



wwPDB X-ray Structure Validation Summary Report

Mar 31, 2014 – 05:27 PM BST

PDB ID : 1PNX
Title : Crystal Structure of the Wild Type Ribosome from E. Coli, 30S Subunit of 70S Ribosome. THIS FILE, 1PNX, CONTAINS ONLY MOLECULES OF THE 30S RIBOSOMAL SUBUNIT. THE 50S SUBUNIT IS IN THE PDB FILE 1PNY.
Authors : Vila-Sanjurjo, A.; Ridgeway, W.K.; Seymaner, V.; Zhang, W.; Santoso, S.; Yu, K.; Cate, J.H.D.
Deposited on : 2003-06-13
Resolution : 9.50 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>

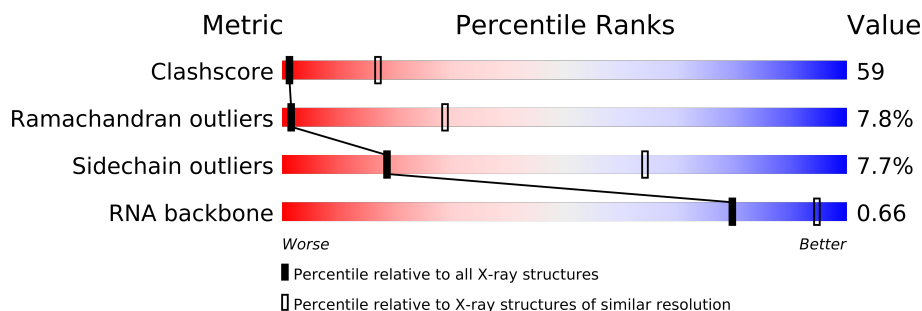
The following versions of software and data (see [references](#)) were used in the production of this report:

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 9.50 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	1010 (15.00-3.54)
Ramachandran outliers	78287	1304 (15.00-3.50)
Sidechain outliers	78261	1278 (15.00-3.50)
RNA backbone	1838	1055 (11.50-2.80)


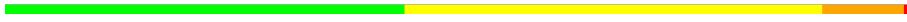
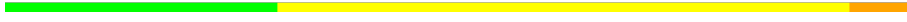

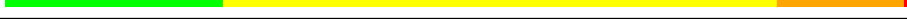
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The 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	1537	
2	B	234	
3	C	206	
4	D	208	
5	E	150	
6	F	101	
7	G	155	
8	H	138	
9	I	127	
10	J	98	
11	K	119	
12	L	124	
13	M	125	
14	N	60	
15	O	88	

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Mol	Chain	Length	Quality of chain
16	P	83	
17	Q	104	
18	R	73	
19	S	80	
20	T	99	

2 Entry composition

There are 20 unique types of molecules in this entry. The entry contains 51951 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 16S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1533	Total	C	N	O	P	0	0	0
			32939	14664	6099	10643	1533			

- 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
			1900	1213	341	341	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
			1612	1016	314	281	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
			1702	1066	339	290	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	150	Total	C	N	O	S	0	0	0
			1146	724	217	201	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
			842	531	155	153	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
			1256	781	252	217	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
			1115	705	215	192	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
			1010	639	198	173				

- 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
			794	499	156	138	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
			884	549	168	164	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
			970	611	195	163	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	125	Total	C	N	O	S	0	0	0
			996	617	207	170	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	60	Total	C	N	O	S	0	0	0
			491	312	104	71	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
			733	459	147	125	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
			700	443	139	117	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Q	104	Total	C	N	O	S	0	0	0
			856	547	161	146	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	R	73	Total	C	N	O	0	0	0
			596	380	118	98			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	S	80	Total	C	N	O	S	0	0	0
			647	414	119	112	2			

