



# wwPDB X-ray Structure Validation Summary Report

Mar 31, 2014 – 05:48 PM BST

PDB ID : 2Y0Y  
Title : THE CRYSTAL STRUCTURE OF EF-TU AND G24A-TRNA-TRP BOUND  
TO A NEAR-COGNATE CODON ON THE 70S RIBOSOME  
Authors : Schmeing, T.M.; Voorhees, R.M.; Ramakrishnan, V.  
Deposited on : 2010-12-07  
Resolution : 3.10 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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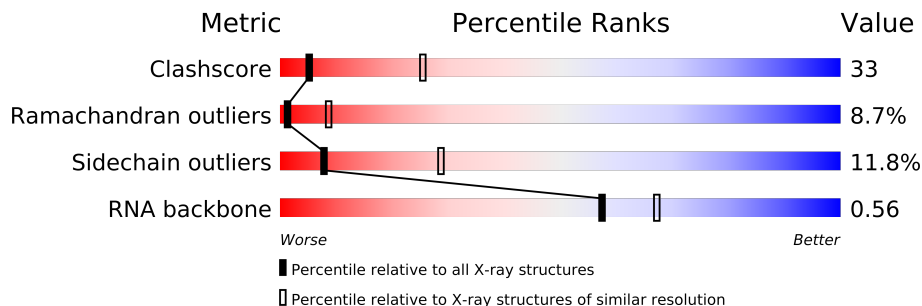
The following versions of software and data (see [references](#)) were used in the production of this report:

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

# 1 Overall quality at a glance

The reported resolution of this entry is 3.10 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	1078 (3.16-3.04)
Ramachandran outliers	78287	1044 (3.16-3.04)
Sidechain outliers	78261	1044 (3.16-3.04)
RNA backbone	1838	1047 (3.60-2.60)

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	
15	O	89	

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Mol	Chain	Length	Quality of chain
16	P	88	
17	Q	105	
18	R	88	
19	S	93	
20	T	106	
21	U	27	
22	V	76	
22	W	76	
23	X	27	
24	Y	77	
25	Z	405	

## 2 Entry composition

There are 28 unique types of molecules in this entry. The entry contains 59791 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	1504	Total	C	N	O	P	0	0	0
			32329	14390	5992	10444	1503			

- 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
			1703	1066	339	291	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
			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	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
			885	549	168	165	3			

- Molecule 12 is a protein called 30S RIBOSOMAL PROTEIN S12.

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

- Molecule 13 is a protein called 30S RIBOSOMAL PROTEIN S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	124	Total	C	N	O	S	0	0	0
			987	611	205	169	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	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	99	Total	C	N	O	S	0	0	0
			823	528	151	142	2			

- Molecule 18 is a protein called 30S RIBOSOMAL PROTEIN S18.

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

- Molecule 19 is a protein called 30S RIBOSOMAL PROTEIN S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	S	78	Total	C	N	O	S	0	0	0
			629	403	114	110	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 THX.

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

- Molecule 22 is a RNA chain called E-SITE TRNA PHE OR P-SITE TRNA PHE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	V	76	Total	C	N	O	P	0	0	0
			1619	723	290	531	75			
22	W	76	Total	C	N	O	P	0	0	0
			1619	723	290	531	75			

- Molecule 23 is a RNA chain called MRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	X	17	Total	C	N	O	P	0	0	0
			361	164	68	113	16			

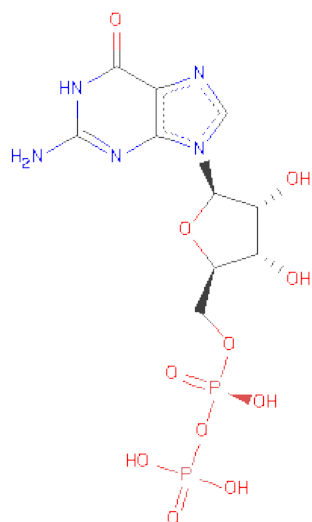
- Molecule 24 is a RNA chain called A-SITE TRNA G24A TRP-TRNA TRP.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
24	Y	77	Total	C	N	O	P	S	0	0	0
			1644	742	289	535	76	2			

- Molecule 25 is a protein called ELONGATION FACTOR TU.

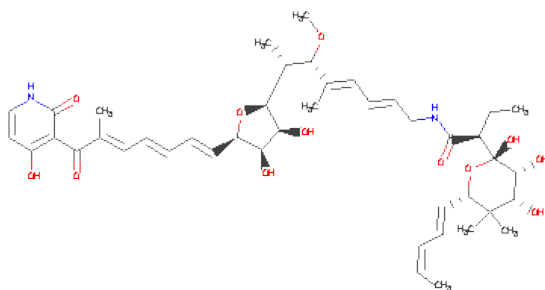
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	Z	385	Total	C	N	O	S	0	0	0
			2984	1885	524	563	12			

- Molecule 26 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>11</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
26	1	1	Total	C	N	O	P	0
			28	10	5	11	2	

- Molecule 27 is KIRROMYCIN (three-letter code: KIR) (formula:  $C_{43}H_{60}N_2O_{12}$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
27	1	1	Total	C	N	O	0	0
			57	43	2	12		

- Molecule 28 is ZINC ION (three-letter code: ZN) (formula: Zn).



