



wwPDB X-ray Structure Validation Summary Report

Mar 31, 2014 – 05:36 PM BST

PDB ID : 2B9O
Title : 30S ribosomal subunit, tRNAs and mRNA from a crystal structure of the whole ribosomal complex with a stop codon in the A-site. This file contains the 30S subunit, tRNAs and mRNA from a crystal structure of the whole ribosomal complex with a stop codon in the A-site and is described in remark 400.
Authors : Petry, S.; Brodersen, D.E.; Murphy IV, F.V.; Dunham, C.M.; Selmer, M.; Tarry, M.J.; Kelley, A.C.; Ramakrishnan, V.
Deposited on : 2005-10-12
Resolution : 6.46 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>

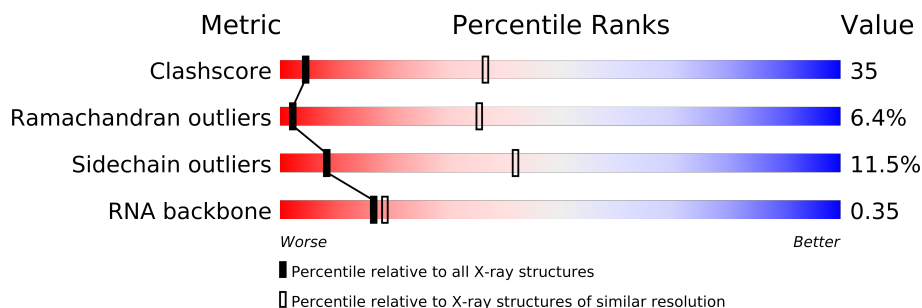
The following versions of software and data (see [references](#)) were used in the production of this report:

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 6.46 Å.



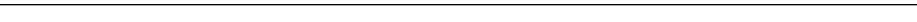


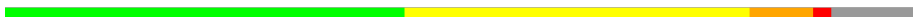


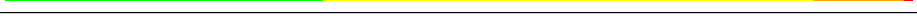



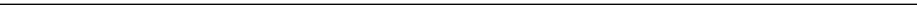


Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	79885	1033 (9.00-3.52)
Ramachandran outliers	78287	1289 (9.00-3.50)
Sidechain outliers	78261	1264 (9.00-3.50)
RNA backbone	1838	1045 (10.00-2.80)


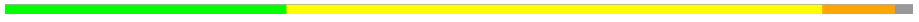


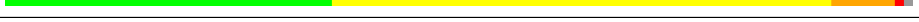

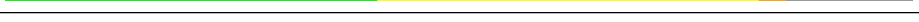

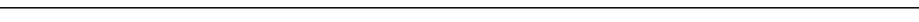
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The 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	1522	
2	V	76	
3	W	76	
4	X	18	
5	B	256	
6	C	239	
7	D	209	
8	E	162	
9	F	101	
10	G	156	
11	H	138	
12	I	128	
13	J	105	
14	K	129	
15	L	135	

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Mol	Chain	Length	Quality of chain
16	M	126	
17	N	61	
18	O	89	
19	P	88	
20	Q	105	
21	R	88	
22	S	93	
23	T	106	
24	U	27	

2 Entry composition

There are 24 unique types of molecules in this entry. The entry contains 55178 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	1515	Total	C	N	O	P	0	0	0
			32551	14490	6022	10525	1514			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	416	G	-	INSERTION	GB 155076
A	905	U	-	INSERTION	GB 155076
A	1395	C	-	INSERTION	GB 155076

- Molecule 2 is a RNA chain called P-site tRNA (Phe).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	V	76	Total	C	N	O	P	0	0	0
			1622	725	293	529	75			

- Molecule 3 is a RNA chain called E-site tRNA (Phe).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	W	76	Total	C	N	O	P	0	0	0
			1638	736	294	533	75			

- Molecule 4 is a RNA chain called 5'-D(*AP*UP*GP*UP*UP*CP*UP*AP*GP*UP*AP*C P*AP*AP*UP*AP*AP*U)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	X	17	Total	C	N	O	P	0	0	11
			136	56	19	44	17			

- Molecule 5 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	B	234	Total	C	N	O	S	0	0	0
			1900	1213	341	341	5			

- Molecule 6 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	C	206	Total	C	N	O	S	0	0	0
			1612	1016	314	281	1			

- Molecule 7 is a protein called 30S ribosomal protein S4.

