



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 08:03 PM 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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

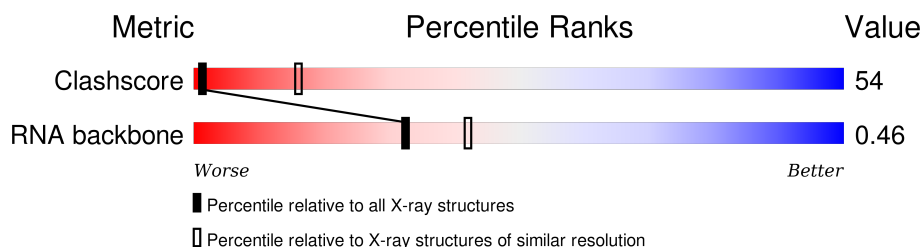
1 Overall quality at a glance

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	102246	1003 (5.30-3.62)
RNA backbone	2183	1090 (6.00-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	0	0	155
			155	155			

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

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

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

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

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

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

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

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

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

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

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

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

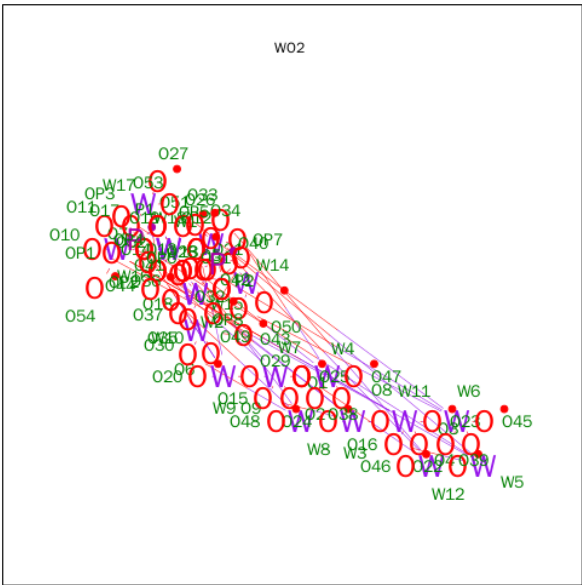
- Molecule 22 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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).

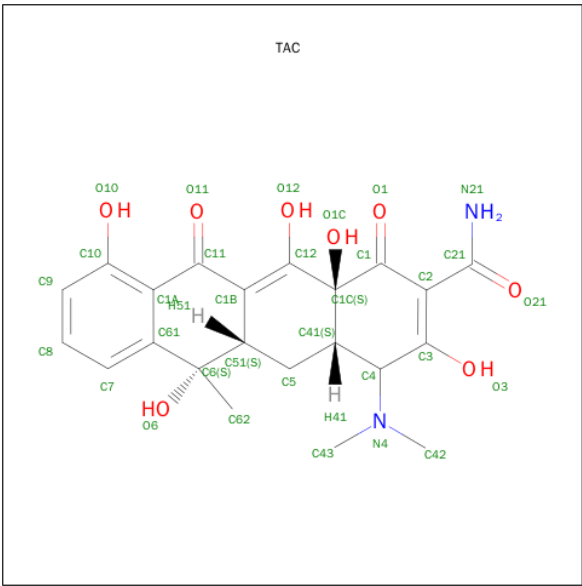
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
23	D	1	Total Zn 1 1	0	0
23	N	1	Total Zn 1 1	0	0

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
24	B	1	Total	O	P	W	0	0
			82	62	2	18		
24	B	1	Total	O	P	W	0	0
			82	62	2	18		
24	A	1	Total	O	P	W	0	0
			82	62	2	18		
24	B	1	Total	O	P	W	0	0
			82	62	2	18		
24	E	1	Total	O	P	W	0	0
			82	62	2	18		
24	G	1	Total	O	P	W	0	0
			82	62	2	18		
24	A	1	Total	O	P	W	0	0
			82	62	2	18		
24	R	1	Total	O	P	W	0	0
			82	62	2	18		
24	J	1	Total	O	P	W	0	0
			82	62	2	18		
24	H	1	Total	O	P	W	0	0
			82	62	2	18		
24	A	1	Total	O	P	W	0	0
			82	62	2	18		
24	D	1	Total	O	P	W	0	0
			82	62	2	18		
24	A	1	Total	O	P	W	0	0
			82	62	2	18		
24	K	1	Total	O	P	W	0	0
			82	62	2	18		

