



wwPDB X-ray Structure Validation Summary Report (i)

Mar 31, 2014 – 06:13 PM BST

PDB ID : 2HGR
Title : 70S T.Th. ribosome functional complex with mRNA and E- and P-site tRNAs at 4.5Å. This entry 2HGr contains 30S ribosomal subunit. The 50S ribosomal subunit can be found in PDB entry 2HGU.
Authors : Jenner, L.; Yusupova, G.; Rees, B.; Moras, D.; Yusupov, M.
Deposited on : 2006-06-27
Resolution : 4.51 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

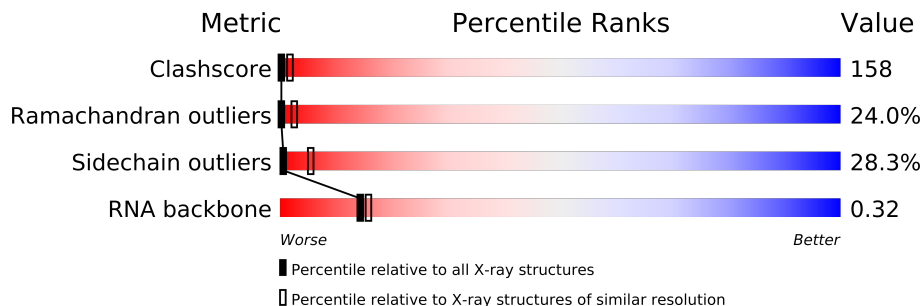
The following versions of software and data (see [references](#)) were used in the production of this report:

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 4.51 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	1300 (5.50-3.50)
Ramachandran outliers	78287	1222 (5.50-3.50)
Sidechain outliers	78261	1203 (5.50-3.50)
RNA backbone	1838	1031 (6.22-2.80)

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. 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	C	76	
3	D	76	
4	1	27	
5	E	256	
6	F	239	
7	G	209	
8	H	162	
9	I	101	
10	J	156	
11	K	138	
12	L	128	
13	M	105	
14	N	129	
15	O	132	

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Mol	Chain	Length	Quality of chain
16	P	126	
17	Q	61	
18	R	89	
19	S	88	
20	T	105	
21	U	88	
22	V	93	
23	W	106	
24	X	27	

2 Entry composition

There are 24 unique types of molecules in this entry. The entry contains 55628 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	1515	Total	C	N	O	P	0	0	0
			32554	14490	6022	10527	1515			

- Molecule 2 is a RNA chain called tRNA fMET (unmodified bases).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	76	Total	C	N	O	P	0	0	0
			1624	723	295	530	76			

- Molecule 3 is a RNA chain called tRNA PHE (unmodified bases).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	76	Total	C	N	O	P	0	0	0
			1623	723	290	534	76			

- Molecule 4 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	1	27	Total	C	N	O	P	0	0	0
			596	267	127	175	27			

- Molecule 5 is a protein called 30S ribosomal protein S2.

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

- Molecule 6 is a protein called 30S ribosomal protein S3.

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

- Molecule 7 is a protein called 30S ribosomal protein S4.

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

- Molecule 8 is a protein called 30S ribosomal protein S5.

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

- Molecule 9 is a protein called 30S ribosomal protein S6.

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

- Molecule 10 is a protein called 30S ribosomal protein S7.

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

- Molecule 11 is a protein called 30S ribosomal protein S8.

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

- Molecule 12 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
12	L	127	Total	C	N	O	0	0	0
			1010	639	197	174			

- Molecule 13 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	98	Total	C	N	O	S	0	0	0
			794	499	156	138	1			

- Molecule 14 is a protein called 30S ribosomal protein S11.

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

- Molecule 15 is a protein called 30S ribosomal protein S12.

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

- Molecule 16 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	P	125	Total	C	N	O	S	0	0	0
			997	617	207	171	2			

- Molecule 17 is a protein called 30S ribosomal protein S14.

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

- Molecule 18 is a protein called 30S ribosomal protein S15.

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

- Molecule 19 is a protein called 30S ribosomal protein S16.

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

- Molecule 20 is a protein called 30S ribosomal protein S17.

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

- Molecule 21 is a protein called 30S ribosomal protein S18.

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

- Molecule 22 is a protein called 30S ribosomal protein S19.

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

- Molecule 23 is a protein called 30S ribosomal protein S20.

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

- Molecule 24 is a protein called 30S ribosomal protein Thx.

