



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 05:56 am GMT

PDB ID : 1I97
Title : CRYSTAL STRUCTURE OF THE 30S RIBOSOMAL SUBUNIT FROM THERMUS THERMOPHILUS IN COMPLEX WITH TETRACYCLINE
Authors : Pioletti, M.; Schlutzen, F.; Harms, J.; Zarivach, R.; Gluehmann, M.; Avila, H.; Bartels, H.; Jacobi, C.; Hartsch, T.; Yonath, A.; Franceschi, F.
Deposited on : 2001-03-18
Resolution : 4.50 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

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

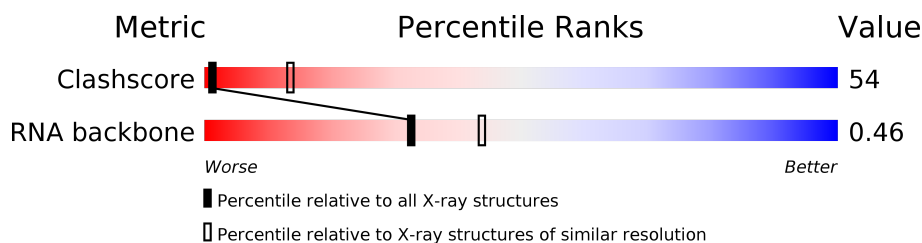
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.50 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	112137	1029 (5.30-3.70)
RNA backbone	2435	1038 (6.00-2.90)

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 ≥ 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	1514	
2	B	255	
3	C	238	
4	D	208	
5	E	161	
6	F	101	
7	G	155	
8	H	138	

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Mol	Chain	Length	Quality of chain
9	I	128	
10	J	104	
11	K	128	
12	L	131	
13	M	125	
14	N	60	
15	O	88	
16	P	88	
17	Q	104	
18	R	87	
19	S	92	
20	T	105	
21	U	26	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	TAC	A	2001	X	-	X	-
25	TAC	A	2003	X	-	X	-
25	TAC	A	2004	X	-	X	-
25	TAC	A	2005	X	-	X	-
25	TAC	A	2006	X	-	X	-
25	TAC	D	2002	X	-	X	-

2 Entry composition

There are 25 unique types of molecules in this entry. The entry contains 36361 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 RRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1514	Total	C	N	O	P	0	0	0
			32534	14482	6022	10517	1513			

- Molecule 2 is a protein called 30S RIBOSOMAL PROTEIN S2.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
2	B	249	Total	C	0	0	249
			249	249			

- Molecule 3 is a protein called 30S RIBOSOMAL PROTEIN S3.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
3	C	206	Total	C	0	0	206
			206	206			

- Molecule 4 is a protein called 30S RIBOSOMAL PROTEIN S4.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
4	D	208	Total	C	0	0	208
			208	208			

- Molecule 5 is a protein called 30S RIBOSOMAL PROTEIN S5.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
5	E	156	Total	C	0	0	156
			156	156			

- Molecule 6 is a protein called 30S RIBOSOMAL PROTEIN S6.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
6	F	101	Total	C	0	0	101
			101	101			

- Molecule 7 is a protein called 30S RIBOSOMAL PROTEIN S7.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
7	G	155	Total C 155 155	0	0	155

- Molecule 8 is a protein called 30S RIBOSOMAL PROTEIN S8.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
8	H	138	Total C 138 138	0	0	138

- Molecule 9 is a protein called 30S RIBOSOMAL PROTEIN S9.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
9	I	127	Total C 127 127	0	0	127

- Molecule 10 is a protein called 30S RIBOSOMAL PROTEIN S10.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
10	J	98	Total C 98 98	0	0	98

- Molecule 11 is a protein called 30S RIBOSOMAL PROTEIN S11.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
11	K	123	Total C 123 123	0	0	123

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
12	L	131	Total C 131 131	0	0	131

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
13	M	93	Total C 93 93	0	0	93

- Molecule 14 is a protein called 30S RIBOSOMAL PROTEIN S14.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
14	N	60	Total C 60 60	0	0	60

- Molecule 15 is a protein called 30S RIBOSOMAL PROTEIN S15.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
15	O	88	Total C 88 88	0	0	88

- Molecule 16 is a protein called 30S RIBOSOMAL PROTEIN S16.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
16	P	88	Total C 88 88	0	0	88