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



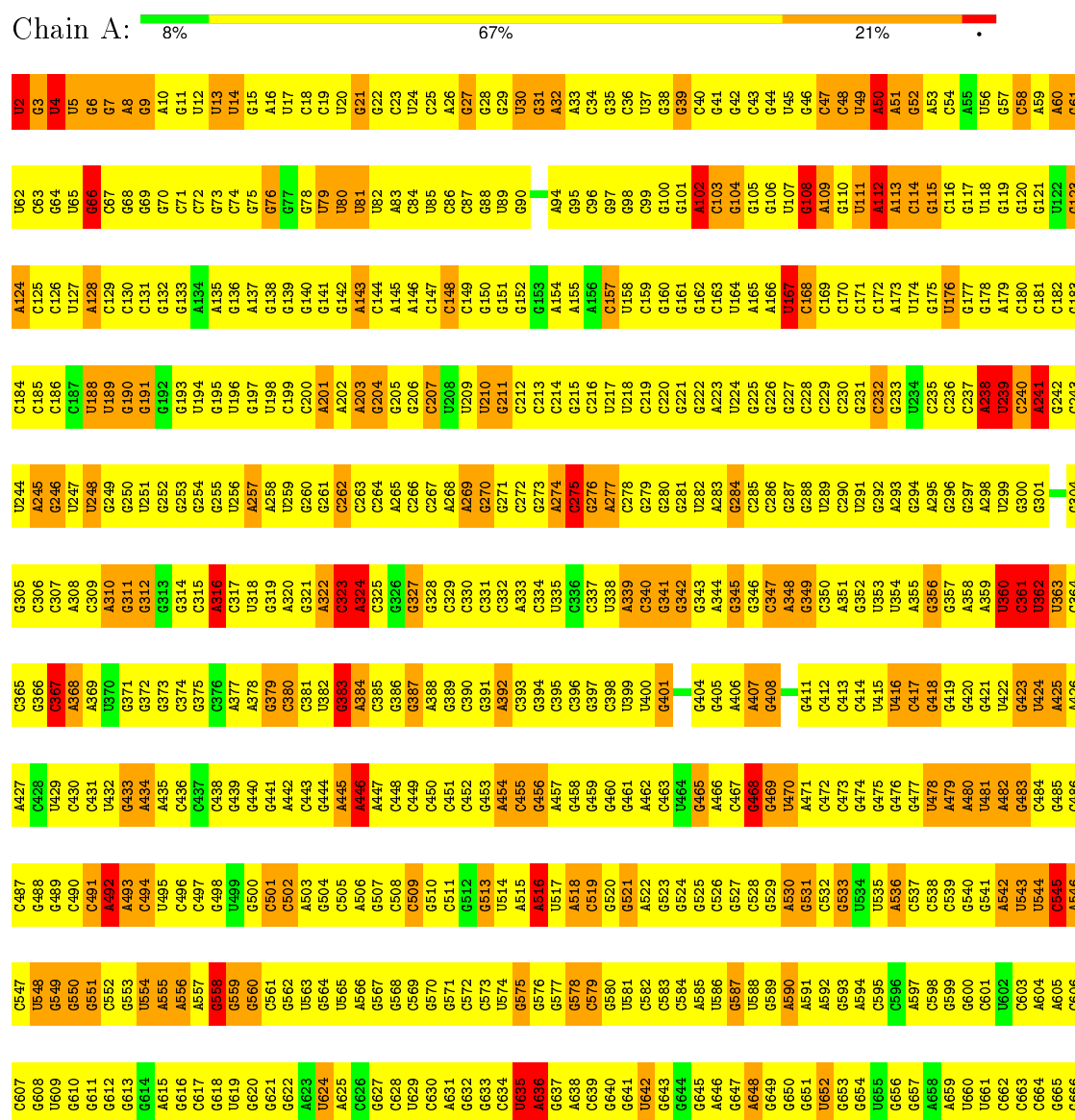
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
25	A	1	Total	C	N	O	0	0
			32	22	2	8		
25	D	1	Total	C	N	O	0	0
			32	22	2	8		
25	A	1	Total	C	N	O	0	0
			32	22	2	8		
25	A	1	Total	C	N	O	0	0
			32	22	2	8		
25	A	1	Total	C	N	O	0	0
			32	22	2	8		
25	A	1	Total	C	N	O	0	0
			32	22	2	8		

