



wwPDB X-ray Structure Validation Summary Report

Mar 31, 2014 – 05:39 PM BST

PDB ID : 3PYN
Title : Crystal structure of a complex containing domain 3 from the PSIV IGR IRES RNA bound to the 70S ribosome. This file contains the 30S subunit of the first 70S ribosome.
Authors : Zhu, J.; Korostelev, A.; Costantino, D.; Noller, H.F.; Kieft, J.S.
Deposited on : 2010-12-13
Resolution : 3.50 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

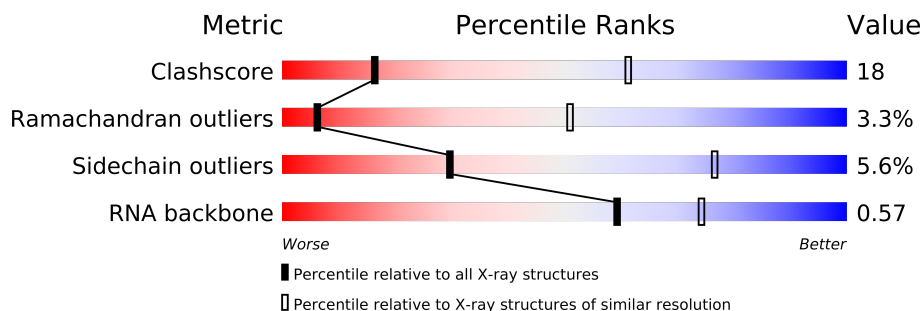
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : **NOT EXECUTED**
Percentile statistics : 21963
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable23004

1 Overall quality at a glance

The reported resolution of this entry is 3.50 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	79885	1039 (3.66-3.34)
Ramachandran outliers	78287	1000 (3.66-3.34)
Sidechain outliers	78261	1000 (3.66-3.34)
RNA backbone	1838	1007 (4.22-2.76)





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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	1506	
2	B	234	
3	C	206	
4	D	208	
5	E	151	
6	F	101	
7	G	155	
8	H	138	
9	I	127	
10	J	98	
11	K	119	
12	L	124	
13	M	116	
14	N	60	
15	O	88	

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Mol	Chain	Length	Quality of chain
16	P	83	
17	Q	99	
18	R	70	
19	S	78	
20	T	99	
21	U	24	
22	V	35	

2 Entry composition

There are 23 unique types of molecules in this entry. The entry contains 52216 atoms, of which 0 are hydrogen and 0 are deuterium.

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 ribosomal RNA 16S.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1506	Total	C	N	O	P	0	0	0
			32372	14409	5999	10459	1505			

- Molecule 2 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	234	Total	C	N	O	S	0	0	0
			1901	1213	341	342	5			

- Molecule 3 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	206	Total	C	N	O	S	0	0	0
			1613	1016	314	282	1			

- Molecule 4 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	208	Total	C	N	O	S	0	0	0
			1703	1066	339	291	7			

- Molecule 5 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	151	Total	C	N	O	S	0	0	0
			1156	729	218	205	4			

- Molecule 6 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			

- Molecule 7 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			

- Molecule 8 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			

- Molecule 9 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	127	Total	C	N	O	S	0	0	0
			1011	639	198	174				

- Molecule 10 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	98	Total	C	N	O	S	0	0	0
			795	499	156	139	1			

- Molecule 11 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	119	Total	C	N	O	S	0	0	0
			885	549	168	165	3			

- Molecule 12 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	124	Total	C	N	O	S	0	0	0
			971	611	195	164	1			

- Molecule 13 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	116	Total	C	N	O	S	0	0	0
			929	574	191	162	2			

- Molecule 14 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			

- Molecule 15 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	O	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			

- Molecule 16 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	P	83	Total	C	N	O	S	0	0	0
			701	443	139	118	1			

- Molecule 17 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Q	99	Total	C	N	O	S	0	0	0
			824	528	152	142	2			

- Molecule 18 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	R	70	Total	C	N	O	0	0	0
			574	367	112	95			