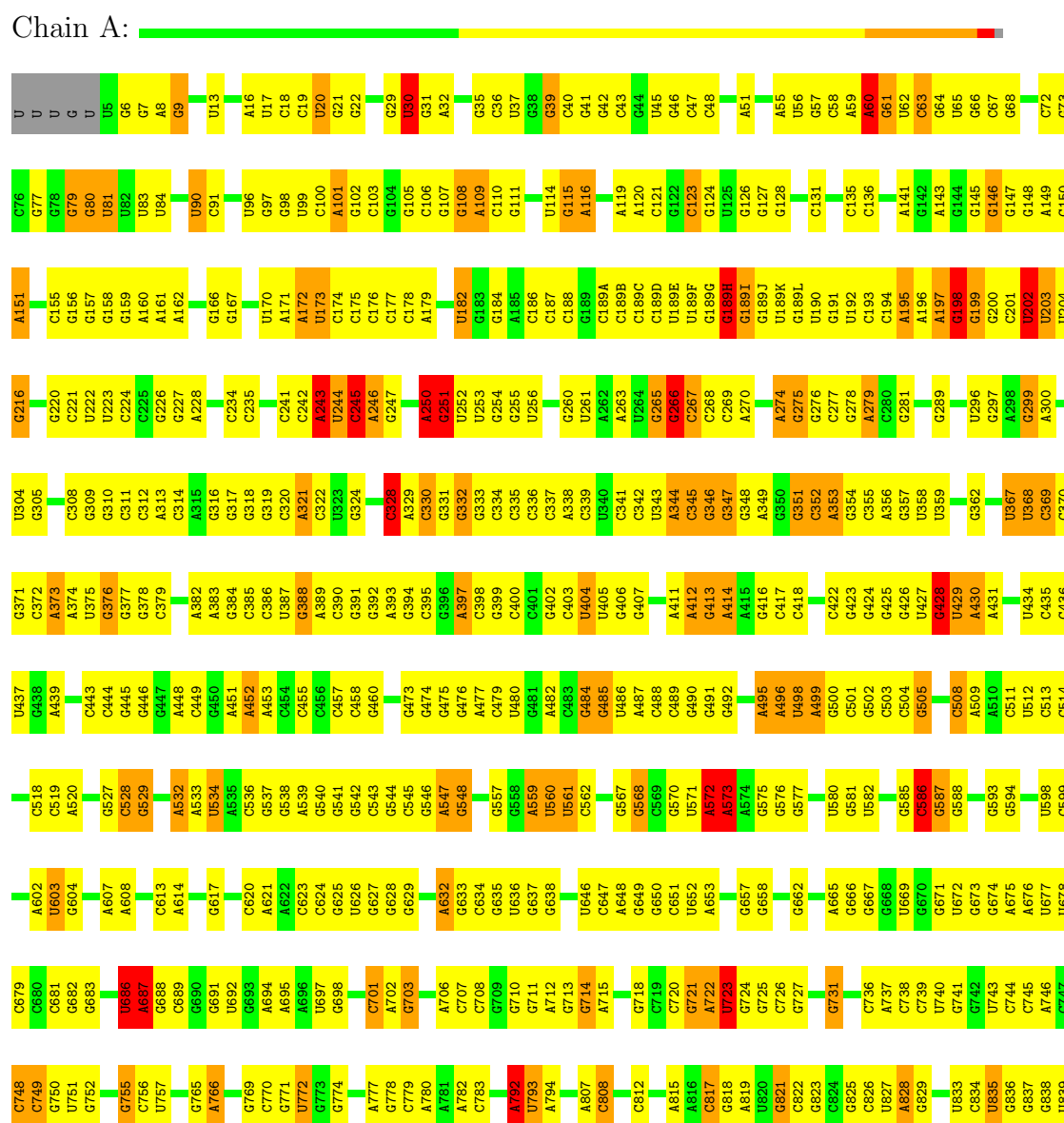
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
28	1	4	Total	Zn	0	0
			4	4		

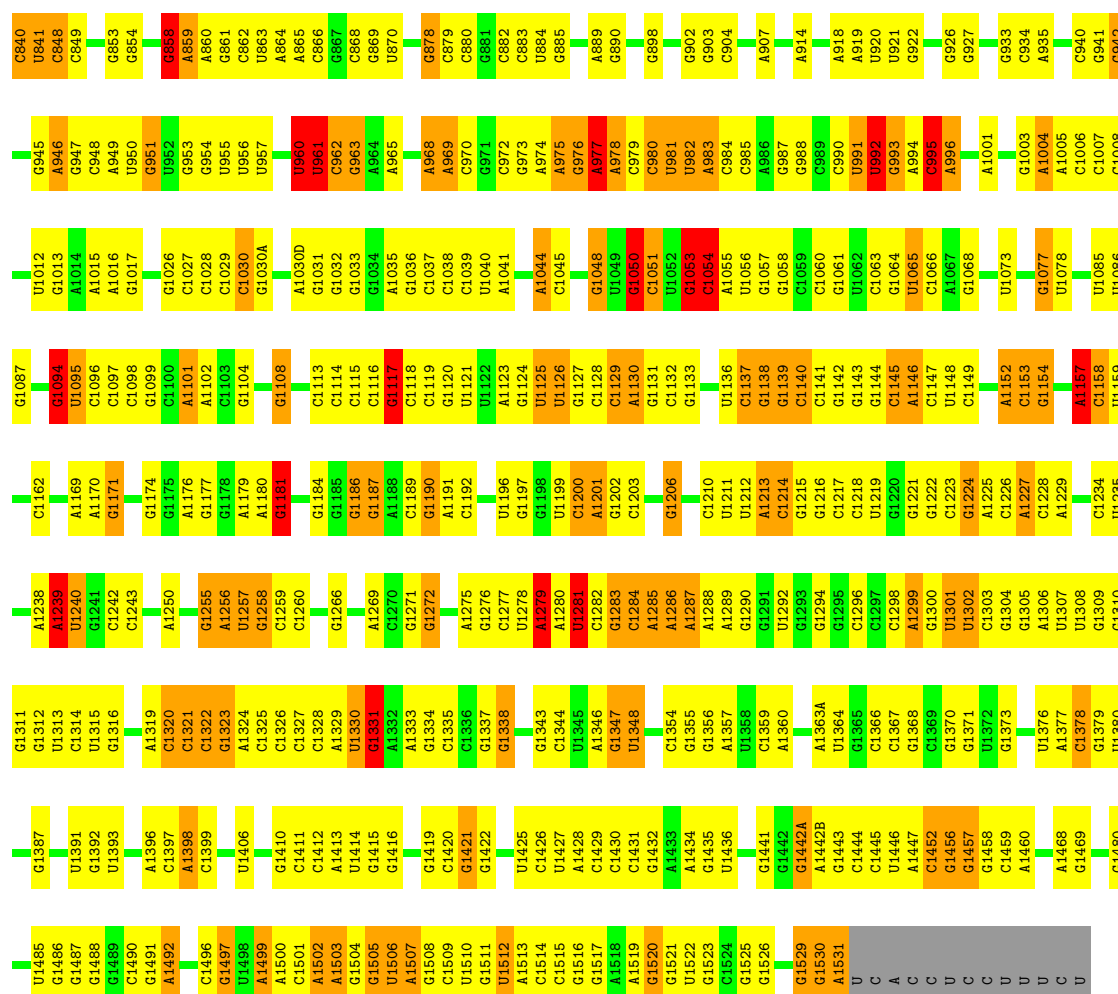
### 3 Residue-property plots

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.

