



wwPDB X-ray Structure Validation Summary Report

Mar 31, 2014 – 05:43 PM BST

PDB ID : 2B9M
Title : 30S ribosomal subunit, tRNAs, mRNA and release factor RF2 from a crystal structure of the whole ribosomal complex. This file contains the 30S ribosomal subunit, tRNAs, mRNA and release factor RF2 from a crystal structure of the whole ribosomal complex". The entire crystal structure contains one 70S ribosome, tRNAs, mRNA and release factor RF2 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 : 6.76 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>

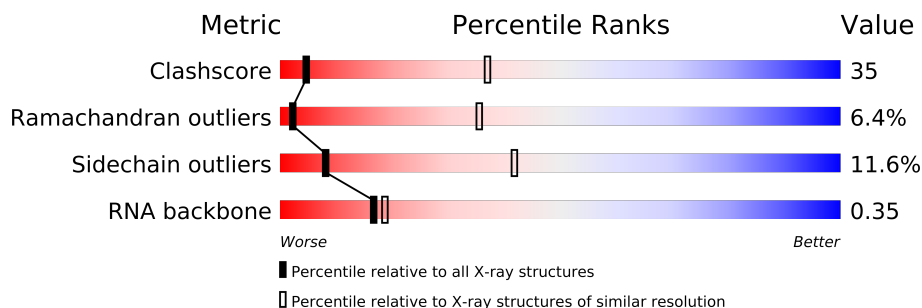
The following versions of software and data (see [references](#)) were used in the production of this report:

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 6.76 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 (10.00-3.52)
Ramachandran outliers	78287	1291 (9.50-3.50)
Sidechain outliers	78261	1265 (9.50-3.50)
RNA backbone	1838	1045 (10.00-2.80)


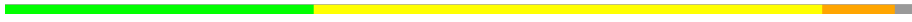


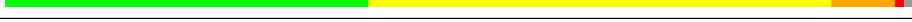

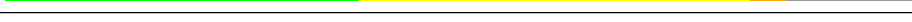

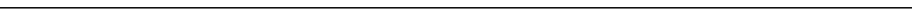

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The 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	

Continued on next page...

Continued from previous page...

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	
25	Y	365	

2 Entry composition

There are 25 unique types of molecules in this entry. The entry contains 55543 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*AP*UP*A
P*CP*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

- 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

- 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

- 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

- 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

- 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

- 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	S	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	S	0	0	0
			208	128	50	30				

- Molecule 25 is a protein called Peptide chain release factor 2.