- Molecule 19 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	S	78	Total	C	N	O	S	0	0	0
			630	403	114	111	2			

- Molecule 20 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	T	99	Total	C	N	O	S	0	0	0
			762	469	162	129	2			

- Molecule 21 is a protein called 30S ribosomal protein Thx.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	U	24	Total	C	N	O	0	0	0
			209	128	50	31			

- Molecule 22 is a RNA chain called domain 3 of PSIC IGR IRES RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	V	35	Total	C	N	O	P	0	0	0
			736	332	128	243	33			

- Molecule 23 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
23	D	1	Total	Zn	0	0
			1	1		
23	N	1	Total	Zn	0	0
			1	1		

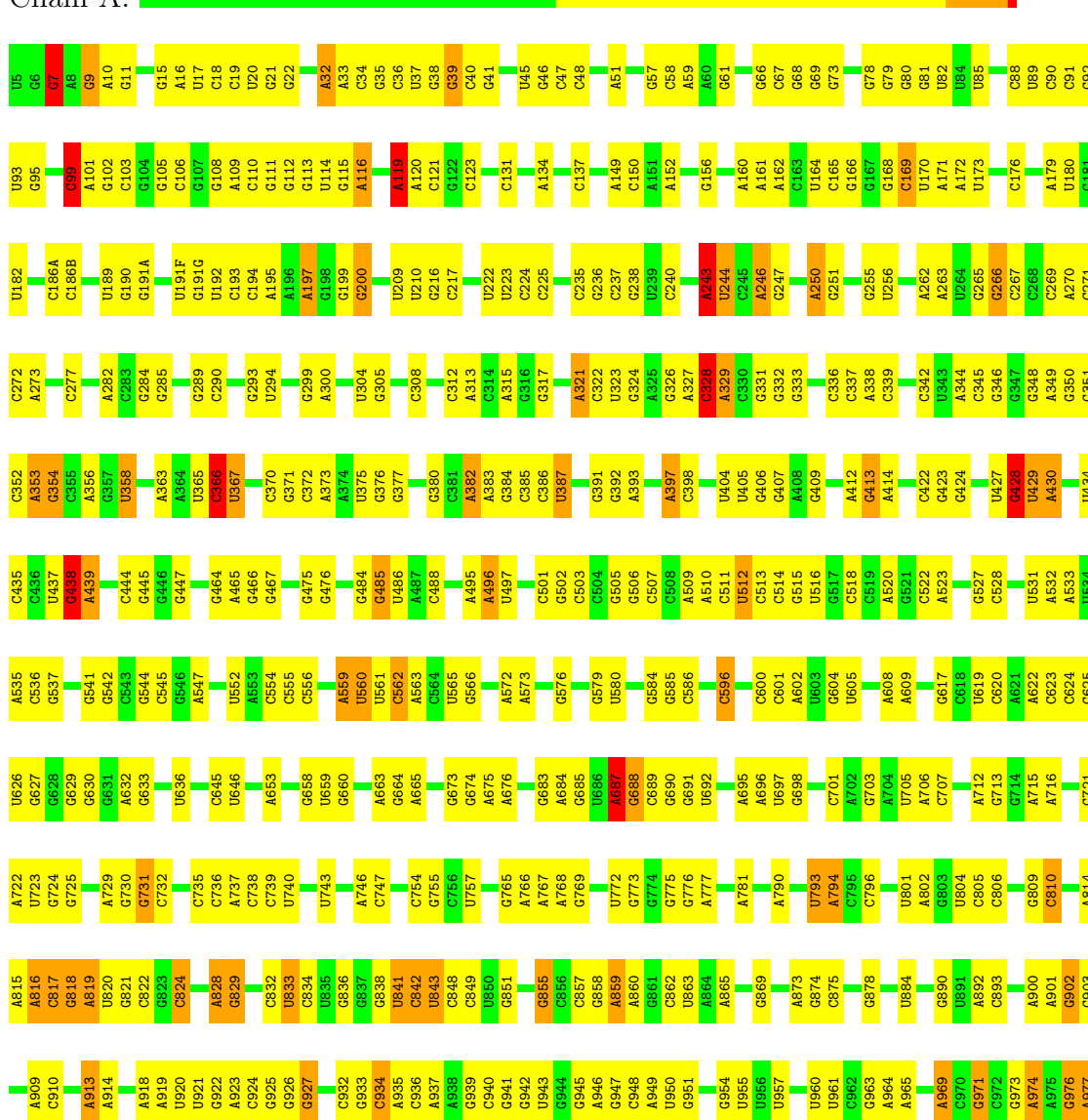
3 Residue-property plots

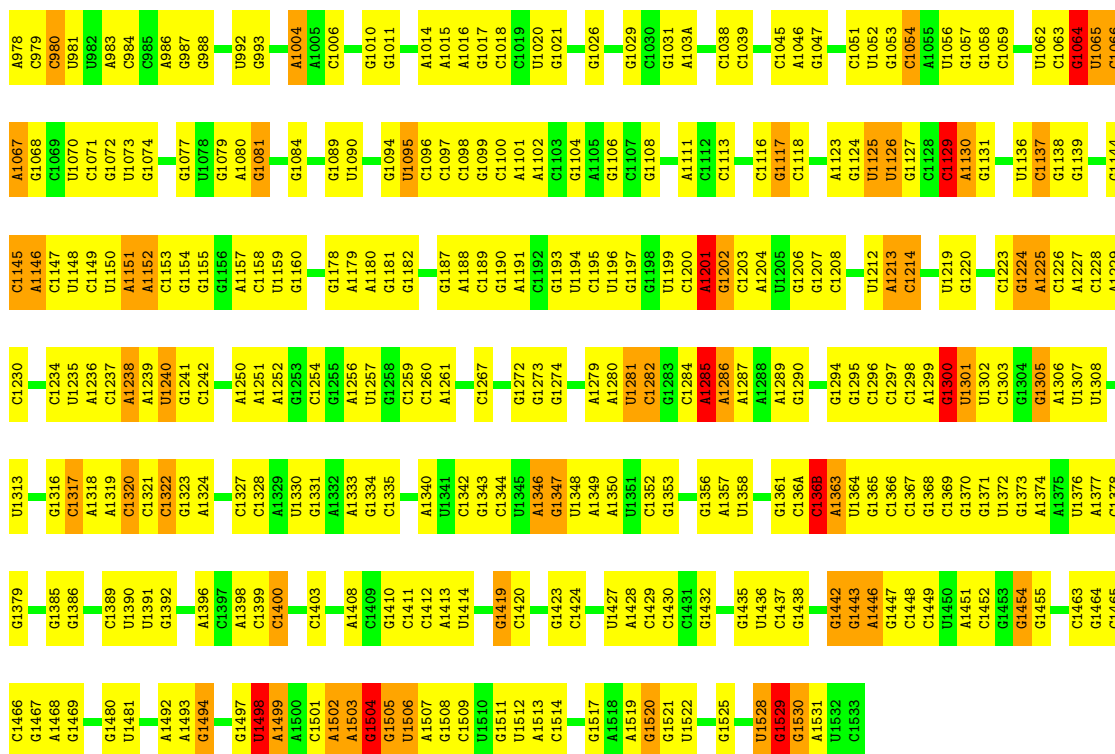
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: ribosomal RNA 16S

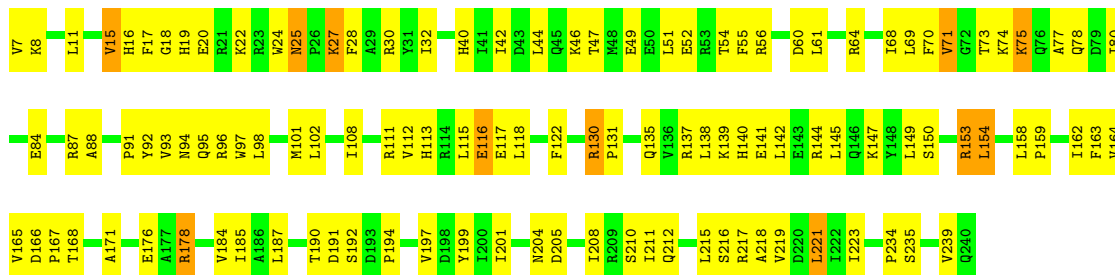
Chain A:





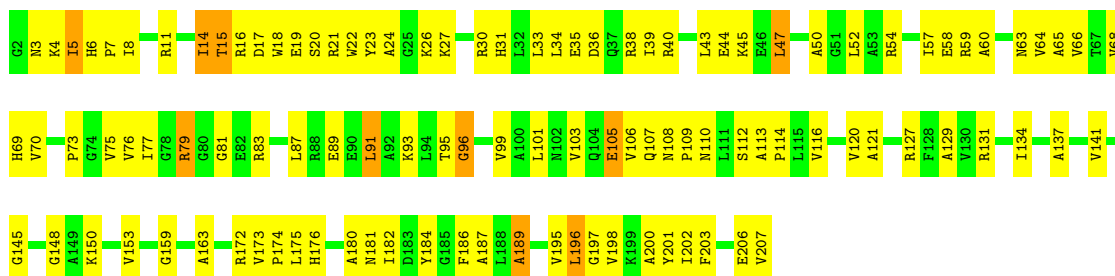
• Molecule 2: 30S ribosomal protein S2

Chain B:



• Molecule 3: 30S ribosomal protein S3

Chain C:



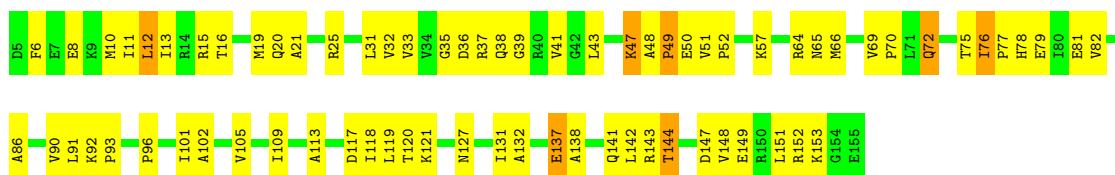
• Molecule 4: 30S ribosomal protein S4

Chain D:



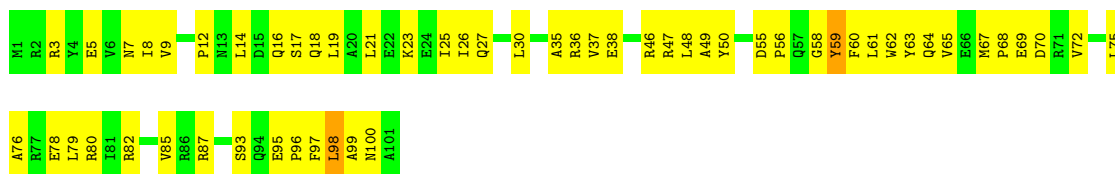
• Molecule 5: 30S ribosomal protein S5

Chain E:



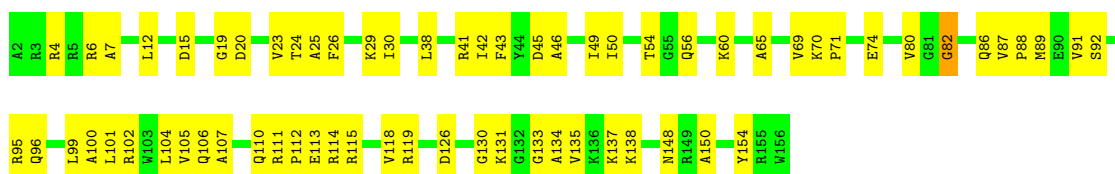
• Molecule 6: 30S ribosomal protein S6

Chain F:



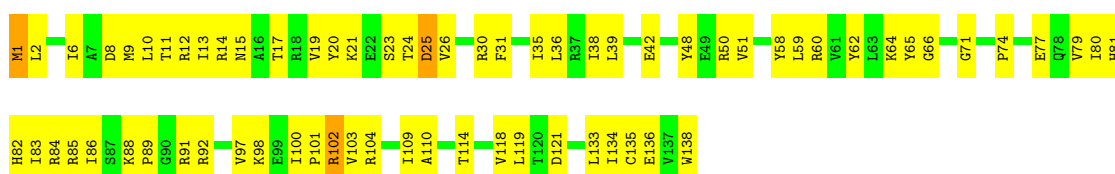
• Molecule 7: 30S ribosomal protein S7

Chain G:



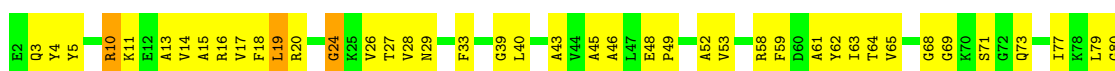
• Molecule 8: 30S ribosomal protein S8

Chain H:



• Molecule 9: 30S ribosomal protein S9

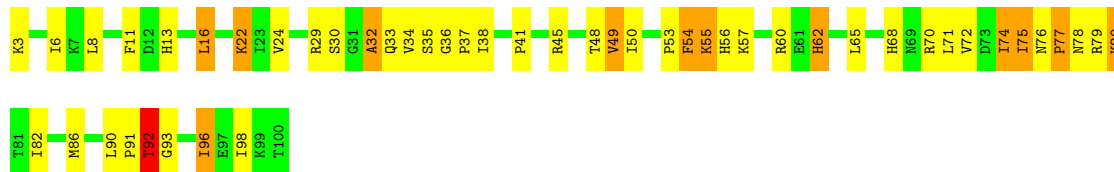
Chain I:





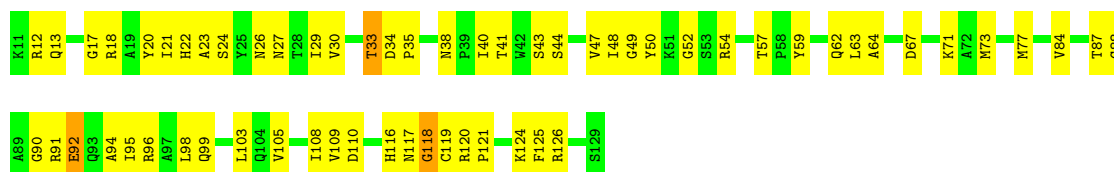
- Molecule 10: 30S ribosomal protein S10

Chain J:



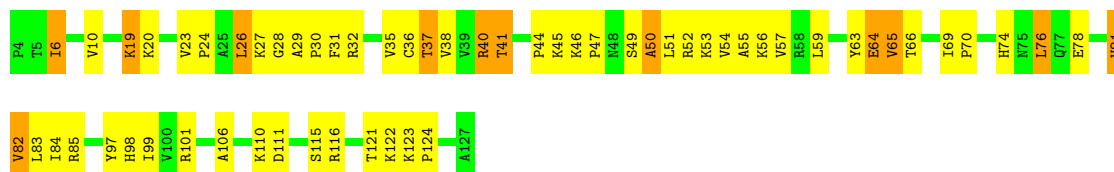
- Molecule 11: 30S ribosomal protein S11

Chain K:



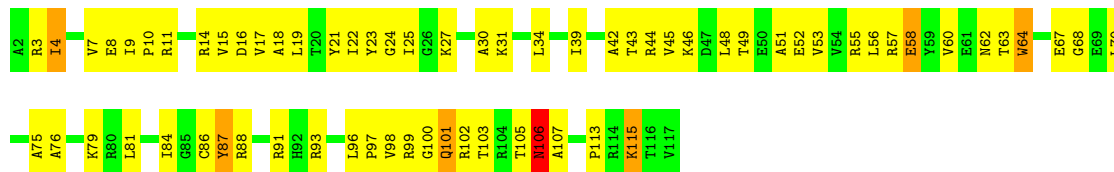
- Molecule 12: 30S ribosomal protein S12