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

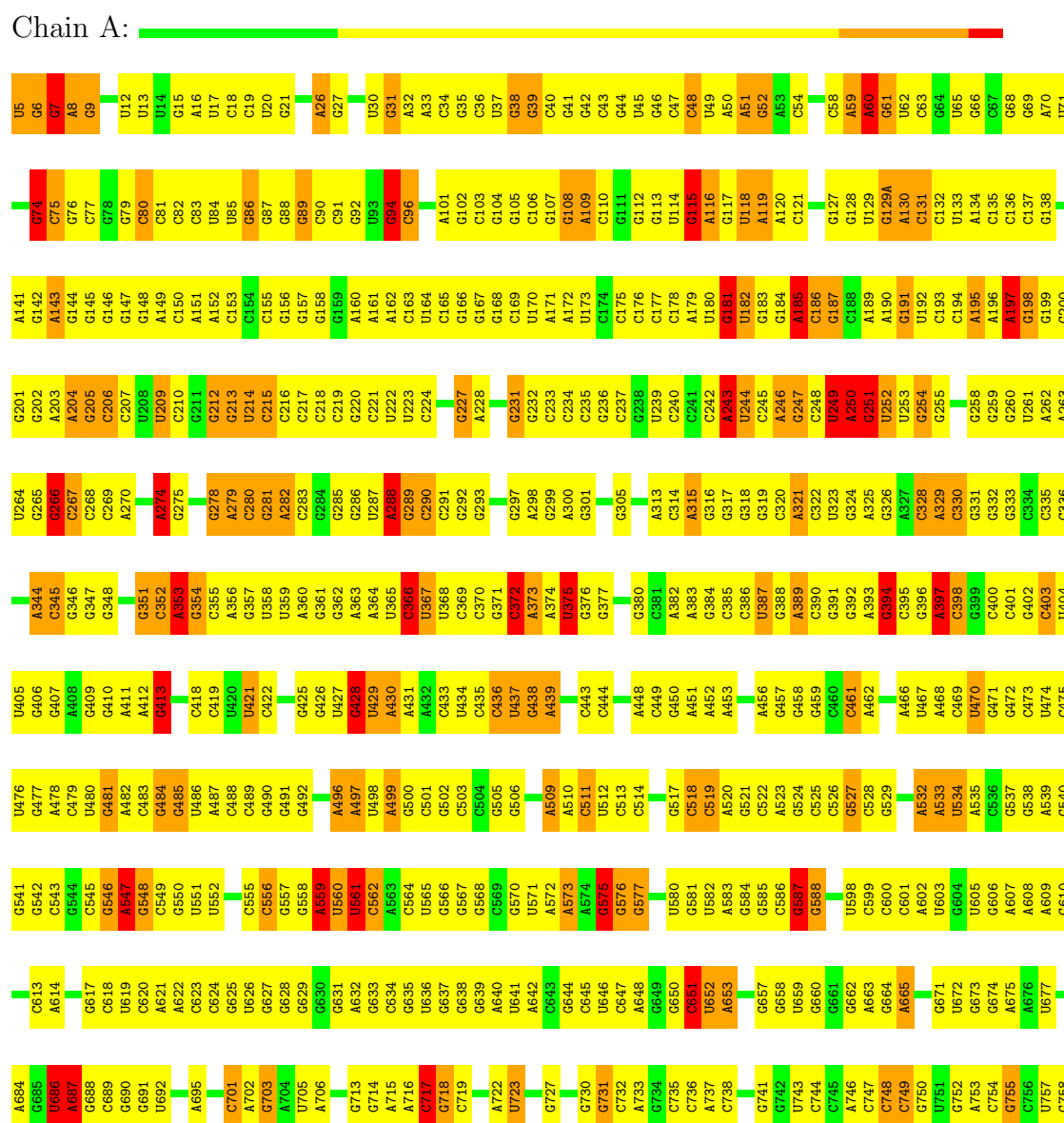
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	T	99	Total	C	N	O	S	0	0	0
			762	469	162	129	2			