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

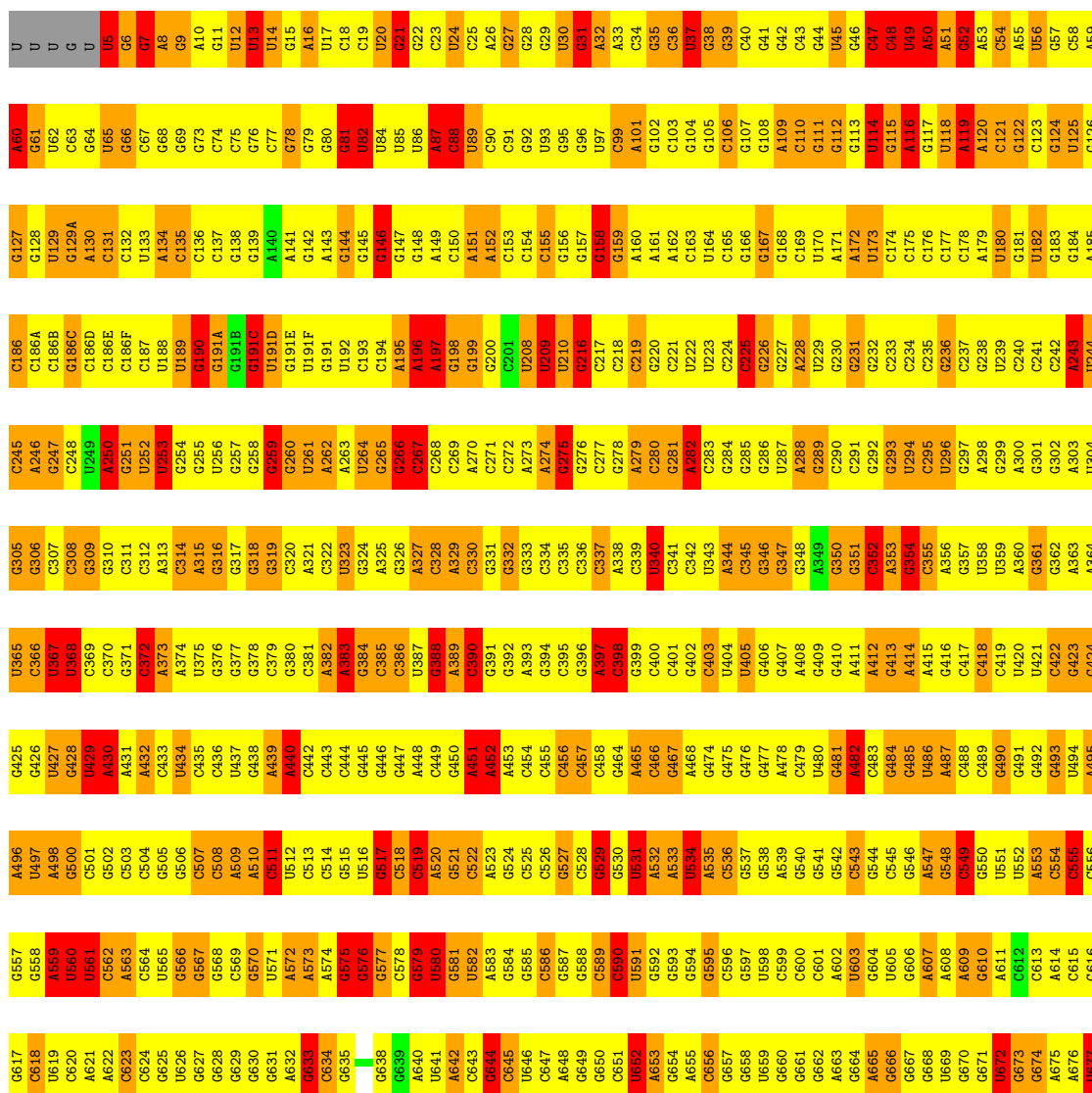
3 Residue-property plots

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 ($\text{RSRZ} > 2$). 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

Chain A: 