Chain L:



- Molecule 13: 30S ribosomal protein S13

Chain M:



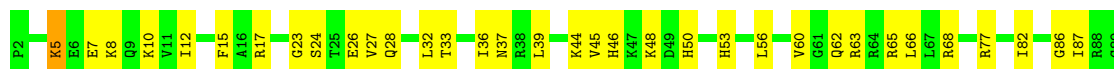
- Molecule 14: 30S ribosomal protein S14 type Z

Chain N:



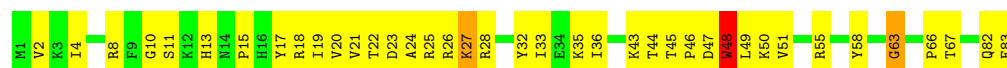
- Molecule 15: 30S ribosomal protein S15

Chain O:



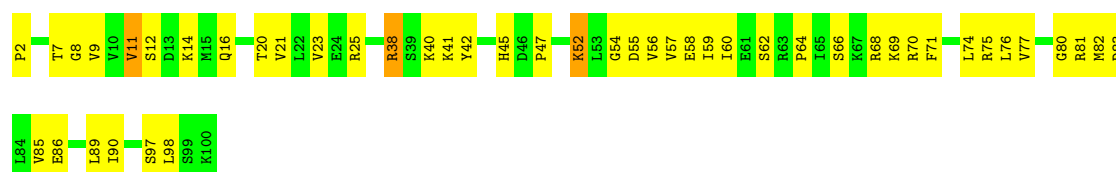
- Molecule 16: 30S ribosomal protein S16

Chain P:



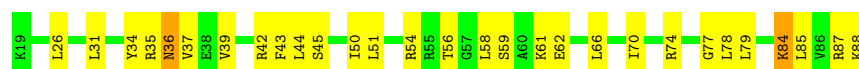
- Molecule 17: 30S ribosomal protein S17

Chain Q:



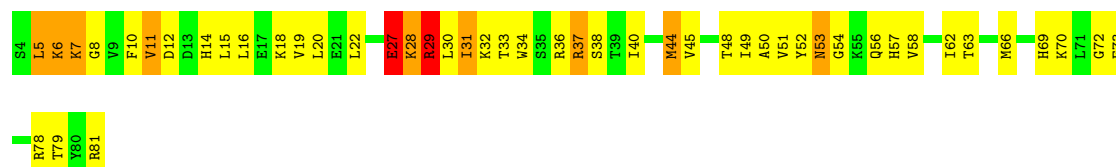
- Molecule 18: 30S ribosomal protein S18

Chain R:



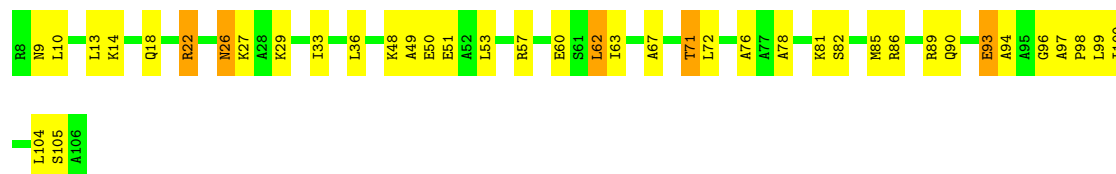
- Molecule 19: 30S ribosomal protein S19

Chain S:



- Molecule 20: 30S ribosomal protein S20

Chain T:



- Molecule 21: 30S ribosomal protein Thx

Chain U:



- Molecule 22: domain 3 of PSIC IGR IRES RNA

Chain V:

U6150	C6155	A6156	A6157	U6161	A6164	G6165	U6166	G6167	G6168	U6169	G6170	U6171	U6172	G6173	C6188	A6189	C6190	A6193
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4 Data and refinement statistics

