



# wwPDB X-ray Structure Validation Summary Report

Sep 15, 2014 – 11:17 AM EDT

PDB ID : 1VVL  
Title : Crystal Structure of Frameshift Suppressor tRNA SufA6 Bound to Codon CCC-U on the Ribosome  
Authors : Maehigashi, T.; Dunkle, J.A.; Dunham, C.M.  
Deposited on : 2013-06-07  
Resolution : 3.22 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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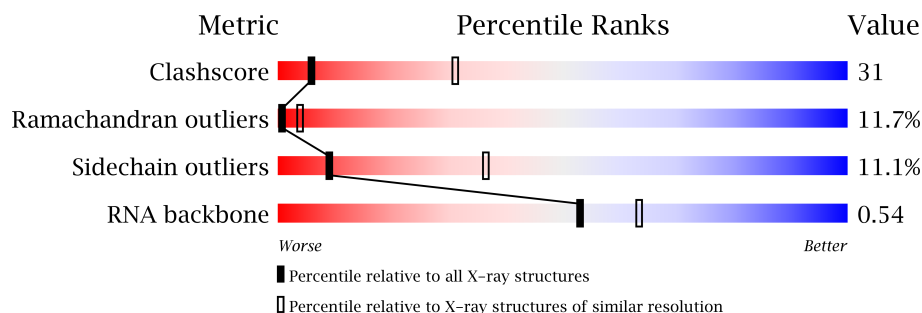
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.16 November 2013  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 21963  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable23489

# 1 Overall quality at a glance

The reported resolution of this entry is 3.22 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	1072 (3.28-3.16)
Ramachandran outliers	78287	1052 (3.28-3.16)
Sidechain outliers	78261	1051 (3.28-3.16)
RNA backbone	1838	1004 (3.74-2.70)





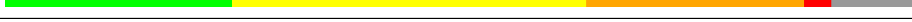

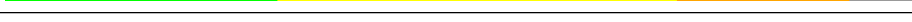

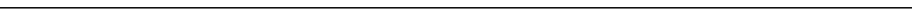

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	B	256	
3	C	239	
4	D	209	
5	E	162	
6	F	101	
7	G	156	
8	H	138	
9	I	128	
10	J	105	
11	K	129	
12	L	132	
13	M	126	
14	N	61	

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Mol	Chain	Length	Quality of chain
15	O	89	
16	P	88	
17	Q	105	
18	R	88	
19	S	93	
20	T	106	
21	U	27	
22	V	77	
23	X	25	
24	Y	18	

## 2 Entry composition

There are 27 unique types of molecules in this entry. The entry contains 53707 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 rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1500	Total	C	N	O	P	0	0	0
			32247	14353	5981	10414	1499			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	237	Total	C	N	O	S	0	0	0
			1924	1228	344	347	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	205	Total	C	N	O	S	0	0	0
			1605	1011	313	280	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
			1155	729	218	204	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
			1010	639	197	174				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	99	Total	C	N	O	S	0	0	0
			801	504	157	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	125	Total	C	N	O	S	0	0	0
			975	614	196	164	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	121	Total	C	N	O	S	0	0	0
			964	597	199	166	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
			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	84	Total	C	N	O	S	0	0	0
			705	446	140	118	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Q	100	Total	C	N	O	S	0	0	0
			834	534	155	143	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	84	Total	C	N	O	S	0	0	0
			674	430	126	116	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
			763	470	162	129	2			

- Molecule 21 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	U	25	Total	C	N	O	0	0	0
			217	134	52	31			

- Molecule 22 is a RNA chain called P-site tRNA fMet.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	V	77	Total	C	N	O	P	0	0	0
			1644	732	297	538	77			

- Molecule 23 is a RNA chain called A-site ASL SufA6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	X	8	Total	C	N	O	P	0	0	0
			167	75	28	56	8			