G1526	C1465	C1400	U1341	G1221	G1160	C1100	U1040	C985	G925	A864	G798	C738	U678
G1527	C1466	G1401	C1342	G1222	C1161	A1101	A1041	A986	G926	A865	G799	C739	C679
U1528	G1467	C1402	G1343	G1223	C1162	A1102	G1042	G987	C927	C866	G800	U740	C680
G1529	A1468	C1403	C1344	G1224	C1163	C1103	C1103	G988	G928	C867	U801	G741	C681
G1530	G1469	G1404	U1345	C1225	C1164	G1104	A1044	C989	G929	C868	A802	G742	G682
A1531	G1470	G1405	U1346	C1226	C1165	A1105	C1045	C990	C930	C869	G803	U743	G683
U1532	G1471	U1406	G1347	C1227	G1166	G1106	A1046	U991	C931	U870	U904	C744	A684
C1533	U1472	C1407	U1348	C1228	A1167	C1107	G1047	U992	C932	U871	C805	C745	G685
U1534	A1473	A1408	A1349	C1229	G1169	G1108	G1048	C993	G933	A872	C906	A746	U686
C1535	G1474	C1409	A1350	G1230	G1170	A1109	U1049	A994	C934	A873	A807	C747	A687
G1536	G1475	G1410	U1351	G1231	G1171	C1110	G1050	C995	A935	G874	C908	C748	C688
U1537	G1476	C1352	G1352	U1232	C1172	A1111	C1051	A996	C936	C875	G809	C749	C689
C1538	C1477	G1353	G1353	G1233	G1173	C1112	U1052	U997	A937	G876	C810	G750	G690
U1539	C1478	A1413	C1354	C1234	G1174	C1113	G1053	C998	A938	C877	C811	U751	C691
C1540	G1479	U1414	U1235	U1235	G1175	C1114	C1054	C998A	G939	G878	C912	G752	C692
U1541	G1480	G1415	G1356	A1236	A1176	A1055	A1055	U999	C940	C879	U813	A753	G693
U1542	U1481	G1416	G1357	C1237	G1177	C1116	U1056	A1000	G941	C880	A814	C754	A694
C	G1482	G1417	U1358	A1238	G1178	G1117	G1057	G1001	G942	G881	A815	G755	A695
U	A1483	C1359	C1359	A1239	A1179	C1118	G1058	G1002	U943	C882	A816	G756	A696
	C1484	A1360	A1360	U1240	A1180	C1119	C1059	G1003	G944	C883	C817	U757	U697
	U1485	C1419	G1361	G1241	A1181	C1120	C1060	A1004	G945	C884	G818	G758	G698
	G1486	G1420	C1362	C1242	G1182	U1121	G1061	A1005	A946	G885	A819	A759	C699
	G1487	G1421	C1362A	C1243	A1183	U1122	U1062	C1006	G947	G886	U820	G760	G700
	G1488	G1423	A1363	C1244	G1184	A1123	C1063	C1007	C948	G887	C821	G761	C701
	G1489	C1424	G1364	A1245	G1185	G1124	G1064	C1008	A949	G888	C822	C762	A702
	C1490	U1425	G1365	G1246	G1186	U1125	U1065	G1009	U950	A889	G823	G763	G703
	G1491	C1426	C1366	U1247	G1187	U1126	C1066	G1010	G951	C890	C824	C764	A704
	A1492	U1427	C1367	U1248	G1188	U1127	A1067	G1011	U952	U891	G825	G765	U705
	A1493	A1428	G1368	C1249	C1189	C1128	G1068	C953	C926	A892	C826	A766	A706
	G1494	C1429	C1369	A1250	G1190	C1129	G1069	G1013	G954	C893	U827	A767	C707
	U1495	C1430	G1370	A1251	A1191	A1130	U1070	A1014	U955	G894	A828	A768	C708
	C1496	C1431	G1371	A1252	C1192	C1131	C1071	A1015	U956	C895	G829	G769	C709
	G1497	G1432	U1372	G1253	G1193	C1132	G1072	A1016	U957	C896	G830	C770	G710
	U1498	A1433	G1373	C1254	U1194	G1133	U1073	G1017	A958	C897	U831	G771	G711
	A1500	A1434	A1374	G1255	C1195	G1134	C832	C1018	A959	G898	C832	U772	A712
	U1501	G1435	A1375	A1256	U1196	U1135	C1075	C1019	U960	C899	U833	G773	G713
	A1502	C1437	U1377	G1257	G1197	U1136	C1076	U1020	U961	A900	C834	G774	G714
	G1503	G1438	C1378	G1258	G1198	C1137	G1077	G1021	C962	A901	U835	G775	A715
	C1504	C1439	G1379	C1259	U1199	G1138	U1078	G1022	G963	G902	G836	G776	A716
	G1505	C1440	U1380	C1260	C1200	G1139	G1079	G1023	A964	G903	G837	A777	C717
	U1506	G1441	U1381	A1261	A1201	C1140	A1080	G1024	A965	G906	C838	G778	G718
	A1507	C1442	C1382	C1262	G1202	C1141	G1081	U1025	G966	A907	C942	C779	C719
	C1508	G1443	C1383	C1263	C1203	G1142	G1082	C1026	C967	A908	U843	A781	G720
	C1509	A1446	C1384	G1265	U1205	G1144	G1083	C1028	A969	A909	C848	A782	G721
	G1510	G1447	G1385	G1266	G1206	C1145	U1085	C1028A	C970	C910	C849	C783	A722
	U1512	C1448	G1386	C1267	G1207	A1146	U1086	C1028B	G971	U911	U850	C784	G724
	A1513	C1449	G1387	A1268	C1208	C1147	G1087	G1029	C972	C912	G851	G785	G725
	C1514	U1450	C1388	A1269	C1209	U1148	G1088	C1030	G973	A913	G852	G786	C726
	U1515	A1451	U1389	C1270	C1210	C1149	G1089	G1031	A974	A914	G853	A787	G727
	C1516	C1452	U1390	G1271	U1211	U1150	U1090	A1032	A975	A915	G854	U788	A728
	G1517	G1453	U1391	G1272	U1212	A1151	U1091	G1032A	G976	G916	G855	U789	A729
	A1518	G1454	C1392	G1273	A1213	A1152	A1092	G1032B	A977	G917	C856	A790	G730
	U1519	C1455	U1393	G1274	C1214	A1093	A1093	C1033	A978	A918	C857	G791	G731
	G1520	A1459	A1394	A1275	G1154	G1154	G1094	G1034	C979	A919	G858	A792	G732
	U1521	C1336	C1395	G1276	G1216	U1155	U1095	A1035	C980	U920	A859	U793	A733
	C1522	G1461	A1386	C1277	C1217	G1156	C1096	G1036	U981	U921	A860	A794	G734
	G1523	C1462	C1397	U1278	A1157	C1157	C1097	C1037	U982	G922	G861	C795	C735
	U1524	C1463	A1398	U1279	U1218	C1158	C1098	C1038	A983	A923	C862	C796	C736
	C1524	G1464	C1399	A1280	G1220	U1159	G1099	C1039	C984	C924	U863	C797	A737