EDS was not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	211.94Å 455.59Å 618.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.50	Depositor
% Data completeness (in resolution range)	99.9 (50.00-3.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.61 (at 3.49Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.5.2)	Depositor
R, R_{free}	0.233 , 0.264	Depositor
Wilson B-factor (Å ²)	106.2	Xtriage
Anisotropy	0.163	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.21$	Xtriage
Outliers	1 of 746568 reflections (0.000%)	Xtriage
Total number of atoms	52216	wwPDB-VP
Average B, all atoms (Å ²)	149.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.63% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.45	0/36238	0.90	34/56561 (0.1%)
2	B	0.21	0/1936	0.38	0/2609
3	C	0.21	0/1637	0.37	0/2205
4	D	0.24	0/1733	0.40	0/2318
5	E	0.24	0/1172	0.41	0/1576
6	F	0.23	0/856	0.42	0/1154
7	G	0.21	0/1276	0.36	0/1709
8	H	0.23	0/1136	0.41	0/1527
9	I	0.22	0/1029	0.38	0/1378
10	J	0.21	0/808	0.39	0/1085
11	K	0.23	0/900	0.40	0/1213
12	L	0.25	0/987	0.46	0/1320
13	M	0.24	0/939	0.41	0/1258
14	N	0.23	0/501	0.37	0/664
15	O	0.24	0/745	0.38	0/992
16	P	0.36	1/717 (0.1%)	0.44	0/963
17	Q	0.24	0/837	0.41	0/1117
18	R	0.24	0/579	0.42	0/768
19	S	0.20	0/643	0.37	0/865
20	T	0.23	0/764	0.39	0/1006
21	U	0.20	0/213	0.37	0/277
22	V	0.43	0/821	0.86	2/1275 (0.2%)
All	All	0.39	1/56467 (0.0%)	0.78	36/83840 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	P	48	TRP	CG-CD1	6.09	1.45	1.36

The worst 5 of 36 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	99	C	P-O3'-C3'	8.79	130.25	119.70
1	A	266	G	P-O3'-C3'	7.94	129.23	119.70
1	A	1498	U	P-O3'-C3'	7.63	128.86	119.70
1	A	243	A	P-O3'-C3'	7.42	128.61	119.70
1	A	438	G	P-O3'-C3'	7.21	128.35	119.70

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	32372	0	16339	680	0
2	B	1901	0	1951	103	0
3	C	1613	0	1677	95	0
4	D	1703	0	1764	98	0
5	E	1156	0	1213	68	0
6	F	843	0	857	46	0
7	G	1257	0	1296	60	0
8	H	1116	0	1177	57	0
9	I	1011	0	1043	62	0
10	J	795	0	840	59	0
11	K	885	0	904	56	0
12	L	971	0	1057	60	0
13	M	929	0	987	62	0
14	N	492	0	529	29	0
15	O	734	0	771	23	0
16	P	701	0	720	30	0
17	Q	824	0	893	42	0
18	R	574	0	644	30	0
19	S	630	0	652	59	0
20	T	762	0	859	32	0
21	U	209	0	221	13	0
22	V	736	0	378	19	0
23	D	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	N	1	0	0	0	0
All	All	52216	0	36772	1611	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 18.

The worst 5 of 1611 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1399:C:H4'	1:A:1400:C:H5'	1.26	1.16
7:G:113:GLU:HB2	7:G:119:ARG:HG2	1.38	1.04
9:I:19:LEU:HD21	9:I:59:PHE:HB3	1.41	1.02
15:O:63:ARG:HH21	15:O:87:ILE:HG21	1.27	0.99
5:E:76:ILE:HG12	5:E:77:PRO:HD2	1.43	0.99

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	B	232/234 (99%)	194 (84%)	32 (14%)	6 (3%)	8	57
3	C	204/206 (99%)	153 (75%)	38 (19%)	13 (6%)	2	29
4	D	206/208 (99%)	172 (84%)	26 (13%)	8 (4%)	5	45
5	E	149/151 (99%)	123 (83%)	22 (15%)	4 (3%)	8	56
6	F	99/101 (98%)	90 (91%)	8 (8%)	1 (1%)	22	78
7	G	153/155 (99%)	132 (86%)	18 (12%)	3 (2%)	11	63
8	H	136/138 (99%)	119 (88%)	17 (12%)	0	100	100
9	I	125/127 (98%)	102 (82%)	20 (16%)	3 (2%)	9	59
10	J	96/98 (98%)	78 (81%)	12 (12%)	6 (6%)	2	29
11	K	117/119 (98%)	97 (83%)	16 (14%)	4 (3%)	6	50
12	L	122/124 (98%)	94 (77%)	22 (18%)	6 (5%)	3	37

