



wwPDB X-ray Structure Validation Summary Report (i)

Mar 31, 2014 – 06:05 PM BST

PDB ID : 2HGP
Title : Crystal structure of the 70S *Thermus thermophilus* ribosome with translocated and rotated Shine-Dalgarno Duplex. This entry 2HGP contains 30S ribosomal subunit. The 50S ribosomal subunit can be found in PDB entry 2HGQ.
Authors : Jenner, L.; Yusupova, G.; Rees, B.; Moras, D.; Yusupov, M.
Deposited on : 2006-06-27
Resolution : 5.50 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>

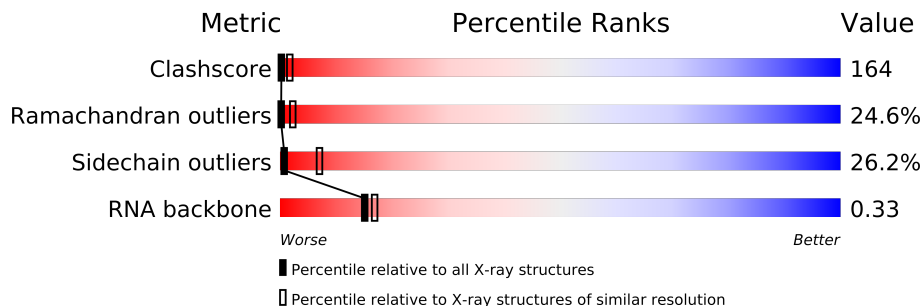
The following versions of software and data (see [references](#)) were used in the production of this report:

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 5.50 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	79885	1008 (7.40-3.52)
Ramachandran outliers	78287	1275 (7.50-3.50)
Sidechain outliers	78261	1251 (7.50-3.50)
RNA backbone	1838	1040 (7.50-2.80)




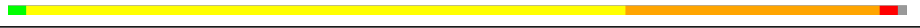
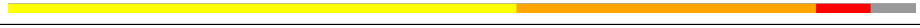



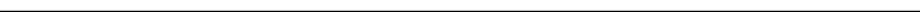
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The 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	1	50	
3	B	76	
3	C	76	
3	D	76	
4	E	256	
5	F	239	
6	G	209	
7	H	162	
8	I	101	
9	J	156	
10	K	138	
11	L	128	
12	M	105	
13	N	129	

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Mol	Chain	Length	Quality of chain
14	O	132	
15	P	126	
16	Q	61	
17	R	89	
18	S	88	
19	T	105	
20	U	88	
21	V	93	
22	W	106	
23	X	27	

2 Entry composition

There are 23 unique types of molecules in this entry. The entry contains 57679 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 ribosomal RNA.

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 mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	1	50	Total	C	N	O	P	0	0	0
			1025	459	128	388	50			

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

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

- Molecule 4 is a protein called 30S ribosomal protein S2.

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

- Molecule 5 is a protein called 30S ribosomal protein S3.

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

- Molecule 6 is a protein called 30S ribosomal protein S4.

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

- Molecule 7 is a protein called 30S ribosomal protein S5.

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

- Molecule 8 is a protein called 30S ribosomal protein S6.

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

- Molecule 9 is a protein called 30S ribosomal protein S7.

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

- Molecule 10 is a protein called 30S ribosomal protein S8.

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

- Molecule 11 is a protein called 30S ribosomal protein S9.

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

- Molecule 12 is a protein called 30S ribosomal protein S10.

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

- Molecule 13 is a protein called 30S ribosomal protein S11.

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

- Molecule 14 is a protein called 30S ribosomal protein S12.

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

- Molecule 15 is a protein called 30S ribosomal protein S13.

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

- Molecule 16 is a protein called 30S ribosomal protein S14.

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

- Molecule 17 is a protein called 30S ribosomal protein S15.

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

- Molecule 18 is a protein called 30S ribosomal protein S16.

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

- Molecule 19 is a protein called 30S ribosomal protein S17.

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

- Molecule 20 is a protein called 30S ribosomal protein S18.

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

- Molecule 21 is a protein called 30S ribosomal protein S19.

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

- Molecule 22 is a protein called 30S ribosomal protein S20.