- Molecule 17 is a protein called 30S RIBOSOMAL PROTEIN S17.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
17	Q	104	Total C 104 104	0	0	104

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
18	R	82	Total C 82 82	0	0	82

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
19	S	80	Total C 80 80	0	0	80

- Molecule 20 is a protein called 30S RIBOSOMAL PROTEIN S20.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
20	T	99	Total C 99 99	0	0	99

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
21	U	24	Total C 24 24	0	0	24

- Molecule 22 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	P	1	Total Mg 1 1	0	0
22	G	1	Total Mg 1 1	0	0
22	Q	2	Total Mg 2 2	0	0
22	D	2	Total Mg 2 2	0	0
22	K	1	Total Mg 1 1	0	0
22	E	1	Total Mg 1 1	0	0
22	A	63	Total Mg 63 63	0	0
22	T	3	Total Mg 3 3	0	0
22	L	1	Total Mg 1 1	0	0

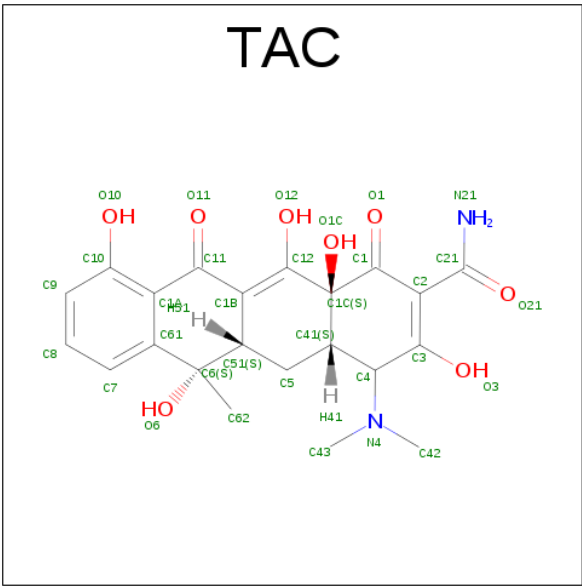
- Molecule 23 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 24 is OCTADECATUNGSTENYL DIPHOSPHATE (three-letter code: WO2) (formula: O₆₂P₂W₁₈).



- Molecule 25 is TETRACYCLINE (three-letter code: TAC) (formula: C₂₂H₂₄N₂O₈).