3 Residue-property plots

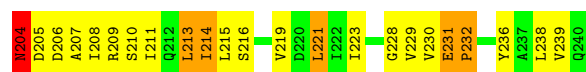
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 ($\text{RSRZ} > 2$). 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: 16S RIBOSOMAL RNA

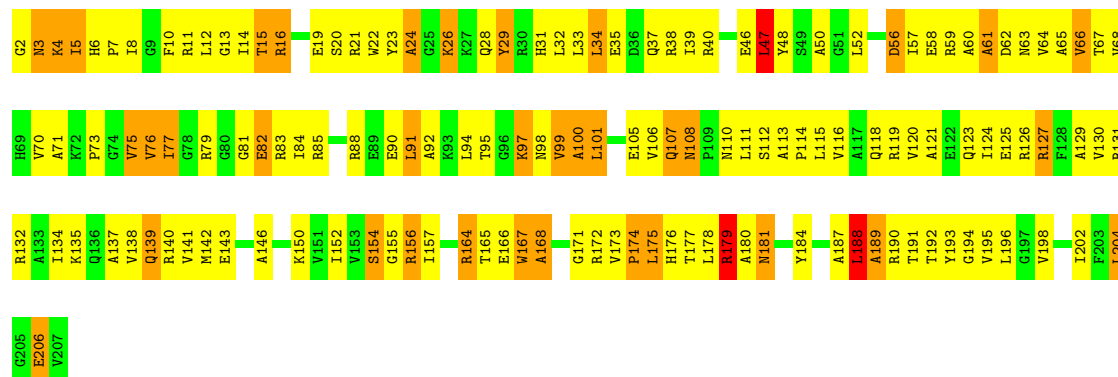






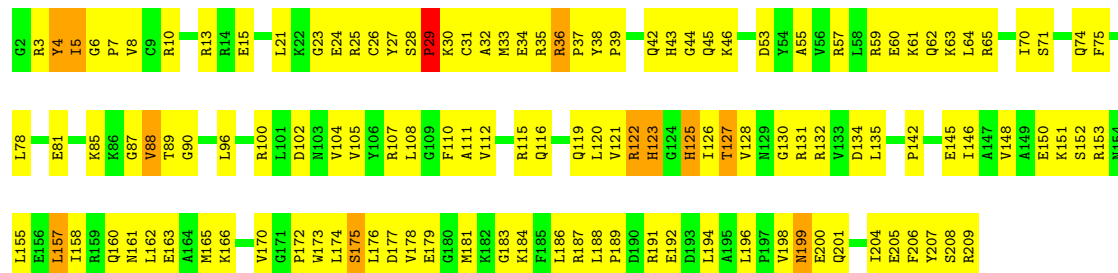
• Molecule 3: 30S ribosomal protein S3

Chain C:



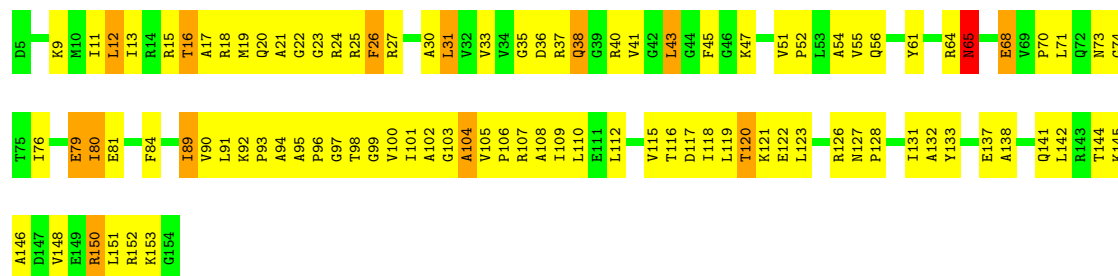
• Molecule 4: 30S ribosomal protein S4

Chain D:



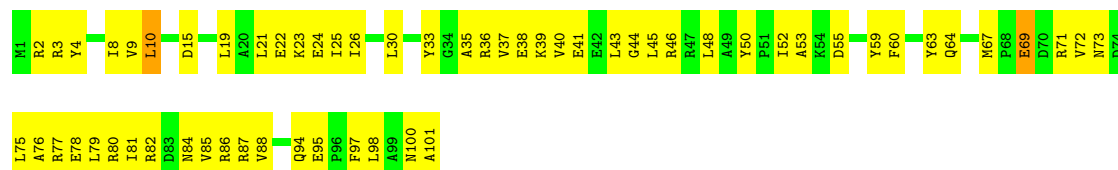
• Molecule 5: 30S ribosomal protein S5

Chain E:

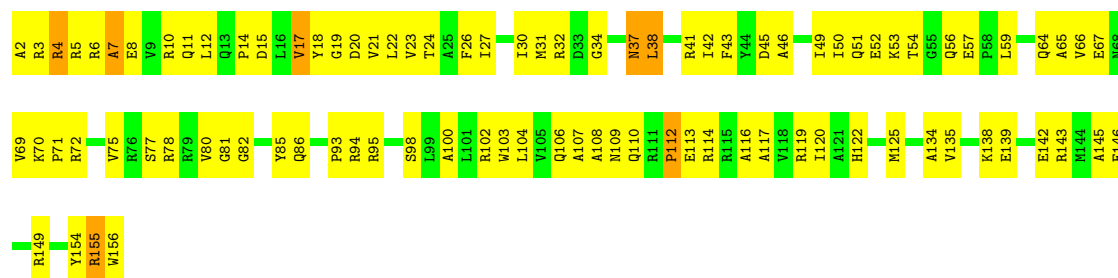


• Molecule 6: 30S ribosomal protein S6

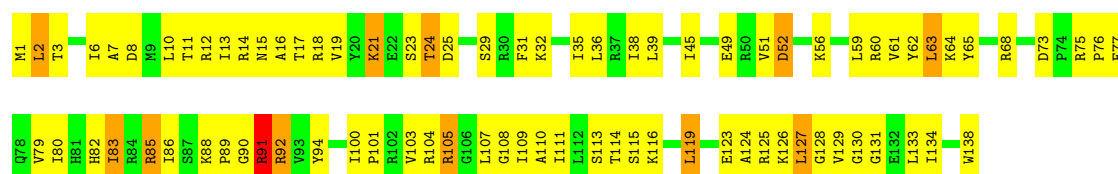
Chain F:



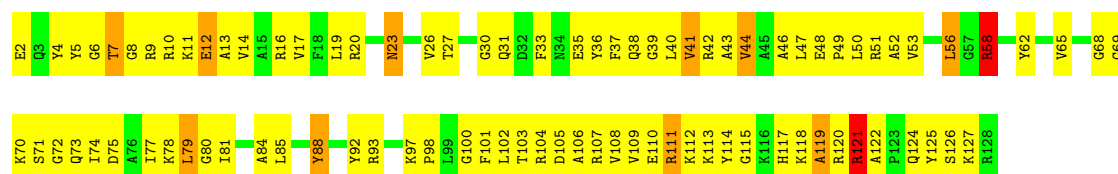
Chain G:



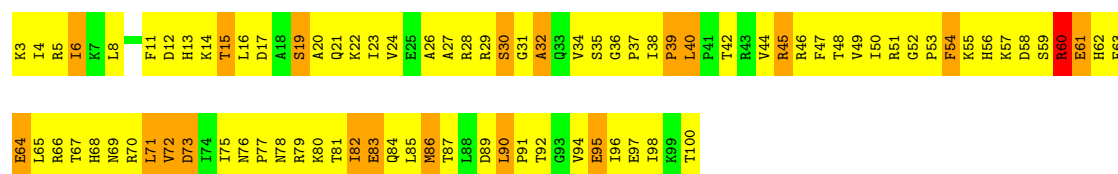
Chain H:



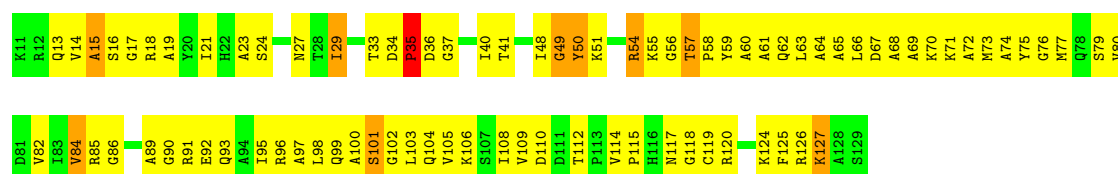
Chain I:



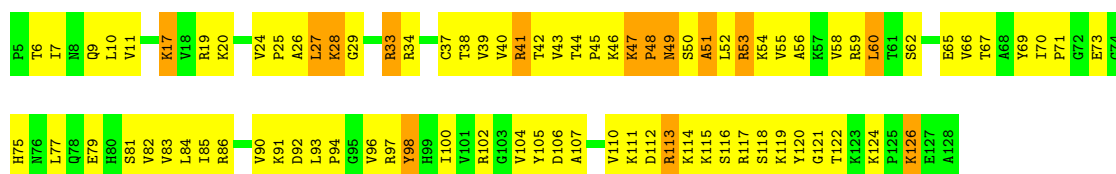
Chain J:



Chain K:

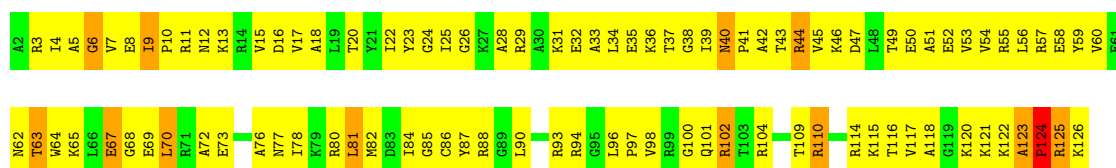


Chain L:



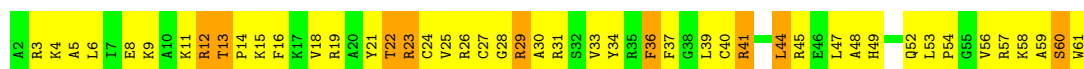
- Molecule 13: 30S ribosomal protein S13

Chain M:



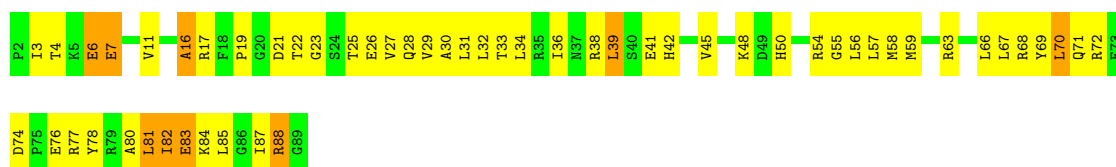
- Molecule 14: 30S ribosomal protein S14

Chain N:



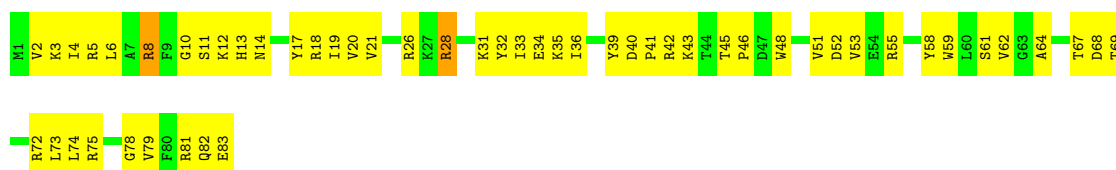
- Molecule 15: 30S ribosomal protein S15

Chain O:



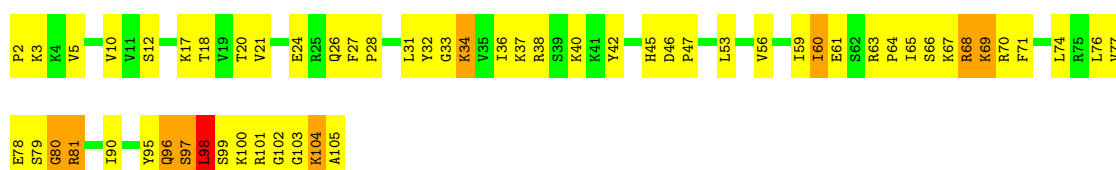
- Molecule 16: 30S ribosomal protein S16

Chain P:



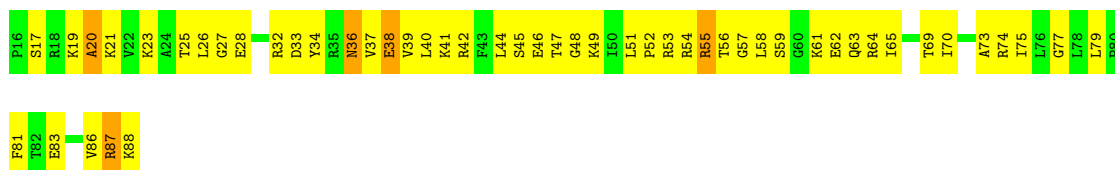
- Molecule 17: 30S ribosomal protein S17

Chain Q:



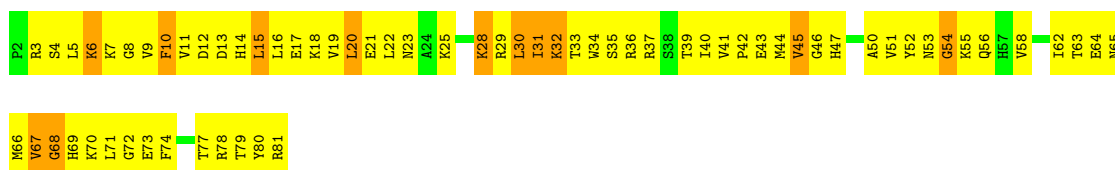
- Molecule 18: 30S ribosomal protein S18

Chain R:



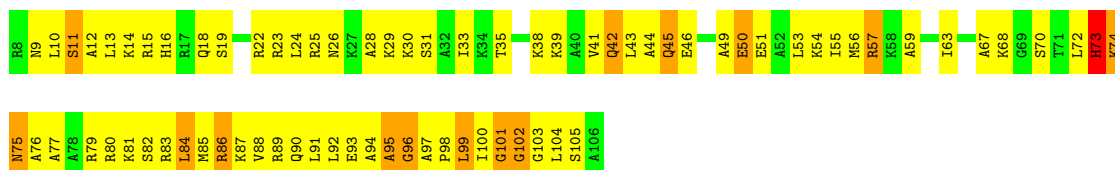
- Molecule 19: 30S ribosomal protein S19

Chain S:



- Molecule 20: 30S ribosomal protein S20

Chain T:



4 Data and refinement statistics

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

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, α , β , γ	683.89Å 683.89Å 386.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	70.00 – 9.50	Depositor
% Data completeness (in resolution range)	92.1 (70.00-9.50)	Depositor
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	9.49 (at 9.99Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.389 , 0.407	Depositor
Wilson B-factor (Å ²)	437.2	Xtriage
Anisotropy	0.460	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 26821 reflections	Xtriage
Total number of atoms	51951	wwPDB-VP
Average B, all atoms (Å ²)	590.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.90% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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	A	1.68	75/36823 (0.2%)	1.26	270/57351 (0.5%)
2	B	0.37	0/1935	0.68	1/2609 (0.0%)
3	C	0.38	0/1636	0.66	0/2205
4	D	0.37	0/1732	0.63	0/2318
5	E	0.49	0/1162	0.79	0/1564
6	F	0.33	0/855	0.62	0/1154
7	G	0.34	0/1275	0.62	0/1709
8	H	0.44	0/1135	0.74	0/1527
9	I	0.36	0/1028	0.62	0/1378
10	J	0.36	0/807	0.71	0/1085
11	K	0.39	0/899	0.70	0/1213
12	L	0.43	0/985	0.73	0/1317
13	M	0.36	0/1006	0.67	0/1344
14	N	0.40	0/500	0.78	0/664
15	O	0.36	0/744	0.63	1/992 (0.1%)
16	P	0.43	0/716	0.76	0/963
17	Q	0.44	0/869	0.75	0/1159
18	R	0.36	0/602	0.63	0/799
19	S	0.35	0/661	0.72	1/890 (0.1%)
20	T	0.39	0/764	0.73	0/1006
All	All	1.38	75/56134 (0.1%)	1.11	273/83247 (0.3%)