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	M	114/116 (98%)	94 (82%)	16 (14%)	4 (4%)	6	50
14	N	58/60 (97%)	50 (86%)	5 (9%)	3 (5%)	3	35
15	O	86/88 (98%)	77 (90%)	7 (8%)	2 (2%)	10	60
16	P	81/83 (98%)	65 (80%)	14 (17%)	2 (2%)	9	57
17	Q	97/99 (98%)	81 (84%)	15 (16%)	1 (1%)	22	78
18	R	68/70 (97%)	53 (78%)	13 (19%)	2 (3%)	7	54
19	S	76/78 (97%)	57 (75%)	14 (18%)	5 (7%)	2	28
20	T	97/99 (98%)	82 (84%)	12 (12%)	3 (3%)	7	53
21	U	22/24 (92%)	17 (77%)	4 (18%)	1 (4%)	4	40
All	All	2338/2378 (98%)	1930 (82%)	331 (14%)	77 (3%)	6	51

5 of 77 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	15	THR
4	D	30	LYS
4	D	137	SER
4	D	138	TYR
4	D	168	ARG

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	B	202/202 (100%)	192 (95%)	10 (5%)	34	79
3	C	160/160 (100%)	154 (96%)	6 (4%)	44	85
4	D	180/180 (100%)	168 (93%)	12 (7%)	23	70
5	E	116/116 (100%)	108 (93%)	8 (7%)	22	69
6	F	90/90 (100%)	85 (94%)	5 (6%)	30	76
7	G	126/126 (100%)	126 (100%)	0	100	100
8	H	119/119 (100%)	114 (96%)	5 (4%)	40	84
9	I	98/98 (100%)	92 (94%)	6 (6%)	26	73

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	J	88/88 (100%)	79 (90%)	9 (10%)	11	48
11	K	90/90 (100%)	86 (96%)	4 (4%)	39	83
12	L	104/104 (100%)	94 (90%)	10 (10%)	12	51
13	M	94/94 (100%)	88 (94%)	6 (6%)	25	72
14	N	49/49 (100%)	47 (96%)	2 (4%)	41	84
15	O	79/79 (100%)	75 (95%)	4 (5%)	33	79
16	P	72/72 (100%)	67 (93%)	5 (7%)	22	69
17	Q	94/94 (100%)	92 (98%)	2 (2%)	66	92
18	R	61/61 (100%)	59 (97%)	2 (3%)	50	88
19	S	69/69 (100%)	60 (87%)	9 (13%)	6	33
20	T	76/76 (100%)	71 (93%)	5 (7%)	24	71
21	U	19/19 (100%)	18 (95%)	1 (5%)	32	78
All	All	1986/1986 (100%)	1875 (94%)	111 (6%)	30	76

5 of 111 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
9	I	104	ARG
11	K	92	GLU
19	S	44	MET
9	I	121	ARG
10	J	62	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 46 such sidechains are listed below:

Mol	Chain	Res	Type
7	G	84	ASN
9	I	117	HIS
19	S	47	HIS
7	G	106	GLN
9	I	23	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1505/1506 (99%)	204 (13%)	35 (2%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
22	V	34/35 (97%)	2 (5%)	2 (5%)
All	All	1539/1541 (99%)	206 (13%)	37 (2%)

5 of 206 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	9	G
1	A	22	G
1	A	32	A
1	A	39	G
1	A	41	G

5 of 37 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	562	C
1	A	1065	U
1	A	1529	G
1	A	687	A
1	A	913	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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 2 ligands modelled in this entry, 2 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.

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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.