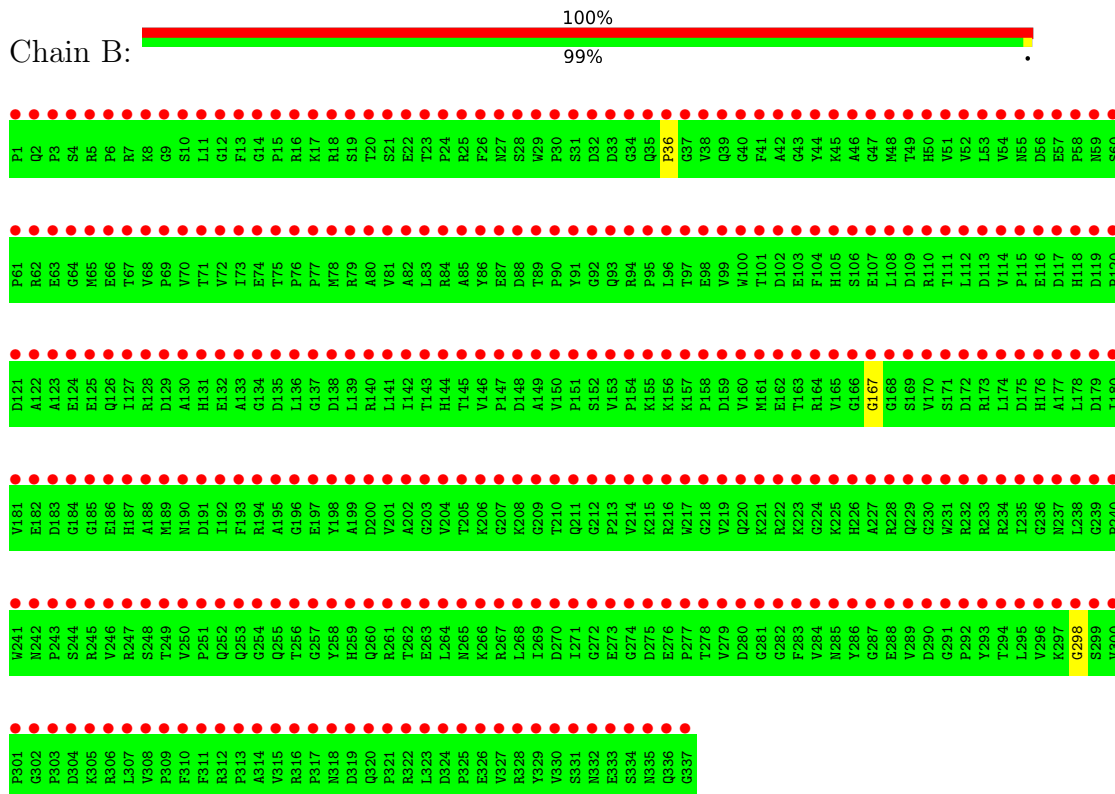




• Molecule 3: RIBOSOMAL PROTEIN L2

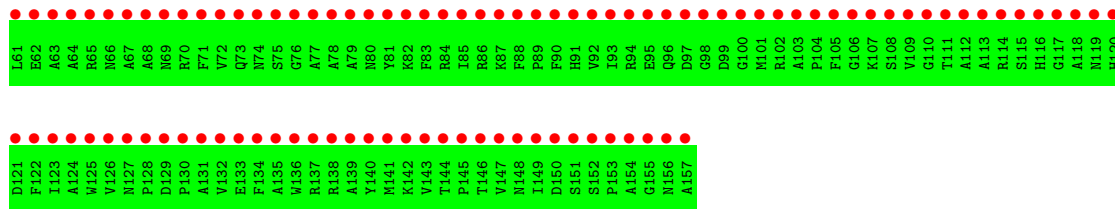


• Molecule 4: RIBOSOMAL PROTEIN L3

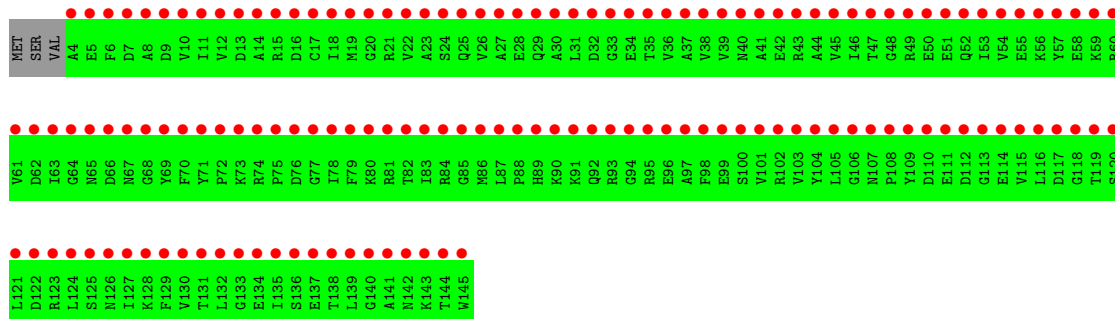


• Molecule 5: RIBOSOMAL PROTEIN L4

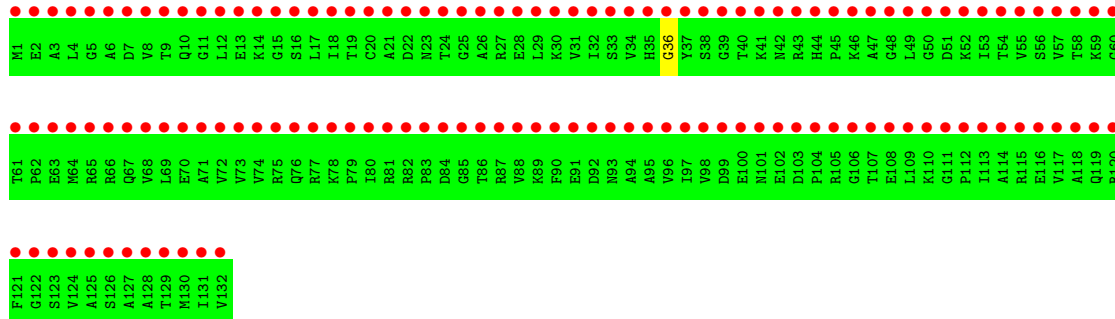




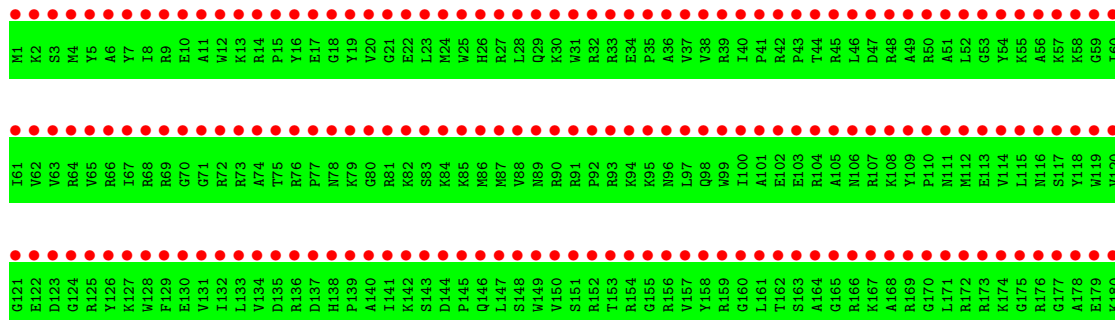
● Molecule 9: RIBOSOMAL PROTEIN L13



● Molecule 10: RIBOSOMAL PROTEIN L14




● Molecule 11: RIBOSOMAL PROTEIN L15E



V181
R162
P183
K4
S184
L185
R186
A187
N188
F189
K190
K191
K192
R193
R194

● Molecule 12: RIBOSOMAL PROTEIN L15

Chain J:  87% 13%

T1 S2 K3 K4 K5 R6 R7 R8 R9 R10 R11 R12 R13 R14 R15 R16 R17 R18 R19 R20 R21 R22 R23 R24 R25 R26 R27 R28 R29 R30 R31 R32 R33 R34 R35 R36 R37 R38 R39 R40 R41 R42 R43 R44 R45 R46 R47 R48 R49 R50 R51 R52 R53 R54 R55 R56 R57 R58 R59 R60