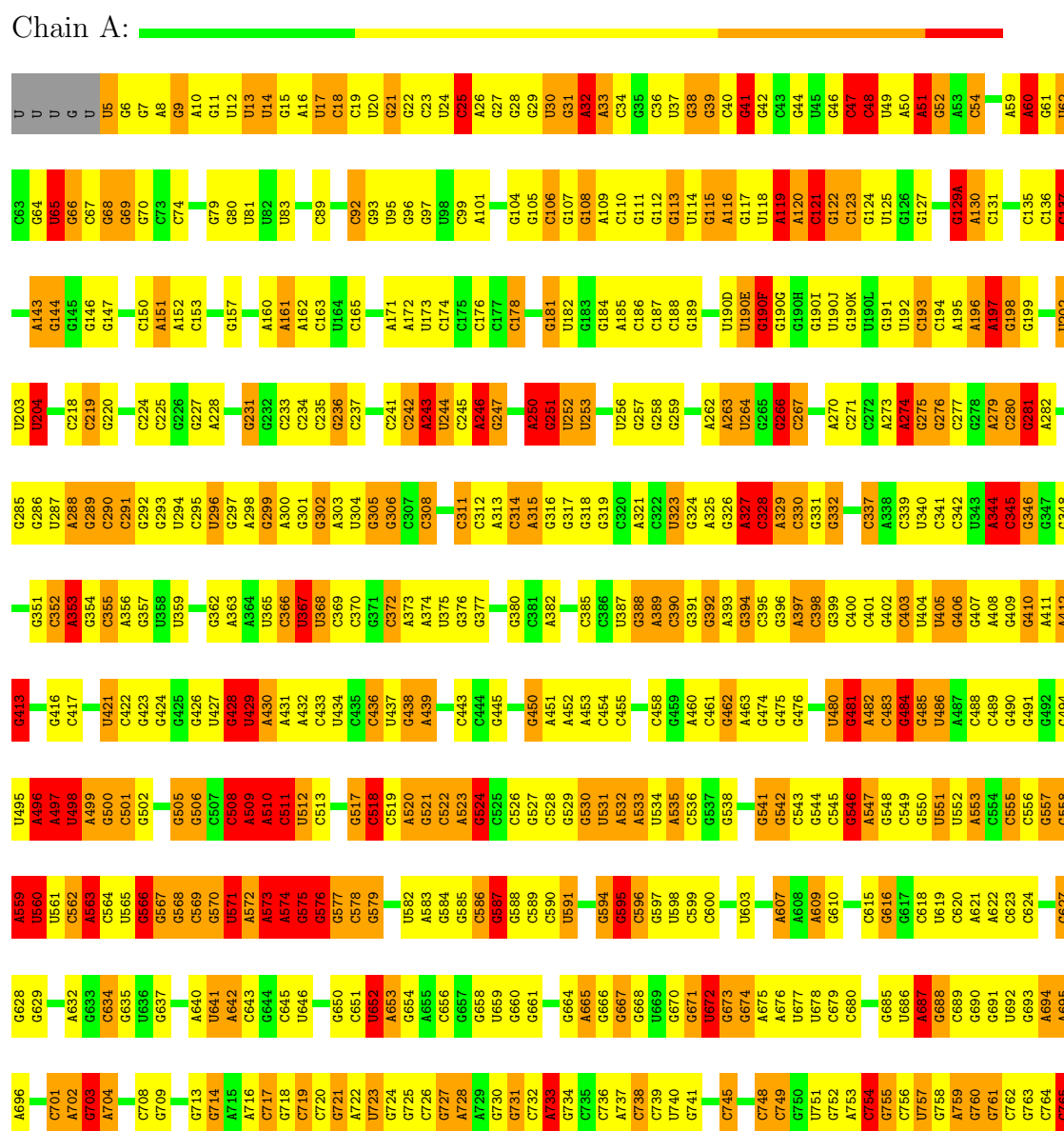
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
25	Y	365	Total	C	0	0	365
			365	365			