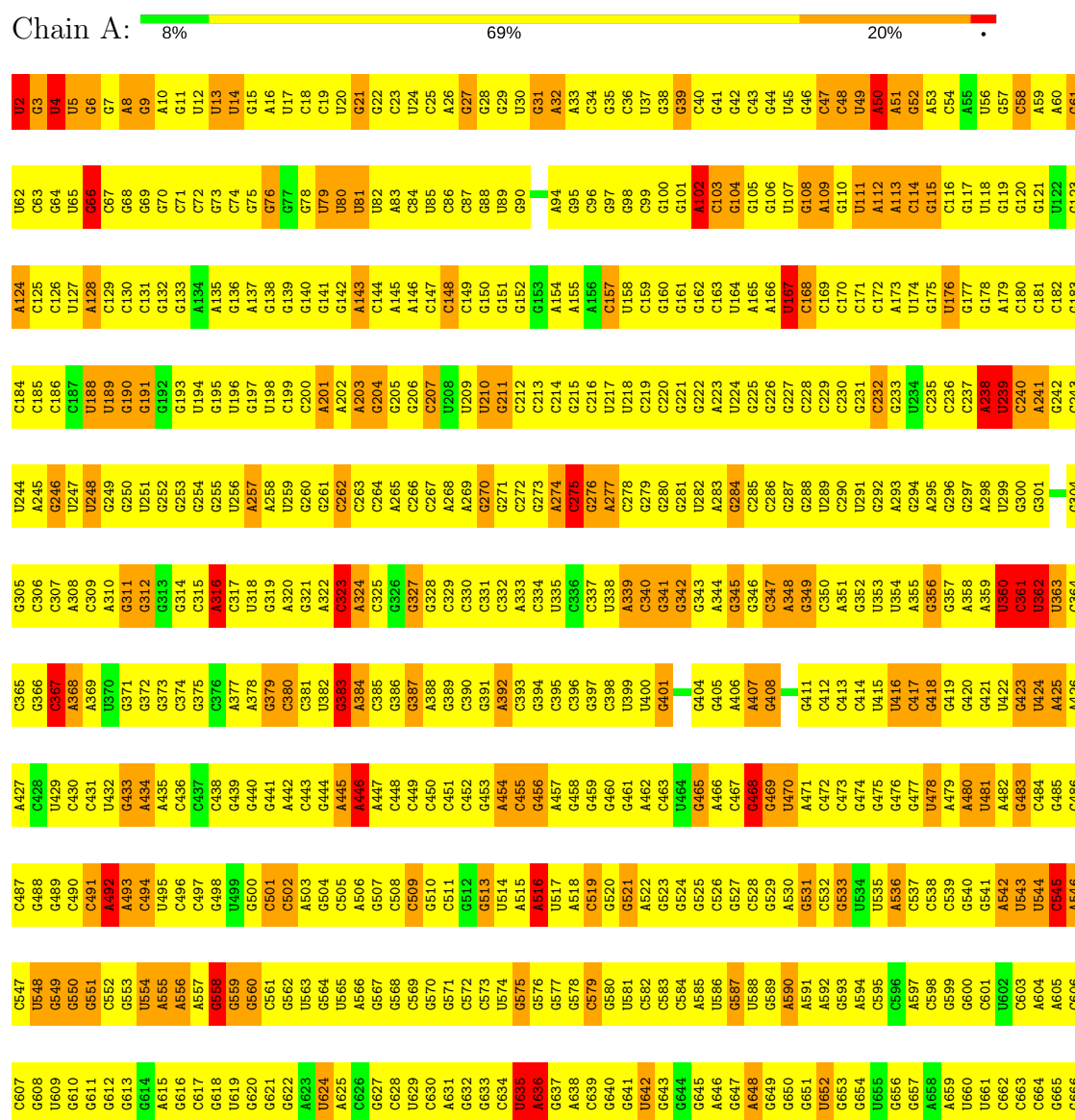
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
25	A	1	Total	C	N	O	0	0
			32	22	2	8		
25	D	1	Total	C	N	O	0	0
			32	22	2	8		
25	A	1	Total	C	N	O	0	0
			32	22	2	8		
25	A	1	Total	C	N	O	0	0
			32	22	2	8		
25	A	1	Total	C	N	O	0	0
			32	22	2	8		
25	A	1	Total	C	N	O	0	0
			32	22	2	8		

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 the various outlier classes 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