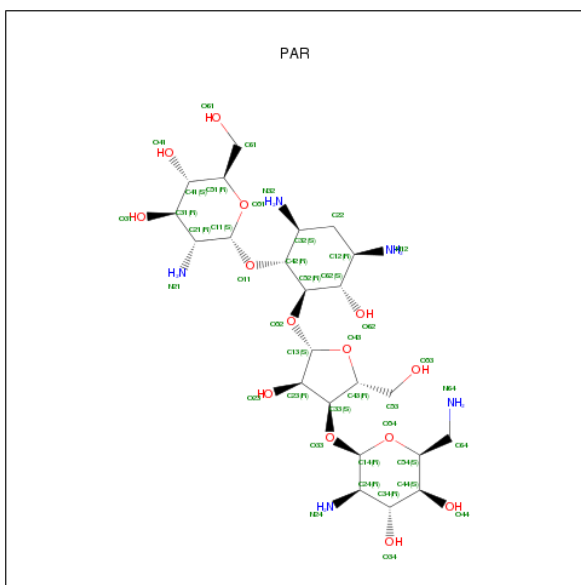
- Molecule 24 is a RNA chain called messenger RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	Y	14	Total	C	N	O	P	0	0	0
			303	135	55	99	14			

- Molecule 25 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
25	H	1	Total	Mg	0	0
			1	1		
25	A	66	Total	Mg	0	0
			66	66		
25	V	2	Total	Mg	0	0
			2	2		
25	F	1	Total	Mg	0	0
			1	1		
25	M	1	Total	Mg	0	0
			1	1		

- Molecule 26 is PAROMOMYCIN (three-letter code: PAR) (formula: C<sub>23</sub>H<sub>45</sub>N<sub>5</sub>O<sub>14</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
26	A	1	Total	C	N	O	0	0
			42	23	5	14		

- Molecule 27 is ZINC ION (three-letter code: ZN) (formula:  $\text{Zn}$ ).

