



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 05:50 am GMT

PDB ID : 1N34  
Title : Structure of the *Thermus thermophilus* 30S ribosomal subunit in the presence of codon and crystallographically disordered near-cognate transfer rna anticodon stem-loop mismatched at the first codon position  
Authors : Ogle, J.M.; Murphy IV, F.V.; Tarry, M.J.; Ramakrishnan, V.  
Deposited on : 2002-10-25  
Resolution : 3.80 Å(reported)

This is a wwPDB X-ray Structure 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/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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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
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

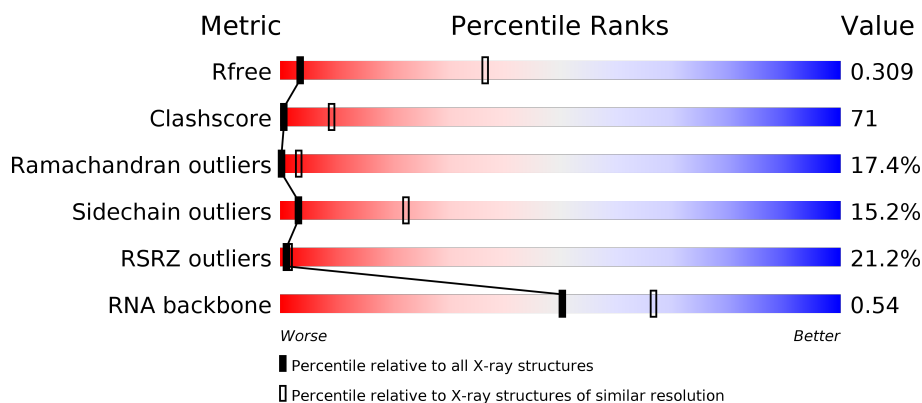
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.80 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))
$R_{free}$	100719	1019 (4.08-3.52)
Clashscore	112137	1030 (4.04-3.56)
Ramachandran outliers	110173	1011 (4.06-3.54)
Sidechain outliers	110143	1005 (4.06-3.54)
RSRZ outliers	101464	1032 (4.08-3.52)
RNA backbone	2435	1016 (4.70-2.90)

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. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1522	<div> <div>38%</div> <div> <div>10%</div> <div>73%</div> <div>15%</div> <div>..</div> </div> </div>
2	Z	6	<div> <div>17%</div> <div>50%</div> <div>33%</div> </div>
3	B	256	<div> <div>2%</div> <div>8%</div> <div>58%</div> <div>24%</div> <div>9%</div> </div>
4	C	239	<div> <div>15%</div> <div>11%</div> <div>51%</div> <div>23%</div> <div>14%</div> </div>

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Mol	Chain	Length	Quality of chain
5	D	208	
6	E	161	
7	F	101	
8	G	155	
9	H	138	
10	I	128	
11	J	104	
12	K	129	
13	L	135	
14	M	126	
15	N	60	
16	O	88	
17	P	88	
18	Q	104	
19	R	88	
20	S	92	
21	T	106	
22	V	26	

## 2 Entry composition [i](#)

There are 23 unique types of molecules in this entry. The entry contains 51757 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	1513	Total	C	N	O	P	42	0	0
			32508	14472	6016	10509	1511			

- Molecule 2 is a RNA chain called A-SITE MESSENGER RNA FRAGMENT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	Z	4	Total	C	N	O	P	0	0	0
			77	36	8	30	3			

- Molecule 3 is a protein called 30S RIBOSOMAL PROTEIN S2.

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

- Molecule 4 is a protein called 30S RIBOSOMAL PROTEIN S3.

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

- Molecule 5 is a protein called 30S RIBOSOMAL PROTEIN S4.

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

- Molecule 6 is a protein called 30S RIBOSOMAL PROTEIN S5.

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

- Molecule 7 is a protein called 30S RIBOSOMAL PROTEIN S6.

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

- Molecule 8 is a protein called 30S RIBOSOMAL PROTEIN S7.

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

- Molecule 9 is a protein called 30S RIBOSOMAL PROTEIN S8.

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

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	25	ASP	GLU	CONFLICT	UNP Q5SHQ2
H	37	ARG	LYS	CONFLICT	UNP Q5SHQ2
H	52	ASP	GLU	CONFLICT	UNP Q5SHQ2
H	61	VAL	ILE	CONFLICT	UNP Q5SHQ2
H	62	TYR	HIS	CONFLICT	UNP Q5SHQ2
H	81	HIS	LYS	CONFLICT	UNP Q5SHQ2
H	88	LYS	ARG	CONFLICT	UNP Q5SHQ2
H	115	SER	PRO	CONFLICT	UNP Q5SHQ2

- Molecule 10 is a protein called 30S RIBOSOMAL PROTEIN S9.