A1470	G1400	A1338	C1278	U1216	G1154	A1092	G1032	U968	C908	U848	C788	C727	A667
G1401	C1402	C1340	A1280	C1218	G1156	C1094	C1033	U969	C909	A849	C789	C728	G668
A1472	C1406	C1341	G1281	A1219	G1159	C1095	C1035	A971	C911	G851	C791	C730	A670
U1407	C1408	C1343	U1282	A1220	G1160	C1096	C1036	C972	C912	G852	C792	C731	G671
A1477	C1409	C1344	C1284	G1222	A1161	C1098	U1038	A973	C913	G853	C793	C732	C672
A1476	A1409	A1345	C1285	C1223	G1162	C1099	C1038	U974	A914	C854	C794	U734	G674
A1478	C1410	C1346	G1286	C1224	G1163	C1100	C1040	C976	A915	G855	C795	G735	G675
C1411	G1347	A1287	A1287	C1225	A1164	C1101	C1041	U977	C917	C857	C796	G735	U676
A1480	C1412	C1348	U1288	A1226	G1165	U1102	C1042	A978	C918	G858	A798	C737	A677
C1413	C1349	C1349	U1289	C1227	G1166	U1104	G1043	C979	C919	C859	A799	C738	A678
G1414	G1350	C1350	G1290	U1228	G1167	A1105	U1044	C980	C920	C860	C800	C739	A679
A1415	C1351	G1351	G1291	A1229	G1168	A1106	C1045	C981	C921	C861	G801	U740	A681
A1416	A1416	C1352	G1292	C1230	A1169	U1107	C1046	A982	C922	G862	A802	C741	G681
G1417	C1353	G1293	A1231	A1231	C1170	U1108	U1047	A983	C923	G863	U803	A742	C682
C1486	U1354	A1294	A1232	A1232	G1171	G1109	C1048	C984	C924	G864	G804	C743	G683
C1487	C1355	C1295	C1295	A1233	A1172	C1110	A1049	G988	C925	G865	C805	G744	C684
C1422	A1488	U1356	U1296	G1234	C1173	C1111	C1050	A989	C926	A866	C745	C684	C684
G1423	A1489	C1357	C1297	C1235	G1174	A1112	C1051	C989	U927	G867	C806	C746	G686
G1424	A1490	C1358	C1298	G1236	U1175	C1113	C1052	U990	C928	U868	C807	C747	A687
C1491	A1491	A1359	A1299	A1237	C1176	G1114	C1053	C991	U929	A869	C808	C748	U688
A1426	C1360	A1300	A1300	U1238	U1177	G1115	U1054	A992	C930	C870	U810	A749	A689
G1427	G1361	C1301	C1301	C1239	G1178	G1116	U1055	A993	C931	C871	A811	A750	C690
C1428	U1362	C1302	C1302	C1240	G1179	U1117	C1056	A994	C932	C872	C812	C751	C691
A1495	C1363	C1303	C1303	C1241	U1180	C1118	C1057	C995	U933	C873	G813	C752	C692
A1496	U1430	C1364	G1304	A1242	C1181	C1119	C1058	C996	U934	C874	U814	C753	G693
C1497	A1365	A1305	A1305	C1243	A1182	G1120	C1059	C997	A935	C875	C815	C754	G694
G1432	C1366	C1306	C1306	C1244	G1183	G1121	U1060	U998	A936	C876	U816	U755	A695
C1433	C1367	C1307	C1307	C1245	C1184	C1122	G1061	C999	U937	A877	C817	C756	G696
G1500	C1368	C1308	C1308	G1246	A1185	C1123	A1062	C1000	U938	C878	U818	C757	G697
C1501	A1435	C1369	C1309	C1247	U1186	G1124	G1063	C1001	C939	A879	C819	C758	A698
G1502	C1436	C1370	A1310	C1248	G1187	G1125	C1064	C1002	C940	G880	C820	C759	A699
A1437	C1371	C1371	C1311	A1249	G1188	G1126	U1065	C1003	A941	C881	G821	A760	C700
A1438	U1372	G1312	G1312	A1250	G1189	C1127	C1066	C1004	A942	U882	U822	C761	G701
C1439	U1373	A1313	A1313	C1251	C1190	A1128	U1067	C1005	C943	G883	C823	C762	C702
G1440	C1374	A1314	A1314	C1252	G1193	C1129	U1068	C1006	C944	A884	U824	A763	C703
C1443	A1376	C1315	C1315	G1253	U1194	U1130	G1069	C1007	A945	A885	C825	A764	C704
G1444	C1377	C1316	C1316	C1257	A1195	C1131	C1070	C1010	A946	A886	C826	A765	A705
A1445	A1378	C1317	G1318	G1258	G1196	U1132	G1071	G1011	C947	C887	U827	C766	C706
C1446	C1379	G1319	C1319	U1259	G1197	A1133	U1072	G1012	C948	U888	C828	C767	G707
G1447	A1380	C1320	A1320	A1260	C1198	G1136	A1074	G1013	C949	C889	C829	C768	C708
C1448	C1381	A1321	A1321	C1261	C1199	G1137	C1075	C1014	C950	A890	G830	C769	C709
C1449	C1382	C1322	U1322	U1262	U1200	G1138	G1076	G1015	A951	A891	C831	U772	G710
G1453	C1383	C1323	C1323	C1263	C1201	A1139	U1077	C1016	A952	A892	C832	U773	A711
C1454	C1384	G1324	G1324	G1264	G1202	C1140	C1078	G1018	A954	G894	C833	C774	G713
C1455	C1385	C1325	C1325	C1265	G1203	U1141	C1079	C1019	A955	A895	C834	A775	C714
C1456	C1386	U1326	A1266	A1266	G1204	G1142	C1080	C1020	C956	A896	A836	C776	C715
C1457	C1387	A1327	A1267	C1267	A1205	C1143	G1081	C1021	C957	U897	C837	A777	C716
U1459	U1388	G1328	A1268	A1268	A1206	C1144	C1082	U1022	C958	U898	G838	C778	G717
U1462	C1391	A1330	C1269	A1270	C1207	C1145	A1083	A1023	C959	G899	C839	C779	C718
C1463	G1392	A1331	C1271	G1271	C1209	C1146	C1084	G1024	A960	U840	U840	C780	C719
G1464	A1395	U1332	G1272	G1272	C1210	C1147	C1085	C1025	C961	C901	A841	G781	A720
C1465	C1396	C1333	C1273	C1211	A1211	G1148	C1086	A1026	C962	C843	C843	G782	C721
G1466	U1397	G1334	G1274	G1274	G1212	U1149	A1087	C1027	A963	G903	C844	G783	C722
C1467	C1398	C1335	C1275	G1213	G1213	A1150	C1088	C1028	G964	G844	C844	U784	U723
G1468	C1399	G1336	G1276	G1214	C1214	A1151	C1089	G1029	C965	G845	C845	A785	G724
A1469	C1400	C1337	C1277	C1215	C1215	G1152	C1090	G1030	C966	G846	C846	G786	G725
C1470	C1401	C1338	C1278	C1216	C1216	C1153	C1091	U1031	C967	C902	C847	U787	U726