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

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

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

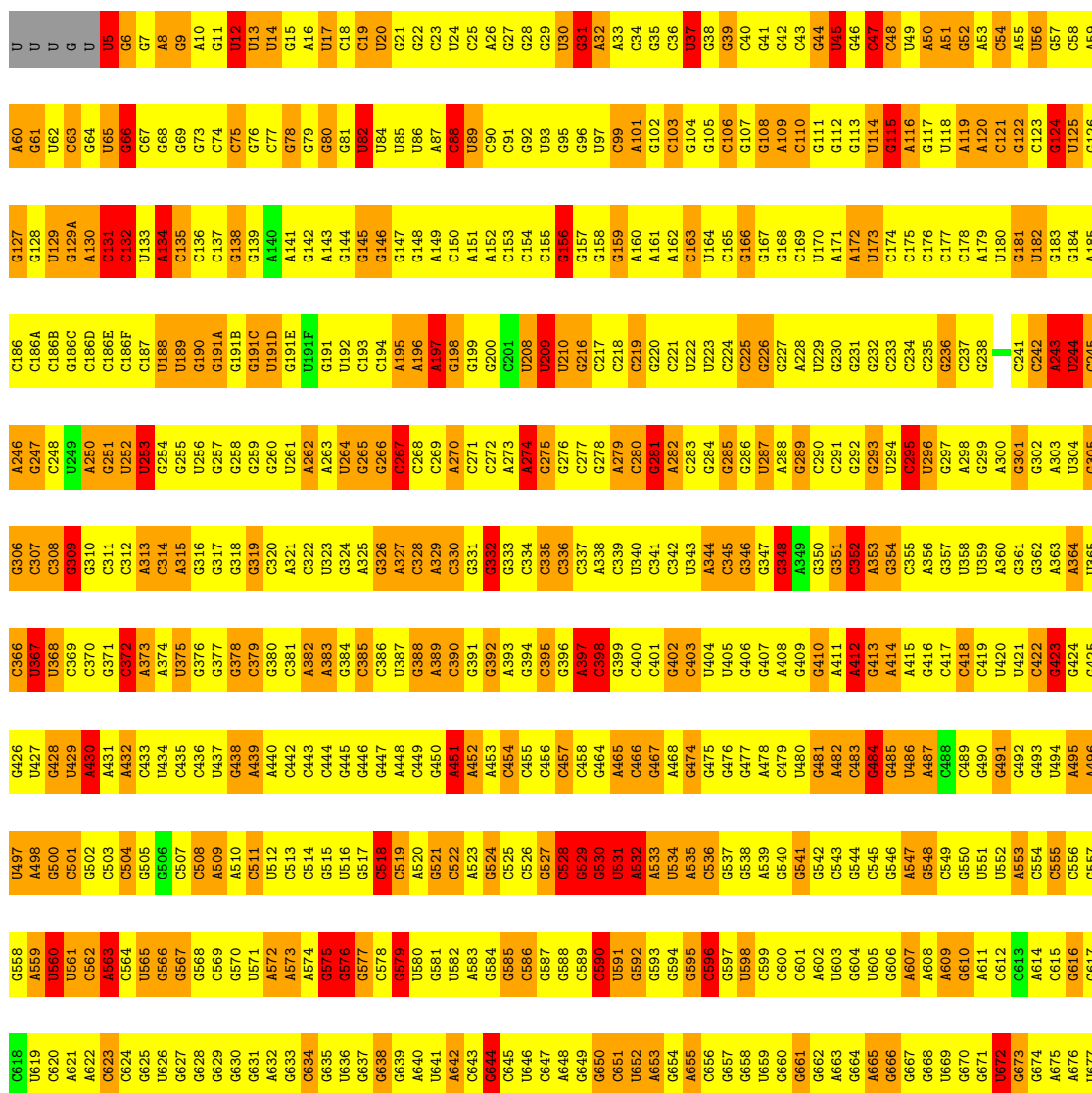
3 Residue-property plots

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 ($RSRZ > 2$). 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 ribosomal RNA

Chain A: 