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

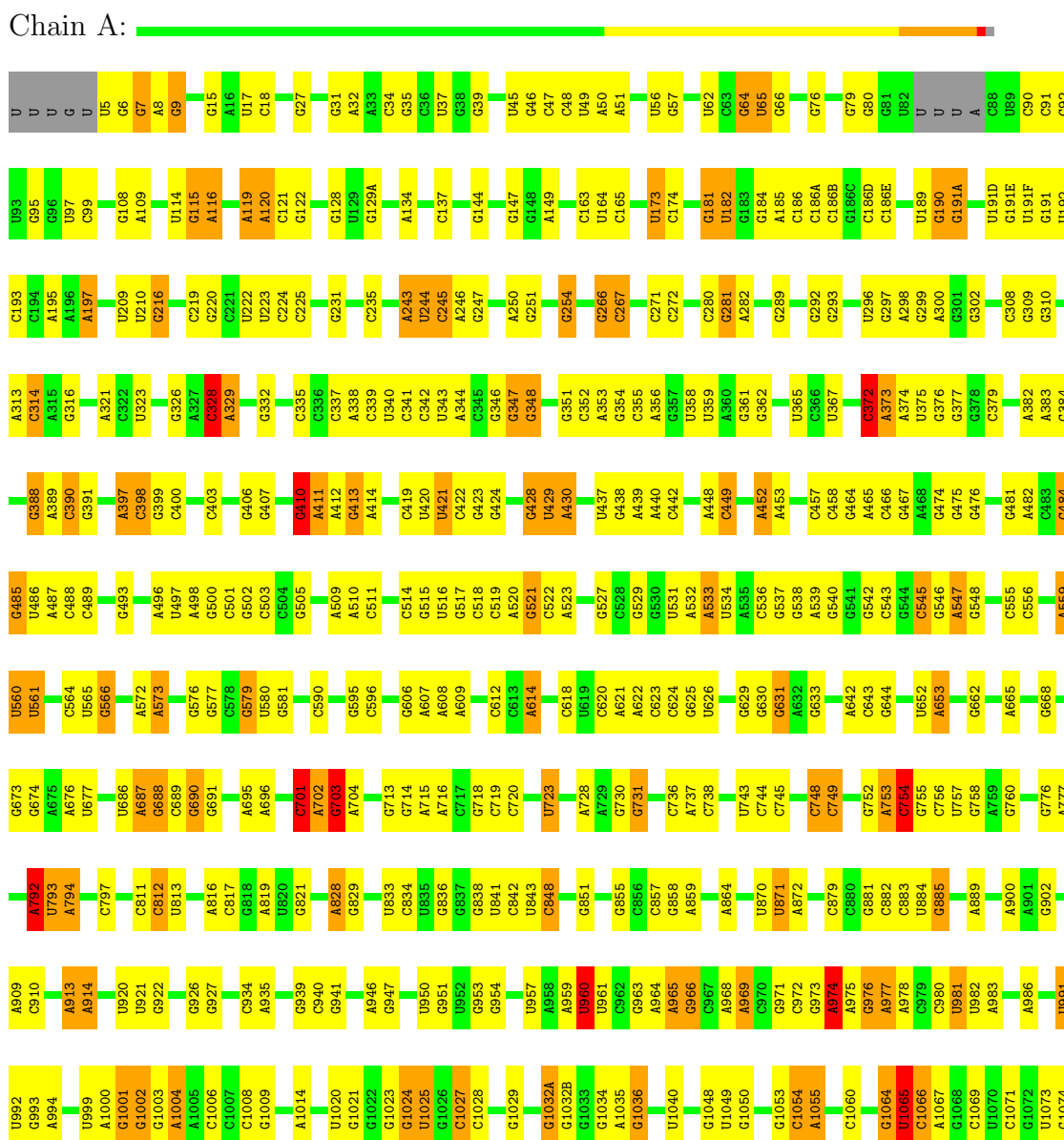


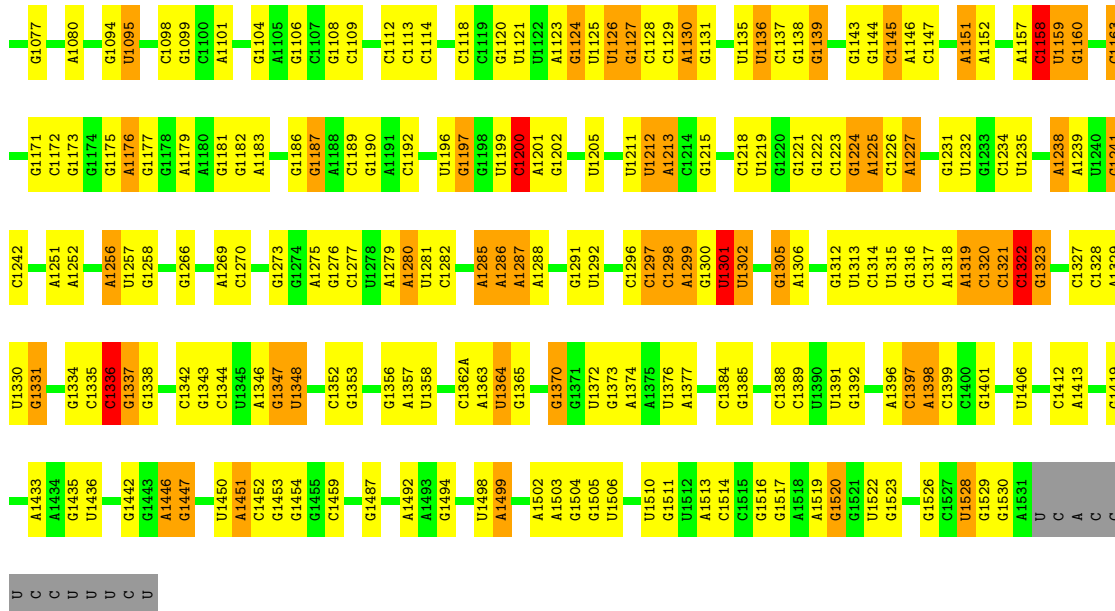
### 3 Residue-property plots

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.