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

- Molecule 11 is a protein called 30S RIBOSOMAL PROTEIN S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	J	98	Total	C	N	O	S	0	0	0
			792	498	156	137	1			

- Molecule 12 is a protein called 30S RIBOSOMAL PROTEIN S11.

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

- Molecule 13 is a protein called 30S RIBOSOMAL PROTEIN S12.

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

- Molecule 14 is a protein called 30S RIBOSOMAL PROTEIN S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	M	118	Total	C	N	O	S	0	0	0
			937	579	193	163	2			

- Molecule 15 is a protein called 30S RIBOSOMAL PROTEIN S14.

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

- Molecule 16 is a protein called 30S RIBOSOMAL PROTEIN S15.

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

- Molecule 17 is a protein called 30S RIBOSOMAL PROTEIN S16.

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

- Molecule 18 is a protein called 30S RIBOSOMAL PROTEIN S17.

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

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	50	LYS	ARG	CONFLICT	UNP Q5SHP7
Q	53	LEU	VAL	CONFLICT	UNP Q5SHP7
Q	62	SER	ALA	CONFLICT	UNP Q5SHP7
Q	79	SER	GLU	CONFLICT	UNP Q5SHP7
Q	82	MET	LEU	CONFLICT	UNP Q5SHP7
Q	90	ILE	VAL	CONFLICT	UNP Q5SHP7
Q	96	GLN	ALA	CONFLICT	UNP Q5SHP7

- Molecule 19 is a protein called 30S RIBOSOMAL PROTEIN S18.

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

- Molecule 20 is a protein called 30S RIBOSOMAL PROTEIN S19.

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

- Molecule 21 is a protein called 30S RIBOSOMAL PROTEIN S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	T	99	Total	C	N	O	S	0	0	0
			763	470	162	129	2			

- Molecule 22 is a protein called 30S RIBOSOMAL PROTEIN THX.

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

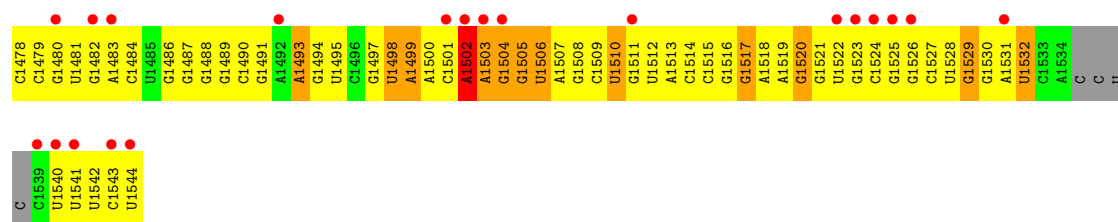
- Molecule 23 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

