



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 21, 2020 – 07:39 PM BST

PDB ID : 1XMO
Title : Crystal Structure of mnm5U34t6A37-tRNA^{Lys}UUU Complexed with AAG-mRNA in the Decoding Center
Authors : Murphy, F.V.; Ramakrishnan, V.; Malkiewicz, A.; Agris, P.F.
Deposited on : 2004-10-04
Resolution : 3.25 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

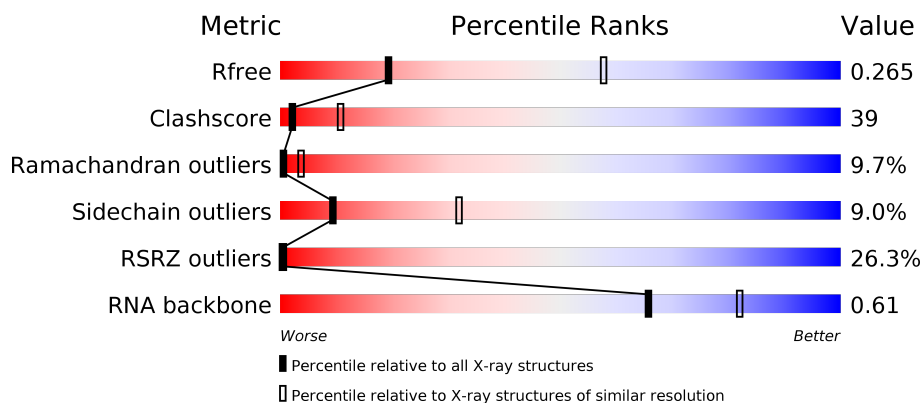
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.25 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



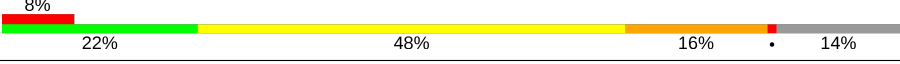
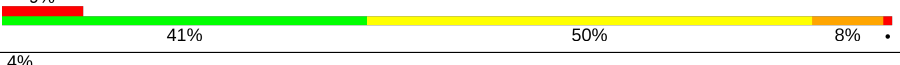
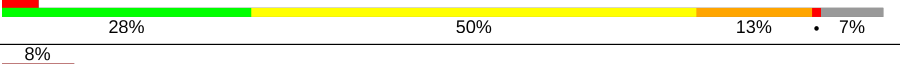
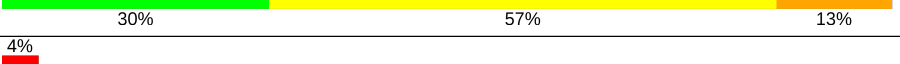
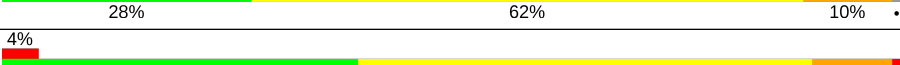
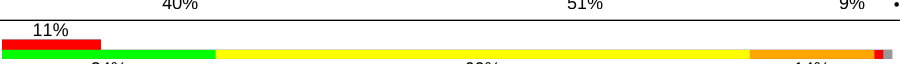
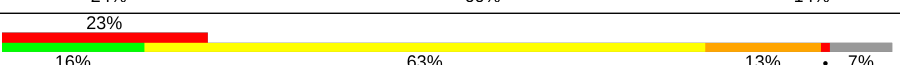
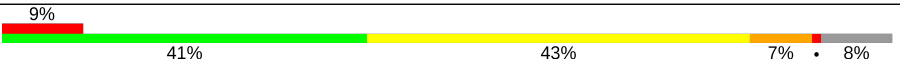
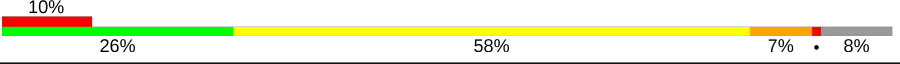
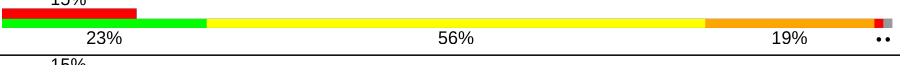
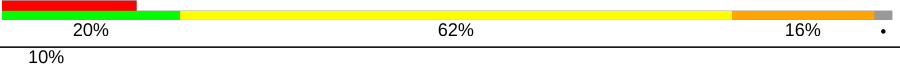
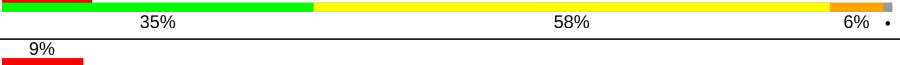

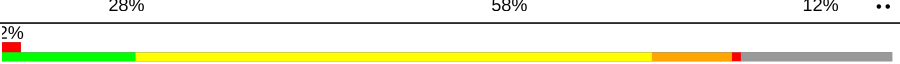
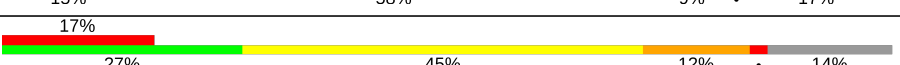
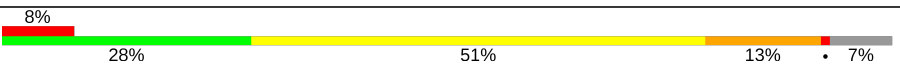
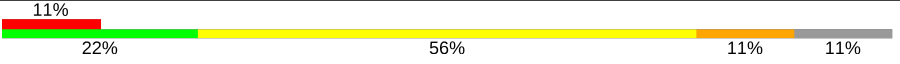
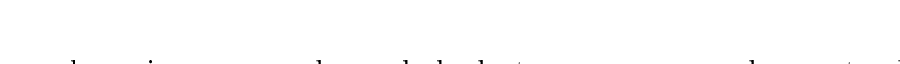
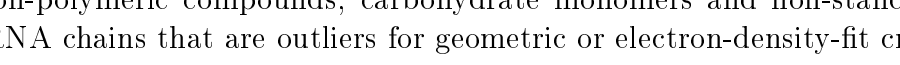
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1191 (3.30-3.22)
Clashscore	141614	1251 (3.30-3.22)
Ramachandran outliers	138981	1229 (3.30-3.22)
Sidechain outliers	138945	1228 (3.30-3.22)
RSRZ outliers	127900	1154 (3.30-3.22)
RNA backbone	3102	1072 (3.62-2.90)