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	A	2	40

The worst 5 of 75 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	59	A	O3'-P	-120.85	0.16	1.61
1	A	1398	A	O3'-P	-86.38	0.57	1.61
1	A	214	U	O3'-P	-73.42	0.73	1.61
1	A	394	G	O3'-P	-71.42	0.75	1.61
1	A	1505	G	O3'-P	-71.04	0.76	1.61

The worst 5 of 273 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	59	A	P-O3'-C3'	-58.31	49.73	119.70
1	A	1490	C	P-O3'-C3'	40.44	168.23	119.70
1	A	651	C	P-O3'-C3'	-39.22	72.64	119.70
1	A	933	G	P-O3'-C3'	-35.50	77.10	119.70
1	A	1238	A	P-O3'-C3'	-35.04	77.65	119.70

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	181	G	C3'
1	A	1528	U	C3'

5 of 40 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	12	U	Sidechain
1	A	187	G	Sidechain
1	A	191	G	Sidechain
1	A	197	A	Sidechain
1	A	231	G	Sidechain

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	32939	0	16653	3366	0
2	B	1900	0	1951	209	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	1612	0	1675	286	0
4	D	1702	0	1767	217	2
5	E	1146	0	1207	255	0
6	F	842	0	855	75	2
7	G	1256	0	1296	138	2
8	H	1115	0	1177	126	0
9	I	1010	0	1043	183	0
10	J	794	0	839	206	2
11	K	884	0	904	81	0
12	L	970	0	1056	151	0
13	M	996	0	1068	169	0
14	N	491	0	529	153	0
15	O	733	0	771	57	0
16	P	700	0	720	78	0
17	Q	856	0	927	187	0
18	R	596	0	668	77	0
19	S	647	0	673	156	0
20	T	762	0	853	286	0
All	All	51951	0	36632	5224	4

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 59.

The worst 5 of 5224 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1278:U:H5''	1:A:1279:A:P	1.31	1.68
1:A:1458:G:C8	1:A:1459:C:H2'	1.27	1.63
1:A:191:G:C6	1:A:192:U:C2	1.90	1.60
1:A:1256:A:H5'	1:A:1258:G:C1'	1.26	1.56
1:A:130:A:C2	1:A:264:U:N1	1.72	1.55

All (4) 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	Distance(Å)	Clash(Å)
4:D:172:PRO:O	6:F:15:ASP:CB[3_555]	1.83	0.37
7:G:51:GLN:NE2	10:J:87:THR:OG1[4_555]	2.08	0.12
4:D:186:LEU:CD1	6:F:15:ASP:OD2[3_555]	2.14	0.06
7:G:57:GLU:OE2	10:J:89:ASP:OD1[4_555]	2.14	0.06