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 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



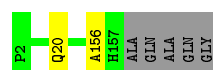
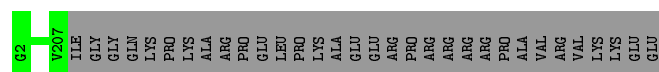
A1470	A1471	A1472	A1473	A1474	A1475	A1476	A1477	A1478	A1479	A1480	A1481	A1482	A1483	A1484	A1485	A1486	A1487	A1488	A1489	A1490	A1491	A1492	A1493	A1494	A1495	A1496	A1497	A1498	A1499	A1500	A1501	A1502	A1503	A1504	A1505	A1506	A1507	A1508	A1509	A1510	A1511	A1512	A1513	A1514	A1515																																																																																																																																																																																																																																																														
G1400	G1401	G1402	G1403	G1404	G1405	G1406	G1407	G1408	G1409	G1410	G1411	G1412	G1413	G1414	G1415	G1416	G1417	G1418	G1419	G1420	G1421	G1422	G1423	G1424	G1425	G1426	G1427	G1428	G1429	G1430	G1431	G1432	G1433	G1434	G1435	G1436	G1437	G1438	G1439	G1440	G1441	G1442	G1443	G1444	G1445	G1446	G1447	G1448																																																																																																																																																																																																																																																											
C1278	C1279	C1280	C1281	C1282	C1283	C1284	C1285	C1286	C1287	C1288	C1289	C1290	C1291	C1292	C1293	C1294	C1295	C1296	C1297	C1298	C1299	C1300	C1301	C1302	C1303	C1304	C1305	C1306	C1307	C1308	C1309	C1310	C1311	C1312	C1313	C1314	C1315	C1316	C1317	C1318	C1319	C1320	C1321	C1322	C1323	C1324	C1325	C1326	C1327	C1328																																																																																																																																																																																																																																																									
U1216	U1217	U1218	U1219	U1220	U1221	U1222	U1223	U1224	U1225	U1226	U1227	U1228	U1229	U1230	U1231	U1232	U1233	U1234	U1235	U1236	U1237	U1238	U1239	U1240	U1241	U1242	U1243	U1244	U1245	U1246	U1247	U1248	U1249	U1250	U1251	U1252	U1253	U1254	U1255	U1256	U1257	U1258	U1259	U1260	U1261	U1262	U1263	U1264	U1265	U1266	U1267	U1268																																																																																																																																																																																																																																																							
G1154	G1155	G1156	G1157	G1158	G1159	G1160	G1161	G1162	G1163	G1164	G1165	G1166	G1167	G1168	G1169	G1170	G1171	G1172	G1173	G1174	G1175	G1176	G1177	G1178	G1179	G1180	G1181	G1182	G1183	G1184	G1185	G1186	G1187	G1188	G1189	G1190	G1191	G1192	G1193	G1194	G1195	G1196	G1197	G1198	G1199	G1200	G1201	G1202	G1203	G1204	G1205	G1206	G1207	G1208																																																																																																																																																																																																																																																					
A1092	A1093	A1094	A1095	A1096	A1097	A1098	A1099	A1100	A1101	A1102	A1103	A1104	A1105	A1106	A1107	A1108	A1109	A1110	A1111	A1112	A1113	A1114	A1115	A1116	A1117	A1118	A1119	A1120	A1121	A1122	A1123	A1124	A1125	A1126	A1127	A1128	A1129	A1130	A1131	A1132	A1133	A1134	A1135	A1136	A1137	A1138	A1139	A1140	A1141	A1142	A1143	A1144	A1145	A1146	A1147	A1148	A1149	A1150	A1151	A1152	A1153																																																																																																																																																																																																																																														