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

Mol	Chain	Length	Quality of chain
1	A	1522	<div> <div>52%</div> <div> <div>28%</div> <div>55%</div> <div>14%</div> <div>••</div> </div> </div>
2	W	3	<div> <div>100%</div> <div> <div>33%</div> <div>67%</div> </div> </div>
3	X	11	<div> <div>27%</div> <div> <div>36%</div> <div>45%</div> <div>18%</div> </div> </div>
4	B	256	<div> <div>7%</div> <div> <div>15%</div> <div>65%</div> <div>9%</div> <div>•</div> <div>9%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
5	C	239	
6	D	209	
7	E	162	
8	F	101	
9	G	156	
10	H	138	
11	I	128	
12	J	105	
13	K	129	
14	L	135	
15	M	126	
16	N	61	
17	O	89	
18	P	88	
19	Q	105	
20	R	88	
21	S	93	
22	T	106	
23	V	27	

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	MG	A	1562	-	-	-	X
25	MG	A	1566	-	-	-	X
25	MG	A	1575	-	-	-	X
25	MG	A	1595	-	-	-	X
25	MG	A	1596	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	MG	A	1607	-	-	-	X
25	MG	A	1622	-	-	-	X
25	MG	A	1634	-	-	-	X
25	MG	A	210	-	-	-	X
25	MG	A	493	-	-	-	X
3	T6A	X	37	X	-	-	-

2 Entry composition [i](#)

There are 26 unique types of molecules in this entry. The entry contains 52063 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1507	Total	C	N	O	P	0	0	0
			32380	14414	5990	10470	1506			

- Molecule 2 is a RNA chain called A-Site Messenger RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	W	3	Total	C	N	O	P	0	0	0
			64	30	15	17	2			

- Molecule 3 is a RNA chain called Anticodon Transfer RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	X	11	Total	C	N	O	P	0	0	0
			239	110	38	81	10			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	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	C	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	D	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	E	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	F	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	G	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	H	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	I	127	Total	C	N	O	0	0	0
			1011	639	198	174			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	K	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	L	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	M	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	N	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	O	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	P	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	Q	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	R	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	S	80	Total	C	N	O	S	0	0	0
			647	414	119	112	2			

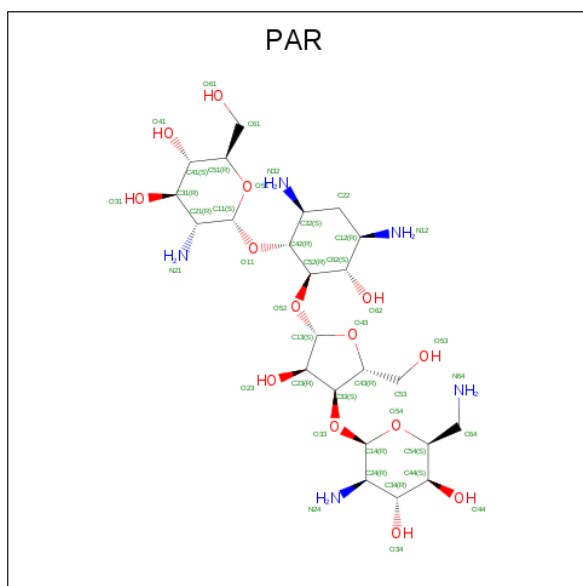
- Molecule 22 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	T	99	Total	C	N	O	S	0	0	0
			762	469	162	129	2			

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

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

- Molecule 24 is PAROMOMYCIN (three-letter code: PAR) (formula: $C_{23}H_{45}N_5O_{14}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
24	A	1	Total	C	N	O	0	0
			42	23	5	14		

- Molecule 25 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
25	X	2	Total	Mg	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
25	J	1	Total 1	Mg 1	0	0
25	A	104	Total 104	Mg 104	0	0