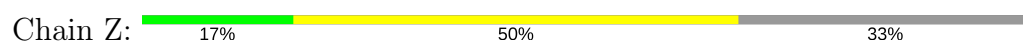




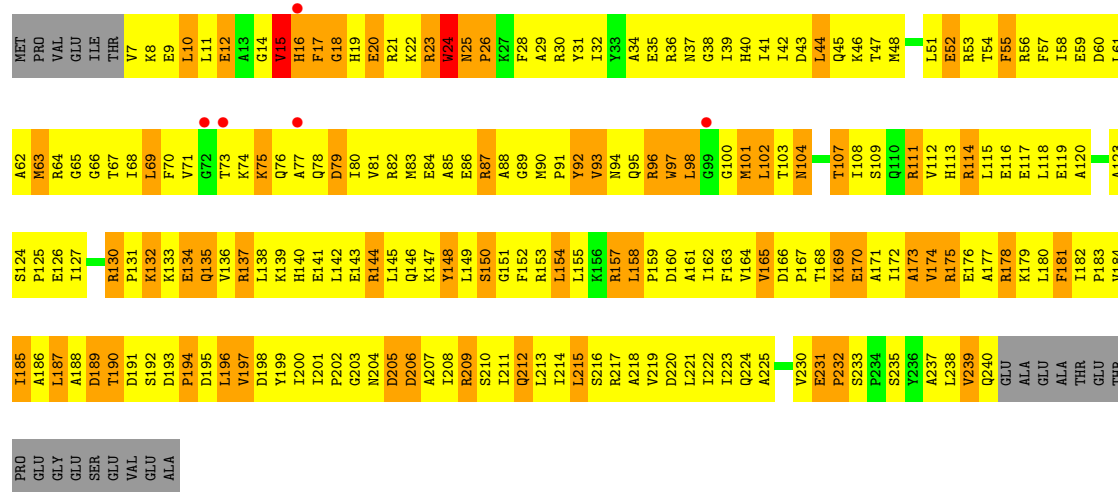
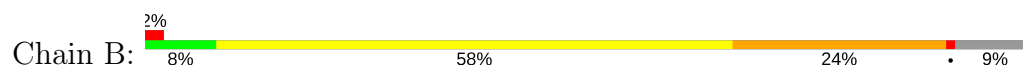
A1413	C1352	G1291	G1231	G1171	G1050	C995	A935	A873	C806	A746	U686	U626
U1414	G1353	U1292	U1232	C1172	C1051	A996	C936	G874	A807	C747	A687	G627
G1415	G1354	G1293	G1233	G1173	U1052	U997	A937	C875	G808	C748	G688	G628
G1416	G1355	G1294	C1234	U1053	G1054	C999	A938	C876	G809	C749	C689	G629
G1417	G1356	G1295	U1235	G1174	C1054	C999	G939	C877	C810	G750	G690	G630
A1418	A1357	G1296	A1236	A1055	A1055	A1000	C940	C878	C811	G751	G691	G631
G1419	U1358	U1358	C1237	G1177	U1056	A1001	G941	C879	C812	G752	U692	A632
C1420	C1359	A1299	A1238	G1178	G1057	G1002	G942	C880	U913	A753	G693	G633
G1421	A1360	G1300	A1239	A1179	G1058	G1003	U943	C881	A814	C754	A694	C634
G1422	G1361	U1301	U1240	A1180	C1059	G1003A	G944	C882	A815	G755	A695	G635
G1423	G1361A	G1302	G1241	G1181	C1060	A1004	G945	C883	A816	G756	A696	U636
C1424	C1362	G1303	C1242	G1182	G1061	C1006	A946	U884	C817	G757	G697	G637
A1425	A1363	G1304	C1243	A1183	U1062	A1005	G947	U885	G818	G758	G698	G638
G1426	U1364	G1305	C1244	G1184	C1063	C1007	C948	G886	A819	U759	G699	G639
U1427	G1365	A1306	A1245	G1185	G1064	G1008	C949	G887	U820	G760	G700	A640
A1428	C1366	U1307	C1246	G1186	U1065	G1009	U950	C888	G821	G761	C701	U641
C1429	C1367	U1308	U1247	G1187	C1066	G1010	G951	A889	C822	G762	A702	A642
G1430	G1368	G1309	A1248	G1188	A1067	G1011	U952	G890	G823	G763	G703	C643
C1431	C1369	G1310	C1249	C1189	G1068	U1012	G953	U891	C824	C764	A704	C644
G1432	G1370	G1311	A1250	G1190	C1069	G1013	G954	A892	G825	C765	U705	C645
G1433	G1371	G1312	A1251	A1191	U1070	A1014	U955	C893	G826	A766	A706	U646
A1434	U1372	U1313	A1252	G1192	C1071	A1015	U956	C894	U827	A767	C707	A647
G1435	G1373	C1314	G1253	G1193	G1072	A1016	U957	C895	A828	A768	C708	A648
U1436	A1374	U1315	C1254	G1194	U1073	G1017	U958	C896	G829	G769	G709	G649
C1437	A1375	G1316	C1255	C1195	G1074	C1018	A959	C897	G830	C770	G710	G650
G1438	U1376	C1317	A1256	U1196	C1075	C1019	U960	C898	U831	G771	G711	C651
C1439	A1377	A1318	U1257	G1197	C1076	U1020	U961	C899	C832	U772	A712	U652
C1440	G1378	A1319	G1258	G1198	C1077	G1021	C962	A900	U833	G773	C713	A653
G1441	G1379	C1320	C1259	U1199	U1078	G1022	G963	A901	U834	G774	G714	G654
G1442	U1380	C1321	C1260	C1200	G1079	G1023	A964	G902	U835	G775	A715	A655
C1443	A1381	C1322	A1261	C1201	A1080	G1024	A965	G903	G836	G776	A716	C656
A1446	C1382	G1323	C1262	G1202	G1081	U1025	G966	C904	G837	A777	C717	G657
G1447	C1383	A1324	C1263	C1203	G1082	G1026	C967	U905	G838	G778	G718	G658
C1448	G1384	C1325	C1264	A1204	U1083	C1027	A968	C906	U839	C779	C719	U659
C1449	G1385	G1326	U1205	G1084	C1028	A1028	A969	A907	C840	A780	C720	G660
U1450	G1386	C1327	G1206	C1145	C1029	G1029	C970	A908	U941	A781	G721	G661
A1451	G1387	C1328	C1267	U1086	G1030	G1030A	G971	A909	C848	A782	A722	G662
C1452	C1388	A1329	U1268	G1207	G1087	G1030B	C972	C910	C849	C783	U723	A663
G1453	C1389	U1330	A1269	C1208	U1088	C1030C	G973	U911	U850	C784	G724	G664
G1454	U1390	G1331	C1270	C1209	G1089	A1030D	A974	C912	G851	G785	G725	A665
G1455	U1391	A1332	G1271	U1211	U1090	A1030D	A975	A913	G852	G786	C726	G666
C1459	G1392	A1333	G1272	U1212	U1091	G1031	G976	A914	G853	A787	G727	G667
A1460	U1393	G1334	G1273	A1213	A1092	G1032	A977	A915	G854	U788	U728	G668
G1461	C1394	C1335	G1274	C1214	A1093	G1033	A978	C916	G855	U789	A729	U669
G1462	C1395	C1336	A1275	G1215	G1094	G1034	C979	G917	G856	A790	G730	G670
A1396	G1396	G1337	G1276	U1095	U1095	A1035	C980	A918	G858	G791	G731	G671
C1463	C1397	G1338	C1277	C1217	C1096	G1036	U981	A919	G859	A792	C732	U672
A1398	A1398	A1339	U1278	C1218	C1097	C1037	U982	U920	A860	U793	A733	G673
C1466	C1399	A1340	A1279	U1219	C1098	C1038	A983	U921	G861	A794	G734	G674
G1467	C1400	U1341	A1280	G1220	G1099	C1039	C984	G922	C862	C795	C735	A675
G1468	G1401	C1342	U1281	G1221	C1100	U1040	C985	A923	U863	C796	C736	A676
C1469	C1402	G1343	C1282	G1222	A1101	A1041	A986	C924	A864	C797	A737	U677
C1470	C1403	C1344	C1283	C1223	A1102	G1042	G987	G925	A865	G798	C738	U678
G1471	G1471	U1345	C1284	G1162	C1103	C1043	G988	G926	C866	G799	C739	C679
U1472	U1405	A1346	A1285	G1164	G1104	A1044	C989	G927	G867	G800	U740	C680
A1473	U1406	G1347	C1286	C1165	A1105	C1045	C990	G928	C868	U801	G741	C681
C1474	C1407	U1348	A1287	G1166	G1106	A1046	U991	G928	C869	A802	G742	G682
G1475	A1408	A1349	A1288	A1167	C1107	A1047	U992	C932	U870	G803	U743	G683
G1476	U1409	A1350	A1289	G1168	G1048	G1048	G993	C933	U871	A684	C744	A684
C1477	C1412	U1351	G1290	A1169	U1049	U1049	A994	C934	A872	C805	C745	G685