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%)	174 (75%)	34 (15%)	24 (10%)	1	19
3	C	204/206 (99%)	135 (66%)	40 (20%)	29 (14%)	0	11
4	D	206/208 (99%)	166 (81%)	31 (15%)	9 (4%)	4	47
5	E	148/150 (99%)	130 (88%)	13 (9%)	5 (3%)	6	55
6	F	99/101 (98%)	79 (80%)	19 (19%)	1 (1%)	22	80
7	G	153/155 (99%)	127 (83%)	16 (10%)	10 (6%)	2	35
8	H	136/138 (99%)	125 (92%)	7 (5%)	4 (3%)	7	58
9	I	125/127 (98%)	88 (70%)	27 (22%)	10 (8%)	1	28
10	J	96/98 (98%)	59 (62%)	20 (21%)	17 (18%)	0	6
11	K	117/119 (98%)	88 (75%)	20 (17%)	9 (8%)	1	29
12	L	120/124 (97%)	96 (80%)	15 (12%)	9 (8%)	2	30
13	M	121/125 (97%)	87 (72%)	26 (22%)	8 (7%)	2	35
14	N	58/60 (97%)	40 (69%)	11 (19%)	7 (12%)	1	14
15	O	86/88 (98%)	70 (81%)	11 (13%)	5 (6%)	3	38
16	P	81/83 (98%)	65 (80%)	15 (18%)	1 (1%)	19	77
17	Q	102/104 (98%)	84 (82%)	10 (10%)	8 (8%)	1	29
18	R	71/73 (97%)	62 (87%)	7 (10%)	2 (3%)	8	59
19	S	78/80 (98%)	48 (62%)	19 (24%)	11 (14%)	0	11
20	T	97/99 (98%)	65 (67%)	20 (21%)	12 (12%)	1	14
All	All	2330/2372 (98%)	1788 (77%)	361 (16%)	181 (8%)	1	29

5 of 181 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	8	LYS
2	B	9	GLU
2	B	15	VAL
2	B	16	HIS

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Mol	Chain	Res	Type
2	B	17	PHE

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%)	180 (89%)	22 (11%)	9	46
3	C	160/160 (100%)	142 (89%)	18 (11%)	9	43
4	D	180/180 (100%)	172 (96%)	8 (4%)	39	82
5	E	115/115 (100%)	100 (87%)	15 (13%)	6	36
6	F	90/90 (100%)	88 (98%)	2 (2%)	64	91
7	G	126/126 (100%)	122 (97%)	4 (3%)	51	87
8	H	119/119 (100%)	109 (92%)	10 (8%)	16	60
9	I	98/98 (100%)	90 (92%)	8 (8%)	17	61
10	J	88/88 (100%)	79 (90%)	9 (10%)	11	49
11	K	90/90 (100%)	84 (93%)	6 (7%)	23	70
12	L	104/104 (100%)	96 (92%)	8 (8%)	18	64
13	M	100/100 (100%)	90 (90%)	10 (10%)	11	50
14	N	49/49 (100%)	47 (96%)	2 (4%)	41	83
15	O	79/79 (100%)	72 (91%)	7 (9%)	14	57
16	P	72/72 (100%)	67 (93%)	5 (7%)	22	68
17	Q	96/96 (100%)	90 (94%)	6 (6%)	25	72
18	R	64/64 (100%)	61 (95%)	3 (5%)	36	80
19	S	71/71 (100%)	68 (96%)	3 (4%)	40	82
20	T	76/76 (100%)	69 (91%)	7 (9%)	13	55
All	All	1979/1979 (100%)	1826 (92%)	153 (8%)	18	64

5 of 153 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	H	2	LEU

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Mol	Chain	Res	Type
9	I	111	ARG
18	R	38	GLU
8	H	52	ASP
8	H	105	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 57 such sidechains are listed below:

Mol	Chain	Res	Type
6	F	64	GLN
9	I	23	ASN
18	R	36	ASN
6	F	94	GLN
7	G	37	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1487/1537 (96%)	218 (14%)	89 (5%)

5 of 218 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	6	G
1	A	8	A
1	A	9	G
1	A	31	G
1	A	32	A

5 of 89 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	559	A
1	A	792	A
1	A	1397	C
1	A	560	U
1	A	687	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 ⓘ

There are no ligands in this entry.

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.