C1524	G1464	C1399	A1340	U1159	G1099	G1039	C984	C924	A864	G798	C738	U678
G1525	C1465	C1400	U1341	G1160	C1100	U1040	C985	G925	A865	G799	C739	C679
G1526	C1466	G1401	C1342	C1161	A1102	A1041	A986	G926	A986	G800	U740	C680
C1527	G1467	C1402	G1343	C1162	A1103	G1042	G987	G927	G867	U801	G741	C681
U1528	A1468	C1403	C1344	C1163	G1103	C1043	G988	G928	C988	A802	G742	G682
G1529	C1469	C1404	U1345	G1164	G1104	A1044	G989	G929	G869	G803	U743	G683
G1530	G1470	G1405	A1346	C1165	A1105	C1045	C990	C930	U870	U804	G744	A684
A1531	U1471	G1406	C1347	C1166	G1106	A1046	U991	C931	U871	C805	C745	G685
U1532	U1472	C1407	U1348	A1167	C1107	G1047	U992	C932	A872	C806	A746	U686
A1534	A1473	A1408	A1349	C1168	G1108	G1048	G993	G933	A873	A807	G747	A687
C1535	G1474	C1409	A1350	A1169	G1109	U1049	A994	C934	G874	C908	C748	G688
C1536	G1475	G1410	U1351	G1170	A1110	G1050	C995	A935	C875	G809	G749	C689
C1537	G1476	C1411	C1352	C1171	A1111	G1051	A996	C936	G876	C810	G750	G690
U1537	C1477	G1412	G1353	C1172	C1112	U1052	U997	A937	C877	C811	U751	G691
C1538	C1478	A1413	C1354	G1173	C1113	G1053	G998	A938	G878	C812	G752	U692
C1539	U1479	G1414	G1355	G1174	C1114	C1054	C998A	A939	G879	U813	A753	G693
U1540	G1480	C1296	C1356	A1176	C1115	A1055	U999	C940	C880	A814	G754	A694
U1541	U1481	G1415	A1357	C1177	C1116	U1056	A1000	G941	G881	A815	G755	A695
U1542	G1482	G1417	U1358	G1178	G1117	G1057	G1001	G942	C882	A816	C756	A696
C	A1483	A1418	C1359	C1179	C1118	G1058	G1002	U943	C883	C817	U757	U697
U	C1484	U1419	A1360	A1180	C1119	C1059	G1003	G944	U884	G818	G758	G698
	U1485	C1420	G1361	G1181	G1120	C1060	A1004	G945	C885	A819	A759	C699
	G1486	G1421	C1362	G1182	U1121	G1061	A1005	G946	G886	U820	G760	G700
	G1487	G1422	C1362A	A1183	U1122	U1062	C1006	G947	G887	G821	G761	C701
	G1488	G1423	A1363	G1184	A1123	C1063	C1007	C948	G888	C822	C762	A702
	G1489	C1424	U1364	C1185	G1124	G1064	C1008	A949	A889	G823	G763	G703
	C1490	U1425	G1365	G1186	U1125	U1065	G1009	U950	G890	C824	C764	A704
	G1491	C1426	U1366	G1187	U1126	C1066	G1010	G951	U891	G825	G765	U705
	A1492	U1427	C1367	A1188	G1127	A1067	G1011	U952	A892	C826	A766	A706
	A1493	A1428	G1368	C1189	C1128	G1068	U1012	G953	C893	U827	A767	C707
	G1494	C1429	C1369	G1190	C1129	C1069	G1013	G954	G894	A828	A768	C708
	U1495	C1430	G1370	A1191	A1130	U1070	A1014	U955	G895	G829	G769	G709
	C1496	C1431	G1371	A1192	G1131	C1071	A1015	U956	C896	G830	C770	G710
	G1497	G1432	U1372	G1193	C1132	G1072	A1016	U957	G897	U831	G771	G711
	U1498	A1433	G1373	U1194	G1133	U1073	C1018	A958	C898	C832	U772	A712
	A1499	A1434	A1374	C1195	G1134	G1074	C1019	U960	A900	C833	G773	G713
	A1500	G1435	A1375	U1196	U1135	C1075	C1019	U960	A901	C834	G774	G714
	C1501	U1436	U1376	G1197	U1136	C1076	U1020	U961	C902	U835	G775	A715
	A1502	C1437	A1377	G1198	C1137	G1077	G1021	C962	G903	G836	A777	C717
	A1503	G1438	C1378	U1199	G1138	U1078	G1022	G963	C903	G837	A778	G718
	G1504	C1439	G1379	C1200	G1139	G1079	G1023	A964	C904	C838	G779	C719
	G1505	C1440	U1380	A1201	C1140	A1080	G1024	A965	U905	U841	C779	C719
	U1506	G1441	U1381	G1202	C1141	G1081	U1025	G966	G906	C942	A780	G720
	A1507	G1442	C1382	C1203	G1142	G1082	G1026	C967	A907	U843	A781	G721
	G1508	G1443	C1383	A1204	G1143	U1083	C1027	A968	A908	C848	A782	A722
	C1509	A1446	C1384	G1205	C1144	C1084	C1028	A969	A909	C849	C783	U723
	U1510	G1447	G1385	G1206	C1145	U1085	C1028A	C970	C910	U850	C784	G724
	G1511	C1448	G1386	C1207	A1146	U1086	C1028B	G971	U911	G851	G785	G725
	U1512	C1449	G1387	C1208	C1147	G1087	G1029	C972	C912	G852	G786	G726
	A1513	U1450	C1388	C1209	U1148	G1088	C1030	G973	A913	G853	A787	G727
	C1514	A1451	C1389	C1210	C1149	G1089	G1031	A974	A914	G854	U788	A728
	G1515	C1452	U1390	U1211	U1150	U1090	A1032	A975	A915	G855	A789	A729
	G1516	A1453	A1391	U1212	A1151	U1091	G1032A	G976	G916	C856	A790	G730
	U1517	G1454	C1392	C1213	A1152	A1092	G1032B	A977	G917	C857	G791	G731
	A1518	G1455	U1393	G1214	C1153	A1093	G1033	A978	A918	G858	A792	C732
	U1519	C1456	C1394	G1215	G1154	G1094	C1034	C979	A919	A859	U793	A733
	G1520	A1460	C1395	G1216	G1155	U1095	A1035	C980	U920	A860	A794	G734
	U1521	G1461	A1396	C1217	G1156	C1096	G1036	U981	U921	G861	C795	C735
	G1522	G1462	C1397	C1218	U1157	C1097	C1037	U982	G922	C862	C796	C736
	G1523	C1463	A1398	U1219	C1158	C1098	C1038	A983	A923	U863	C797	A737