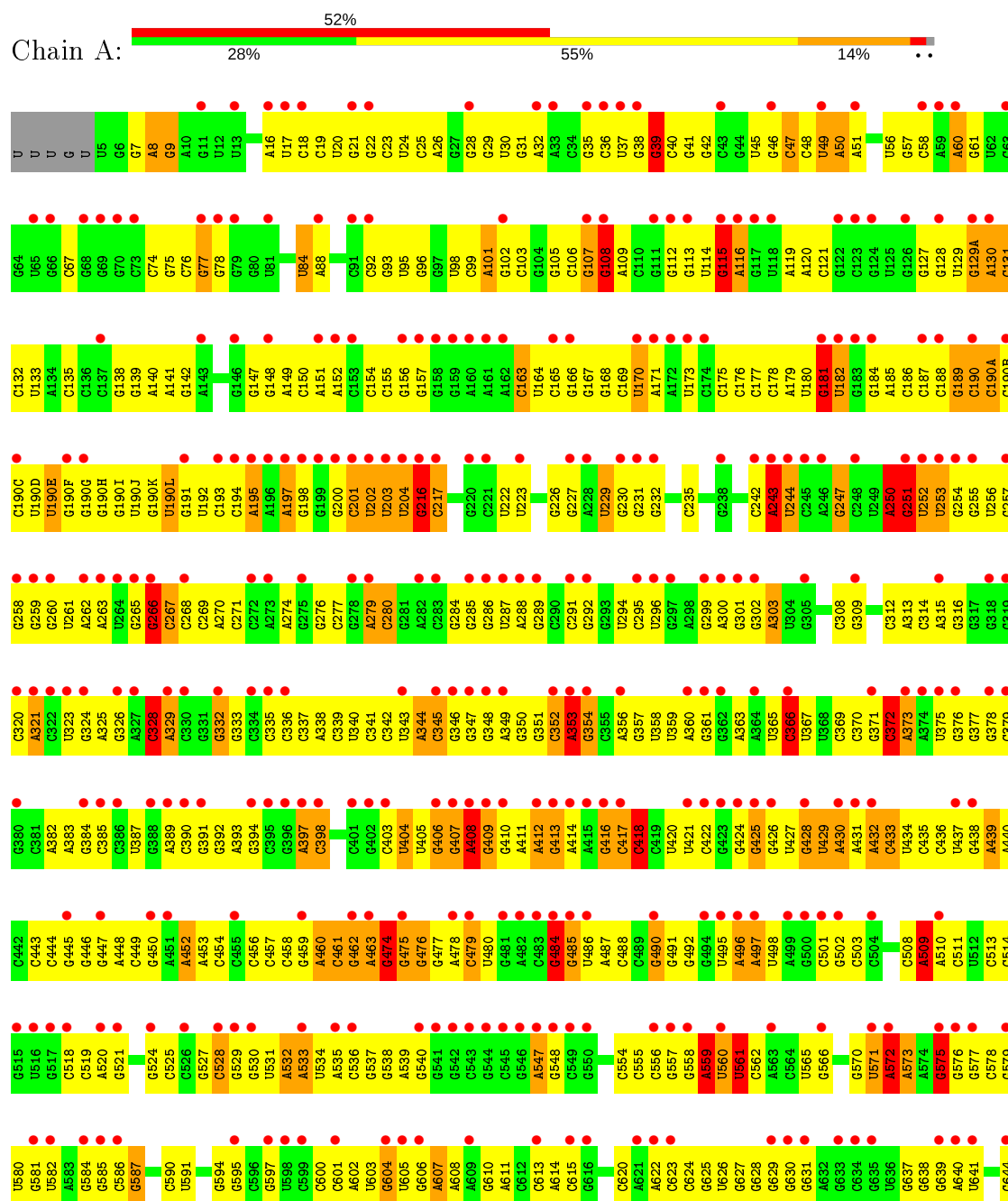
- Molecule 26 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

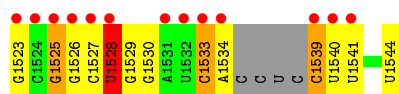
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