C1032	C1033	C1034	G1035	C1036	C1037	C1038	C1039	C1040	C1041	C1042	C1043	C1044	C1045	C1046	C1047	C1048	A1049	C1050	C1051	C1052	C1053	C1054	C1055	C1056	C1057	C1058	C1059	C1060	C1061	C1062	C1063	C1064	C1065	C1066	C1067	C1068	C1069	C1070	C1071	C1072	C1073	C1074	C1075	C1076	C1077	C1078	C1079	C1080	C1081	C1082	A1083	C1084	C1085	C1086	C1087	C1088	C1089	C1090	C1091																																																																																																																																																																																																																																																
U968	U969	U970	A971	C972	C973	C974	C975	C976	C977	A978	C979	C980	C981	C982	C983	C984		C985	C986	C987	C988	C989	C990	C991	C992	C993	C994	C995	C996	C997	C998	C999	C1000	C1001	C1002	C1003	C1004	C1005	C1006	C1007	C1008	C1009	C1010	C1011	C947	C948	C949	C950	C951	C952	C953	C954	C955	C956	C957	C958	C959	C960	C961	C962	C963	C964	C965	C966	C967																																																																																																																																																																																																																																										
C908	C909	C910	C911	C912	C913	C914	C915	C916	C917	C918	C919	C920	C921	C922	C923	C924	C925	C926	C927	C928	C929	C930	C931	C932	C933	C934	C935	C936	C937	C938	C939	C940	C941	C942	C943	C944	C945	C946	C947	C948	C949	C950	C951	C952	C953	C954	C955	C956	C957	C958	C959	C960	C961	C962	C963	C964	C965	C966	C967																																																																																																																																																																																																																																																
U848	U849	U850	C851	C852	C853	C854	C855	C856	C857	C858	C859	C860	U861	C862	C863	C864	C865	C866	C867	U868	C869	C870	C871	C872	C873	C874	C875	C876	C877	C878	C879	C880	C881	C882	C883	C884	C885	C886	C887	C888	C889	C890	C891	C892	C893	C894	C895	C896	C897	C898	C899	C900	C901	C902	C903	C904	C905	C906	C907	C908	C909	C910	C911	C912	C913	C914	C915	C916	C917	C918	C919	C920	C921	C922	C923	C924	C925	C926	C927	C928	C929	C930	C931	C932	C933	C934	C935	C936	C937	C938	C939	C940	C941	C942	C943	C944	C945	C946	C947	C948	C949	C950	C951	C952	C953	C954	C955	C956	C957	C958	C959	C960	C961	C962	C963	C964	C965	C966	C967																																																																																																																																																																																				
C788	C789	C790	C791	C792	C793	C794	C795	C796	C797	C798	C799	C800	C801	C802	C803	C804	C805	C806	C807	C808	C809	U810	U811	C812	C813	C814	C815	U816	C817	U818	C819	C820	C821	C822	C823	C824	C825	C826	C827	C828	C829	C830	C831	C832	C833	C834	C835	C836	C837	C838	C839	C840	C841	C842	C843	C844	C845	C846	C847	C848	C849	C850	C851	C852	C853	C854	C855	C856	C857	C858	C859	C860	C861	C862	C863	C864	C865	C866	C867	C868	C869	C870	C871	C872	C873	C874	C875	C876	C877	C878	C879	C880	C881	C882	C883	C884	C885	C886	