• Molecule 2: mRNA

Chain 1:





- Molecule 3: tRNA PHE (unmodified bases)

Chain C:



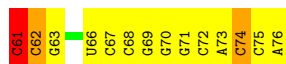
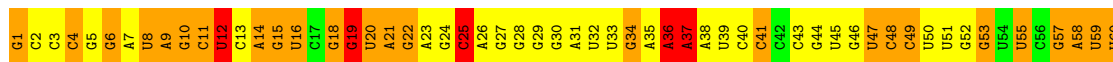
- Molecule 3: tRNA PHE (unmodified bases)

Chain D:



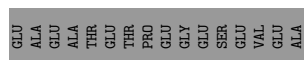
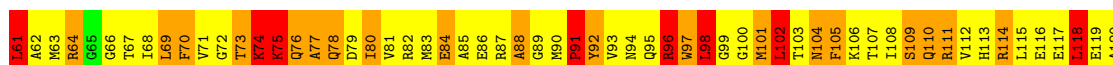
- Molecule 3: tRNA PHE (unmodified bases)

Chain B:



- Molecule 4: 30S ribosomal protein S2

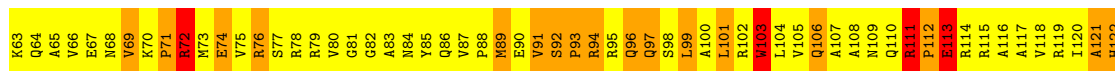
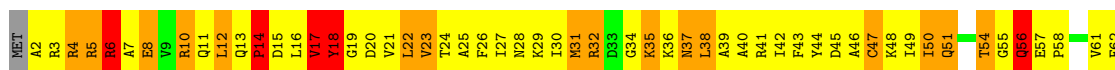
Chain E:



- Molecule 5: 30S ribosomal protein S3

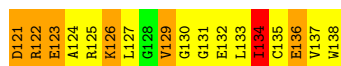
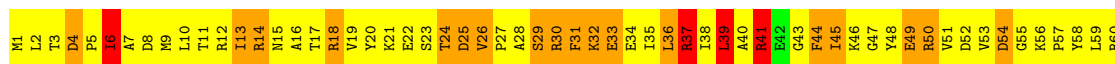
Chain F:





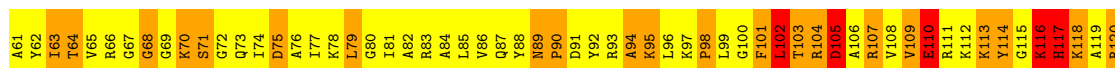
• Molecule 10: 30S ribosomal protein S8

Chain K:



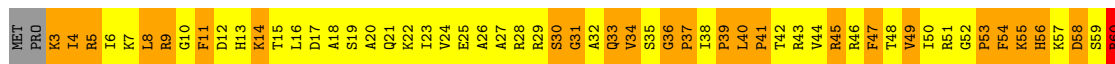
• Molecule 11: 30S ribosomal protein S9

Chain L:



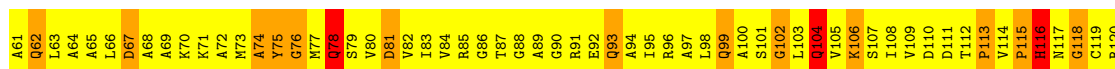
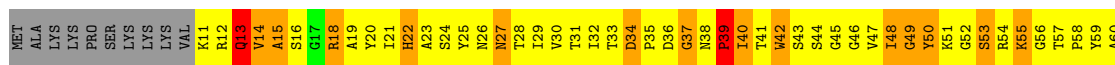
• Molecule 12: 30S ribosomal protein S10

Chain M:



• Molecule 13: 30S ribosomal protein S11

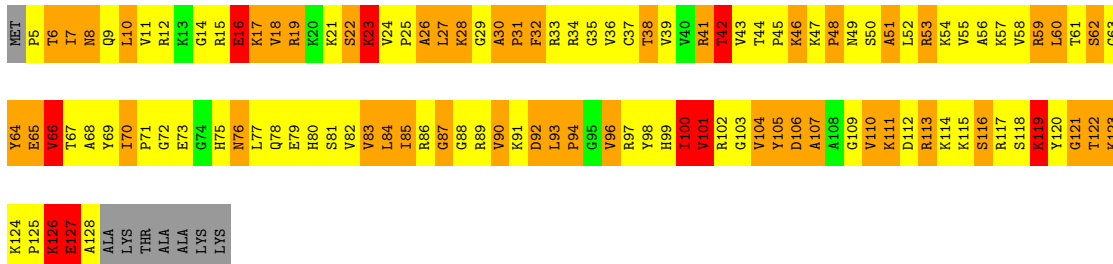
Chain N:





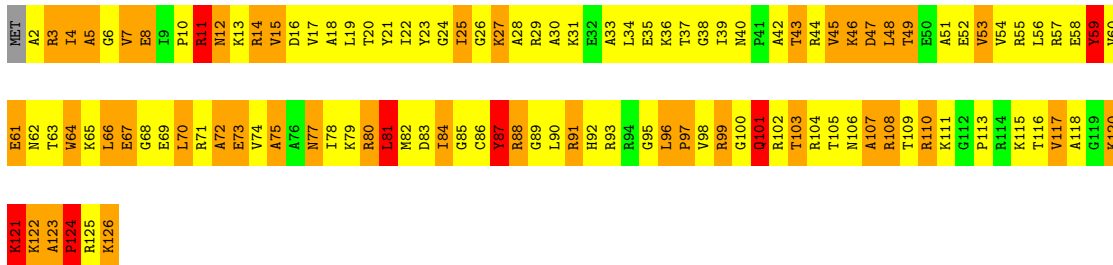
- Molecule 14: 30S ribosomal protein S12

Chain 0:



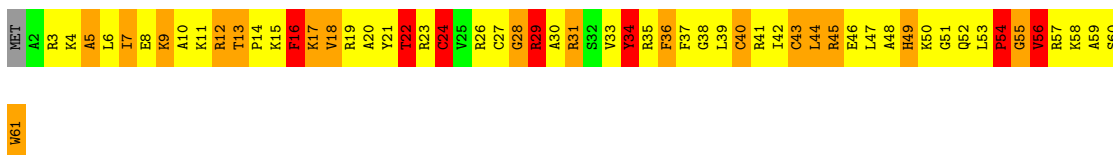
- Molecule 15: 30S ribosomal protein S13

Chain P:



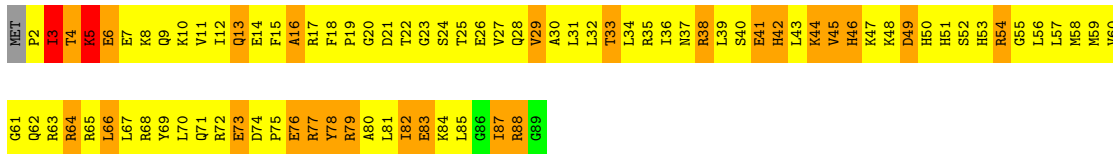
- Molecule 16: 30S ribosomal protein S14

Chain Q:



- Molecule 17: 30S ribosomal protein S15

Chain R:



- Molecule 18: 30S ribosomal protein S16

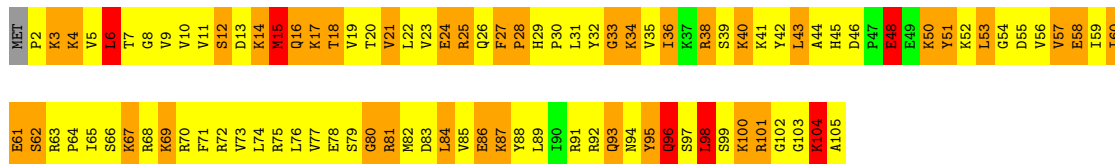
Chain S:





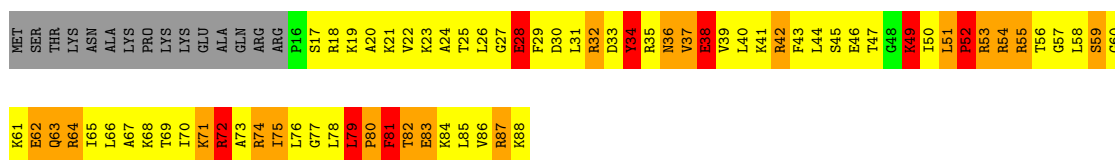
• Molecule 19: 30S ribosomal protein S17

Chain T:



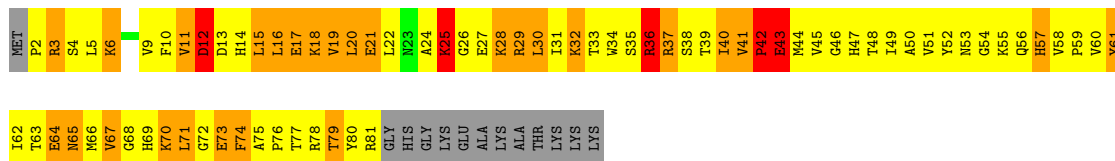
• Molecule 20: 30S ribosomal protein S18

Chain U:



• Molecule 21: 30S ribosomal protein S19

Chain V:



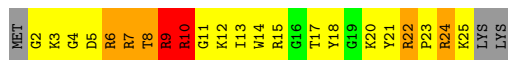
• Molecule 22: 30S ribosomal protein S20

Chain W:



• Molecule 23: 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	508.54Å 508.54Å 806.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	300.00 – 5.50	Depositor
% Data completeness (in resolution range)	96.7 (300.00-5.50)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.00 (at 4.88Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.243 , 0.326	Depositor
Wilson B-factor (Å ²)	108.9	Xtriage
Anisotropy	0.045	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.37$	Xtriage
Outliers	1 of 226745 reflections (0.000%)	Xtriage
Total number of atoms	57679	wwPDB-VP
Average B, all atoms (Å ²)	232.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.63% 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	0.87	32/36438 (0.1%)	1.08	147/56869 (0.3%)
2	1	0.67	1/1133 (0.1%)	0.93	2/1753 (0.1%)
3	B	0.70	1/1813 (0.1%)	1.02	9/2823 (0.3%)
3	C	0.98	2/1813 (0.1%)	0.93	2/2823 (0.1%)
3	D	0.69	1/1813 (0.1%)	0.92	2/2823 (0.1%)
4	E	0.64	0/1935	1.00	4/2609 (0.2%)
5	F	0.55	0/1636	0.92	4/2205 (0.2%)
6	G	0.64	1/1733 (0.1%)	0.98	3/2318 (0.1%)
7	H	0.63	0/1162	1.01	3/1564 (0.2%)
8	I	0.60	0/856	0.95	0/1154
9	J	0.57	0/1276	0.90	3/1709 (0.2%)
10	K	0.62	0/1136	1.01	3/1527 (0.2%)
11	L	0.54	0/1029	0.83	0/1379
12	M	0.48	0/807	0.89	1/1085 (0.1%)
13	N	0.62	0/900	0.98	0/1213
14	O	0.60	0/986	1.00	3/1320 (0.2%)
15	P	0.50	0/1008	0.91	2/1347 (0.1%)
16	Q	0.55	0/501	0.96	1/664 (0.2%)
17	R	0.62	0/745	0.95	0/992
18	S	0.62	0/716	0.95	1/963 (0.1%)
19	T	0.68	1/870 (0.1%)	0.99	2/1159 (0.2%)
20	U	0.59	0/603	1.01	1/799 (0.1%)
21	V	0.51	0/661	0.92	0/890
22	W	0.65	0/765	1.00	2/1007 (0.2%)
23	X	0.45	0/212	0.80	0/277
All	All	0.78	39/62547 (0.1%)	1.03	195/93272 (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.