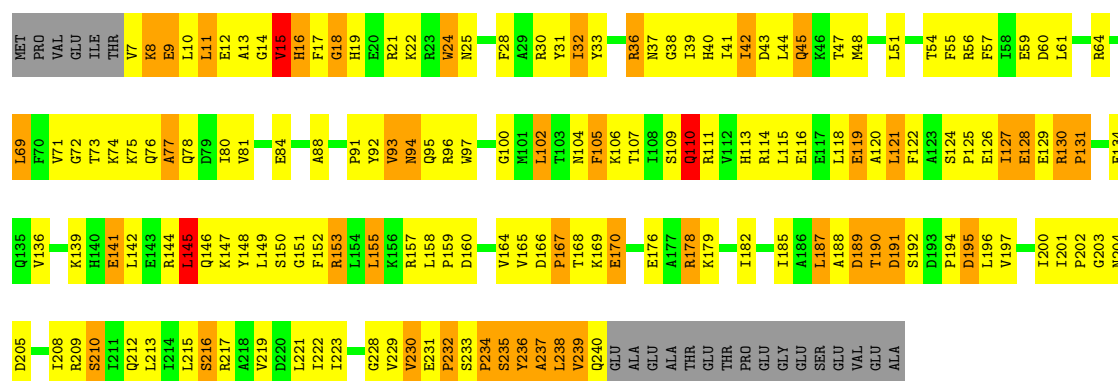
#### • Molecule 1: 16S rRNA





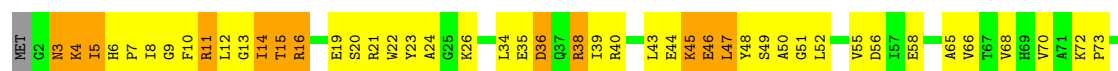
## • Molecule 2: 30S RIBOSOMAL PROTEIN S2

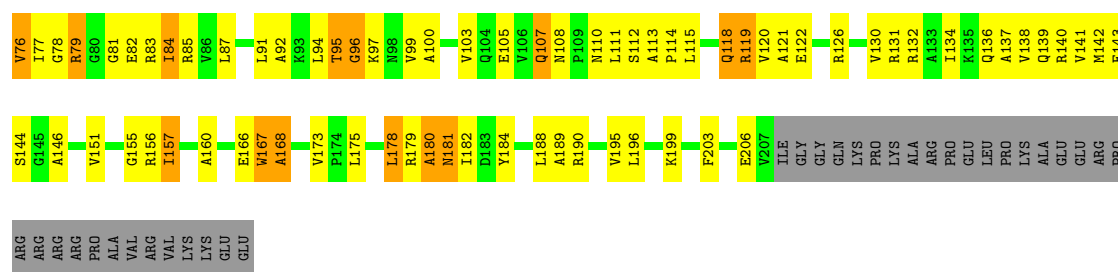
Chain B:



## • Molecule 3: 30S RIBOSOMAL PROTEIN S3

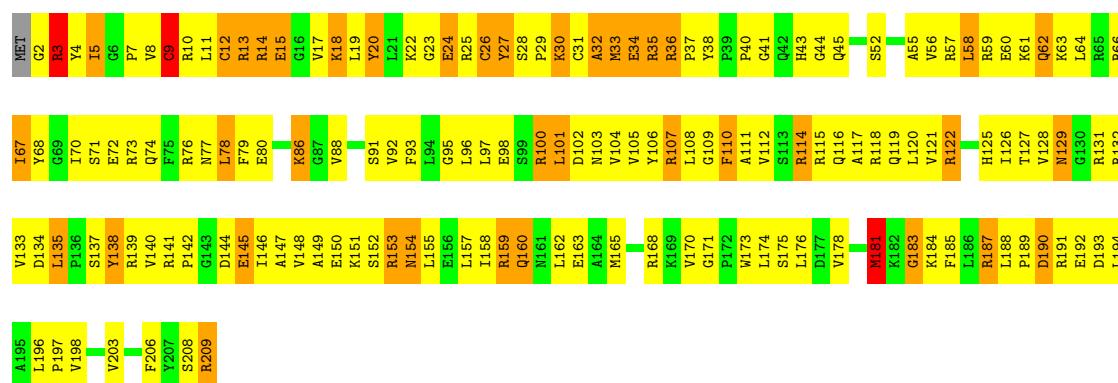
Chain C:





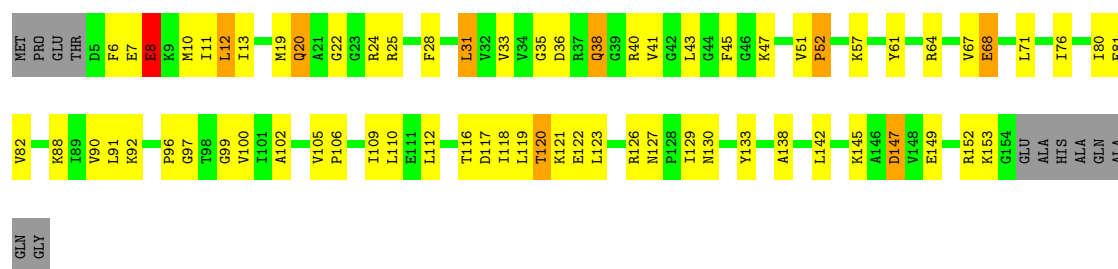
### • Molecule 4: 30S RIBOSOMAL PROTEIN S4