• Molecule 2: tRNA fMET (unmodified bases)

Chain C:



C1 G2 G3 G4 G5 G6 G7 G8 G9 G10 G11 G12 G13 G14 G15 G16 G17 G18 G19 U20 U21 A21 A22 G23 G24 U25 G26 G27 G28 G29 G30 G31 G32 G33 G34 A35 A36 A37 A38 A39 C40 C41 C42 C43 C44 C45 G46 G47 C48 C49 U50 C51 G52 G53 U54 U55 C56 A57 A58 A59 U60

C61 C62 G63 G64 C65 C66 C67 C68 C69 G70 G71 A72 A73 C74 C75 A76

• Molecule 3: tRNA PHE (unmodified bases)

Chain D:

G1 G2 G3 G4 A5 G6 G7 G8 G9 G10 G11 G12 G13 G14 G15 G16 G17 G18 G19 U20 U21 A21 A22 G23 G24 C25 C26 A27 U27 G28 G29 C29 G30 G31 G32 G33 G34 A35 A36 A37 A38 A39 C40 C41 C42 C43 C44 C45 G46 G47 C48 C49 G50 C51 G52 G53 U54 U55 C56 G57 A58 A59 U60

C61 C62 G63 G64 U65 C66 C67 C68 C69 G70 G71 A72 A73 C74 C75 A76

• Molecule 4: mRNA

Chain 1:

G1 G2 C3 G4 A5 G6 G7 G8 G9 G10 G11 U11 U12 G13 A13 A14 A15 A16 A17 U17 G18 A19 A20 A21 A22 A23 A24 A25 A26 A27

• Molecule 5: 30S ribosomal protein S2

Chain E:

MET PRD VAL GLU ILE THR V7 K8 E9 L11 L12 G12 A12 A13 A14 A15 A16 A17 F17 G18 H19 E20 E21 R22 K23 R24 W24 N25 P26 K27 A28 A29 G30 R30 Y31 Y32 Y33 Y34 A35 E36 R36 R37 N37 G38 L39 H40 T41 T42 T43 D43 T103 T104 R104 F105 K46 T47 M48 T108 S109 E109 Q110 R111 V112 H113 R114 T54 T55 F55 E56 F57 L58 E59 D60

L61 A62 M63 G64 G65 G66 T67 L68 L69 F70 V71 G72 G73 A74 G75 G76 A77 G78 D79 I80 V81 R82 M83 E84 A85 E86 E87 A88 G89 M90 R91 Y92 Y93 Y94 Q95 Q96 R96 W97 L98 G99 M101 T102 T103 T104 F105 F106 T107 T108 S109 Q110 R111 V112 H113 R114 T54 T55 F55 E56 F57 L58 E59 D60