A61 A62 I64 I65 D66 D67 E68 E69 E70 E71 E72 E73 E74 E75 E76 E77 E78 E79 E80 E81 E82 E83 VAL A24 G25 H26 G27 G28 G29 PHE R40 Q150 ARG G31 A151 D82 D83 A33 G34 R94 R95 D96 D97 V98 V99 E98 E99 A100 F40 D101 H41 D102 M42 ASP A103 H43 E44 F45 Y105 L106 K107 G47 K48 V108 L109 S49 G50 G51 F51 A111 G112 Q113 P54 P55 Q55 H116 E117 T118 L119 E59 E60

L121 A122 D123 K4 S126 F127 G128 A129 R130 R131 R132 R133 R134 E135 E136 A137 G138 G139 V140 E141 L142 L143 T144 D145 L146 E147 E148 R149 Q150 A151 GLU ALA GLU THR GLU ASP ALA ASP ALA ASP GLU

● Molecule 13: RIBOSOMAL PROTEIN L18

Chain K:  100% 100%

A1 T2 G3 P4 R5 R6 R7 R8 R9 R10 R11 R12 R13 R14 R15 R16 R17 R18 R19 R20 R21 R22 R23 R24 R25 R26 R27 R28 R29 R30 R31 R32 R33 R34 R35 R36 R37 R38 R39 R40 R41 R42 R43 R44 R45 R46 R47 R48 R49 R50 R51 R52 R53 R54 R55 R56 R57 R58 R59 R60