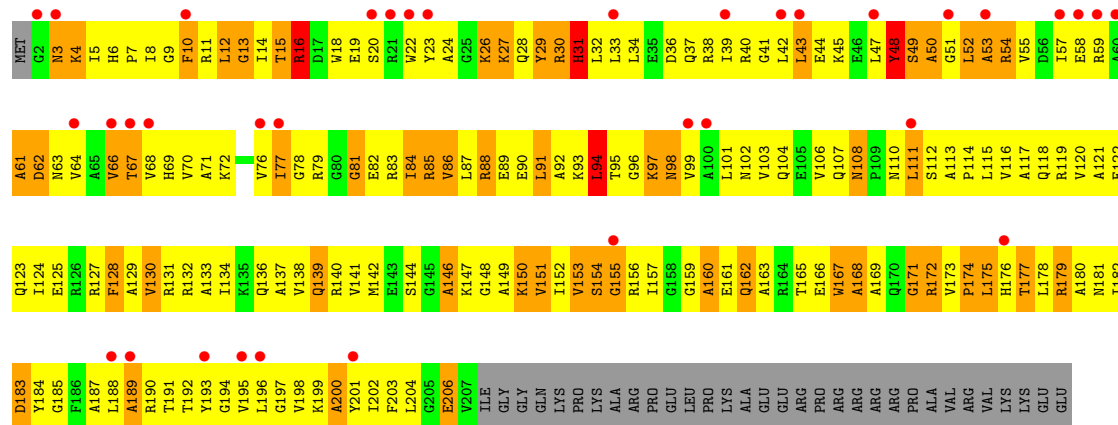
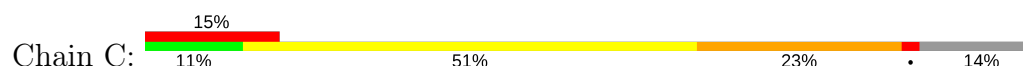
• Molecule 2: A-SITE MESSENGER RNA FRAGMENT