- Molecule 1: 16S ribosomal RNA



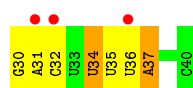
G1461	G1392	A1382	G1270	C1208	C1145	U1085	C1029	A968	C904	G836	G769	A706	G645
G1462	U1393	A1383	G1271	C1209	A1146	U1086	G1030	A969	U905	G837	G770	C707	U646
G1463	A1394	C1394	G1272	C1210	C1147	G1087	C	C970	G906	G838	G775	C708	C647
G1464	C1395	C1395	U1211	U1211	U1148	G1088	G	G971	A907	U839	G776	C709	A648
G1465	A1396	C1396	G1273	U1212	C1149	G1089	A	C972	A908	U840	A777	G710	G649
G1466	C1397	C1397	U1213	U1213	U1150	U1090	G1031	G973	A909	U841	A778	G711	G650
G1467	A1398	C1398	G1274	C1214	A1151	U1091	G1032	A974	C910	C848	C779	A712	C651
G1468	C1399	A1399	G1275	G1215	A1152	U1092	G1033	A975	U911	C849	A780	G713	U652
G1469	C1400	A1340	U1276	G1216	C1153	A1093	G1034	G976	C912	U850	A781	G714	A653
G1470	C1401	U1341	A1277	C1217	G1154	U1094	G1035	G977	A913	G851	A782	A715	G654
G1471	C1402	C1342	A1280	C1218	G1155	U1095	A1035	A978	A914	G852	A783	A716	A655
G1472	C1403	G1343	U1281	U1219	A1156	C1096	G1036	C979	A915	G853	C717	G717	C656
G1473	C1404	C1344	U1282	G1220	A1157	C1097	G1037	C980	A916	G854	C718	G718	C657
G1474	G1405	U1345	G1283	G1221	C1158	C1098	C1038	U981	G917	G855	G785	C719	G658
G1475	U1406	A1346	A1284	G1222	U1159	C1099	C1039	U982	A918	C856	G786	C720	U659
G1476	C1407	C1347	A1285	C1223	G1160	C1100	U1040	U983	A919	C857	A787	G721	G660
G1477		U1348	A1286	G1224	C1161	A1101	A1041	C984	U920	G858	U788	G722	G661
G1478		A1349	A1287	C1225	C1162	A1102	G1042	C985	U921	A859	U789	A723	U662
G1479	C1412	C1350	A1288	G1226	C1163	C1103	C1043	A986	G922	A860	A790	G724	A663
G1480	A1413	U1351	A1289	A1227	G1164	G1104	A1044	G987	A923	G861	G791	G725	G664
G1481	U1414	C1352	G1290	C1228	C1165	U1105	C1045	G988	C924	C862	A792	G726	A665
G1482	A1483	G1353	G1291	A1229	G1166	G1106	A1046	C989	G925	U863	U793	G727	G666
G1483	C1484	C1354	U1292	C1230	A1167	C1107	G1047	C990	A864	U864	A794	A728	G667
G1484	G1417	G1355	G1293	G1231	A1168	G1108	G1048	U991	G927	A865	C795	G729	C668
G1485	A1418	C1356	G1294	U1232	A1169	C1109	U1049	U992	G928	C866	C796	A730	U669
G1486	G1487	A1357	G1295	G1233	G1171	A1110	G1050	G993	G929	C867	C797	G731	G670
G1487		U1358	C1296	C1234		A1111	C1051	A994	C934	C868	G798	C732	G671
G1488	G1421	C1359	C1297	U1235	G1174	C1112	U1052	C995	A935	C869	G799	C735	U672
G1489	G1422	A1360	G1298	C1236	A1175	C1113	G1053	A996	A936	U870	G800	C736	G673
G1490	C1423	C1361	A1299	C1237	A1176	C1114	C1054	U1000	A937	U871	U801	A737	G674
G1491	G1424	C	U1300	A1238	G1177	C1115	A1055	A1001	A938	A872	A802	C738	A675
G1492	U1425	C1362	U1301	U1239	G1178	C1116	U1056	G	A939	A873	G803	C739	U676
G1493	C1426	A1363	U1302	U1240	A1179	G1117	U1057	U1002	A940	G874	U804	C740	U677
G1494	U1427	C1364	C1303	G1241	C1180	C1118	G1058	G1003	G941	C875	C806	G741	U678
G1495	A1428	U1365	G1304	C1242	G1181	C1119	U1059	G1004	G942	C876	A807	G742	C680
G1496	C1429	C1366	G1305	C1243	G1182	G1120	G1060	A1005	U943	C877	G807	G743	C681
G1497	G1430	C1367	A1306	C1244	G1183	U1121	G1061	C1006	G944	C878	C811	U743	G682
G1498	C1431	C1368	U1307		G1184	U1122	U1062	C1007	G945	C879	C812	C744	G683
G1499	G1432	C1369	U1307	A1248	G1185	A1123	G1063	C1008	A946	C880	U813	C745	A684
A1500		A1433	G1311	C1249	G1186	G1124	C1064	C1009	A947	C881	U814	A746	G685
G1501	A1501	C1370	G1312	A1250	C	U1125	U1065	G1010	C948	C882	A815	C747	U686
A1502	C1503	G1371	U1313	A1251	C1189	U1126	C1066	G1011	A949	C883	A816	C748	C687
G1503	U1504	U1372	C1314	A1252	C1190	G1127	A1067	U1012	U950	G884	C817	G750	G688
G1504	C1437	G1373	U1315	G1253	A1191	C1128	G1068	G1013	G951	G885	G818	U751	C689
G1505	G1438	A1374	G1316	C1254	C1192	C129	C1069	G1014	U952	G886	A819	G752	G690
U1506	U1507	C1375	C1317	U1255	G1193	A1130	U1070	A1015	G953	G887	U820	A753	G691
G1508	C1440	A1376	C1318	A1256	U1194	G1131	C1071	A1016	G954	G888	G821	G754	U692
U1510	G1442	C1377	A1319	U1257	C1195	C1132	G1072	G1017	U955	A889	G822	G755	G693
G1443	A1443	G1378	G1320	G1258	U1196	G1133	U1073	C1018		G890	G823	G756	A694
A1446	A1446	U1380	C1321	G1259	G1197	U1134	G1074	C1019	A958	U891	C825	C757	A695
G1447		U1381	C1322	C1260	G1198	U1135	C1075	U1020	A959	G895	C826	U757	A696
		C1382	G1323	A1261	U1199	U1136	G1076	G1021	U960	C896	A828	G758	U697
U1450	A1451	C1383	A1324	C1262	C1200	C1137	U1077	G1022	U961	C897	A759	G760	G698
A1451	C1452	G1384	C1325	C1263	A1201	G1138	U1078	G1023	C962	C898	G829	G761	
G1452	G1453	U1385	G1326	C1264	C1203	G1139	G1079	G1024	G963	C899	U831		C701
G1453	C1454	G1386	C1327	G1265	C1204	C1140	A1080	U1025	A964	C900	C832	G765	A702
A1515	G1454	C1387	C1328	G1266	A1204	C1141	G1081	U1026	A965	A901	C833	A766	G703
G1516	U1455	C1388	A1329	C1267	U1205	G1142	G1082	G1027	A966	G902	C834	A767	U704
G1517	C1456	U1389	U1330	A1268	G1206	G1143	U1083	G1028	C967	G903	U835	A768	U705
G1518	G1457	A1390	G1331	A1269	G1207	G1144	G1084						