L121 F122 A123 S124 I125 E126 L127 E128 E129 F130 R131 R132 K132 K133 E134 Q135 V136 L137 R138 L139 H140 H141 L142 L143 E144 R145 L146 Q147 K148 Y149 L149 M150 S150 F151 F152 R153 L154 L155 Q156 K156 R157 L158 P159 D160 A161 T162 T163 F163 V164 V165 D166 D167 P167 G228 T168 K169 V209 E170 A171 E172 A173 P174 R175 R176 A177 R178 V239 R179 A180

F181 I182 P183 V184 I185 E186 L187 A188 D189 T190 D191 S192 D193 F194 D195 V196 V197 Y198 Y199 I200 I201 G202 G203 R204 D205 D206 A207 T208 R209 S210 T211 Q212 L213 L214 L215 S216 R217 A218 V219 D220 L221 T222 T223 Q224 A225 R226 G227 G228 V229 V230 E231 P232 S233 P234 S235 Y236 A237 V238 V239 Q240

GLU ALA GLU ALA THR GLU THR PRO GLU GLU GLU SER GLU VAL ALA

• Molecule 6: 30S ribosomal protein S3

Chain F:

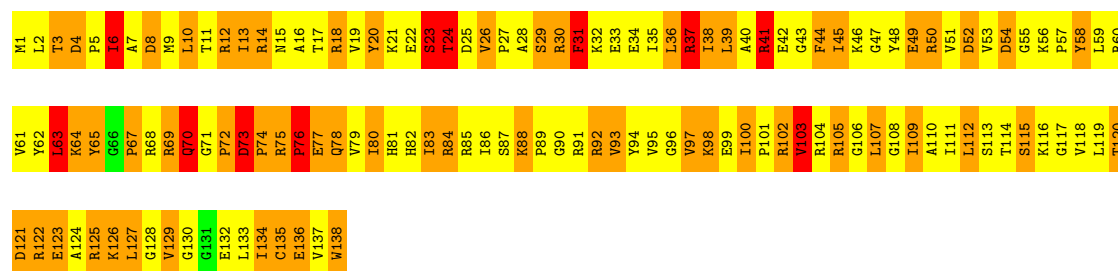
MET G2 N3 K4 I5 H6 P7 I8 G9 F10 R11 L12 G13 L14 T15 R16 D17 W18 E19 S20 R21 W22 Y23 R24 G25 G26 K27 L28 Q28 Y29 R30 R31 L32 L33 L34 E35 D36 Q37 Q38 R39 I39 R40 G41 L42 L43 E44 K45 E46 Y48 S49 A50 A51 G51 L52 A53 A54 P54 V55 D56 I57 E58 R59 A60

A61 D62 N63 V64 A65 H66 T67 V68 H69 V70 A71 G72 P73 G74 V75 V76 I77 G78 R79 G80 G81 E82 R83 S84 I85 R86 L87 R88 E89 E90 E91 L91 A92 I93 S94 T95 G96 G97 N98 G99 A100 L101 Q102 V103 Q104 T105 V106 Q107 N108 P109 A110 L111 L112 A113 P114 L115 V116 L117 R118 R119 A120

A121 E122 Q123 I124 E125 R126 T127 F128 A129 V130 R131 R132 A133 P134 K135 Q136 A137 V138 G139 R140 V141 E142 M143 S144 G145 A146 L147 R148 E149 E150 E151 L152 I153 S154 T155 R156 I157 G158 G159 A160 E161 Q162 A163 R164 T165 E166 W167 A168 N169 Q170 G171 R172 V173 P174 L175 L176 R177 L178 R179 A180

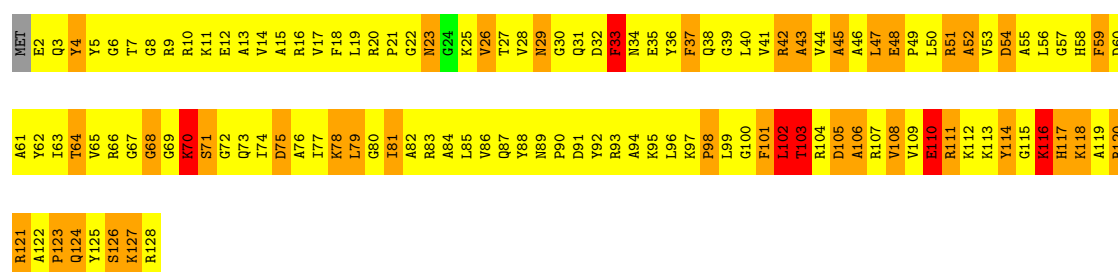
- Molecule 11: 30S ribosomal protein S8

Chain K:



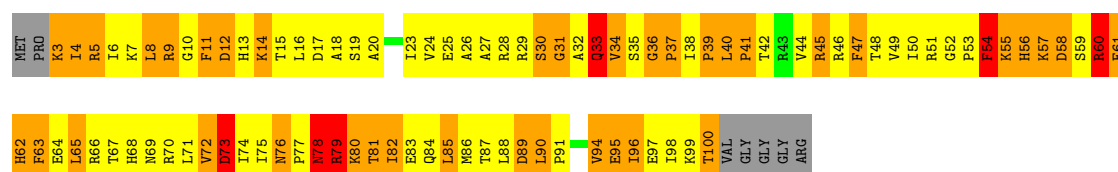
- Molecule 12: 30S ribosomal protein S9

Chain L:



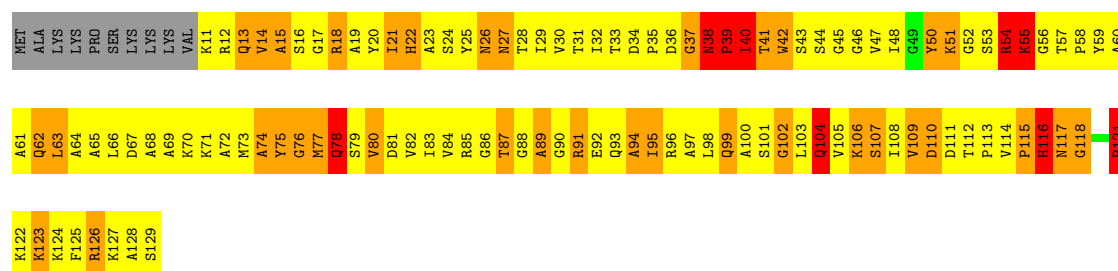
- Molecule 13: 30S ribosomal protein S10

Chain M:



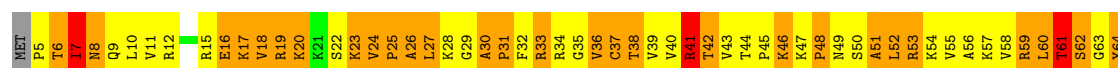
- Molecule 14: 30S ribosomal protein S11

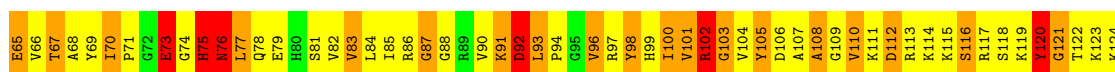
Chain N:



- Molecule 15: 30S ribosomal protein S12

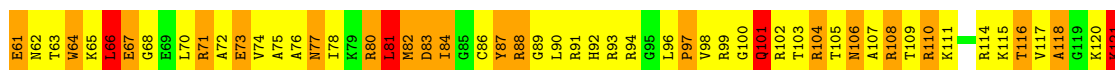
Chain O:





- Molecule 16: 30S ribosomal protein S13

Chain P:



- Molecule 17: 30S ribosomal protein S14

Chain Q:



- Molecule 18: 30S ribosomal protein S15

Chain R:



- Molecule 19: 30S ribosomal protein S16

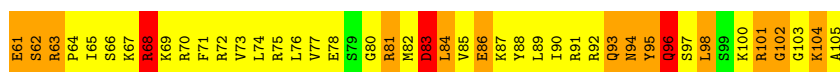
Chain S:



- Molecule 20: 30S ribosomal protein S17

Chain T:





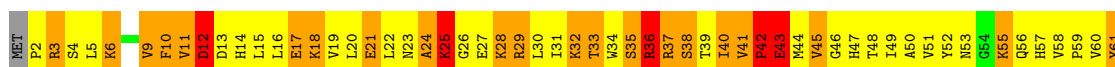
- Molecule 21: 30S ribosomal protein S18

Chain U:



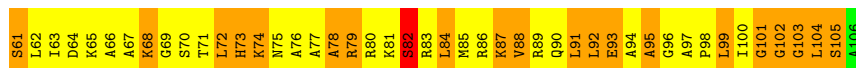
- Molecule 22: 30S ribosomal protein S19

Chain V:



- Molecule 23: 30S ribosomal protein S20

Chain W:



- Molecule 24: 30S ribosomal protein Thx

Chain X:



4 Data and refinement statistics

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

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, α , β , γ	508.65Å 508.65Å 803.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	300.00 – 4.51	Depositor
% Data completeness (in resolution range)	90.3 (300.00-4.51)	Depositor
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.00 (at 4.02Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.298 , 0.345	Depositor
Wilson B-factor (Å ²)	198.7	Xtriage
Anisotropy	0.113	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.55$, $\langle L^2 \rangle = 0.39$	Xtriage
Outliers	0 of 441813 reflections	Xtriage
Total number of atoms	55628	wwPDB-VP
Average B, all atoms (Å ²)	257.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.62% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