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

- Molecule 8 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	E	150	Total	C	N	O	S	0	0	0
			1146	724	217	201	4			

- Molecule 9 is a protein called 30S ribosomal protein S6.

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

- Molecule 10 is a protein called 30S ribosomal protein S7.

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

- Molecule 11 is a protein called 30S ribosomal protein S8.

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

- Molecule 12 is a protein called 30S ribosomal protein S9.

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

- Molecule 13 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	J	98	Total	C	N	O	S			
			794	499	156	138	1	0	0	0

- Molecule 14 is a protein called 30S ribosomal protein S11.

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

- Molecule 15 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	L	124	Total	C	N	O	S			
			970	611	195	163	1	0	0	0

- Molecule 16 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	M	125	Total	C	N	O	S			
			997	617	207	171	2	0	0	0

- Molecule 17 is a protein called 30S ribosomal protein S14.

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

- Molecule 18 is a protein called 30S ribosomal protein S15.

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

- Molecule 19 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	P	83	Total	C	N	O	S	0	0	0
			700	443	139	117	1			

- Molecule 20 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	Q	104	Total	C	N	O	S	0	0	0
			857	547	161	147	2			

- Molecule 21 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	R	73	Total	C	N	O		0	0	0
			597	380	118	99				

- Molecule 22 is a protein called 30S ribosomal protein S19.

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

- Molecule 23 is a protein called 30S ribosomal protein S20.

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

- Molecule 24 is a protein called 30S ribosomal protein Thx.