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Mol	Chain	#Chirality outliers	#Planarity outliers
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Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	175
2	1	0	3
3	B	0	6
3	C	0	8
3	D	0	8
6	G	0	1
8	I	0	1
13	N	0	1
15	P	0	1
16	Q	0	1
All	All	0	205

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1064	G	C5-C6	-9.61	1.32	1.42
1	A	530	G	N9-C4	-9.56	1.30	1.38
1	A	1493	A	C5-C6	8.51	1.48	1.41
1	A	1494	G	C5-C6	8.33	1.50	1.42
1	A	1492	A	N9-C4	8.30	1.42	1.37

The worst 5 of 195 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1064	G	N1-C2-N2	-71.65	51.71	116.20
1	A	1064	G	N3-C2-N2	57.72	160.30	119.90
1	A	1064	G	N1-C2-N3	-25.51	108.59	123.90
3	B	18	G	OP2-P-O3'	14.85	137.87	105.20
1	A	1064	G	C2-N3-C4	14.60	119.20	111.90

There are no chirality outliers.

5 of 205 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	12	U	Sidechain
1	A	17	U	Sidechain
1	A	31	G	Sidechain
1	A	37	U	Sidechain
1	A	45	U	Sidechain

5.2 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	32554	0	16431	6696	0
2	1	1025	0	511	175	0
3	B	1623	0	821	149	0
3	C	1623	0	821	283	0
3	D	1623	0	821	235	0
4	E	1900	0	1951	1040	0
5	F	1612	0	1677	721	0
6	G	1703	0	1763	869	0
7	H	1146	0	1207	588	0
8	I	843	0	857	384	0
9	J	1257	0	1296	577	0
10	K	1116	0	1177	735	0
11	L	1010	0	1037	470	0
12	M	794	0	840	358	0
13	N	885	0	904	471	0
14	O	970	0	1057	512	0
15	P	997	0	1072	496	0
16	Q	492	0	529	278	0
17	R	734	0	771	331	0
18	S	700	0	720	353	0
19	T	857	0	930	450	0
20	U	597	0	668	369	0
21	V	647	0	673	312	0
22	W	763	0	861	374	0
23	X	208	0	221	83	0
All	All	57679	0	39616	15868	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 164.

The worst 5 of 15868 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:38:G:N2	1:A:397:A:H5''	1.43	1.32
9:J:78:ARG:O	9:J:84:ASN:HA	1.33	1.28

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1443:G:H4'	1:A:1446:A:C5'	1.68	1.24
1:A:901:A:C2	1:A:902:G:H1'	1.74	1.22
1:A:1062:U:H2'	1:A:1063:C:C5	1.74	1.21