A61 H62 S63 S64 D65 L66 A67 E68 Y69 G70 W71 W72 E73 A74 P74 F75 W76 G77 N77 M78 P79 S80 Q140 R141 Q22 R143 L83 T84 G85 L86 L87 L88 A88 G89 R90 L90 R91 A92 Q93 L94 E95 A96 E97 V97 L98 Y189 A100 V101 D102 F103 I104 G105 L106 N107 P109 T110 P111 G112 S113 K114 D115 V115 F116 A117 L118 Q119 L120 E120

G121 A122 I123 D124 A125 G126 L127 D128 I129 R130 H131 M132 R133 D134 V135 W136 A137 D138 W139 Q140 R141 Q22 R143 L83 T84 G85 L86 L87 L88 A88 G89 R90 L90 R91 A92 Q93 L94 E95 A96 E97 V97 L98 Y189 A100 V101 D102 F103 I104 G105 L106 N107 P109 T110 P111 G112 S113 K114 D115 V115 F116 A117 L118 Q119 L120 E120

D181
G182
D183
I184
E185
L186

● Molecule 14: RIBOSOMAL PROTEIN L18E

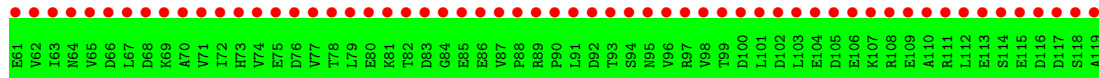
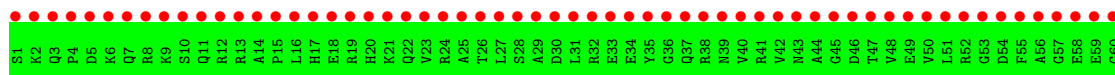
Chain L:  100% 100%