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	0.93	38/36438 (0.1%)	1.05	172/56869 (0.3%)
2	C	0.93	2/1814 (0.1%)	1.01	4/2825 (0.1%)
3	D	1.47	34/1813 (1.9%)	1.27	21/2823 (0.7%)
4	I	0.81	1/673 (0.1%)	1.07	3/1048 (0.3%)
5	E	0.63	0/1935	1.01	4/2609 (0.2%)
6	F	0.53	0/1636	0.93	4/2205 (0.2%)
7	G	0.67	1/1733 (0.1%)	1.10	7/2318 (0.3%)
8	H	0.70	0/1162	1.08	4/1564 (0.3%)
9	I	0.69	0/856	1.03	3/1154 (0.3%)
10	J	0.54	0/1276	0.87	0/1709
11	K	0.73	0/1136	1.08	3/1527 (0.2%)
12	L	0.51	0/1029	0.84	1/1379 (0.1%)
13	M	0.50	0/807	0.85	0/1085
14	N	0.67	0/900	1.06	0/1213
15	O	0.67	0/986	1.09	3/1320 (0.2%)
16	P	0.51	0/1008	0.91	2/1347 (0.1%)
17	Q	0.53	0/501	1.02	3/664 (0.5%)
18	R	0.67	0/745	0.98	0/992
19	S	0.72	0/716	1.04	4/963 (0.4%)
20	T	0.67	0/870	1.05	2/1159 (0.2%)
21	U	0.65	0/603	1.12	3/799 (0.4%)
22	V	0.49	0/661	0.91	1/890 (0.1%)
23	W	0.66	0/765	1.05	1/1007 (0.1%)
24	X	0.47	0/212	0.82	0/277
All	All	0.86	76/60275 (0.1%)	1.04	245/89746 (0.3%)

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	241

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	C	0	9
3	D	0	12
4	1	0	5
7	G	0	1
8	H	0	1
11	K	0	2
14	N	0	1
15	O	0	1
20	T	0	1
24	X	0	1
All	All	0	275

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	173	U	O3'-P	19.14	1.84	1.61
1	A	196	A	O3'-P	-18.33	1.39	1.61
1	A	37	U	N3-C4	-14.53	1.25	1.38
3	D	65	U	C2-N3	13.82	1.47	1.37
3	D	65	U	N3-C4	13.08	1.50	1.38

The worst 5 of 245 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	37	U	N3-C4-O4	-25.04	101.87	119.40
1	A	173	U	P-O3'-C3'	17.00	140.10	119.70
1	A	961	U	N1-C1'-C2'	12.14	129.78	114.00
1	A	1494	G	N9-C1'-C2'	11.89	129.45	114.00
1	A	576	G	N9-C1'-C2'	11.62	129.11	114.00

There are no chirality outliers.

5 of 275 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	12	U	Sidechain
1	A	16	A	Sidechain
1	A	21	G	Sidechain
1	A	24	U	Sidechain
1	A	7	G	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	32554	0	16429	6669	0
2	C	1624	0	826	297	0
3	D	1623	0	809	257	0
4	I	596	0	296	65	0
5	E	1900	0	1951	928	0
6	F	1612	0	1677	661	0
7	G	1703	0	1763	807	0
8	H	1146	0	1207	482	0
9	I	843	0	857	397	0
10	J	1257	0	1296	519	0
11	K	1116	0	1177	666	0
12	L	1010	0	1037	457	0
13	M	794	0	840	327	0
14	N	885	0	904	410	0
15	O	970	0	1057	413	0
16	P	997	0	1072	432	0
17	Q	492	0	529	264	0
18	R	734	0	771	349	0
19	S	700	0	720	348	0
20	T	857	0	930	385	0
21	U	597	0	668	357	0
22	V	647	0	673	241	0
23	W	763	0	861	330	0
24	X	208	0	221	87	0
All	All	55628	0	38571	14835	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 158.