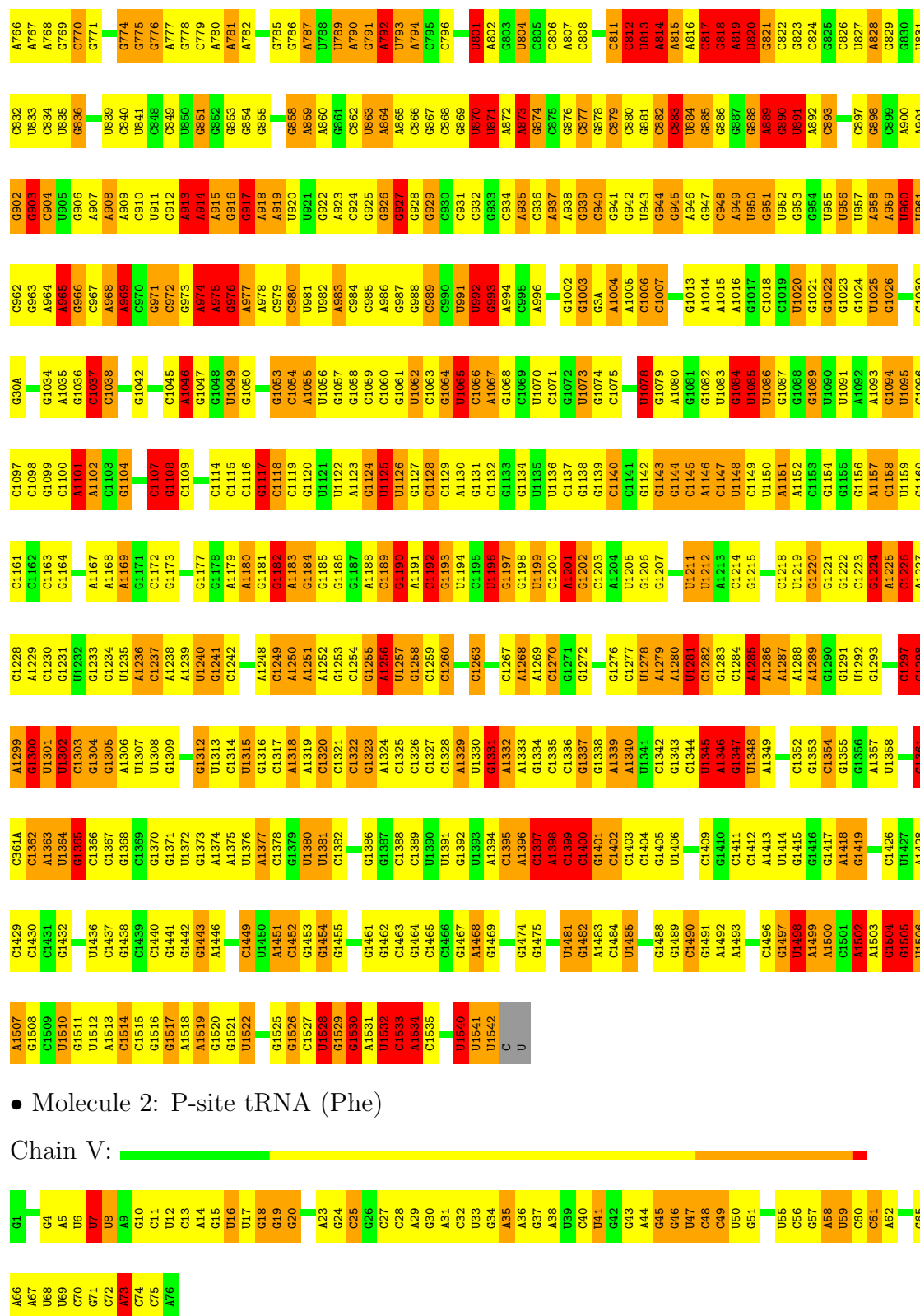
3 Residue-property plots

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

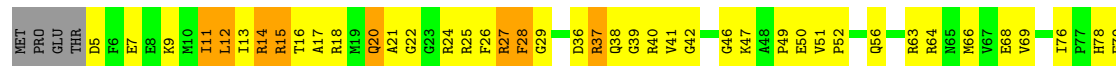






• Molecule 8: 30S ribosomal protein S5

Chain E:



• Molecule 9: 30S ribosomal protein S6

Chain F:



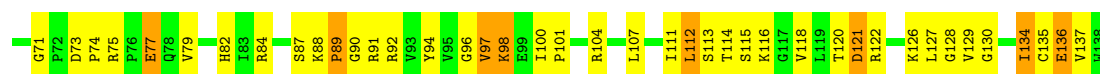
• Molecule 10: 30S ribosomal protein S7

Chain G:



• Molecule 11: 30S ribosomal protein S8

Chain H:



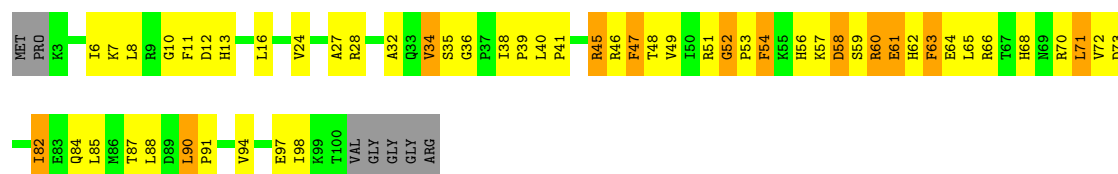
• Molecule 12: 30S ribosomal protein S9

Chain I:



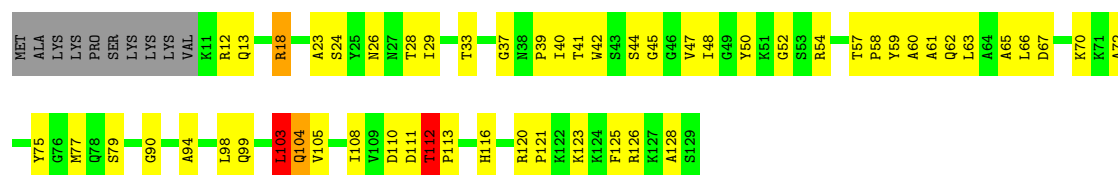
• Molecule 13: 30S ribosomal protein S10

Chain J:



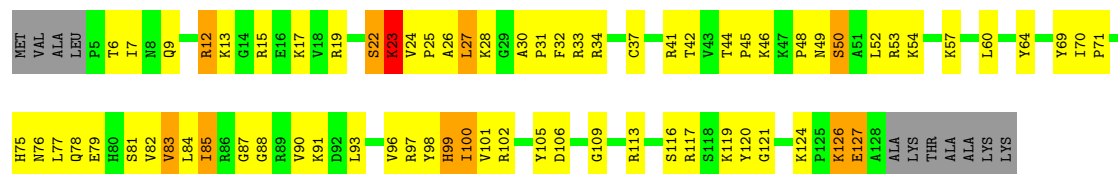
• Molecule 14: 30S ribosomal protein S11

Chain K:



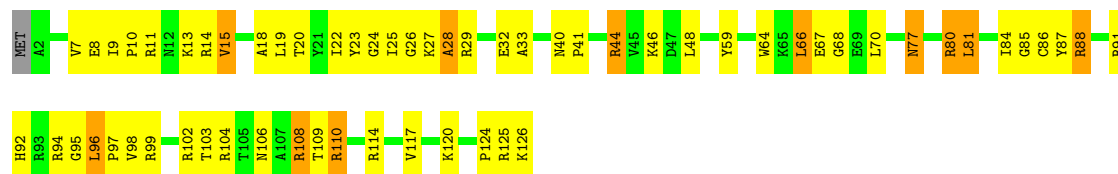
• Molecule 15: 30S ribosomal protein S12

Chain L:



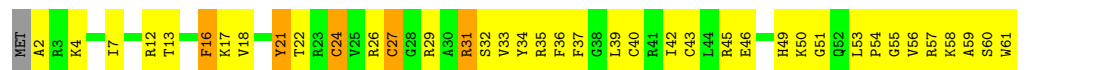
• Molecule 16: 30S ribosomal protein S13

Chain M:



• Molecule 17: 30S ribosomal protein S14

Chain N:



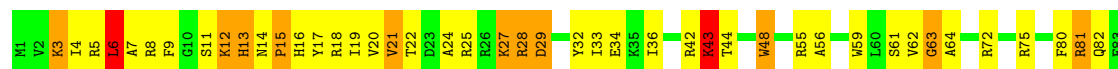
• Molecule 18: 30S ribosomal protein S15

Chain O:



• Molecule 19: 30S ribosomal protein S16

Chain P:



ALA
ARG
GLU
GLY
ALA

- Molecule 20: 30S ribosomal protein S17

Chain Q:

MET P2 K3 K4 V5 G8 V9 V10 V11 M15 T18 V19 T20 T21 V22 V23 E24 E25 H29 G33 K34 V35 I36 I37 R38 R39 S39 K40 K41 Y42 Y43 A44 H45 D46 P47 E48 G54 D55 V56 V57 E58 I59 I60 E61 S62 R63 P64 I65 S66 K67 R68 K69 R70 L74

R75 L76 V77 E78 S79 G80 R81 L84 V85 E86 K87 Y88 L89 I90 R91 Q92 Q93 N94 Y95 Q96 S97 S99 K100 R101 G102 G103 K104 A105

- Molecule 21: 30S ribosomal protein S18

Chain R:

MET SER THR LYS ASN ALA LYS PRO LYS LYS GLU GLN ARG ARG P16 K21 E28 P29 D30 L31 R32 R33 Y34 R35 N36 V37 L40 E46 T47 G48 K49 R53 R54 R55 L58 S59 G60 K61 E62 L66 I70 K71 R72 A73 R74 I75 L76 G77 L78 P80

F81 T82 E83 K84 L85 V86 R87 K88

- Molecule 22: 30S ribosomal protein S19

Chain S:

MET P2 R3 S4 L5 K6 K7 G8 F10 D13 H14 L15 L16 E17 K18 K25 L30 T33 N34 S35 R36 R37 S38 T39 I40 E43 M44 Y45 G46 H47 Y52 N53 G54 K55 Q56 V60 Y61 T62 T63 E64 N65 M66 K70 L71 G72 E73 F74 T77 R78 T79

Y80 R81 GLY HIS GLY LYS GLU ALA THR LYS LYS

- Molecule 23: 30S ribosomal protein S20

Chain T:

MET ALA GLN LYS PRO LYS R8 Q18 R23 R26 R27 A28 K29 K30 I33 K34 V41 Q45 K48 A49 E50 E60 S61 L62 I63 D64 K65 A66 A67 K68 G69 S70 T71 L72 H73 K74 N75 A76 A77 A78 R79 R80 K81 S82 R83 L84 M85 R86 K87 V88 R89

Q90 L91 L92 G96 A97 P98 L99 I100 G101 G102 G103 L104 S105 A106

- Molecule 24: 30S ribosomal protein Thx

Chain U:

MET G2 K3 G4 D5 R6 R10 G11 K12 R15 G16 T17 Y18 G19 K20 Y21 R22 P23 R24 K25 LYS

- Molecule 25: Peptide chain release factor 2

Chain Y:

There are no outlier residues recorded for this chain.

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	520.21Å 520.21Å 365.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.35 – 6.76	Depositor
% Data completeness (in resolution range)	96.2 (43.35-6.76)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.19	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.11 (at 6.14Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.341 , 0.356	Depositor
Wilson B-factor (Å ²)	233.6	Xtriage
Anisotropy	0.105	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.37$, $\langle L^2 \rangle = 0.20$	Xtriage
Outliers	0 of 112763 reflections	Xtriage
Total number of atoms	55543	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 2.50% 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	1.34	66/36411 (0.2%)	1.47	428/56769 (0.8%)
2	V	1.58	5/1814 (0.3%)	1.08	11/2827 (0.4%)
3	W	1.77	16/1737 (0.9%)	1.68	30/2690 (1.1%)
4	X	0.18	0/139	0.66	0/213
5	B	0.61	2/1935 (0.1%)	0.61	0/2609
6	C	0.43	1/1636 (0.1%)	1.10	6/2205 (0.3%)
7	D	0.79	5/1733 (0.3%)	1.09	11/2318 (0.5%)
8	E	0.92	1/1162 (0.1%)	0.63	2/1564 (0.1%)
9	F	0.35	0/856	0.54	0/1154
10	G	0.33	0/1276	0.76	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	0.64	1/900 (0.1%)	0.56	0/1213
15	L	0.99	1/986 (0.1%)	0.70	1/1320 (0.1%)
16	M	0.35	0/1006	0.56	0/1341
17	N	0.49	0/501	0.64	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	1.20	3/870 (0.3%)	1.54	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	0.31	0/764	0.57	1/1006 (0.1%)
24	U	0.34	0/212	0.49	0/277
All	All	1.18	101/59635 (0.2%)	1.30	501/88672 (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
6	C	0	1
14	K	0	1
20	Q	0	1
All	All	1	8

The worst 5 of 101 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1037	C	O3'-P	-82.19	0.62	1.61
1	A	1255	G	O3'-P	-72.80	0.73	1.61
1	A	1224	G	O3'-P	43.87	2.13	1.61
1	A	1046	A	O3'-P	43.16	2.12	1.61
1	A	1107	C	O3'-P	42.57	2.12	1.61