S1 K2 T3 M4 P5 R6 L7 S8 S9 S10 I11 I12 A13 D13 L14 K15 S16 S17 A18 A19 R20 S21 S22 G23 G24 A24 V25 W26 G27 D28 R29 V30 A31 R32 L33 E34 A35 P36 R37 R38 T39 H40 A41 E42 V43 M44 L45 G46 R47 I48 S49 R50 Y51 A52 Q53 E54 I114 D55 E56 T57 V58 V59 Q119 L120 E120

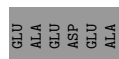
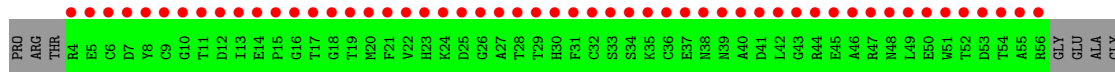
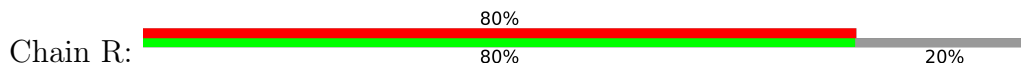
P61 G62 K63 V64 L65 G66 S67 G68 G69 L70 Q71 Q72 K73 D73 V74 W75 V76 A77 A78 V79 D80 S81 S82 S83 G84 A85 A86 T87 R88 I89 R90 Q91 V92 L93 G94 E95 A96 P96 R97 R98 E99 Q100 A101 I102 E103 N104 N105 P106 E107 G108 S109 H110 V111 A112 Q113 I114 D115 E116 T117 V118 V119 Q119 L120 E120

● Molecule 15: RIBOSOMAL PROTEIN L19

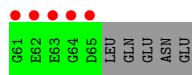
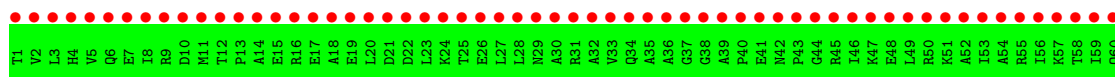
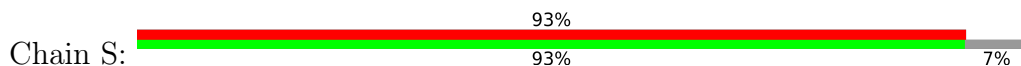
Chain M:  96% 3%



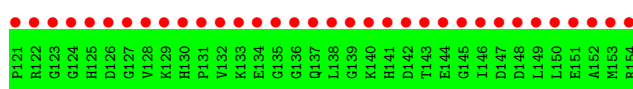
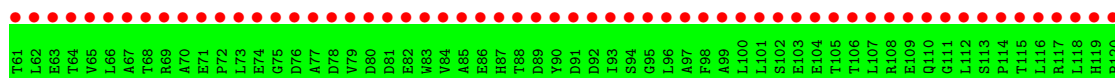
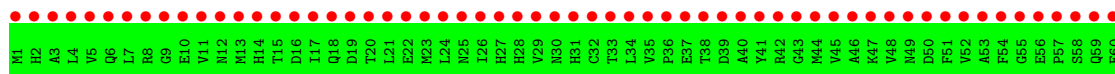
● Molecule 20: RIBOSOMAL PROTEIN L24E



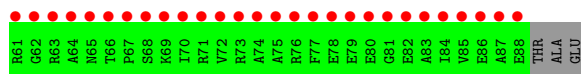
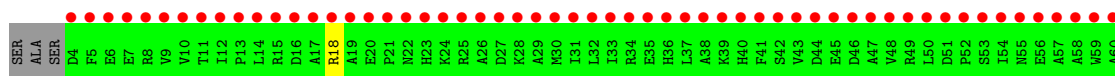
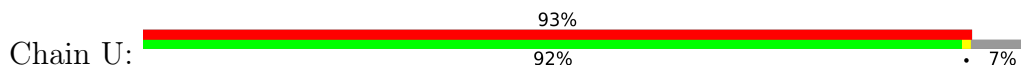
● Molecule 21: RIBOSOMAL PROTEIN L29