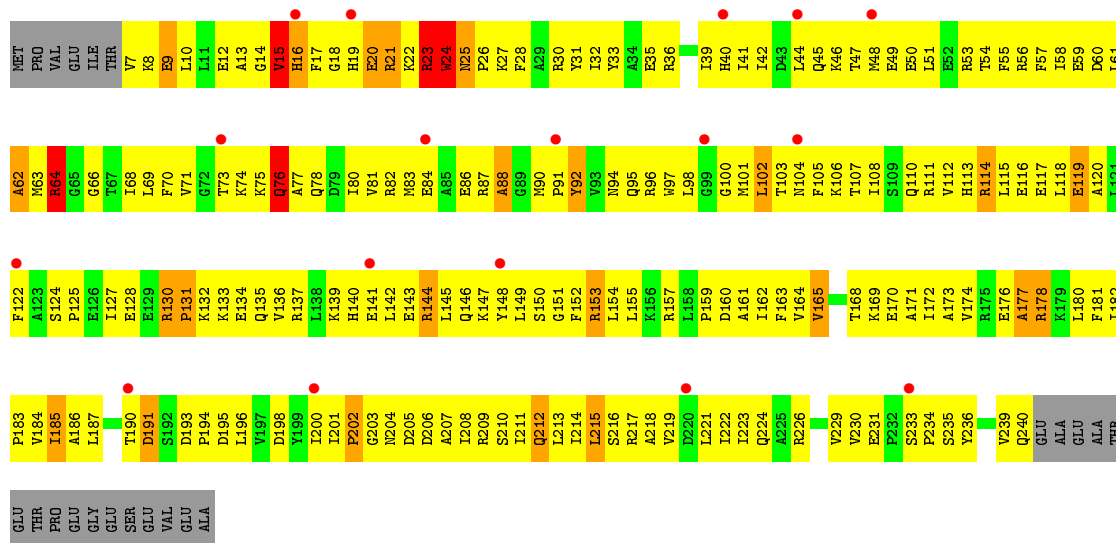
• Molecule 2: A-Site Messenger RNA



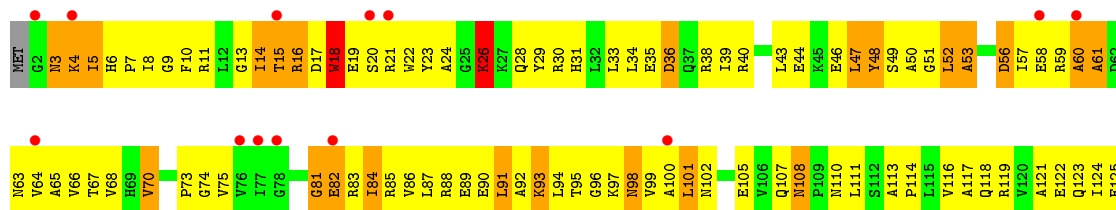
• Molecule 3: Anticodon Transfer RNA

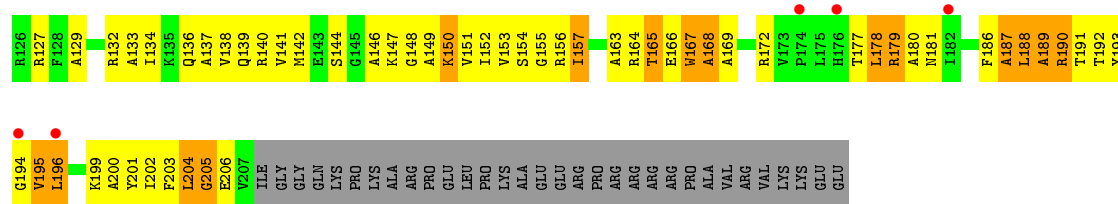


• Molecule 4: 30S ribosomal protein S2

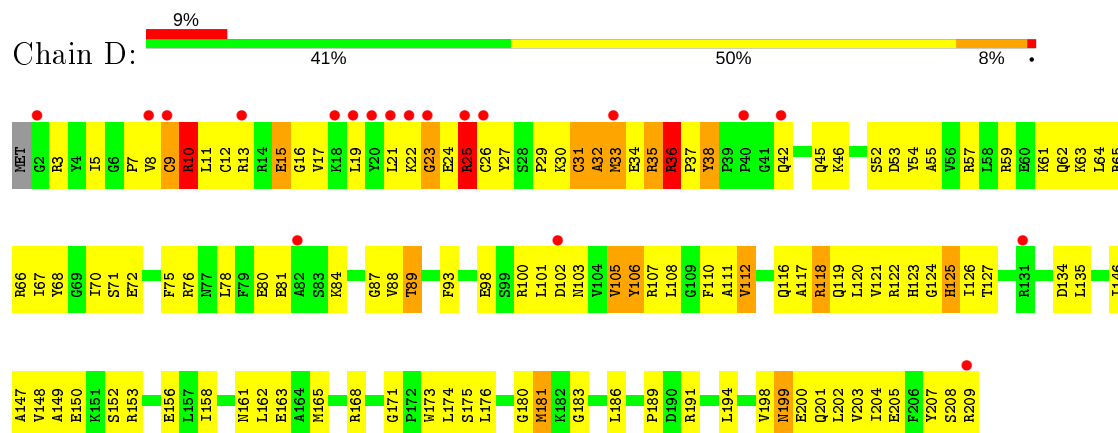


• Molecule 5: 30S ribosomal protein S3

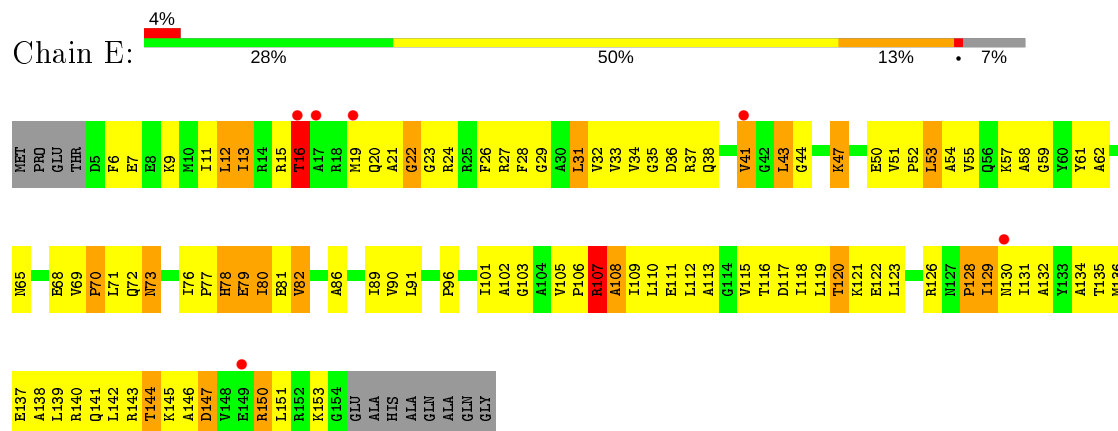




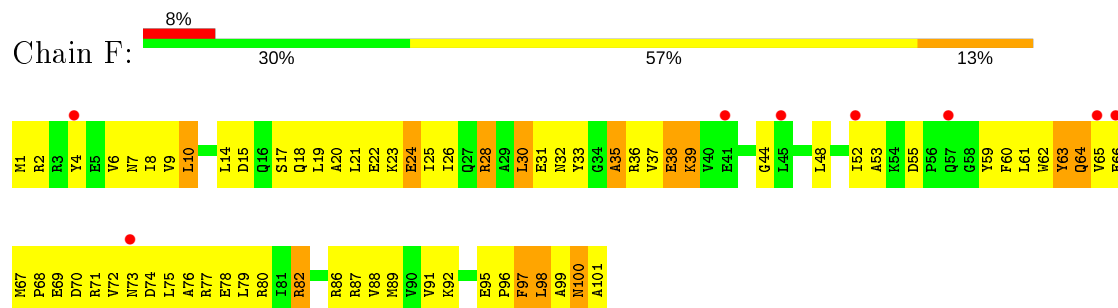
• Molecule 6: 30S ribosomal protein S4