The worst 5 of 501 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	W	33	U	P-O3'-C3'	27.30	152.45	119.70
3	W	35	A	P-O3'-C3'	27.16	152.29	119.70
20	Q	22	LEU	O-C-N	27.15	166.15	122.70
1	A	1073	U	P-O3'-C3'	-25.83	88.70	119.70
2	V	73	A	P-O3'-C3'	-24.87	89.86	119.70

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	W	37	YYG	C15

5 of 8 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	16464	2019	0
2	V	1622	0	820	134	0
3	W	1638	0	836	141	0
4	X	136	0	63	22	0
5	B	1900	0	1950	92	0
6	C	1612	0	1675	113	0
7	D	1703	0	1760	288	0
8	E	1146	0	1206	59	0
9	F	843	0	857	49	0
10	G	1257	0	1295	94	0
11	H	1116	0	1177	99	0
12	I	1011	0	1040	89	0
13	J	794	0	840	105	0
14	K	885	0	904	55	0
15	L	970	0	1056	74	0
16	M	997	0	1070	175	0
17	N	492	0	529	95	0
18	O	734	0	771	30	0
19	P	700	0	720	78	0
20	Q	857	0	928	53	0
21	R	597	0	668	52	0
22	S	647	0	672	215	0
23	T	762	0	859	33	0
24	U	208	0	221	75	0
25	Y	365	0	0	0	0
All	All	55543	0	38381	3223	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 3223 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1320:C:C1'	22:S:73:GLU:HG2	1.23	1.60
1:A:409:G:H5''	7:D:25:ARG:CB	1.29	1.57
16:M:92:HIS:CD2	16:M:98:VAL:HG21	1.42	1.55
1:A:986:A:C1'	22:S:55:LYS:HA	1.31	1.54
3:W:37:YYG:H192	10:G:84:ASN:CA	1.12	1.54

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%)	34 (15%)	15 (6%)	2	35
6	C	204/239 (85%)	165 (81%)	23 (11%)	16 (8%)	1	28
7	D	206/209 (99%)	156 (76%)	33 (16%)	17 (8%)	1	26
8	E	148/162 (91%)	115 (78%)	29 (20%)	4 (3%)	8	60
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%)	87 (70%)	30 (24%)	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%)	92 (75%)	13 (11%)	17 (14%)	0	11
16	M	119/126 (94%)	95 (80%)	19 (16%)	5 (4%)	4	47
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%)	10 (12%)	7 (9%)	1	25
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	51
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
All	All	2352/2541 (93%)	1841 (78%)	360 (15%)	151 (6%)	2	35

5 of 151 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%)	91 (76%)	28 (24%)	1	9
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
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%)	1767 (88%)	231 (12%)	8	42

5 of 231 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	84	ARG

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

Mol	Chain	Res	Type
9	F	94	GLN
12	I	3	GLN
22	S	56	GLN
10	G	68	ASN
12	I	87	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1496/1522 (98%)	518 (34%)	159 (10%)
2	V	75/76 (98%)	17 (22%)	2 (2%)
3	W	68/76 (89%)	13 (19%)	4 (5%)
4	X	5/18 (27%)	0	0
All	All	1644/1692 (97%)	548 (33%)	165 (10%)

5 of 548 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
1	A	12	U

5 of 165 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	701	C
1	A	872	A
1	A	1502	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	718	G
1	A	792	A

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	1.11	4 (10%)	50,62,65	11.14	11 (22%)
3	PSU	W	39	3	19,21,22	0.92	1 (5%)	23,30,33	0.88	1 (4%)
3	PSU	W	55	3	19,21,22	1.15	4 (21%)	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 9 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	-2.73	1.33	1.38
3	W	37	YYG	C2-N1	-2.40	1.36	1.39
3	W	37	YYG	P-OP1	2.38	1.49	1.46
3	W	55	PSU	C6-C5	-2.32	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	-75.59	130.22	134.24
3	W	37	YYG	C11-C12-N1	18.56	111.39	104.24
3	W	37	YYG	C24-O23-C21	5.81	123.15	115.66
3	W	37	YYG	C13-C12-C11	-5.33	123.54	131.05
3	W	37	YYG	O23-C21-N20	4.02	118.46	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.