C887	C888	C889	C890	C891	C892	C893	C894	C895	C896	C897	C898	C899	C900	C901	C902	C903	C904	C905	C906	C907	C908	C909	C910	C911	C912	C913	C914	C915	C916	C917	C918	C919	C920	C921	C922	C923	C924	C925	C926	C927	C928	C929	C930	C931	C932	C933	C934	C935	C936	C937	C938	C939	C940	C941	C942	C943	C944	C945	C946	C947	C948	C949	C950	C951	C952	C953	C954	C955	C956	C957	C958	C959	C960	C961	C962	C963	C964	C965	C966	C967																																																																																																																								
C727	C728	C729	C730	C731	C732	C733	U734	C735	C736	C737	C738	C739	U740	C741	C742	C743	C744	C745	C746	C747	C748	U749	U750	C751	C752	C753	C754	C755	C756	C757	C758	C759	C760	C761	C762	C763	C764	C765	C766	C767	C768	C769		U772	C773	C774	C775	C776	C777	C778	C779	C780	C781	C782	C783	C784	C785	C786	C787	C788	C789	C790	C791	C792	C793	C794	C795	C796	C797	C798	C799	C800	C801	C802	C803	C804	C805	C806	C807	C808	C809	C810	C811	C812	C813	C814	C815	C816	C817	C818	C819	C820	C821	C822	C823	C824	C825	C826	C827	C828	C829	C830	C831	C832	C833	C834	C835	C836	C837	C838	C839	C840	C841	C842	C843	C844	C845	C846	C847	C848	C849	C850	C851	C852	C853	C854	C855	C856	C857	C858	C859	C860	C861	C862	C863	C864	C865	C866	C867	C868	C869	C870	C871	C872	C873	C874	C875	C876	C877	C878	C879	C880	C881	C882	C883	C884	C885	C886	C887	C888	C889	C890	C891	C892	C893	C894	C895	C896	C897	C898	C899	C900	C901	C902	C903	C904	C905	C906	C907	C908	C909	C910	C911	C912	C913	C914	C915	C916	C917	C918	C919	C920	C921	C922	C923	C924	C925	C926	C927	C928	C929	C930	C931	C932	C933	C934	C935	C936	C937	C938	C939	C940	C941	C942	C943	C944	C945	C946	C947	C948	C949	C950	C951	C952	C953	C954	C955	C956	C957	C958	C959	C960	C961	C962	C963	C964	C965	C966	C967																																																												
A667	A668	A669	A670	A671	A672	A673	A674	A675	A676	A677	A678	A679	A680	A681	A682	A683	A684	A685	A686	A687	A688	A689	A690	A691	A692	A693	A694	A695	A696	A697	A698	A699	C700	C701	C702	C703	C704	C705	C706	C707	C708	C709	C710	C711	C712	C713	C714	C715	C716	C717	C718	C719	C720	C721	C722	C723	C724	C725	C726	C727	C728	C729	C730	C731	C732	C733	C734	C735	C736	C737	C738	C739	C740	C741	C742	C743	C744	C745	C746	C747	C748	C749	C750	C751	C752	C753	C754	C755	C756	C757	C758	C759	C760	C761	C762	C763	C764	C765	C766	C767	C768	C769		U772	C773	C774	C775	C776	C777	C778	C779	C780	C781	C782	C783	C784	C785	C786	C787	C788	C789	C790	C791	C792	C793	C794	C795	C796	C797	C798	C799	C800	C801	C802	C803	C804	C805	C806	C807	C808	C809	C810	C811	C812	C813	C814	C815	C816	C817	C818	C819	C820	C821	C822	C823	C824	C825	C826	C827	C828	C829	C830	C831	C832	C833	C834	C835	C836	C837	C838	C839	C840	C841	C842	C843	C844	C845	C846	C847	C848	C849	C850	C851	C852	C853	C854	C855	C856	C857	C858	C859	C860	C861	C862	C863	C864	C865	C866	C867	C868	C869	C870	C871	C872	C873	C874	C875	C876	C877	C878	C879	C880	C881	C882	C883	C884	C885	C886	C887	C888	C889	C890	C891	C892	C893	C894	C895	C896	C897	C898	C899	C900	C901	C902	C903	C904	C905	C906	C907	C908	C909	C910	C911	C912	C913	C914	C915	C916	C917	C918	C919	C920	C921	C922	C923	C924	C925	C926	C927	C928	C929	C930	C931	C932	C933	C934	C935	C936	C937	C938	C939	C940	C941	C942	C943	C944	C945	C946	C947	C948	C949	C950	C951	C952	C953	C954	C955	C956	C957	C958	C959	C960	C961	C962	C963	C964	C965	C966	C967