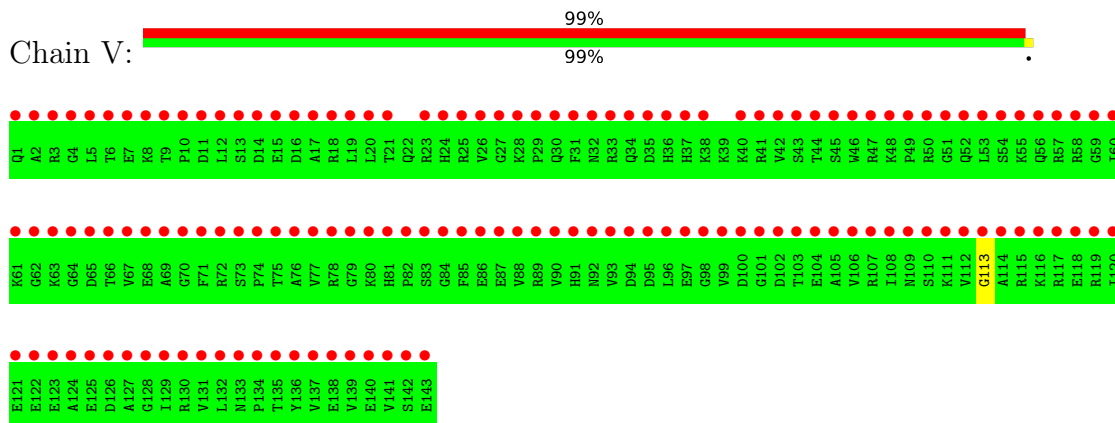
● Molecule 22: RIBOSOMAL PROTEIN L30



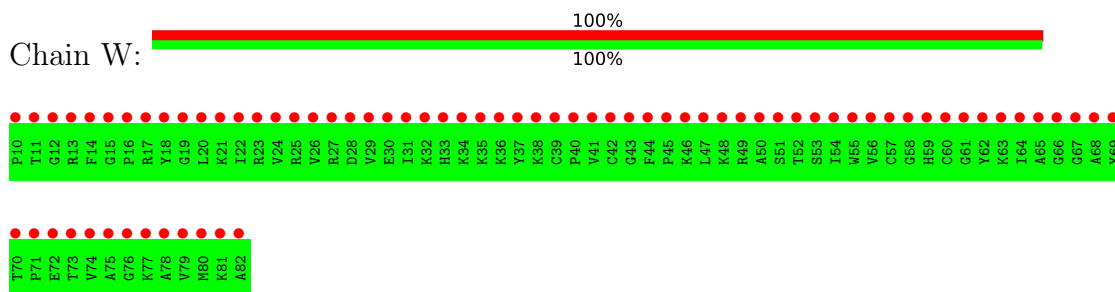
● Molecule 23: RIBOSOMAL PROTEIN L31E



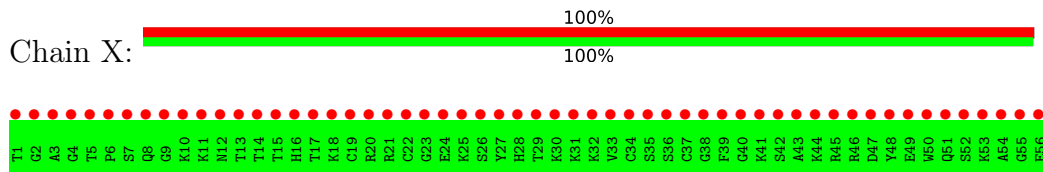
- Molecule 24: RIBOSOMAL PROTEIN L32E



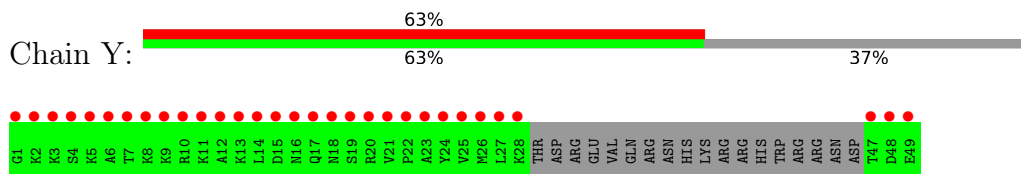
- Molecule 25: RIBOSOMAL PROTEIN L37AE



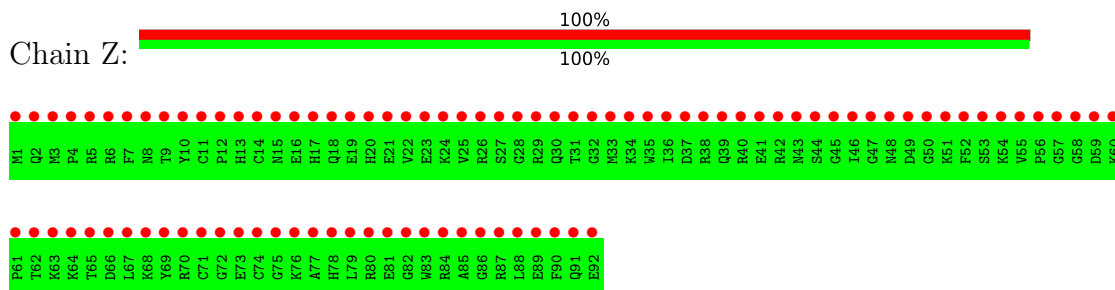
- Molecule 26: RIBOSOMAL PROTEIN L37E



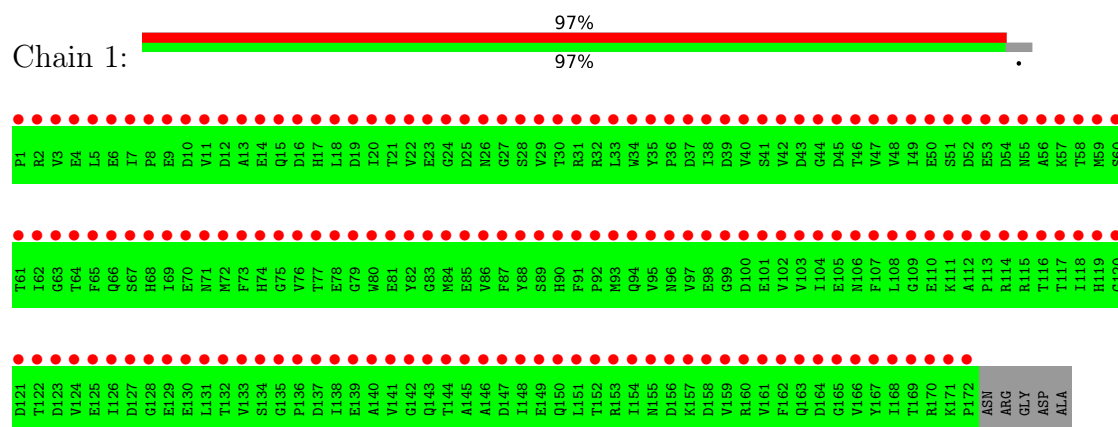
- Molecule 27: RIBOSOMAL PROTEIN L39E



- Molecule 28: RIBOSOMAL PROTEIN L44E



- Molecule 29: RIBOSOMAL PROTEIN L6



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	211.66Å 299.67Å 573.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	90.00 – 2.40 90.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	82.3 (90.00-2.40) 95.1 (90.00-2.40)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.28 (at 2.40Å)	Xtrriage
Refinement program	CNS, TNT & CNS	Depositor
R, R_{free}	0.252 , 0.261 0.346 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	42.3	Xtrriage
Anisotropy	0.271	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 276.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.77	EDS