• Molecule 7: 30S ribosomal protein S5

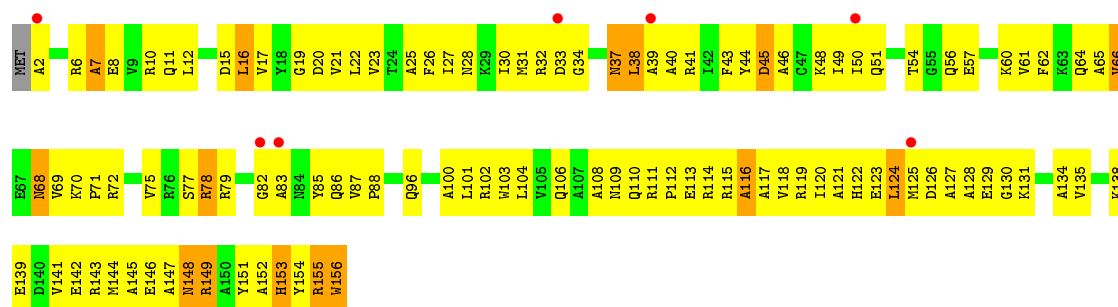


• Molecule 8: 30S ribosomal protein S6

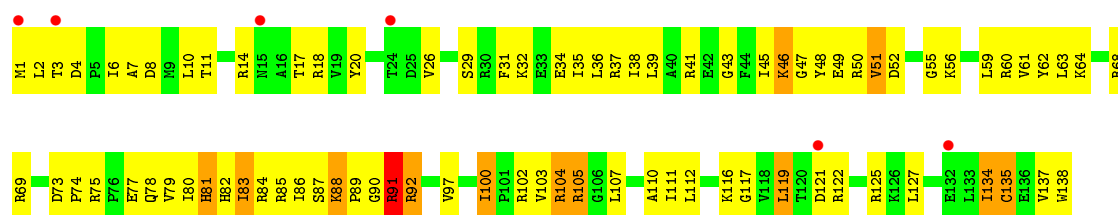


• Molecule 9: 30S ribosomal protein S7

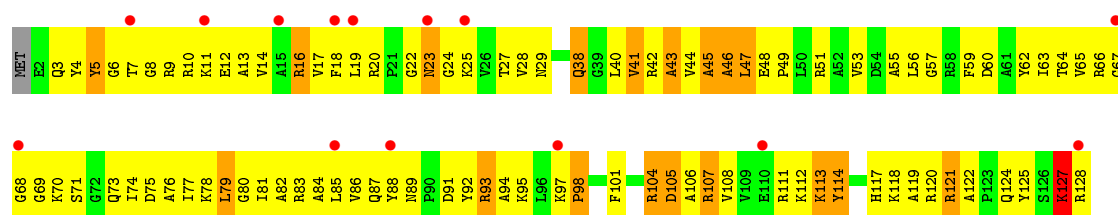




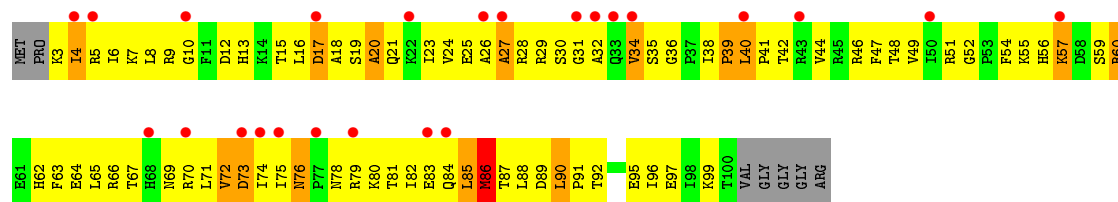
• Molecule 10: 30S ribosomal protein S8



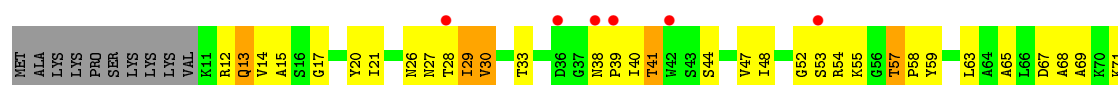
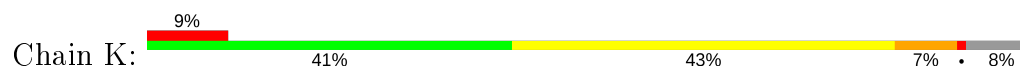
• Molecule 11: 30S ribosomal protein S9