● Molecule 2: 30S RIBOSOMAL PROTEIN S2

Chain B:

97%

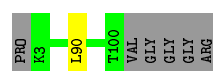




There are no outlier residues recorded for this chain.

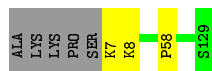


There are no outlier residues recorded for this chain.



- Molecule 11: 30S RIBOSOMAL PROTEIN S11

Chain K:  94% . .



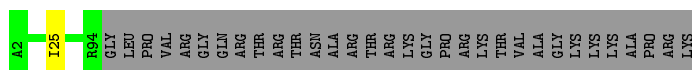
- Molecule 12: 30S RIBOSOMAL PROTEIN S12

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.

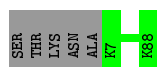
- Molecule 17: 30S RIBOSOMAL PROTEIN S17

Chain Q:  99% .



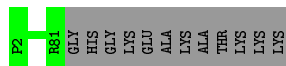
- Molecule 18: 30S RIBOSOMAL PROTEIN S18

Chain R:  94% 6%



- Molecule 19: 30S RIBOSOMAL PROTEIN S19

Chain S:
87% 13%



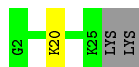
- Molecule 20: 30S RIBOSOMAL PROTEIN S20

Chain T:
94% 6%



- Molecule 21: 30S RIBOSOMAL PROTEIN THX

Chain U:
88% 8%



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be 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 [i](#)

5.1 Standard geometry [i](#)

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 [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1513/1514 (99%)	322 (21%)	119 (7%)

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

5 of 119 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	545	C
1	A	800	C
1	A	1345	A
1	A	558	G
1	A	684	C

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 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	-	54,116,116	54.93	10 (18%)	6,348,348	12.83	2 (33%)
24	WO2	A	1580	-	54,116,116	54.93	10 (18%)	6,348,348	12.83	2 (33%)
24	WO2	A	1581	-	54,116,116	54.94	10 (18%)	6,348,348	12.83	2 (33%)
24	WO2	A	1582	-	54,116,116	54.93	10 (18%)	6,348,348	12.82	2 (33%)
25	TAC	A	2001	22	33,35,35	1.89	7 (21%)	44,58,58	2.03	9 (20%)
25	TAC	A	2003	-	33,35,35	1.90	7 (21%)	44,58,58	2.05	10 (22%)
25	TAC	A	2004	-	33,35,35	1.90	7 (21%)	44,58,58	2.04	9 (20%)
25	TAC	A	2005	-	33,35,35	1.88	7 (21%)	44,58,58	2.04	9 (20%)
25	TAC	A	2006	-	33,35,35	1.89	7 (21%)	44,58,58	2.05	9 (20%)
24	WO2	B	1001	-	54,116,116	54.94	10 (18%)	6,348,348	12.83	2 (33%)
24	WO2	B	1002	-	54,116,116	54.94	11 (20%)	6,348,348	12.83	2 (33%)
24	WO2	B	1004	-	54,116,116	54.92	11 (20%)	6,348,348	12.82	2 (33%)
24	WO2	D	1012	-	54,116,116	54.92	10 (18%)	6,348,348	12.82	2 (33%)
25	TAC	D	2002	-	33,35,35	1.89	7 (21%)	44,58,58	2.04	9 (20%)
24	WO2	E	1005	-	54,116,116	54.92	11 (20%)	6,348,348	12.82	2 (33%)
24	WO2	G	1006	-	54,116,116	54.94	10 (18%)	6,348,348	12.83	2 (33%)
24	WO2	H	1010	-	54,116,116	54.94	10 (18%)	6,348,348	12.84	2 (33%)
24	WO2	J	1009	-	54,116,116	54.93	10 (18%)	6,348,348	12.83	2 (33%)
24	WO2	K	1014	-	54,116,116	54.93	10 (18%)	6,348,348	12.83	2 (33%)
24	WO2	R	1008	-	54,116,116	54.94	10 (18%)	6,348,348	12.84	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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 185 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	2004	TAC	C1B-C11	-3.51	1.39	1.47
25	A	2006	TAC	C1B-C11	-3.50	1.39	1.47
25	D	2002	TAC	C1B-C11	-3.48	1.39	1.47
25	A	2003	TAC	C1B-C11	-3.47	1.39	1.47
25	A	2005	TAC	C1B-C11	-3.47	1.39	1.47

The worst 5 of 83 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	R	1008	WO2	OP6-P2-OP5	-29.13	61.91	111.62
24	H	1010	WO2	OP6-P2-OP5	-29.12	61.93	111.62
24	A	1581	WO2	OP6-P2-OP5	-29.12	61.94	111.62
24	A	1580	WO2	OP6-P2-OP5	-29.12	61.94	111.62
24	A	1579	WO2	OP6-P2-OP5	-29.12	61.94	111.62

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
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 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.