Chain D:



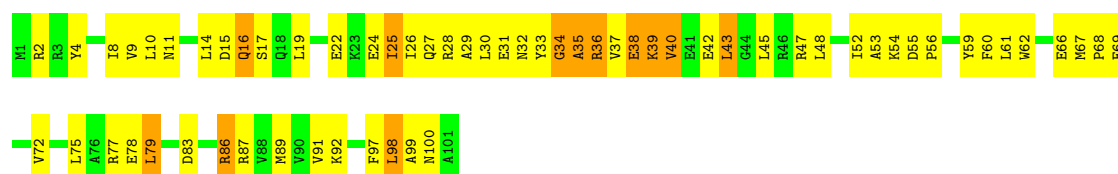
### • Molecule 5: 30S RIBOSOMAL PROTEIN S5

Chain E:



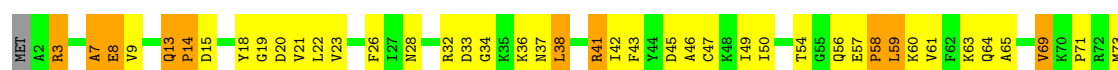
### • Molecule 6: 30S RIBOSOMAL PROTEIN S6

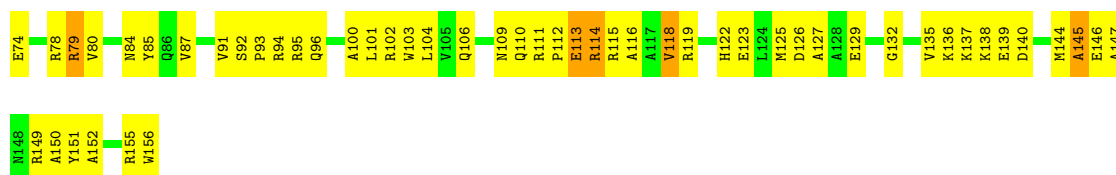
Chain F:



### • Molecule 7: 30S RIBOSOMAL PROTEIN S7

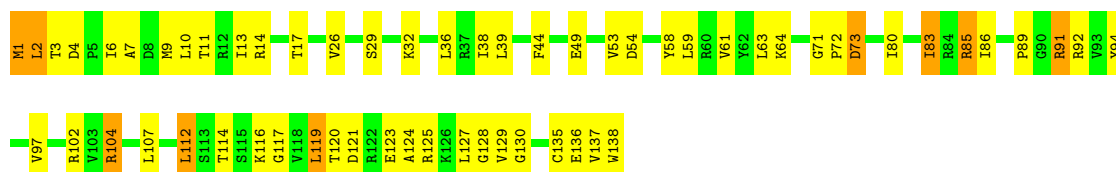
Chain G:





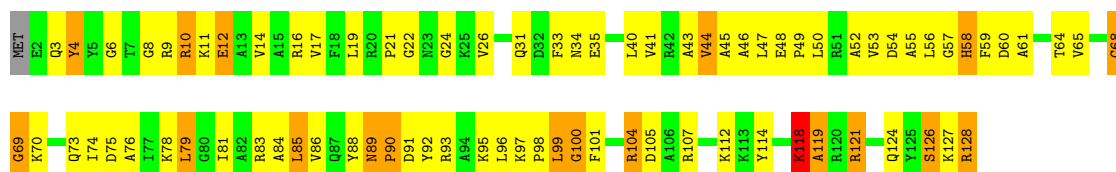
• Molecule 8: 30S RIBOSOMAL PROTEIN S8

Chain H:



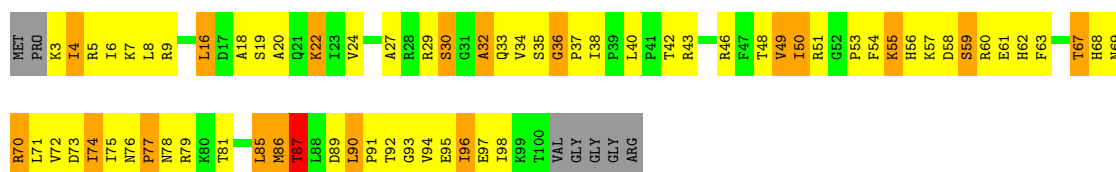
• Molecule 9: 30S RIBOSOMAL PROTEIN S9

Chain I:



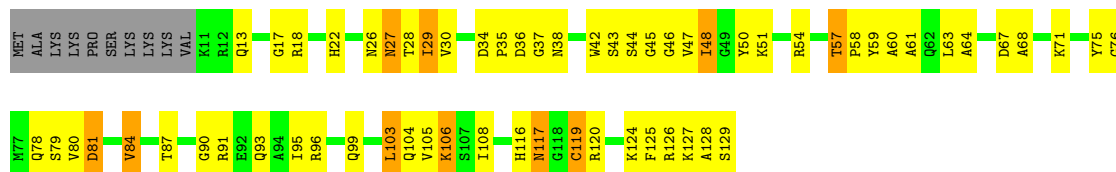
• Molecule 10: 30S RIBOSOMAL PROTEIN S10

Chain J:



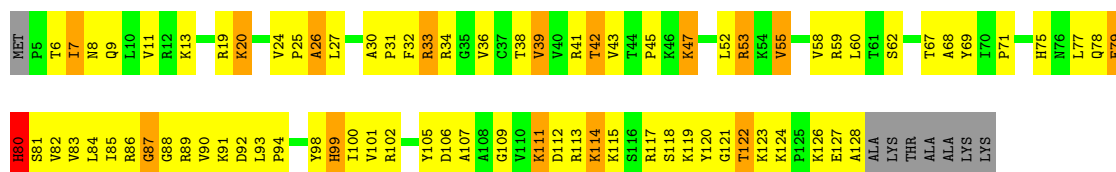
• Molecule 11: 30S RIBOSOMAL PROTEIN S11

Chain K:



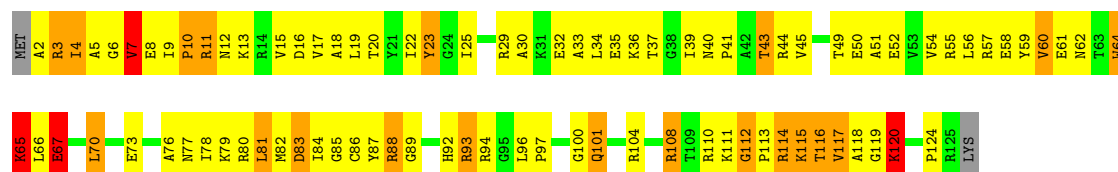
• Molecule 12: 30S RIBOSOMAL PROTEIN S12

Chain L:



- Molecule 13: 30S RIBOSOMAL PROTEIN S13

Chain M:



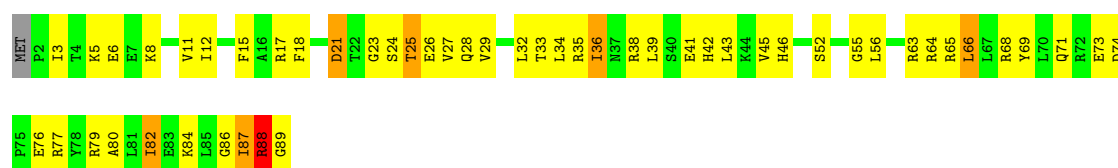
- Molecule 14: 30S RIBOSOMAL PROTEIN S14

Chain N:



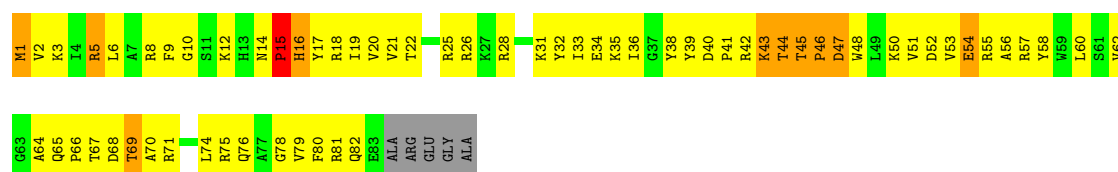
- Molecule 15: 30S RIBOSOMAL PROTEIN S15

Chain O:



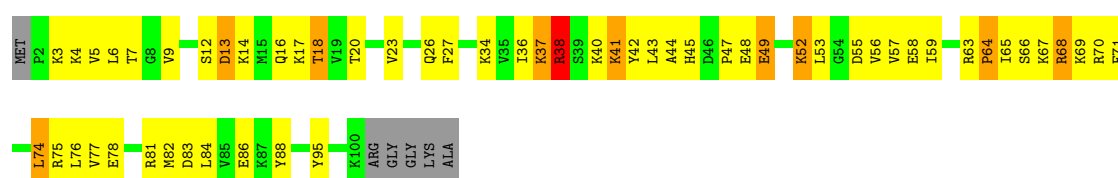
- Molecule 16: 30S RIBOSOMAL PROTEIN S16

Chain P:



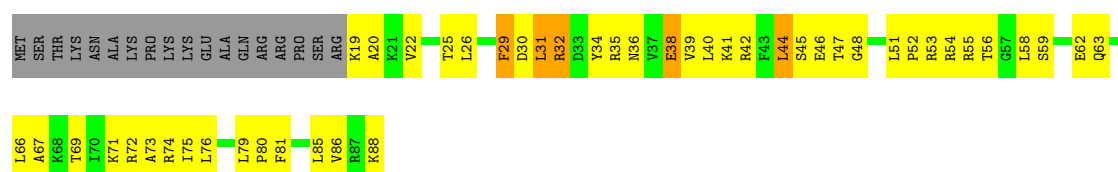
- Molecule 17: 30S RIBOSOMAL PROTEIN S17

Chain Q:



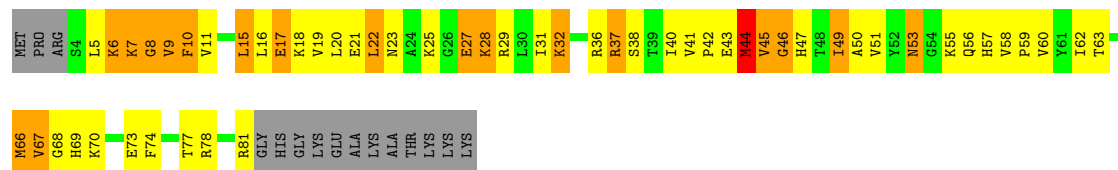
- Molecule 18: 30S RIBOSOMAL PROTEIN S18

Chain R:



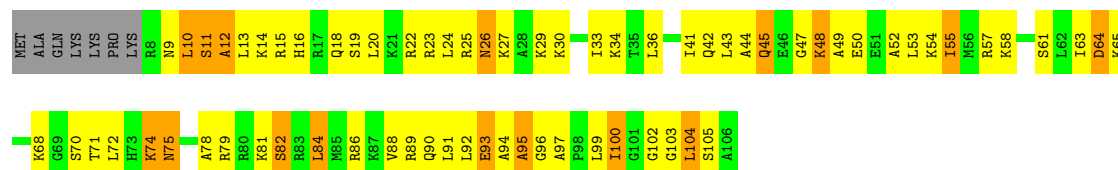
- Molecule 19: 30S RIBOSOMAL PROTEIN S19

Chain S:



- Molecule 20: 30S RIBOSOMAL PROTEIN S20

Chain T:



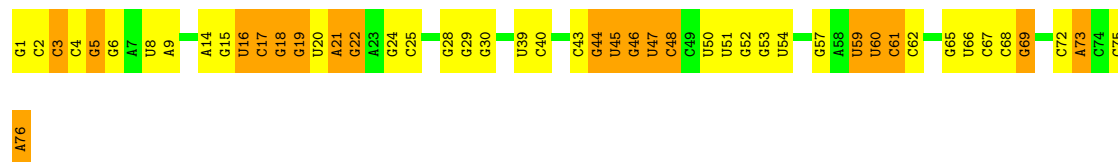
- Molecule 21: 30S RIBOSOMAL PROTEIN THX