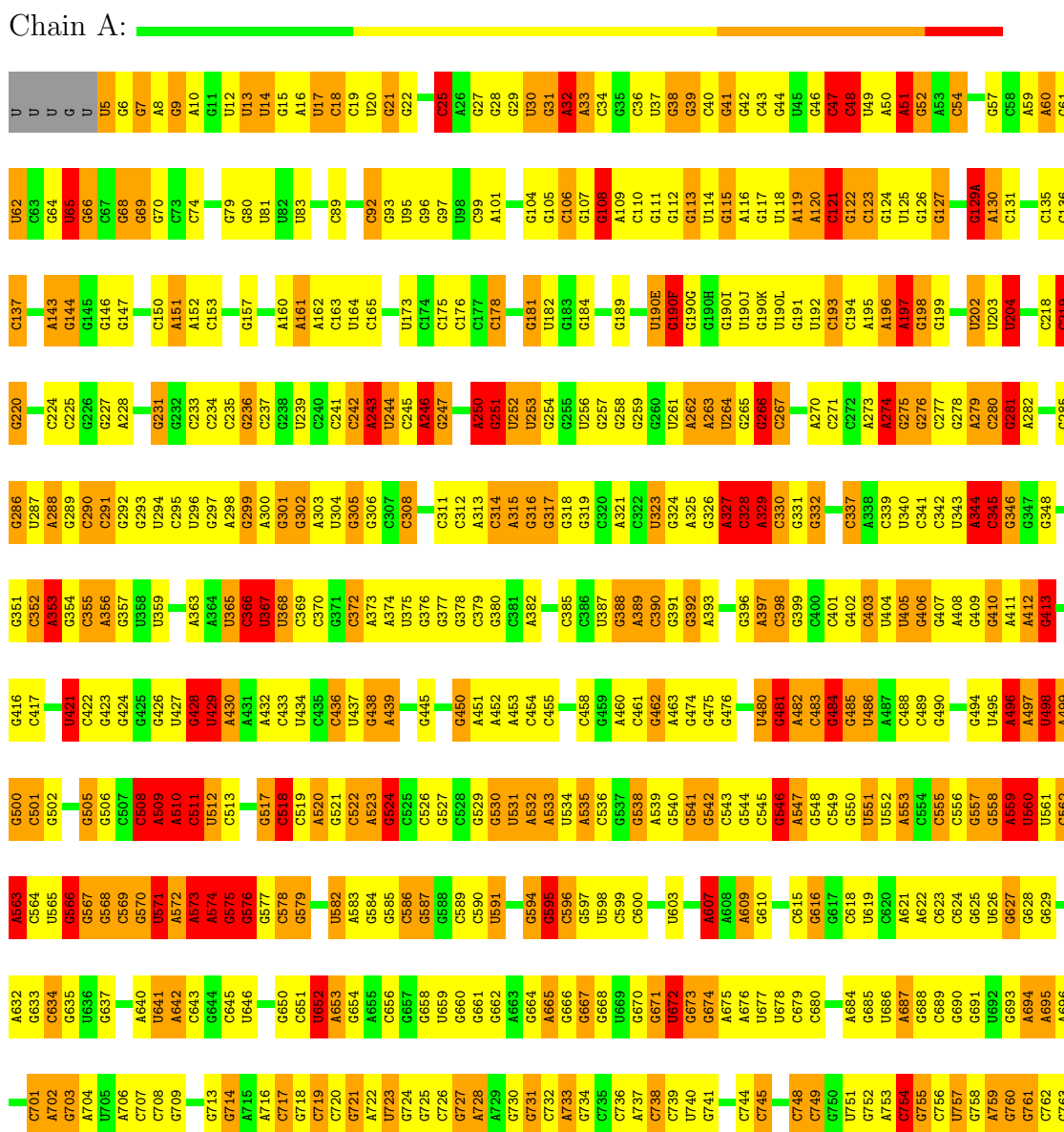
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	U	24	Total	C	N	O		0	0	0
			208	128	50	30				

3 Residue-property plots

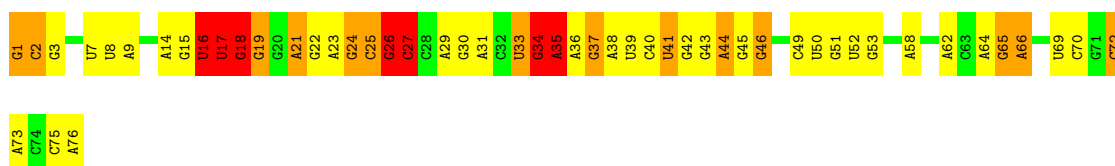
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

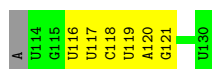






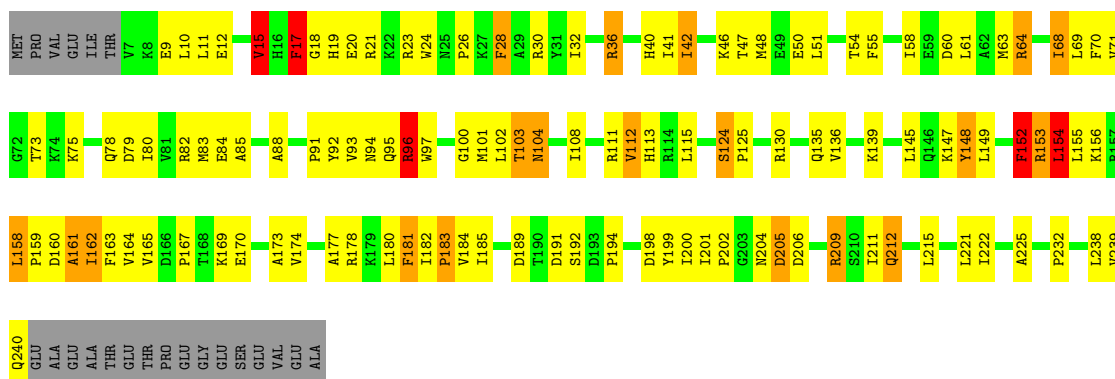
- Molecule 4: 5'-D(*AP*UP*GP*UP*UP*CP*UP*AP*GP*UP*AP*CP*AP*AP*UP*AP*AP*U)-3'