Total number of atoms	64281	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.51% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.40	0/64945	0.66	119/101281 (0.1%)
2	9	0.36	0/2905	0.68	7/4528 (0.2%)
All	All	0.40	0/67850	0.66	126/105809 (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	18	45
2	9	2	0
All	All	20	45

There are no bond length outliers.

The worst 5 of 126 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	0	2749	U	C2'-C3'-O3'	16.23	133.85	109.50
1	0	904	U	C2'-C3'-O3'	15.24	132.35	109.50
1	0	1981	A	C2'-C3'-O3'	15.00	132.00	109.50
2	9	3	A	C2'-C3'-O3'	14.05	130.57	109.50
1	0	894	A	C2'-C3'-O3'	13.75	130.13	109.50

5 of 20 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	0	191	A	C3'
1	0	282	C	C3'
1	0	600	G	C3'

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Mol	Chain	Res	Type	Atom
1	0	894	A	C3'
1	0	904	U	C3'

5 of 45 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	138	U	Sidechain
1	0	189	A	Sidechain
1	0	262	A	Sidechain
1	0	270	U	Sidechain
1	0	333	G	Sidechain

5.2 Too-close contacts [i](#)

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	58012	0	29282	980	0
2	9	2600	0	1326	62	0
3	A	237	0	0	1	0
4	B	337	0	0	2	0
5	C	246	0	0	0	0
6	D	140	0	0	0	0
7	E	118	0	0	1	0
8	F	157	0	0	0	0
9	G	142	0	0	0	0