Chain U:



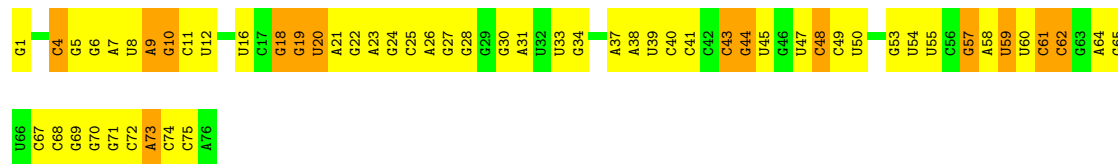
- Molecule 22: E-SITE TRNA PHE OR P-SITE TRNA PHE

Chain V:



- Molecule 22: E-SITE TRNA PHE OR P-SITE TRNA PHE

Chain W:



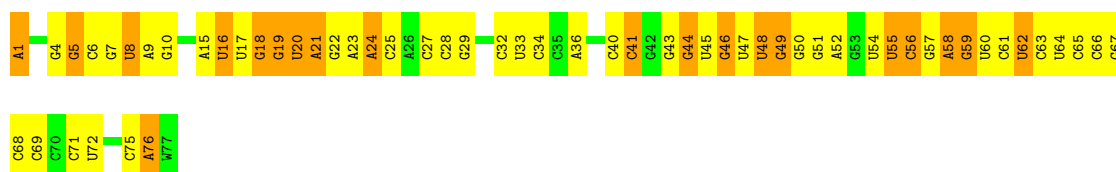
- Molecule 23: MRNA

Chain X:



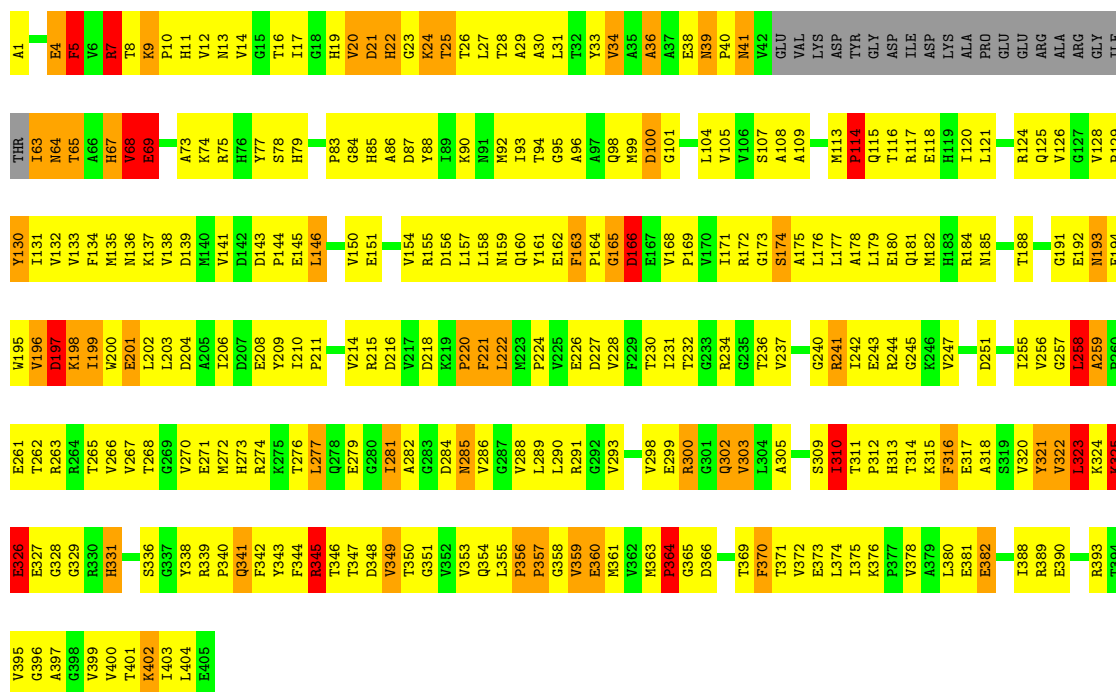
- Molecule 24: A-SITE TRNA G24A TRP-TRNA TRP

Chain Y:



• Molecule 25: ELONGATION FACTOR TU

Chain Z:





## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	289.90Å 269.40Å 404.50Å 90.00° 91.51° 90.00°	Depositor
Resolution (Å)	50.00 – 3.10	Depositor
% Data completeness (in resolution range)	98.7 (50.00-3.10)	Depositor
$R_{merge}$	0.02	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.18 (at 2.81Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.238 , 0.275	Depositor
Wilson B-factor (Å <sup>2</sup> )	65.1	Xtriage
Anisotropy	0.052	Xtriage
Estimated twinning fraction	0.024 for h,-k,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	2 of 1394902 reflections (0.000%)	Xtriage
Total number of atoms	59791	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.01% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities 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: OMC, GDP, ZN, H2U, KIR, MIA, 4SU, 7MG, 5MU, 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	0.67	10/36190 (0.0%)	0.79	44/56486 (0.1%)
2	B	0.55	0/1935	0.76	0/2609
3	C	0.65	1/1636 (0.1%)	0.83	0/2205
4	D	0.48	1/1733 (0.1%)	0.75	1/2318 (0.0%)
5	E	0.65	1/1162 (0.1%)	0.81	0/1564
6	F	0.50	0/856	0.70	1/1154 (0.1%)
7	G	0.52	0/1276	0.73	1/1709 (0.1%)
8	H	0.57	0/1136	0.80	0/1527
9	I	0.55	0/1029	0.82	0/1379
10	J	0.55	0/807	0.85	0/1085
11	K	0.60	1/900 (0.1%)	0.80	0/1213
12	L	0.52	0/986	0.82	1/1320 (0.1%)
13	M	0.51	0/998	0.80	0/1336
14	N	0.70	1/501 (0.2%)	0.98	1/664 (0.2%)
15	O	0.52	0/745	0.77	0/992
16	P	0.46	0/716	0.74	0/963
17	Q	0.54	0/836	0.76	0/1117
18	R	0.56	0/579	0.73	0/768
19	S	0.55	0/642	0.76	0/865
20	T	0.42	0/765	0.69	0/1007
21	U	0.55	0/212	0.87	0/277
22	V	0.68	0/1809	0.79	0/2819
22	W	0.47	0/1809	0.74	0/2819
23	X	0.79	0/405	0.91	2/629 (0.3%)
24	Y	0.49	1/1618 (0.1%)	0.71	0/2514
25	Z	0.84	12/3042 (0.4%)	0.99	15/4129 (0.4%)
All	All	0.64	28/64323 (0.0%)	0.79	66/95468 (0.1%)