Chain X:



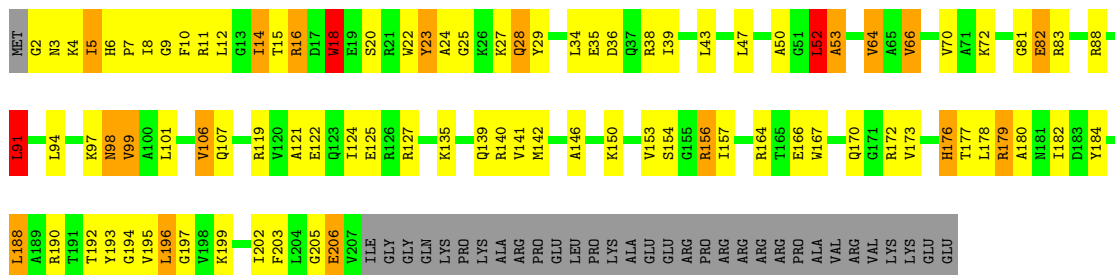
- Molecule 5: 30S ribosomal protein S2

Chain B:



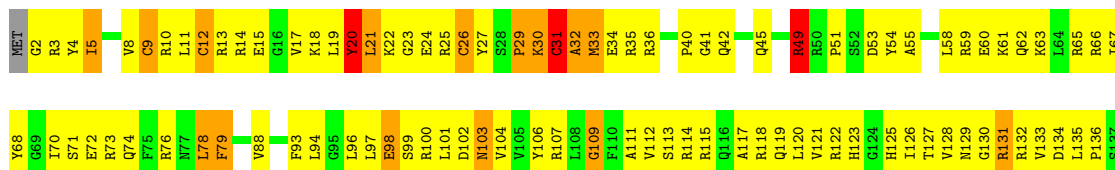
- Molecule 6: 30S ribosomal protein S3

Chain C:



- Molecule 7: 30S ribosomal protein S4

Chain D:





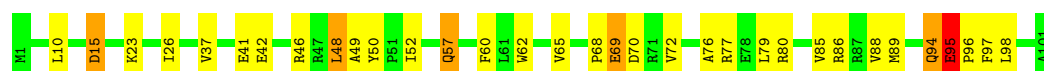
• Molecule 8: 30S ribosomal protein S5

Chain E:



• Molecule 9: 30S ribosomal protein S6

Chain F:



• Molecule 10: 30S ribosomal protein S7

Chain G:



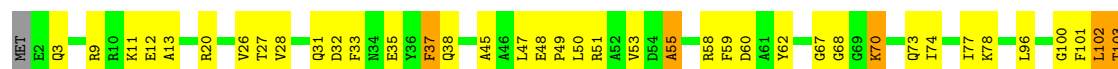
• Molecule 11: 30S ribosomal protein S8

Chain H:



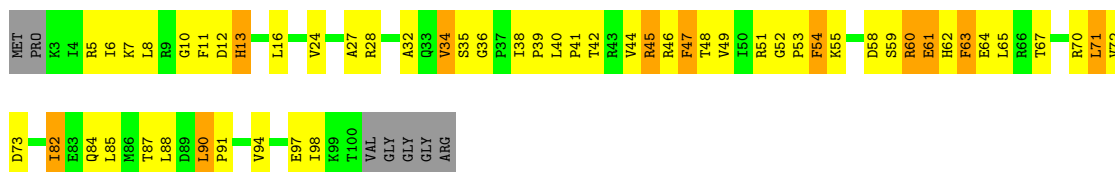
• Molecule 12: 30S ribosomal protein S9

Chain I:



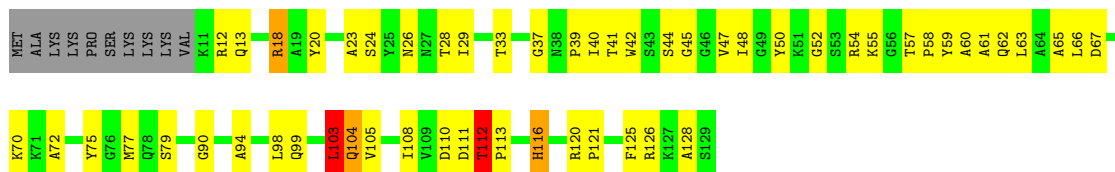
• Molecule 13: 30S ribosomal protein S10

Chain J:



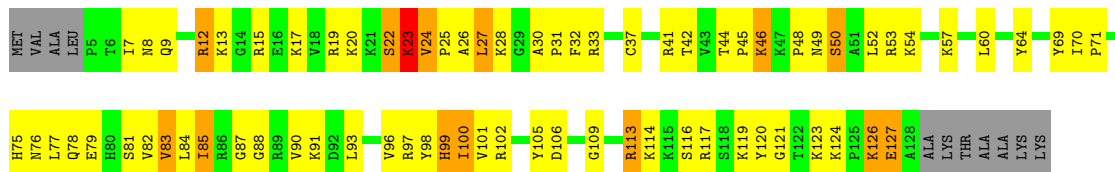
- Molecule 14: 30S ribosomal protein S11

Chain K:



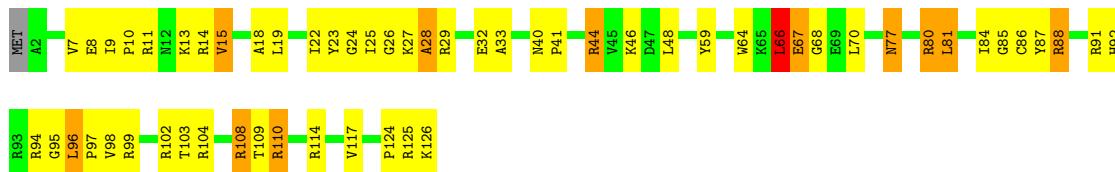
- Molecule 15: 30S ribosomal protein S12

Chain L:



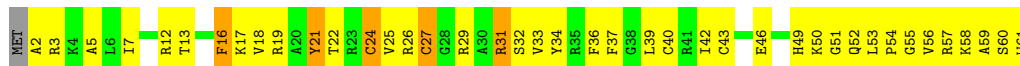
- Molecule 16: 30S ribosomal protein S13

Chain M:



- Molecule 17: 30S ribosomal protein S14

Chain N:



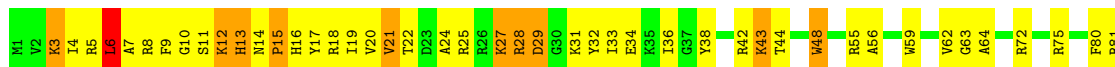
- Molecule 18: 30S ribosomal protein S15

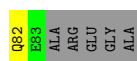
Chain O:



- Molecule 19: 30S ribosomal protein S16

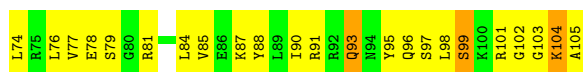
Chain P:





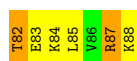
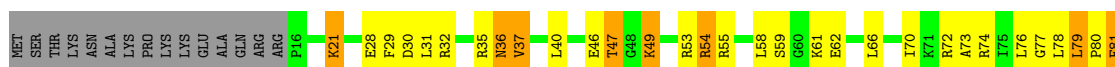
- Molecule 20: 30S ribosomal protein S17

Chain Q:



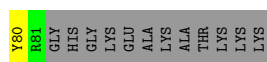
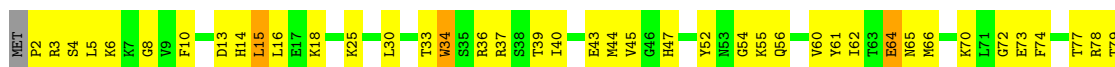
- Molecule 21: 30S ribosomal protein S18

Chain R:



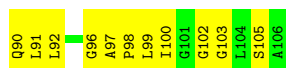
- Molecule 22: 30S ribosomal protein S19

Chain S:



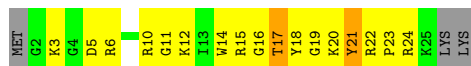
- Molecule 23: 30S ribosomal protein S20

Chain T:



- Molecule 24: 30S ribosomal protein Thx

Chain U:



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	517.41Å 517.41Å 365.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 6.46	Depositor
% Data completeness (in resolution range)	99.9 (40.00-6.46)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.87 (at 6.19Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.354 , 0.361	Depositor
Wilson B-factor (Å ²)	240.8	Xtriage
Anisotropy	0.222	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 123103 reflections	Xtriage
Total number of atoms	55178	wwPDB-VP
Average B, all atoms (Å ²)	354.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.58% 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: YYG, PSU

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	1.32	68/36413 (0.2%)	1.49	439/56777 (0.8%)
2	V	0.74	3/1812 (0.2%)	1.20	8/2819 (0.3%)
3	W	1.81	19/1739 (1.1%)	2.15	47/2698 (1.7%)
4	X	0.18	0/139	0.67	0/213
5	B	0.60	2/1935 (0.1%)	0.61	0/2609
6	C	0.73	2/1636 (0.1%)	0.61	4/2205 (0.2%)
7	D	0.70	4/1733 (0.2%)	1.03	11/2318 (0.5%)
8	E	0.83	1/1162 (0.1%)	0.63	1/1564 (0.1%)
9	F	0.35	0/856	0.54	0/1154
10	G	0.34	0/1276	0.59	3/1709 (0.2%)
11	H	0.41	0/1136	0.66	0/1527
12	I	0.34	0/1029	0.54	0/1378
13	J	0.35	0/807	0.56	0/1085
14	K	0.59	1/900 (0.1%)	0.54	0/1213
15	L	1.33	1/986 (0.1%)	1.11	3/1320 (0.2%)
16	M	0.92	1/1007 (0.1%)	0.59	1/1344 (0.1%)
17	N	0.49	1/501 (0.2%)	0.65	1/664 (0.2%)
18	O	0.32	0/745	0.54	0/992
19	P	0.40	0/716	0.59	1/963 (0.1%)
20	Q	1.23	2/870 (0.2%)	1.38	6/1159 (0.5%)
21	R	0.40	0/603	0.70	0/799
22	S	0.34	0/661	0.53	0/890
23	T	0.32	0/764	0.57	1/1006 (0.1%)
24	U	0.33	0/212	0.49	0/277
All	All	1.15	105/59638 (0.2%)	1.33	526/88683 (0.6%)

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
3	W	1	5
5	B	0	1
6	C	0	1
7	D	0	1
14	K	0	1
15	L	0	1
20	Q	0	1
All	All	1	11

The worst 5 of 105 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1278	U	O3'-P	-56.53	0.93	1.61
1	A	1337	G	O3'-P	-53.91	0.96	1.61
1	A	1004	A	O3'-P	48.18	2.19	1.61
1	A	1224	G	O3'-P	47.01	2.17	1.61
1	A	219	C	O3'-P	46.80	2.17	1.61

The worst 5 of 526 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	W	65	G	P-O3'-C3'	-50.68	58.88	119.70
2	V	65	G	P-O3'-C3'	39.88	167.56	119.70
1	A	1255	G	P-O3'-C3'	-38.36	73.67	119.70
1	A	983	A	P-O3'-C3'	-29.74	84.01	119.70
3	W	33	U	P-O3'-C3'	27.31	152.47	119.70