• Molecule 3: 30S RIBOSOMAL PROTEIN S2



• Molecule 4: 30S RIBOSOMAL PROTEIN S3



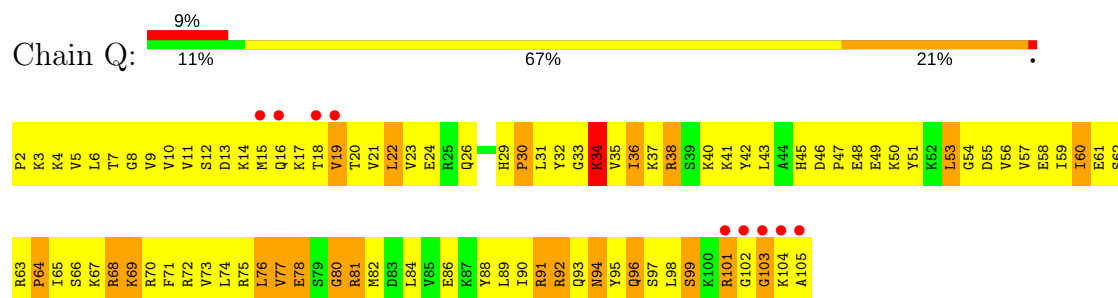
• Molecule 5: 30S RIBOSOMAL PROTEIN S4



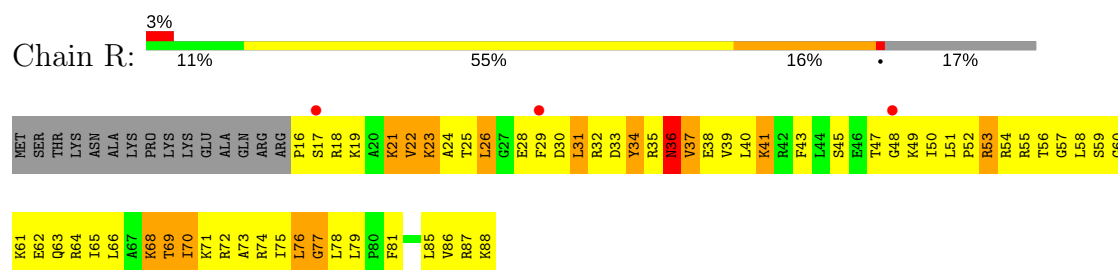




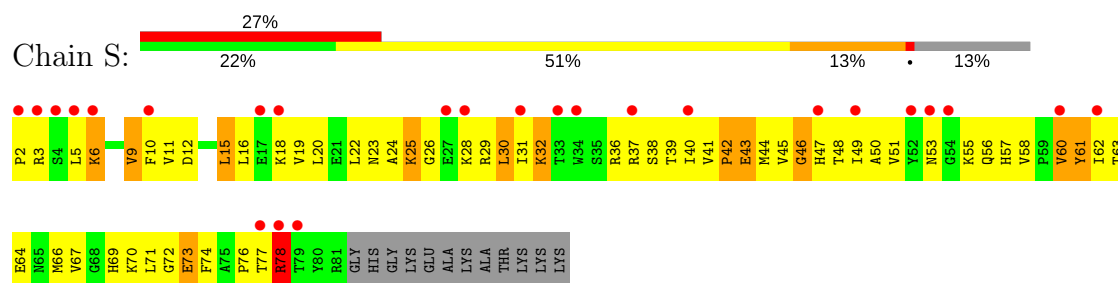
● Molecule 18: 30S RIBOSOMAL PROTEIN S17