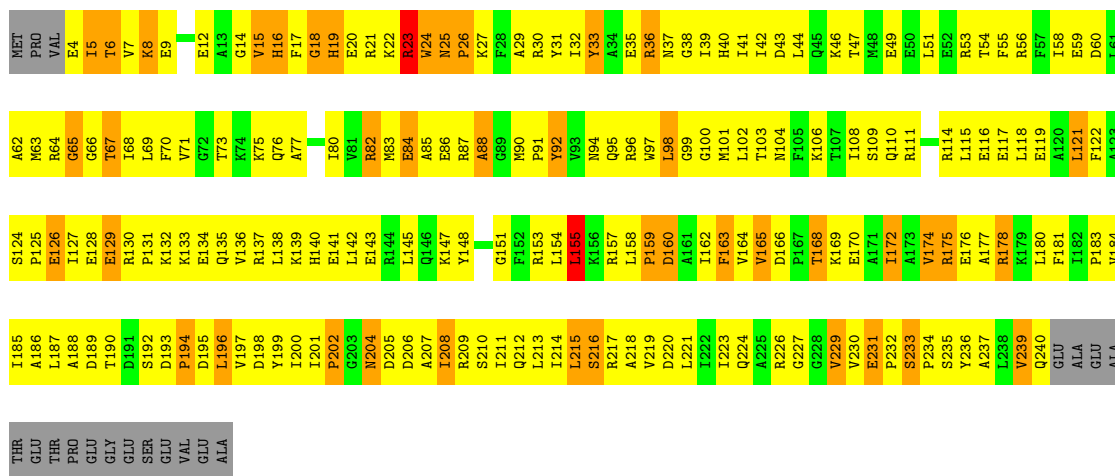
#### • Molecule 1: 16S rRNA





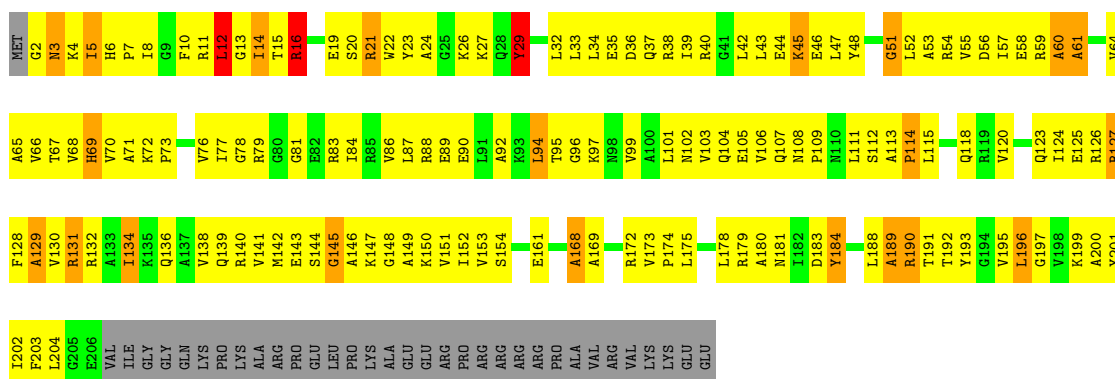
- Molecule 2: 30S ribosomal protein S2

Chain B:



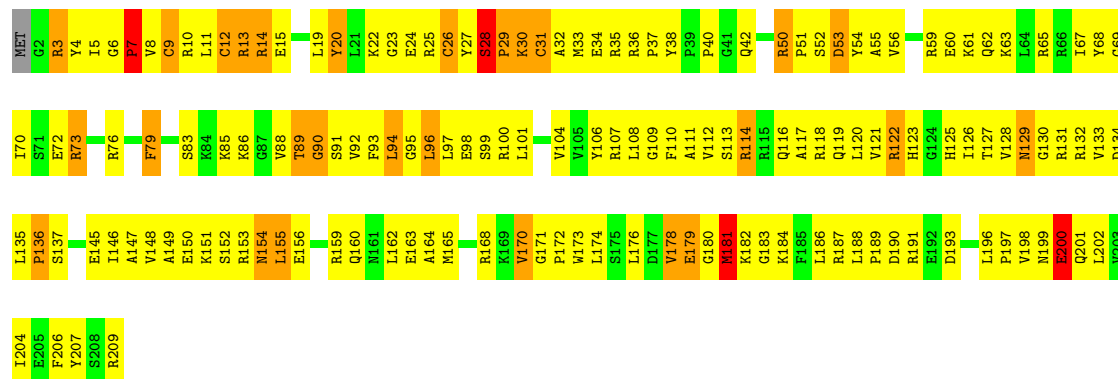
- Molecule 3: 30S ribosomal protein S3

Chain C:



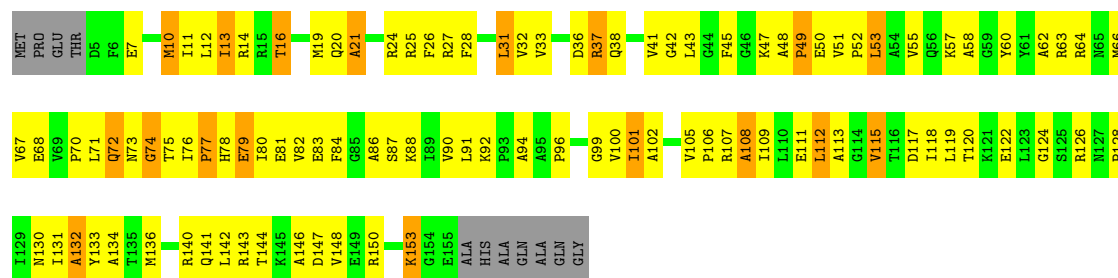
- Molecule 4: 30S ribosomal protein S4

Chain D:



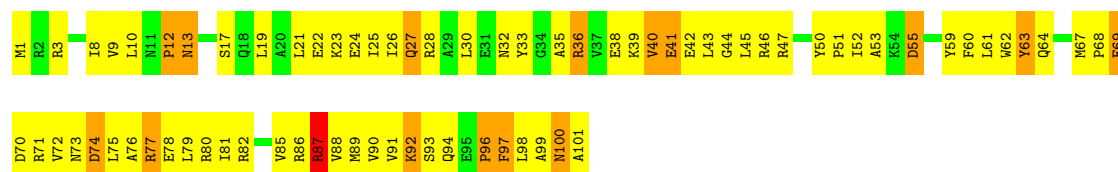
- Molecule 5: 30S ribosomal protein S5

Chain E:



- Molecule 6: 30S ribosomal protein S6

Chain F:



- Molecule 7: 30S ribosomal protein S7

Chain G:



- Molecule 8: 30S ribosomal protein S8

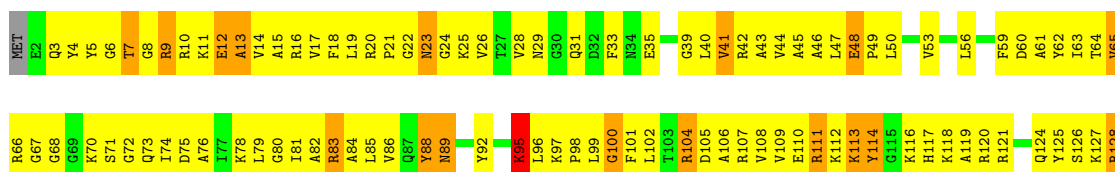
Chain H:





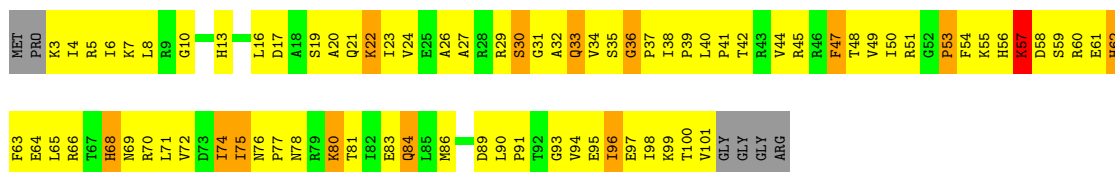
• Molecule 9: 30S ribosomal protein S9

Chain I:



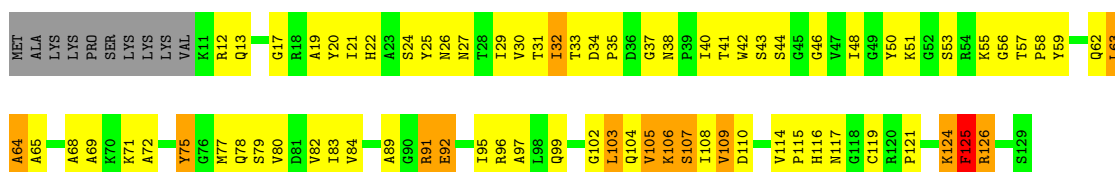
• Molecule 10: 30S ribosomal protein S10

Chain J:



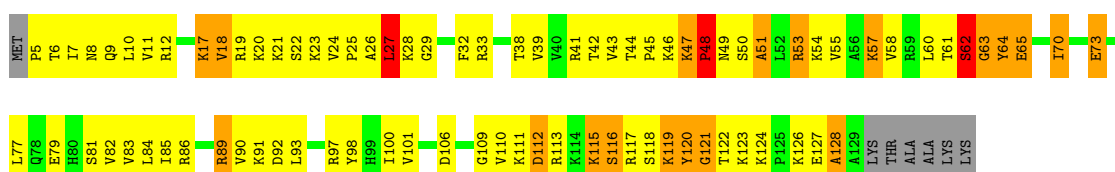
• Molecule 11: 30S ribosomal protein S11

Chain K:



• Molecule 12: 30S ribosomal protein S12

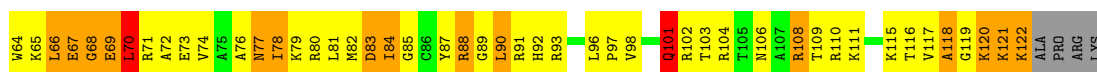
Chain L:



• Molecule 13: 30S ribosomal protein S13

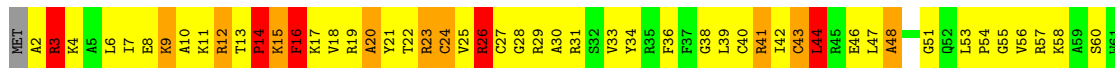
Chain M:





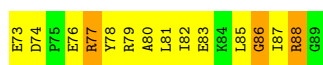
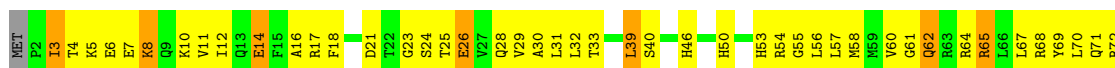
- Molecule 14: 30S ribosomal protein S14

Chain N:



- Molecule 15: 30S ribosomal protein S15

Chain O:



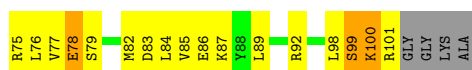
- Molecule 16: 30S ribosomal protein S16

Chain P:



- Molecule 17: 30S ribosomal protein S17

Chain Q:



- Molecule 18: 30S ribosomal protein S18

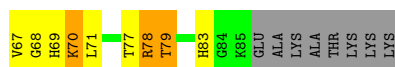
Chain R:



- Molecule 19: 30S ribosomal protein S19

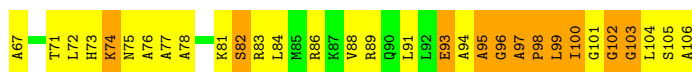
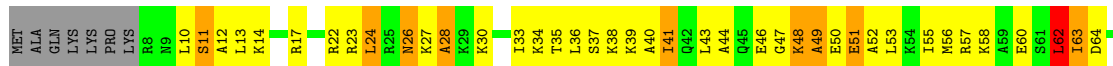
Chain S:





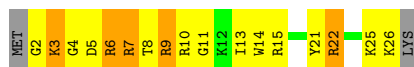
- Molecule 20: 30S ribosomal protein S20

Chain T:



- Molecule 21: 30S ribosomal protein S21

Chain U:



- Molecule 22: P-site tRNA fMet

Chain V:



- Molecule 23: A-site ASL SufA6

Chain X:



- Molecule 24: messenger RNA

Chain Y:



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	210.20Å 450.23Å 621.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.97 – 3.22	Depositor
% Data completeness (in resolution range)	98.5 (34.97-3.22)	Depositor
$R_{merge}$	0.25	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.229 , 0.260	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	53707	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	106.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG, PAR, 1MG

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	0.31	0/36098	0.86	46/56341 (0.1%)
2	B	0.35	0/1959	0.65	0/2642
3	C	0.36	0/1629	0.60	0/2195
4	D	0.41	0/1733	0.68	1/2318 (0.0%)
5	E	0.38	0/1171	0.66	0/1576
6	F	0.43	0/856	0.68	0/1154
7	G	0.37	0/1276	0.60	0/1709
8	H	0.40	0/1136	0.69	0/1527
9	I	0.36	0/1029	0.67	0/1379
10	J	0.35	0/814	0.61	0/1095
11	K	0.40	0/900	0.67	0/1213
12	L	0.45	0/991	1.00	4/1327 (0.3%)
13	M	0.34	0/974	0.66	0/1303
14	N	0.42	0/501	0.68	0/664
15	O	0.39	0/745	0.67	0/992
16	P	0.36	0/721	0.67	0/970
17	Q	0.37	0/847	0.68	0/1131
18	R	0.39	0/579	0.72	0/768
19	S	0.36	0/689	0.84	2/926 (0.2%)
20	T	0.33	0/765	0.69	0/1007
21	U	0.37	0/221	0.63	0/288
22	V	0.52	0/1836	0.99	5/2859 (0.2%)
23	X	0.39	0/185	0.72	0/285
24	Y	0.52	0/311	0.88	0/483
All	All	0.34	0/57966	0.82	58/86152 (0.1%)

There are no bond length outliers.