● Molecule 2: 30S RIBOSOMAL PROTEIN S2

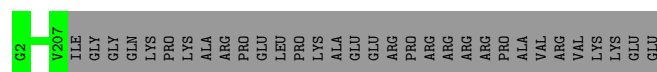
Chain B:

97%



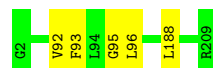
- Molecule 3: 30S RIBOSOMAL PROTEIN S3

Chain C:  87% 13%



- Molecule 4: 30S RIBOSOMAL PROTEIN S4

Chain D: 98%



• Molecule 5: 30S RIBOSOMAL PROTEIN S5

Chain E: 96%



- Molecule 6: 30S RIBOSOMAL PROTEIN S6

Chain F: 100%

There are no outlier residues recorded for this chain.

- Molecule 7: 30S RIBOSOMAL PROTEIN S7

Chain G: 99%



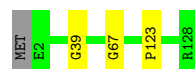
- Molecule 8: 30S RIBOSOMAL PROTEIN S8

Chain H: 100%

There are no outlier residues recorded for this chain.

• Molecule 9: 30S RIBOSOMAL PROTEIN S9

Chain I: 97% ..



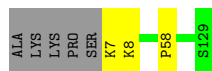
● Molecule 10: 30S RIBOSOMAL PROTEIN S10

Chain J:  93% • 6%



- Molecule 11: 30S RIBOSOMAL PROTEIN S11

Chain K:  94%



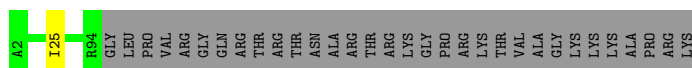
- Molecule 12: 30S RIBOSOMAL PROTEIN S12

Chain L:  99%



- Molecule 13: 30S RIBOSOMAL PROTEIN S13

Chain M:  74% 26%



- Molecule 14: 30S RIBOSOMAL PROTEIN S14

Chain N:  98%



- Molecule 15: 30S RIBOSOMAL PROTEIN S15

Chain O:  99%



- Molecule 16: 30S RIBOSOMAL PROTEIN S16

Chain P:  100%

There are no outlier residues recorded for this chain.

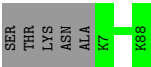
- Molecule 17: 30S RIBOSOMAL PROTEIN S17

Chain Q:  99%

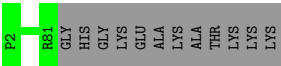
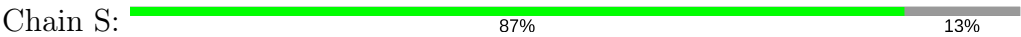


- Molecule 18: 30S RIBOSOMAL PROTEIN S18

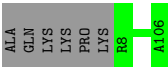
Chain R:  94% 6%



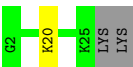
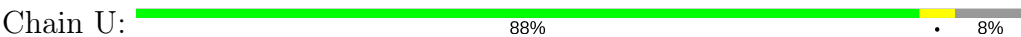
• Molecule 19: 30S RIBOSOMAL PROTEIN S19



• Molecule 20: 30S RIBOSOMAL PROTEIN S20



• Molecule 21: 30S RIBOSOMAL PROTEIN THX



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	406.90 Å 406.90 Å 175.20 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.00 – 4.50	Depositor
% Data completeness (in resolution range)	(Not available) (35.00-4.50)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.223 , 0.254	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	36361	wwPDB-VP
Average B, all atoms (Å ²)	77.0	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, WO2, MG, TAC

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	0.65	6/36417 (0.0%)	0.96	88/56838 (0.2%)