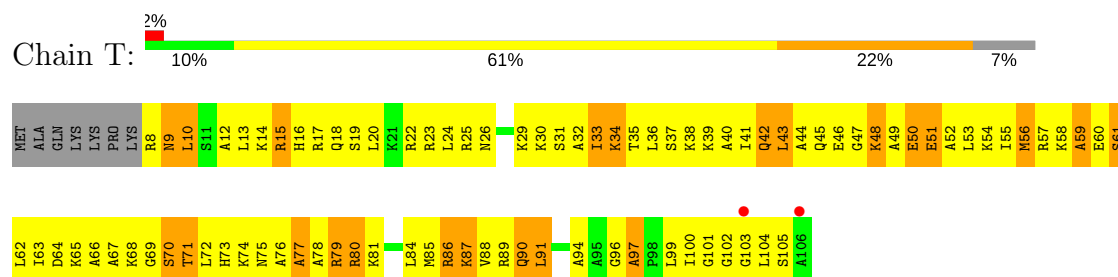
● Molecule 19: 30S RIBOSOMAL PROTEIN S18



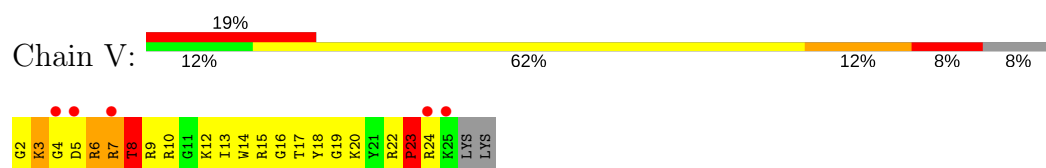
• Molecule 20: 30S RIBOSOMAL PROTEIN S19



- Molecule 21: 30S RIBOSOMAL PROTEIN S20



• Molecule 22: 30S RIBOSOMAL PROTEIN THX



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	401.84Å 401.84Å 173.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	141.42 – 3.80 148.30 – 3.78	Depositor EDS
% Data completeness (in resolution range)	92.6 (141.42-3.80) 92.4 (148.30-3.78)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.94 (at 3.78Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.241 , 0.312 0.242 , 0.309	Depositor DCC
$R_{free}$ test set	6382 reflections (5.20%)	DCC
Wilson B-factor (Å <sup>2</sup> )	122.1	Xtriage
Anisotropy	0.327	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 194.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.84	EDS
Total number of atoms	51757	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	101.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.15% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.60	1/36387 (0.0%)	0.76	22/56789 (0.0%)
2	Z	0.62	0/84	0.87	0/128
3	B	0.42	0/1935	0.73	0/2609
4	C	0.37	0/1636	0.70	0/2205
5	D	0.44	0/1733	0.73	0/2318
6	E	0.52	0/1162	0.83	0/1564
7	F	0.37	0/856	0.69	0/1154
8	G	0.35	0/1276	0.66	0/1709
9	H	0.57	0/1136	0.87	0/1527
10	I	0.36	0/1029	0.66	0/1378
11	J	0.36	0/805	0.68	0/1082
12	K	0.42	0/900	0.71	0/1213
13	L	0.41	0/986	0.76	0/1320
14	M	0.36	0/947	0.68	0/1270
15	N	0.38	0/501	0.74	0/664
16	O	0.44	0/745	0.67	0/992
17	P	0.47	0/716	0.71	0/963
18	Q	0.56	0/870	0.83	1/1159 (0.1%)
19	R	0.41	0/603	0.71	0/799
20	S	0.35	0/661	0.67	0/890
21	T	0.37	0/765	0.73	0/1007
22	V	0.40	0/212	0.71	0/277
All	All	0.54	1/55945 (0.0%)	0.75	23/83017 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	2	42

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Mol	Chain	#Chirality outliers	#Planarity outliers
17	P	0	1
All	All	2	43

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	858	G	C5-C6	-6.02	1.36	1.42

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	51	A	C2'-C3'-O3'	9.80	131.06	109.50
1	A	266	G	C2'-C3'-O3'	9.28	129.91	109.50
1	A	1498	U	C2'-C3'-O3'	9.05	129.41	109.50
1	A	1085	U	C2'-C3'-O3'	7.77	126.60	109.50
1	A	575	G	C2'-C3'-O3'	7.36	125.69	109.50