The worst 5 of 58 bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	L	47	LYS	C-N-CD	-20.48	75.56	120.60
22	V	17	C	C2-N1-C1'	11.77	131.75	118.80
1	A	1322	C	C2-N1-C1'	9.46	129.20	118.80
12	L	47	LYS	C-N-CA	8.81	159.00	122.00
22	V	17	C	C6-N1-C1'	-8.74	110.32	120.80

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	32247	0	16278	483	0
2	B	1924	0	1975	287	0
3	C	1605	0	1668	207	0
4	D	1703	0	1764	240	0
5	E	1155	0	1213	136	0
6	F	843	0	857	94	0
7	G	1257	0	1296	145	0
8	H	1116	0	1175	140	0
9	I	1010	0	1037	141	0
10	J	801	0	849	148	0
11	K	885	0	904	100	0
12	L	975	0	1062	104	0
13	M	964	0	1034	151	0
14	N	492	0	530	98	0
15	O	734	0	771	75	0
16	P	705	0	725	112	0
17	Q	834	0	904	83	0
18	R	574	0	644	66	0
19	S	674	0	699	103	0
20	T	763	0	860	105	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	U	217	0	234	26	0
22	V	1644	0	836	23	0
23	X	167	0	87	12	0
24	Y	303	0	154	11	0
25	A	66	0	0	0	0
25	F	1	0	0	0	0
25	H	1	0	0	0	0
25	M	1	0	0	0	0
25	V	2	0	0	0	0
26	A	42	0	45	1	0
27	D	1	0	0	0	0
27	N	1	0	0	0	0
All	All	53707	0	37601	2831	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 31.

The worst 5 of 2831 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
10:J:49:VAL:HG21	14:N:41:ARG:CB	1.49	1.42
10:J:49:VAL:CG2	14:N:41:ARG:CB	2.04	1.36
4:D:22:LYS:HG3	4:D:26:CYS:SG	1.70	1.31
10:J:49:VAL:CG2	14:N:41:ARG:HB2	1.62	1.29
14:N:25:VAL:HG23	14:N:38:GLY:O	1.37	1.25

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	235/256 (92%)	153 (65%)	52 (22%)	30 (13%)	0 3
3	C	203/239 (85%)	128 (63%)	56 (28%)	19 (9%)	1 8

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	D	206/209 (99%)	136 (66%)	50 (24%)	20 (10%)	1	7
5	E	149/162 (92%)	103 (69%)	31 (21%)	15 (10%)	1	7
6	F	99/101 (98%)	66 (67%)	24 (24%)	9 (9%)	1	8
7	G	153/156 (98%)	102 (67%)	36 (24%)	15 (10%)	1	7
8	H	136/138 (99%)	92 (68%)	29 (21%)	15 (11%)	1	5
9	I	125/128 (98%)	77 (62%)	32 (26%)	16 (13%)	0	3
10	J	97/105 (92%)	68 (70%)	20 (21%)	9 (9%)	1	8
11	K	117/129 (91%)	87 (74%)	21 (18%)	9 (8%)	1	11
12	L	123/132 (93%)	85 (69%)	24 (20%)	14 (11%)	1	4
13	M	119/126 (94%)	71 (60%)	28 (24%)	20 (17%)	0	1
14	N	58/61 (95%)	31 (53%)	15 (26%)	12 (21%)	0	0
15	O	86/89 (97%)	61 (71%)	19 (22%)	6 (7%)	2	14
16	P	82/88 (93%)	48 (58%)	23 (28%)	11 (13%)	0	2
17	Q	98/105 (93%)	75 (76%)	15 (15%)	8 (8%)	1	10
18	R	68/88 (77%)	46 (68%)	14 (21%)	8 (12%)	1	4
19	S	82/93 (88%)	47 (57%)	17 (21%)	18 (22%)	0	0
20	T	97/106 (92%)	63 (65%)	16 (16%)	18 (19%)	0	1
21	U	23/27 (85%)	15 (65%)	4 (17%)	4 (17%)	0	1
All	All	2356/2538 (93%)	1554 (66%)	526 (22%)	276 (12%)	1	4