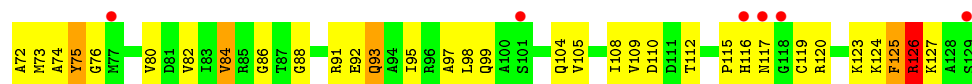


• Molecule 12: 30S ribosomal protein S10

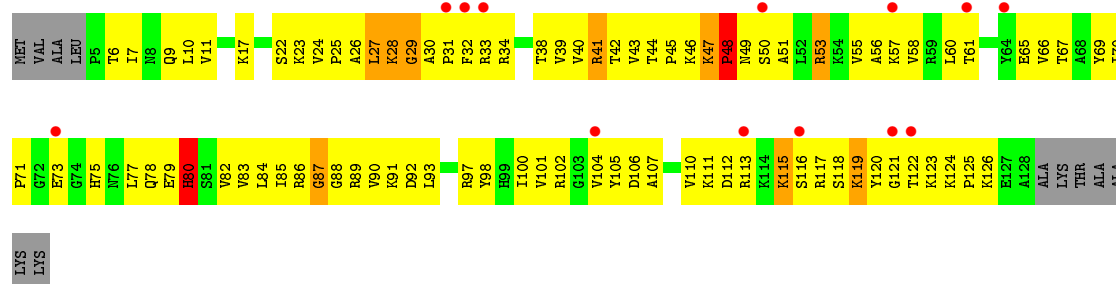


• Molecule 13: 30S ribosomal protein S11

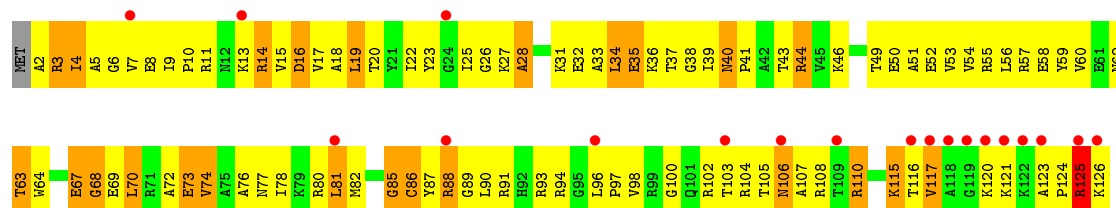




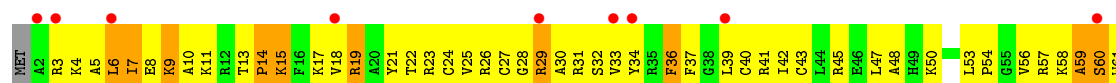
• Molecule 14: 30S ribosomal protein S12



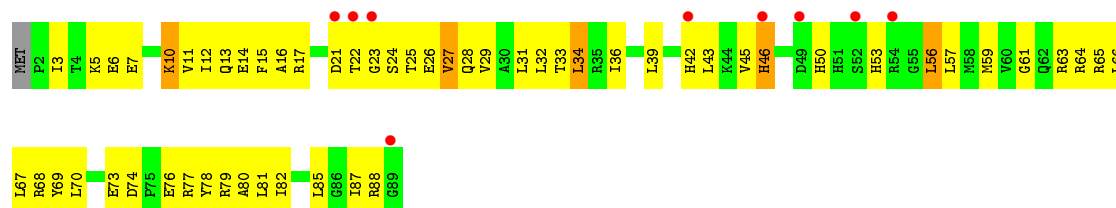
• Molecule 15: 30S ribosomal protein S13



• Molecule 16: 30S ribosomal protein S14

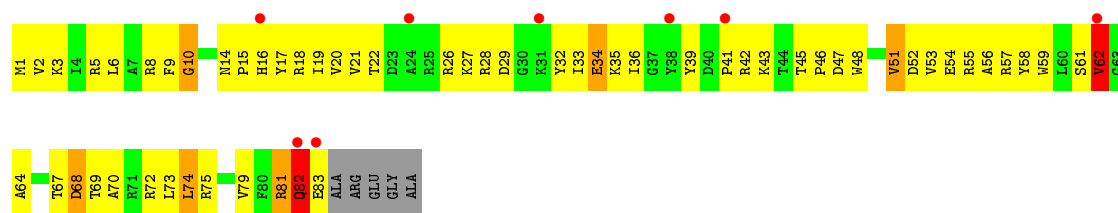


• Molecule 17: 30S ribosomal protein S15

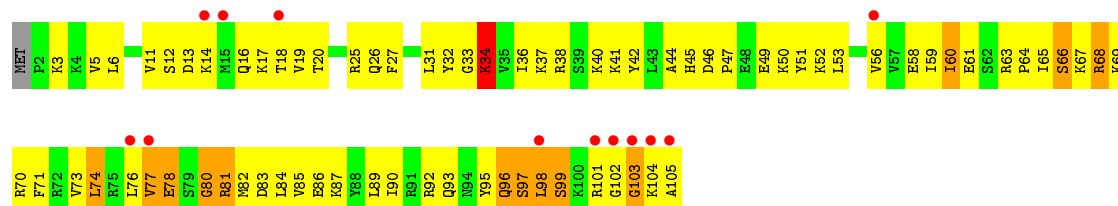


• Molecule 18: 30S ribosomal protein S16

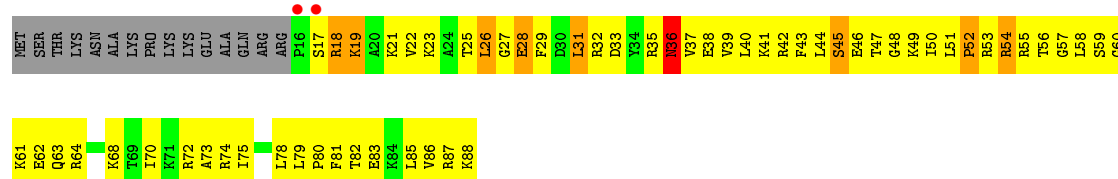
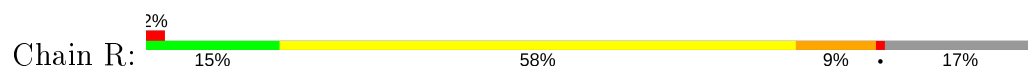