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	51	A	C3'
1	A	1498	U	C3'

5 of 43 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	127	G	Sidechain
1	A	148	G	Sidechain
1	A	197	A	Sidechain
1	A	28	G	Sidechain
1	A	90	U	Sidechain

## 5.2 Too-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 hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	32508	0	16414	2480	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	Z	77	0	42	5	0
3	B	1900	0	1951	427	0
4	C	1612	0	1677	396	0
5	D	1703	0	1765	380	0
6	E	1146	0	1207	261	0
7	F	843	0	857	159	0
8	G	1257	0	1296	257	0
9	H	1116	0	1177	235	0
10	I	1011	0	1043	246	0
11	J	792	0	835	245	0
12	K	885	0	904	142	0
13	L	970	0	1057	183	0
14	M	937	0	995	167	0
15	N	492	0	533	140	0
16	O	734	0	771	142	0
17	P	700	0	720	175	0
18	Q	857	0	930	180	0
19	R	597	0	668	143	0
20	S	647	0	673	114	0
21	T	763	0	861	174	0
22	V	208	0	221	53	0
23	D	1	0	0	0	0
23	N	1	0	0	0	0
All	All	51757	0	36597	6246	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 71.

The worst 5 of 6246 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:818:G:O2'	1:A:819:A:H5''	1.44	1.17
1:A:1064:G:H4'	1:A:1065:U:H5'	1.28	1.15
1:A:1443:G:H5''	1:A:1446:A:H5'	1.21	1.14
19:R:53:ARG:HH21	19:R:60:GLY:N	1.46	1.14
6:E:13:ILE:HG22	6:E:30:ALA:HA	1.22	1.13

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	
3	B	232/256 (91%)	134 (58%)	71 (31%)	27 (12%)	0	8
4	C	204/239 (85%)	95 (47%)	64 (31%)	45 (22%)	0	1
5	D	206/208 (99%)	109 (53%)	63 (31%)	34 (16%)	0	4
6	E	148/161 (92%)	98 (66%)	30 (20%)	20 (14%)	0	5
7	F	99/101 (98%)	56 (57%)	30 (30%)	13 (13%)	0	6
8	G	153/155 (99%)	68 (44%)	47 (31%)	38 (25%)	0	1
9	H	136/138 (99%)	91 (67%)	28 (21%)	17 (12%)	0	7
10	I	125/128 (98%)	70 (56%)	27 (22%)	28 (22%)	0	1
11	J	96/104 (92%)	51 (53%)	26 (27%)	19 (20%)	0	2
12	K	117/129 (91%)	72 (62%)	31 (26%)	14 (12%)	0	7
13	L	122/135 (90%)	81 (66%)	22 (18%)	19 (16%)	0	4
14	M	116/126 (92%)	66 (57%)	33 (28%)	17 (15%)	0	5
15	N	58/60 (97%)	25 (43%)	8 (14%)	25 (43%)	0	0
16	O	86/88 (98%)	42 (49%)	30 (35%)	14 (16%)	0	4
17	P	81/88 (92%)	44 (54%)	20 (25%)	17 (21%)	0	2
18	Q	102/104 (98%)	60 (59%)	27 (26%)	15 (15%)	0	5
19	R	71/88 (81%)	36 (51%)	24 (34%)	11 (16%)	0	4
20	S	78/92 (85%)	45 (58%)	24 (31%)	9 (12%)	0	8
21	T	97/106 (92%)	34 (35%)	42 (43%)	21 (22%)	0	1
22	V	22/26 (85%)	10 (46%)	7 (32%)	5 (23%)	0	1
All	All	2349/2532 (93%)	1287 (55%)	654 (28%)	408 (17%)	0	3

5 of 408 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	B	20	GLU

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Mol	Chain	Res	Type
3	B	158	LEU
3	B	232	PRO
3	B	239	VAL
4	C	4	LYS