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	1	90
5	E	0	1
22	V	0	1
23	X	0	2
25	Z	0	2
All	All	1	96

The worst 5 of 28 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	Z	69	GLU	CB-CG	16.36	1.83	1.52
25	Z	68	VAL	CA-C	12.52	1.85	1.52
1	A	858	G	C5-C6	-9.64	1.32	1.42
25	Z	5	PHE	CE2-CZ	8.25	1.53	1.37
25	Z	1	ALA	CA-CB	7.97	1.69	1.52

The worst 5 of 66 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	Z	356	PRO	C-N-CD	-26.29	62.77	120.60
25	Z	197	ASP	CB-CG-OD2	-14.50	105.25	118.30
25	Z	69	GLU	N-CA-CB	-13.90	85.58	110.60
25	Z	197	ASP	CB-CG-OD1	10.73	127.96	118.30
25	Z	69	GLU	CA-CB-CG	10.09	135.61	113.40

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	508	C	C3'

5 of 96 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	108	G	Sidechain
1	A	123	C	Sidechain
1	A	13	U	Sidechain
1	A	189(G)	G	Sidechain
1	A	20	U	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	32329	0	16318	1019	0
2	B	1900	0	1951	204	0
3	C	1612	0	1677	145	0
4	D	1703	0	1763	229	0
5	E	1146	0	1207	75	0
6	F	843	0	857	71	0
7	G	1257	0	1296	88	0
8	H	1116	0	1177	64	0
9	I	1010	0	1037	111	0
10	J	794	0	840	126	0
11	K	885	0	904	67	0
12	L	970	0	1057	112	0
13	M	987	0	1059	121	0
14	N	492	0	531	62	0
15	O	734	0	771	47	0
16	P	700	0	720	92	0
17	Q	823	0	891	70	0
18	R	574	0	644	51	0
19	S	629	0	652	81	0
20	T	763	0	861	105	0
21	U	208	0	221	32	0
22	V	1619	0	822	71	0
22	W	1619	0	822	69	0
23	X	361	0	184	27	0
24	Y	1644	0	853	66	0
25	Z	2984	0	2997	433	0
26	1	28	0	12	12	0
27	1	57	0	59	11	0
28	1	4	0	0	2	0
All	All	59791	0	42183	3364	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 33.

The worst 5 of 3364 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
25:Z:69:GLU:CG	25:Z:69:GLU:CB	1.83	1.52
25:Z:68:VAL:CA	25:Z:68:VAL:C	1.85	1.45
4:D:20:TYR:HA	4:D:26:CYS:SG	1.73	1.26
25:Z:198:LYS:HA	25:Z:198:LYS:NZ	1.49	1.24
25:Z:198:LYS:HE3	25:Z:201:GLU:OE1	1.35	1.22

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	232/256 (91%)	168 (72%)	35 (15%)	29 (12%)	1	3
3	C	204/239 (85%)	161 (79%)	29 (14%)	14 (7%)	2	13
4	D	206/209 (99%)	139 (68%)	44 (21%)	23 (11%)	1	5
5	E	148/162 (91%)	138 (93%)	8 (5%)	2 (1%)	16	58
6	F	99/101 (98%)	78 (79%)	15 (15%)	6 (6%)	2	16
7	G	153/156 (98%)	121 (79%)	20 (13%)	12 (8%)	1	11
8	H	136/138 (99%)	124 (91%)	8 (6%)	4 (3%)	7	38
9	I	125/128 (98%)	85 (68%)	26 (21%)	14 (11%)	1	5
10	J	96/105 (91%)	72 (75%)	15 (16%)	9 (9%)	1	7
11	K	117/129 (91%)	103 (88%)	13 (11%)	1 (1%)	25	71
12	L	122/132 (92%)	97 (80%)	15 (12%)	10 (8%)	1	10
13	M	122/126 (97%)	75 (62%)	31 (25%)	16 (13%)	0	3
14	N	58/61 (95%)	40 (69%)	10 (17%)	8 (14%)	0	2
15	O	86/89 (97%)	68 (79%)	13 (15%)	5 (6%)	3	18
16	P	81/88 (92%)	50 (62%)	21 (26%)	10 (12%)	1	3
17	Q	97/105 (92%)	84 (87%)	9 (9%)	4 (4%)	4	27
18	R	68/88 (77%)	52 (76%)	12 (18%)	4 (6%)	2	17
19	S	76/93 (82%)	50 (66%)	16 (21%)	10 (13%)	0	2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	T	97/106 (92%)	62 (64%)	24 (25%)	11 (11%)	1	4
21	U	22/27 (82%)	16 (73%)	3 (14%)	3 (14%)	0	2
25	Z	381/405 (94%)	272 (71%)	66 (17%)	43 (11%)	1	4
All	All	2726/2943 (93%)	2055 (75%)	433 (16%)	238 (9%)	1	9

5 of 238 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	8	LYS
2	B	9	GLU
2	B	15	VAL
2	B	127	ILE
2	B	131	PRO