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	
4	E	232/256 (91%)	114 (49%)	42 (18%)	76 (33%)	0	0
5	F	204/239 (85%)	107 (52%)	46 (22%)	51 (25%)	0	2
6	G	206/209 (99%)	96 (47%)	57 (28%)	53 (26%)	0	2
7	H	148/162 (91%)	93 (63%)	38 (26%)	17 (12%)	1	15
8	I	99/101 (98%)	58 (59%)	19 (19%)	22 (22%)	0	3
9	J	153/156 (98%)	73 (48%)	45 (29%)	35 (23%)	0	3
10	K	136/138 (99%)	68 (50%)	35 (26%)	33 (24%)	0	2
11	L	125/128 (98%)	62 (50%)	33 (26%)	30 (24%)	0	3
12	M	96/105 (91%)	52 (54%)	20 (21%)	24 (25%)	0	2
13	N	117/129 (91%)	65 (56%)	29 (25%)	23 (20%)	0	4
14	O	122/132 (92%)	50 (41%)	30 (25%)	42 (34%)	0	0
15	P	123/126 (98%)	56 (46%)	34 (28%)	33 (27%)	0	2
16	Q	58/61 (95%)	24 (41%)	16 (28%)	18 (31%)	0	1
17	R	86/89 (97%)	36 (42%)	35 (41%)	15 (17%)	0	6
18	S	81/88 (92%)	42 (52%)	24 (30%)	15 (18%)	0	5
19	T	102/105 (97%)	62 (61%)	23 (22%)	17 (17%)	0	7
20	U	71/88 (81%)	26 (37%)	26 (37%)	19 (27%)	0	2
21	V	78/93 (84%)	32 (41%)	23 (30%)	23 (30%)	0	1
22	W	97/106 (92%)	38 (39%)	32 (33%)	27 (28%)	0	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
23	X	22/27 (82%)	9 (41%)	6 (27%)	7 (32%)	0	1
All	All	2356/2538 (93%)	1163 (49%)	613 (26%)	580 (25%)	0	2

5 of 580 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	E	8	LYS
4	E	11	LEU
4	E	13	ALA
4	E	15	VAL
4	E	16	HIS

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	
4	E	202/220 (92%)	138 (68%)	64 (32%)	0	4
5	F	160/188 (85%)	123 (77%)	37 (23%)	1	9
6	G	180/181 (99%)	131 (73%)	49 (27%)	0	6
7	H	115/123 (94%)	78 (68%)	37 (32%)	0	4
8	I	90/90 (100%)	61 (68%)	29 (32%)	0	4
9	J	126/127 (99%)	93 (74%)	33 (26%)	1	7
10	K	119/119 (100%)	86 (72%)	33 (28%)	0	6
11	L	98/99 (99%)	73 (74%)	25 (26%)	1	8
12	M	88/92 (96%)	67 (76%)	21 (24%)	1	9
13	N	90/99 (91%)	74 (82%)	16 (18%)	2	19
14	O	104/109 (95%)	81 (78%)	23 (22%)	1	11
15	P	100/101 (99%)	75 (75%)	25 (25%)	1	8
16	Q	49/50 (98%)	36 (74%)	13 (26%)	1	7
17	R	79/80 (99%)	64 (81%)	15 (19%)	2	16
18	S	72/74 (97%)	49 (68%)	23 (32%)	0	4
19	T	96/97 (99%)	67 (70%)	29 (30%)	0	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	U	64/77 (83%)	48 (75%)	16 (25%)	1	8
21	V	71/80 (89%)	55 (78%)	16 (22%)	1	10
22	W	76/82 (93%)	59 (78%)	17 (22%)	1	11
23	X	19/22 (86%)	17 (90%)	2 (10%)	10	47
All	All	1998/2110 (95%)	1475 (74%)	523 (26%)	1	7

5 of 523 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
9	J	111	ARG
11	L	47	LEU
20	U	74	ARG
9	J	143	ARG
10	K	54	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 81 such sidechains are listed below:

Mol	Chain	Res	Type
9	J	97	GLN
11	L	23	ASN
19	T	93	GLN
9	J	106	GLN
9	J	153	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1515/1522 (99%)	463 (30%)	137 (9%)
2	1	49/50 (98%)	21 (42%)	4 (8%)
3	B	75/76 (98%)	32 (42%)	1 (1%)
3	C	75/76 (98%)	23 (30%)	4 (5%)
3	D	75/76 (98%)	23 (30%)	1 (1%)
All	All	1789/1800 (99%)	562 (31%)	147 (8%)

5 of 562 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	6	G

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Mol	Chain	Res	Type
1	A	8	A
1	A	9	G
1	A	14	U
1	A	19	C

5 of 147 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	723	U
1	A	889	A
1	A	1529	G
1	A	753	A
1	A	816	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.