10	H	132	0	0	1	0
11	I	194	0	0	0	0
12	J	143	0	0	0	0
13	K	186	0	0	0	0
14	L	115	0	0	0	0
15	M	143	0	0	0	0
16	N	95	0	0	0	0
17	O	150	0	0	0	0
18	P	78	0	0	0	0
19	Q	119	0	0	0	0
20	R	53	0	0	0	0
21	S	65	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	T	154	0	0	0	0
23	U	85	0	0	1	0
24	V	143	0	0	2	0
25	W	73	0	0	0	0
26	X	56	0	0	0	0
27	Y	31	0	0	0	0
28	Z	92	0	0	0	0
29	1	172	0	0	0	0
30	0	1	0	0	0	0
31	0	2	0	0	0	0
32	R	1	0	0	0	0
32	W	1	0	0	0	0
32	X	1	0	0	0	0
32	Z	1	0	0	0	0
33	0	6	0	0	0	0
All	All	64281	0	30608	1044	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 11.

The worst 5 of 1044 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)
2:9:76:G:H3'	2:9:77:A:H5''	1.29	1.10
1:0:1682:A:H2	1:0:1696:U:H3	1.05	1.01
1:0:795:G:H2'	1:0:817:G:H22	1.25	1.00
1:0:326:G:H1	1:0:330:C:H5	1.03	1.00
1:0:1355:A:O2'	1:0:1356:A:H3'	1.60	1.00

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2697/2922 (92%)	341 (12%)	107 (3%)
2	9	122/122 (100%)	17 (13%)	5 (4%)
All	All	2819/3044 (92%)	358 (12%)	112 (3%)

5 of 358 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	0	11	A
1	0	31	C
1	0	60	A
1	0	67	A
1	0	70	A

5 of 112 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	1591	A
2	9	55	U
1	0	1981	A
2	9	28	U
1	0	2749	U