5 of 276 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	6	THR
2	B	15	VAL
2	B	26	PRO
2	B	84	GLU
2	B	88	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	
2	B	205/220 (93%)	181 (88%)	24 (12%)	8	34
3	C	159/188 (85%)	143 (90%)	16 (10%)	11	41
4	D	180/181 (99%)	160 (89%)	20 (11%)	9	36
5	E	116/123 (94%)	108 (93%)	8 (7%)	22	65
6	F	90/90 (100%)	76 (84%)	14 (16%)	4	17
7	G	126/127 (99%)	114 (90%)	12 (10%)	12	44
8	H	119/119 (100%)	106 (89%)	13 (11%)	9	37
9	I	98/99 (99%)	87 (89%)	11 (11%)	9	36
10	J	89/92 (97%)	81 (91%)	8 (9%)	14	48
11	K	90/99 (91%)	81 (90%)	9 (10%)	11	41
12	L	104/109 (95%)	90 (86%)	14 (14%)	6	26
13	M	97/101 (96%)	81 (84%)	16 (16%)	3	14
14	N	49/50 (98%)	40 (82%)	9 (18%)	2	11
15	O	79/80 (99%)	73 (92%)	6 (8%)	19	60
16	P	72/74 (97%)	63 (88%)	9 (12%)	7	30
17	Q	95/97 (98%)	89 (94%)	6 (6%)	25	69
18	R	61/77 (79%)	54 (88%)	7 (12%)	8	35
19	S	73/80 (91%)	62 (85%)	11 (15%)	4	19
20	T	76/82 (93%)	68 (90%)	8 (10%)	10	39
21	U	20/22 (91%)	19 (95%)	1 (5%)	34	78
All	All	1998/2110 (95%)	1776 (89%)	222 (11%)	9	36

5 of 222 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	H	69	ARG
10	J	84	GLN
19	S	13	ASP
8	H	119	LEU
9	I	95	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
7	G	28	ASN

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Mol	Chain	Res	Type
7	G	148	ASN
19	S	65	ASN
7	G	37	ASN
7	G	86	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1499/1522 (98%)	296 (19%)	46 (3%)
22	V	76/77 (98%)	30 (39%)	1 (1%)
23	X	7/25 (28%)	5 (71%)	1 (14%)
24	Y	13/18 (72%)	5 (38%)	1 (7%)
All	All	1595/1642 (97%)	336 (21%)	49 (3%)

5 of 336 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	32	A

5 of 49 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	595	G
1	A	792	A
1	A	1528	U
1	A	701	C
1	A	812	C

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

1 non-standard protein/DNA/RNA residue is 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	$\# Z  > 2$
24	1MG	Y	37	24	24,26,27	3.02	6 (25%)	34,39,42	3.99	12 (35%)

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
24	1MG	Y	37	24	-	0/8/25/26	0/3/3/3

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	Y	37	1MG	C4-N3	8.23	1.49	1.35
24	Y	37	1MG	C2-N1	7.46	1.47	1.37
24	Y	37	1MG	C2-N2	6.66	1.48	1.33
24	Y	37	1MG	P-OP1	4.81	1.52	1.46
24	Y	37	1MG	C5-N7	-3.70	1.33	1.38

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	Y	37	1MG	C6-C5-N7	-17.40	133.31	134.24
24	Y	37	1MG	C6-N1-C2	11.86	123.96	120.71
24	Y	37	1MG	N2-C2-N1	3.91	123.76	118.45
24	Y	37	1MG	N3-C4-N9	3.77	132.43	126.91
24	Y	37	1MG	C8-N9-C4	3.31	109.65	106.96

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 74 ligands modelled in this entry, 73 are monoatomic - leaving 1 for Mogul analysis.

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$
26	PAR	A	1667	-	45,45,45	1.31	7 (15%)	67,67,67	1.40	8 (11%)

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
26	PAR	A	1667	-	-	0/18/94/94	0/4/4/4

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	A	1667	PAR	C52-C42	3.21	1.58	1.52
26	A	1667	PAR	C64-C54	2.90	1.59	1.51
26	A	1667	PAR	O54-C14	2.87	1.49	1.41
26	A	1667	PAR	O51-C11	2.31	1.47	1.41
26	A	1667	PAR	C11-C21	2.18	1.56	1.52

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	A	1667	PAR	O52-C13-C23	4.73	115.94	107.50
26	A	1667	PAR	C14-O54-C54	3.86	121.19	113.73
26	A	1667	PAR	O33-C14-C24	3.34	114.68	108.08
26	A	1667	PAR	O11-C42-C52	3.14	115.41	107.42
26	A	1667	PAR	O11-C42-C32	-3.03	101.73	108.97

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.