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	0	69

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	822	U	O3'-P	17.42	1.82	1.61
1	A	1178	G	O3'-P	10.60	1.73	1.61
1	A	872	G	O3'-P	8.69	1.71	1.61
1	A	4	U	N1-C2	6.91	1.44	1.38
1	A	1330	A	O3'-P	6.03	1.68	1.61

The worst 5 of 88 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	239	U	P-O3'-C3'	49.44	179.03	119.70
1	A	871	G	P-O3'-C3'	-44.80	65.94	119.70
1	A	919	G	P-O3'-C3'	43.73	172.17	119.70
1	A	872	G	P-O3'-C3'	-26.95	87.36	119.70
1	A	820	G	P-O3'-C3'	-26.57	87.81	119.70

There are no chirality outliers.

5 of 69 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	2	U	Sidechain
1	A	21	G	Sidechain
1	A	27	G	Sidechain
1	A	4	U	Sidechain
1	A	50	A	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	32534	0	16424	2783	0
2	B	249	0	0	1	0
3	C	206	0	0	0	0
4	D	208	0	0	12	0
5	E	156	0	0	2	0
6	F	101	0	0	0	0
7	G	155	0	0	2	0
8	H	138	0	0	0	0
9	I	127	0	0	5	0
10	J	98	0	0	1	0
11	K	123	0	0	5	0
12	L	131	0	0	1	0
13	M	93	0	0	1	0
14	N	60	0	0	1	0
15	O	88	0	0	1	0
16	P	88	0	0	0	0
17	Q	104	0	0	3	0
18	R	82	0	0	0	0
19	S	80	0	0	0	0
20	T	99	0	0	0	0
21	U	24	0	0	1	0
22	A	63	0	0	0	0
22	D	2	0	0	0	0
22	E	1	0	0	0	0
22	G	1	0	0	0	0
22	K	1	0	0	0	0
22	L	1	0	0	0	0
22	P	1	0	0	0	0
22	Q	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	T	3	0	0	0	0
23	D	1	0	0	0	0
23	N	1	0	0	0	0
24	A	328	0	0	0	0
24	B	246	0	0	1	0
24	D	82	0	0	0	0
24	E	82	0	0	1	0
24	G	82	0	0	3	0
24	H	82	0	0	0	0
24	J	82	0	0	1	0
24	K	82	0	0	4	0
24	R	82	0	0	0	0
25	A	160	0	115	159	0
25	D	32	0	23	12	0
All	All	36361	0	16562	2812	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 54.

The worst 5 of 2812 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:239:U:H1'	25:A:2005:TAC:C9	1.30	1.54
1:A:872:G:C5	1:A:873:C:C5	2.02	1.46
4:D:92:VAL:CA	25:D:2002:TAC:H423	1.41	1.46
1:A:872:G:C5	1:A:873:C:C6	2.11	1.38
1:A:239:U:H1'	25:A:2005:TAC:C8	1.52	1.36

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1513/1514 (99%)	322 (21%)	0

5 of 322 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	3	G
1	A	4	U
1	A	5	U
1	A	6	G
1	A	8	A

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 97 ligands modelled in this entry, 77 are monoatomic - leaving 20 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$
24	WO2	A	1579	-	60,116,116	51.46	8 (13%)	6,348,348	13.00	2 (33%)
24	WO2	A	1580	-	60,116,116	51.46	8 (13%)	6,348,348	13.00	2 (33%)
24	WO2	A	1581	-	60,116,116	51.46	8 (13%)	6,348,348	13.00	2 (33%)
24	WO2	A	1582	-	60,116,116	51.46	8 (13%)	6,348,348	13.00	2 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	TAC	A	2001	22	33,35,35	1.87	7 (21%)	41,58,58	2.13	8 (19%)
25	TAC	A	2003	-	33,35,35	1.89	7 (21%)	41,58,58	2.14	8 (19%)
25	TAC	A	2004	-	33,35,35	1.88	7 (21%)	41,58,58	2.14	8 (19%)
25	TAC	A	2005	-	33,35,35	1.87	7 (21%)	41,58,58	2.13	8 (19%)
25	TAC	A	2006	-	33,35,35	1.88	7 (21%)	41,58,58	2.15	8 (19%)
24	WO2	B	1001	-	60,116,116	51.46	8 (13%)	6,348,348	13.00	2 (33%)
24	WO2	B	1002	-	60,116,116	51.46	8 (13%)	6,348,348	13.00	2 (33%)
24	WO2	B	1004	-	60,116,116	51.45	8 (13%)	6,348,348	12.99	2 (33%)
24	WO2	D	1012	-	60,116,116	51.45	8 (13%)	6,348,348	12.99	2 (33%)
25	TAC	D	2002	-	33,35,35	1.88	7 (21%)	41,58,58	2.14	8 (19%)
24	WO2	E	1005	-	60,116,116	51.44	8 (13%)	6,348,348	12.99	2 (33%)
24	WO2	G	1006	-	60,116,116	51.46	8 (13%)	6,348,348	13.00	2 (33%)
24	WO2	H	1010	-	60,116,116	51.47	8 (13%)	6,348,348	13.01	2 (33%)
24	WO2	J	1009	-	60,116,116	51.46	8 (13%)	6,348,348	13.00	2 (33%)
24	WO2	K	1014	-	60,116,116	51.46	8 (13%)	6,348,348	13.00	2 (33%)
24	WO2	R	1008	-	60,116,116	51.47	8 (13%)	6,348,348	13.02	2 (33%)