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 7 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	0	2706/2922 (92%)	1.36	593 (21%) 2 2	12, 29, 60, 87	0
2	9	122/122 (100%)	2.27	57 (46%) 0 0	22, 42, 67, 106	0
3	A	237/239 (99%)	7.71	237 (100%) 0 0	16, 35, 64, 78	0
4	B	337/337 (100%)	8.99	337 (100%) 0 0	18, 42, 65, 72	0
5	C	246/246 (100%)	7.23	242 (98%) 0 0	14, 31, 54, 76	0
6	D	140/176 (79%)	11.34	140 (100%) 0 0	49, 80, 90, 94	0
7	E	118/119 (99%)	8.39	117 (99%) 0 0	32, 51, 69, 72	0
8	F	157/157 (100%)	11.04	157 (100%) 0 0	33, 56, 81, 93	0
9	G	142/145 (97%)	7.95	142 (100%) 0 0	22, 38, 58, 68	0
10	H	132/132 (100%)	8.13	132 (100%) 0 0	20, 37, 55, 63	0
11	I	194/194 (100%)	9.04	194 (100%) 0 0	22, 36, 54, 66	0
12	J	143/164 (87%)	9.34	143 (100%) 0 0	21, 46, 73, 85	0
13	K	186/186 (100%)	11.32	186 (100%) 0 0	40, 65, 83, 87	0
14	L	115/115 (100%)	7.27	115 (100%) 0 0	28, 38, 55, 65	0
15	M	143/148 (96%)	7.40	142 (99%) 0 0	24, 38, 49, 58	0
16	N	95/95 (100%)	7.68	95 (100%) 0 0	20, 32, 53, 65	0
17	O	150/154 (97%)	6.95	150 (100%) 0 0	19, 31, 49, 58	0
18	P	78/84 (92%)	8.00	78 (100%) 0 0	27, 38, 63, 65	0
19	Q	119/119 (100%)	7.80	119 (100%) 0 0	28, 39, 56, 67	0
20	R	53/66 (80%)	8.02	53 (100%) 0 0	29, 43, 55, 58	0
21	S	65/70 (92%)	8.86	65 (100%) 0 0	35, 51, 77, 83	0
22	T	154/154 (100%)	7.75	154 (100%) 0 0	24, 35, 51, 56	0
23	U	85/91 (93%)	10.14	85 (100%) 0 0	29, 47, 73, 80	0
24	V	143/143 (100%)	8.04	141 (98%) 0 0	18, 33, 62, 76	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	W	73/73 (100%)	8.39	73 (100%) 0 0	36, 43, 57, 62	0
26	X	56/56 (100%)	8.33	56 (100%) 0 0	17, 27, 35, 41	0
27	Y	31/49 (63%)	7.48	31 (100%) 0 0	25, 33, 55, 61	0
28	Z	92/92 (100%)	8.41	92 (100%) 0 0	23, 40, 51, 63	0
29	1	172/177 (97%)	8.80	172 (100%) 0 0	31, 48, 64, 71	0
All	All	6484/6825 (95%)	5.45	4298 (66%) 0 0	12, 36, 70, 106	0

The worst 5 of 4298 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
23	U	80	GLU	56.9
10	H	61	THR	45.8
9	G	4	ALA	43.4
3	A	35	GLY	41.6
4	B	156	LYS	39.0

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 oligosaccharides 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
32	CD	X	102	1/1	0.82	0.11	48,48,48,48	0
30	K	0	2924	1/1	0.87	0.24	30,30,30,30	0
31	MG	0	2926	1/1	0.94	0.09	30,30,30,30	0
32	CD	R	101	1/1	0.96	0.06	39,39,39,39	0
32	CD	W	103	1/1	0.96	0.05	30,30,30,30	0
31	MG	0	2925	1/1	0.96	0.07	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
32	CD	Z	104	1/1	0.97	0.16	54,54,54,54	0

6.5 Other polymers [i](#)

There are no such residues in this entry.