The worst 5 of 14835 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:582:U:H5'	18:R:64:ARG:NH2	1.46	1.31
1:A:37:U:O4	1:A:397:A:N1	1.59	1.30
5:E:82:ARG:HD2	5:E:92:TYR:OH	1.34	1.27

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:123:C:O2'	1:A:290:C:H1'	1.32	1.24
1:A:901:A:C2	1:A:902:G:H1'	1.72	1.24

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	
5	E	232/256 (91%)	112 (48%)	47 (20%)	73 (32%)	0	0
6	F	204/239 (85%)	115 (56%)	43 (21%)	46 (22%)	0	3
7	G	206/209 (99%)	103 (50%)	61 (30%)	42 (20%)	0	4
8	H	148/162 (91%)	92 (62%)	34 (23%)	22 (15%)	0	9
9	I	99/101 (98%)	58 (59%)	19 (19%)	22 (22%)	0	3
10	J	153/156 (98%)	74 (48%)	40 (26%)	39 (26%)	0	2
11	K	136/138 (99%)	71 (52%)	32 (24%)	33 (24%)	0	2
12	L	125/128 (98%)	64 (51%)	33 (26%)	28 (22%)	0	3
13	M	96/105 (91%)	55 (57%)	14 (15%)	27 (28%)	0	1
14	N	117/129 (91%)	62 (53%)	30 (26%)	25 (21%)	0	4
15	O	122/132 (92%)	62 (51%)	22 (18%)	38 (31%)	0	0
16	P	123/126 (98%)	63 (51%)	36 (29%)	24 (20%)	0	5
17	Q	58/61 (95%)	28 (48%)	14 (24%)	16 (28%)	0	1
18	R	86/89 (97%)	40 (46%)	33 (38%)	13 (15%)	0	9
19	S	81/88 (92%)	45 (56%)	21 (26%)	15 (18%)	0	5
20	T	102/105 (97%)	63 (62%)	22 (22%)	17 (17%)	0	7
21	U	71/88 (81%)	30 (42%)	18 (25%)	23 (32%)	0	0
22	V	78/93 (84%)	32 (41%)	18 (23%)	28 (36%)	0	0
23	W	97/106 (92%)	32 (33%)	36 (37%)	29 (30%)	0	1
24	X	22/27 (82%)	9 (41%)	8 (36%)	5 (23%)	0	3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	2356/2538 (93%)	1210 (51%)	581 (25%)	565 (24%)	0 2

5 of 565 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	E	13	ALA
5	E	15	VAL
5	E	17	PHE
5	E	19	HIS
5	E	20	GLU

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
5	E	202/220 (92%)	135 (67%)	67 (33%)	0 3
6	F	160/188 (85%)	123 (77%)	37 (23%)	1 10
7	G	180/181 (99%)	127 (71%)	53 (29%)	0 5
8	H	115/123 (94%)	75 (65%)	40 (35%)	0 3
9	I	90/90 (100%)	64 (71%)	26 (29%)	0 5
10	J	126/127 (99%)	95 (75%)	31 (25%)	1 9
11	K	119/119 (100%)	76 (64%)	43 (36%)	0 2
12	L	98/99 (99%)	76 (78%)	22 (22%)	1 11
13	M	88/92 (96%)	65 (74%)	23 (26%)	1 7
14	N	90/99 (91%)	62 (69%)	28 (31%)	0 4
15	O	104/109 (95%)	77 (74%)	27 (26%)	1 7
16	P	100/101 (99%)	79 (79%)	21 (21%)	1 12
17	Q	49/50 (98%)	37 (76%)	12 (24%)	1 9
18	R	79/80 (99%)	56 (71%)	23 (29%)	0 5
19	S	72/74 (97%)	48 (67%)	24 (33%)	0 3
20	T	96/97 (99%)	71 (74%)	25 (26%)	1 7
21	U	64/77 (83%)	41 (64%)	23 (36%)	0 2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
22	V	71/80 (89%)	57 (80%)	14 (20%)	2	15
23	W	76/82 (93%)	56 (74%)	20 (26%)	1	7
24	X	19/22 (86%)	13 (68%)	6 (32%)	0	4
All	All	1998/2110 (95%)	1433 (72%)	565 (28%)	0	5

5 of 565 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	K	4	ASP
12	L	124	GLN
21	U	81	PHE
11	K	26	VAL
11	K	107	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 86 such sidechains are listed below:

Mol	Chain	Res	Type
10	J	11	GLN
11	K	70	GLN
20	T	93	GLN
10	J	68	ASN
10	J	106	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1515/1522 (99%)	479 (31%)	151 (9%)
2	C	75/76 (98%)	30 (40%)	7 (9%)
3	D	75/76 (98%)	27 (36%)	3 (4%)
4	1	26/27 (96%)	11 (42%)	1 (3%)
All	All	1691/1701 (99%)	547 (32%)	162 (9%)

5 of 547 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	6	G
1	A	8	A
1	A	9	G
1	A	13	U

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Mol	Chain	Res	Type
1	A	14	U

5 of 162 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	723	U
1	A	873	A
1	A	1529	G
1	A	748	C
1	A	815	A

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 ⓘ

There are no ligands in this entry.

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.