### 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	
3	B	202/220 (92%)	156 (77%)	46 (23%)	1	8
4	C	160/188 (85%)	140 (88%)	20 (12%)	5	29
5	D	180/180 (100%)	150 (83%)	30 (17%)	2	19
6	E	115/122 (94%)	90 (78%)	25 (22%)	1	9
7	F	90/90 (100%)	81 (90%)	9 (10%)	9	39
8	G	126/126 (100%)	111 (88%)	15 (12%)	6	32
9	H	119/119 (100%)	102 (86%)	17 (14%)	4	25
10	I	98/99 (99%)	79 (81%)	19 (19%)	1	12
11	J	87/91 (96%)	70 (80%)	17 (20%)	1	12
12	K	90/99 (91%)	76 (84%)	14 (16%)	3	22
13	L	104/111 (94%)	94 (90%)	10 (10%)	10	41
14	M	94/101 (93%)	85 (90%)	9 (10%)	10	41
15	N	49/49 (100%)	35 (71%)	14 (29%)	0	3
16	O	79/79 (100%)	68 (86%)	11 (14%)	4	27
17	P	72/74 (97%)	59 (82%)	13 (18%)	2	15
18	Q	96/96 (100%)	83 (86%)	13 (14%)	4	27
19	R	64/77 (83%)	59 (92%)	5 (8%)	15	51
20	S	71/79 (90%)	63 (89%)	8 (11%)	7	34
21	T	76/82 (93%)	71 (93%)	5 (7%)	19	57
22	V	19/21 (90%)	17 (90%)	2 (10%)	8	37

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1991/2103 (95%)	1689 (85%)	302 (15%)	3 22

5 of 302 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	G	56	GLN
10	I	91	ASP
18	Q	93	GLN
8	G	94	ARG
9	H	84	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 65 such sidechains are listed below:

Mol	Chain	Res	Type
7	F	94	GLN
8	G	122	HIS
19	R	36	ASN
8	G	37	ASN
8	G	86	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1511/1522 (99%)	234 (15%)	0
2	Z	3/6 (50%)	0	0
All	All	1514/1528 (99%)	234 (15%)	0

5 of 234 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	8	A
1	A	9	G
1	A	31	G
1	A	32	A
1	A	39	G

There are no RNA pucker outliers to report.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	1511/1522 (99%)	1.96	573 (37%) 0 1	15, 89, 187, 199	0
2	Z	4/6 (66%)	1.03	0 100 100	168, 184, 185, 199	0
3	B	234/256 (91%)	0.02	5 (2%) 64 54	23, 99, 178, 199	0
4	C	206/239 (86%)	0.91	35 (16%) 2 2	46, 134, 198, 199	0
5	D	208/208 (100%)	0.21	9 (4%) 36 28	14, 86, 165, 189	0
6	E	150/161 (93%)	0.12	4 (2%) 55 44	6, 56, 121, 160	0
7	F	101/101 (100%)	0.53	10 (9%) 8 7	44, 111, 171, 185	0
8	G	155/155 (100%)	0.15	7 (4%) 34 27	43, 141, 195, 199	0
9	H	138/138 (100%)	0.06	2 (1%) 75 67	3, 46, 115, 127	0
10	I	127/128 (99%)	0.92	28 (22%) 1 1	40, 146, 195, 199	0
11	J	98/104 (94%)	1.78	41 (41%) 0 1	63, 154, 199, 199	0
12	K	119/129 (92%)	0.39	11 (9%) 10 8	16, 93, 164, 199	0
13	L	124/135 (91%)	0.35	10 (8%) 13 10	19, 96, 159, 196	0
14	M	118/126 (93%)	0.59	16 (13%) 3 4	61, 125, 173, 199	0
15	N	60/60 (100%)	2.04	25 (41%) 0 1	42, 134, 185, 199	0
16	O	88/88 (100%)	0.17	6 (6%) 18 13	25, 70, 145, 189	0
17	P	83/88 (94%)	0.20	1 (1%) 79 71	12, 69, 141, 188	0
18	Q	104/104 (100%)	0.28	9 (8%) 11 9	2, 69, 140, 199	0
19	R	73/88 (82%)	0.33	3 (4%) 38 30	27, 87, 168, 194	0
20	S	80/92 (86%)	1.82	25 (31%) 0 1	55, 152, 198, 199	0
21	T	99/106 (93%)	-0.02	2 (2%) 65 56	24, 82, 169, 199	0
22	V	24/26 (92%)	1.16	5 (20%) 1 1	39, 125, 181, 195	0
All	All	3904/4060 (96%)	1.06	827 (21%) 1 1	2, 98, 186, 199	0

The worst 5 of 827 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1221	G	10.4
4	C	2	GLY	10.3
1	A	1053	G	9.4
20	S	2	PRO	9.0
5	D	42	GLN	8.5

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
23	ZN	D	306	1/1	0.88	0.39	0.16	78,78,78,78	0
23	ZN	N	307	1/1	0.99	0.11	-1.23	78,78,78,78	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.