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	W	37	YYG	C15

5 of 11 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	W	16	U	Sidechain
3	W	17	U	Sidechain
3	W	18	G	Sidechain
3	W	19	G	Sidechain
3	W	62	A	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	32551	0	16459	2025	0
2	V	1622	0	821	167	0
3	W	1638	0	837	201	0
4	X	136	0	63	26	0
5	B	1900	0	1950	97	0
6	C	1612	0	1675	99	0
7	D	1703	0	1761	289	0
8	E	1146	0	1206	68	0
9	F	843	0	857	30	0
10	G	1257	0	1295	102	0
11	H	1116	0	1177	100	0
12	I	1011	0	1040	80	0
13	J	794	0	840	81	0
14	K	885	0	904	53	0
15	L	970	0	1056	72	0
16	M	997	0	1070	143	0
17	N	492	0	529	82	0
18	O	734	0	771	28	0
19	P	700	0	720	70	0
20	Q	857	0	928	80	0
21	R	597	0	668	40	0
22	S	647	0	673	155	0
23	T	762	0	859	37	0
24	U	208	0	221	84	0
All	All	55178	0	38380	3246	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 35.

The worst 5 of 3246 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:409:G:H5''	7:D:25:ARG:CB	1.17	1.63
1:A:1268:A:H4'	24:U:20:LYS:CA	1.27	1.60
2:V:31:A:C5'	12:I:127:LYS:HD2	1.21	1.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:V:31:A:P	12:I:127:LYS:HE3	1.43	1.58
2:V:35:A:C2	4:X:118:C:N3	1.70	1.57

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	
5	B	232/256 (91%)	183 (79%)	33 (14%)	16 (7%)	2	32
6	C	204/239 (85%)	166 (81%)	24 (12%)	14 (7%)	2	32
7	D	206/209 (99%)	157 (76%)	33 (16%)	16 (8%)	1	28
8	E	148/162 (91%)	116 (78%)	29 (20%)	3 (2%)	11	67
9	F	99/101 (98%)	85 (86%)	10 (10%)	4 (4%)	5	49
10	G	153/156 (98%)	131 (86%)	18 (12%)	4 (3%)	8	60
11	H	136/138 (99%)	101 (74%)	25 (18%)	10 (7%)	2	30
12	I	125/128 (98%)	86 (69%)	31 (25%)	8 (6%)	2	35
13	J	96/105 (91%)	73 (76%)	14 (15%)	9 (9%)	1	23
14	K	117/129 (91%)	88 (75%)	22 (19%)	7 (6%)	2	37
15	L	122/135 (90%)	90 (74%)	13 (11%)	19 (16%)	0	8
16	M	121/126 (96%)	95 (78%)	20 (16%)	6 (5%)	3	42
17	N	58/61 (95%)	42 (72%)	12 (21%)	4 (7%)	2	32
18	O	86/89 (97%)	76 (88%)	9 (10%)	1 (1%)	19	77
19	P	81/88 (92%)	64 (79%)	11 (14%)	6 (7%)	2	30
20	Q	102/105 (97%)	78 (76%)	18 (18%)	6 (6%)	2	38
21	R	71/88 (81%)	54 (76%)	11 (16%)	6 (8%)	1	26
22	S	78/93 (84%)	60 (77%)	15 (19%)	3 (4%)	5	50
23	T	97/106 (92%)	79 (81%)	12 (12%)	6 (6%)	2	36
24	U	22/27 (82%)	17 (77%)	3 (14%)	2 (9%)	1	24

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	2354/2541 (93%)	1841 (78%)	363 (15%)	150 (6%)	2	35

5 of 150 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	B	24	TRP
5	B	104	ASN
5	B	153	ARG
5	B	154	LEU
5	B	161	ALA