### 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	202/220 (92%)	178 (88%)	24 (12%)	8	27
3	C	160/188 (85%)	142 (89%)	18 (11%)	9	32
4	D	180/181 (99%)	151 (84%)	29 (16%)	3	13
5	E	115/123 (94%)	106 (92%)	9 (8%)	18	57
6	F	90/90 (100%)	79 (88%)	11 (12%)	7	26
7	G	126/127 (99%)	113 (90%)	13 (10%)	10	36
8	H	119/119 (100%)	108 (91%)	11 (9%)	13	45
9	I	98/99 (99%)	89 (91%)	9 (9%)	13	45
10	J	88/92 (96%)	77 (88%)	11 (12%)	7	25
11	K	90/99 (91%)	77 (86%)	13 (14%)	5	19
12	L	104/109 (95%)	91 (88%)	13 (12%)	7	25
13	M	99/101 (98%)	85 (86%)	14 (14%)	5	20
14	N	49/50 (98%)	42 (86%)	7 (14%)	5	19
15	O	79/80 (99%)	69 (87%)	10 (13%)	6	24

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	P	72/74 (97%)	68 (94%)	4 (6%)	30	70
17	Q	94/97 (97%)	87 (93%)	7 (7%)	20	59
18	R	61/77 (79%)	54 (88%)	7 (12%)	8	31
19	S	69/80 (86%)	58 (84%)	11 (16%)	4	13
20	T	76/82 (93%)	66 (87%)	10 (13%)	6	23
21	U	19/22 (86%)	17 (90%)	2 (10%)	10	35
25	Z	322/338 (95%)	282 (88%)	40 (12%)	7	25
All	All	2312/2448 (94%)	2039 (88%)	273 (12%)	8	29

5 of 273 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
9	I	128	ARG
12	L	42	THR
25	Z	199	ILE
10	J	49	VAL
11	K	48	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 66 such sidechains are listed below:

Mol	Chain	Res	Type
10	J	13	HIS
11	K	116	HIS
25	Z	64	ASN
10	J	56	HIS
10	J	78	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1503/1522 (98%)	227 (15%)	50 (3%)
22	V	75/76 (98%)	20 (26%)	0
22	W	75/76 (98%)	20 (26%)	0
23	X	17/27 (62%)	8 (47%)	1 (5%)
24	Y	74/77 (96%)	24 (32%)	1 (1%)
All	All	1744/1778 (98%)	299 (17%)	52 (2%)

5 of 299 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	9	G
1	A	31	G
1	A	32	A
1	A	39	G
1	A	47	C

5 of 52 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	534	U
1	A	587	G
1	A	1285	A
1	A	547	A
1	A	573	A

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

9 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	$\# Z  > 2$
24	H2U	Y	16	24	19,21,22	1.11	1 (5%)	27,30,33	1.68	4 (14%)
24	H2U	Y	17	24	19,21,22	1.04	2 (10%)	27,30,33	1.76	6 (22%)
24	H2U	Y	20	24	19,21,22	1.06	2 (10%)	27,30,33	1.89	6 (22%)
24	OMC	Y	32	24	20,22,23	1.29	2 (10%)	25,31,34	0.98	2 (8%)
24	MIA	Y	37	24	29,31,32	1.26	2 (6%)	41,44,47	1.66	6 (14%)
24	7MG	Y	46	24	24,26,27	2.49	3 (12%)	34,39,42	1.95	6 (17%)
24	5MU	Y	54	24	20,22,23	0.87	1 (5%)	25,32,35	1.36	3 (12%)
24	PSU	Y	55	24	19,21,22	1.95	2 (10%)	23,30,33	1.04	2 (8%)
24	4SU	Y	8	24	19,21,22	2.19	5 (26%)	23,30,33	20.48	4 (17%)

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	H2U	Y	16	24	-	0/8/38/39	0/2/2/2
24	H2U	Y	17	24	-	0/8/38/39	0/2/2/2
24	H2U	Y	20	24	-	0/8/38/39	0/2/2/2
24	OMC	Y	32	24	-	0/8/27/28	0/2/2/2
24	MIA	Y	37	24	-	0/16/33/34	0/1/3/3
24	7MG	Y	46	24	-	0/8/37/38	0/1/3/3
24	5MU	Y	54	24	-	0/6/25/26	0/2/2/2
24	PSU	Y	55	24	-	0/8/25/26	0/2/2/2
24	4SU	Y	8	24	-	0/6/25/26	0/2/2/2

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	Y	46	7MG	C8-N9	-10.00	1.38	1.46
24	Y	55	PSU	C6-N1	7.84	1.39	1.32
24	Y	8	4SU	C6-C5	5.67	1.45	1.36
24	Y	46	7MG	C8-N7	-5.17	1.31	1.45
24	Y	37	MIA	C2-S10	4.34	1.79	1.75

The worst 5 of 39 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	Y	8	4SU	C4-N3-C2	98.04	125.79	121.60
24	Y	46	7MG	N7-C8-N9	7.61	113.14	103.08
24	Y	37	MIA	C11-S10-C2	6.64	107.05	102.26
24	Y	54	5MU	C6-N1-C2	-4.74	121.06	122.41
24	Y	20	H2U	C4-N3-C2	-4.61	121.84	125.83

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 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 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	GDP	1	1	-	30,30,30	1.04	2 (6%)	44,47,47	2.92	9 (20%)
27	KIR	1	2	-	59,59,59	3.70	25 (42%)	82,84,84	1.88	16 (19%)

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	GDP	1	1	-	-	0/16/32/32	0/1/3/3
27	KIR	1	2	-	-	0/53/98/98	0/3/3/3

The worst 5 of 27 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	1	2	KIR	O18-C17	-13.85	1.22	1.44
27	1	2	KIR	O30-C30	-11.19	1.18	1.42
27	1	2	KIR	O34-C33	-10.24	1.30	1.44
27	1	2	KIR	C45-C28	8.53	1.64	1.54
27	1	2	KIR	C22-C21	6.52	1.39	1.34

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	1	1	GDP	C6-C5-N7	-15.38	132.07	134.14
27	1	2	KIR	C45-C28-C27	6.77	113.03	108.10
27	1	2	KIR	C3-C2-N1	5.56	120.08	115.40
26	1	1	GDP	PA-O3A-PB	-5.15	116.58	131.68
27	1	2	KIR	O29-C29-O34	-4.75	102.49	110.22

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.