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	WO2	A	1579	-	-	0/0/624/624	0/0/35/35
24	WO2	A	1580	-	-	0/0/624/624	0/0/35/35
24	WO2	A	1581	-	-	0/0/624/624	0/0/35/35
24	WO2	A	1582	-	-	0/0/624/624	0/0/35/35
25	TAC	A	2001	22	1/1/13/13	0/8/74/74	0/4/4/4
25	TAC	A	2003	-	1/1/13/13	0/8/74/74	0/4/4/4
25	TAC	A	2004	-	1/1/13/13	0/8/74/74	0/4/4/4
25	TAC	A	2005	-	1/1/13/13	0/8/74/74	0/4/4/4
25	TAC	A	2006	-	1/1/13/13	0/8/74/74	0/4/4/4
24	WO2	B	1001	-	-	0/0/624/624	0/0/35/35
24	WO2	B	1002	-	-	0/0/624/624	0/0/35/35
24	WO2	B	1004	-	-	0/0/624/624	0/0/35/35
24	WO2	D	1012	-	-	0/0/624/624	0/0/35/35
25	TAC	D	2002	-	1/1/13/13	0/8/74/74	0/4/4/4
24	WO2	E	1005	-	-	0/0/624/624	0/0/35/35
24	WO2	G	1006	-	-	0/0/624/624	0/0/35/35

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	WO2	H	1010	-	-	0/0/624/624	0/0/35/35
24	WO2	J	1009	-	-	0/0/624/624	0/0/35/35
24	WO2	K	1014	-	-	0/0/624/624	0/0/35/35
24	WO2	R	1008	-	-	0/0/624/624	0/0/35/35

The worst 5 of 154 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	2004	TAC	C1B-C11	-3.47	1.39	1.47
25	A	2006	TAC	C1B-C11	-3.46	1.39	1.47
25	D	2002	TAC	C1B-C11	-3.44	1.39	1.47
25	A	2003	TAC	C1B-C11	-3.43	1.39	1.47
25	A	2005	TAC	C1B-C11	-3.43	1.39	1.47

The worst 5 of 76 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	R	1008	WO2	OP6-P2-OP5	-29.53	61.91	111.56
24	H	1010	WO2	OP6-P2-OP5	-29.52	61.93	111.56
24	A	1581	WO2	OP6-P2-OP5	-29.52	61.94	111.56
24	A	1580	WO2	OP6-P2-OP5	-29.52	61.94	111.56
24	A	1579	WO2	OP6-P2-OP5	-29.51	61.94	111.56

5 of 6 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
25	A	2006	TAC	C4
25	A	2003	TAC	C4
25	D	2002	TAC	C4
25	A	2004	TAC	C4
25	A	2005	TAC	C4

There are no torsion outliers.

There are no ring outliers.

11 monomers are involved in 181 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	A	2001	TAC	14	0
25	A	2003	TAC	32	0
25	A	2004	TAC	50	0
25	A	2005	TAC	42	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	A	2006	TAC	21	0
24	B	1001	WO2	1	0
25	D	2002	TAC	12	0
24	E	1005	WO2	1	0
24	G	1006	WO2	3	0
24	J	1009	WO2	1	0
24	K	1014	WO2	4	0

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

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.