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	
5	B	202/220 (92%)	173 (86%)	29 (14%)	5	31
6	C	160/188 (85%)	146 (91%)	14 (9%)	14	57
7	D	180/181 (99%)	162 (90%)	18 (10%)	11	50
8	E	115/123 (94%)	94 (82%)	21 (18%)	2	17
9	F	90/90 (100%)	83 (92%)	7 (8%)	18	63
10	G	126/127 (99%)	116 (92%)	10 (8%)	18	62
11	H	119/119 (100%)	92 (77%)	27 (23%)	1	10
12	I	98/99 (99%)	90 (92%)	8 (8%)	17	60
13	J	88/92 (96%)	77 (88%)	11 (12%)	7	38
14	K	90/99 (91%)	85 (94%)	5 (6%)	30	75
15	L	104/111 (94%)	93 (89%)	11 (11%)	10	47
16	M	100/101 (99%)	87 (87%)	13 (13%)	6	36
17	N	49/50 (98%)	43 (88%)	6 (12%)	7	39
18	O	79/80 (99%)	70 (89%)	9 (11%)	8	42
19	P	72/74 (97%)	62 (86%)	10 (14%)	5	33
20	Q	96/97 (99%)	87 (91%)	9 (9%)	13	53
21	R	64/77 (83%)	57 (89%)	7 (11%)	9	46

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
22	S	71/80 (89%)	64 (90%)	7 (10%)	11	50
23	T	76/82 (93%)	68 (90%)	8 (10%)	10	47
24	U	19/22 (86%)	19 (100%)	0	100	100
All	All	1998/2112 (95%)	1768 (88%)	230 (12%)	8	42

5 of 230 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	H	18	ARG
12	I	47	LEU
21	R	54	ARG
11	H	37	ARG
11	H	77	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 49 such sidechains are listed below:

Mol	Chain	Res	Type
10	G	64	GLN
12	I	3	GLN
22	S	47	HIS
10	G	106	GLN
12	I	87	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1497/1522 (98%)	520 (34%)	164 (10%)
2	V	73/76 (96%)	16 (21%)	1 (1%)
3	W	70/76 (92%)	16 (22%)	3 (4%)
4	X	5/18 (27%)	0	0
All	All	1645/1692 (97%)	552 (33%)	168 (10%)

5 of 552 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	6	G
1	A	7	G
1	A	8	A
1	A	9	G

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Mol	Chain	Res	Type
1	A	12	U

5 of 168 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	702	A
1	A	873	A
1	A	1490	C
1	A	721	G
1	A	793	U

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

3 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	YYG	W	37	10,3	40,42,43	1.10	4 (10%)	50,62,65	11.21	11 (22%)
3	PSU	W	39	3	19,21,22	0.90	1 (5%)	23,30,33	0.88	1 (4%)
3	PSU	W	55	3	19,21,22	1.13	3 (15%)	23,30,33	1.06	2 (8%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	YYG	W	37	10,3	1/1/8/9	0/25/42/43	0/1/4/4
3	PSU	W	39	3	-	0/8/25/26	0/2/2/2
3	PSU	W	55	3	-	0/8/25/26	0/2/2/2

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	W	37	YYG	C6-N1	2.76	1.42	1.35
3	W	39	PSU	C6-C5	-2.72	1.33	1.38
3	W	37	YYG	P-OP1	2.43	1.49	1.46
3	W	37	YYG	C2-N1	-2.38	1.36	1.39
3	W	55	PSU	C6-C5	-2.37	1.34	1.38

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	W	37	YYG	C6-C5-N7	-76.04	130.19	134.24
3	W	37	YYG	C11-C12-N1	18.61	111.41	104.24
3	W	37	YYG	C24-O23-C21	5.80	123.13	115.66
3	W	37	YYG	C13-C12-C11	-5.34	123.52	131.05
3	W	37	YYG	O23-C21-N20	4.04	118.48	110.72

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	W	37	YYG	C15

There are no torsion outliers.

There are no ring outliers.

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.