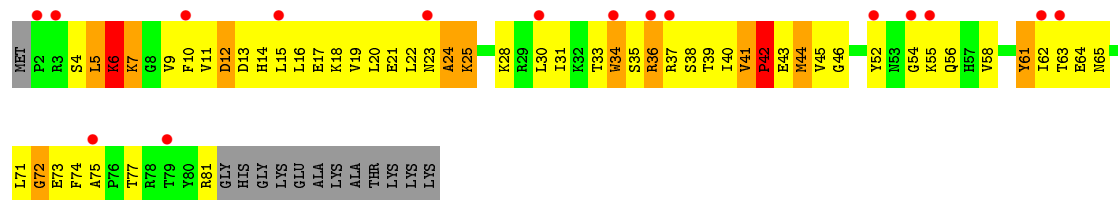
• Molecule 19: 30S ribosomal protein S17



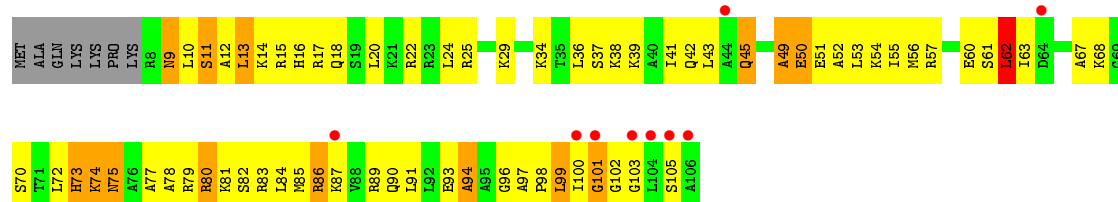
• Molecule 20: 30S ribosomal protein S18



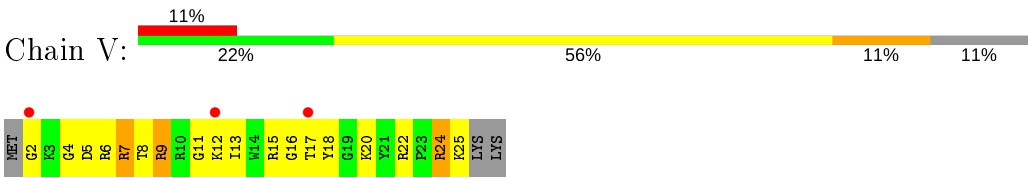
• Molecule 21: 30S ribosomal protein S19



• Molecule 22: 30S ribosomal protein S20



● Molecule 23: 30S ribosomal protein Thx



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	400.81Å 400.81Å 176.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	99.00 – 3.25 200.41 – 3.23	Depositor EDS
% Data completeness (in resolution range)	5.0 (99.00-3.25) 88.5 (200.41-3.23)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.14	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.05 (at 3.26Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.231 , 0.284 0.215 , 0.265	Depositor DCC
R_{free} test set	10562 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	85.2	Xtriage
Anisotropy	0.267	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 146.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	52063	wwPDB-VP
Average B, all atoms (Å ²)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.22% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG, T6A, PAR, MNU

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	0.57	2/36244 (0.0%)	0.74	36/56567 (0.1%)
2	W	0.55	0/72	0.95	1/111 (0.9%)
3	X	0.41	0/203	0.78	0/311
4	B	0.34	0/1935	0.65	0/2609
5	C	0.36	0/1636	0.63	0/2205
6	D	0.39	0/1733	0.65	0/2318
7	E	0.44	0/1162	0.74	0/1564
8	F	0.32	0/856	0.59	0/1154
9	G	0.35	0/1276	0.61	0/1709
10	H	0.44	0/1136	0.75	0/1527
11	I	0.35	0/1029	0.63	0/1378
12	J	0.35	0/805	0.69	0/1082
13	K	0.41	0/900	0.68	0/1213
14	L	0.45	0/986	0.77	0/1320
15	M	0.35	0/1008	0.67	0/1347
16	N	0.43	0/501	0.74	0/664
17	O	0.36	0/745	0.63	0/992
18	P	0.47	0/716	0.74	0/963
19	Q	0.47	0/870	0.77	0/1159
20	R	0.35	0/603	0.65	0/799
21	S	0.32	0/661	0.63	0/890
22	T	0.41	0/764	0.77	0/1006
23	V	0.42	0/212	0.72	0/277
All	All	0.52	2/56053 (0.0%)	0.73	37/83165 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	4	60
3	X	1	0
All	All	5	60

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1361	G	C3'-O3'	5.22	1.49	1.42
1	A	1361	G	O3'-P	5.14	1.67	1.61

The worst 5 of 37 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	575	G	C2'-C3'-O3'	9.66	130.74	109.50
1	A	115	G	C2'-C3'-O3'	9.52	130.44	109.50
1	A	559	A	C2'-C3'-O3'	9.37	130.12	109.50
1	A	243	A	C2'-C3'-O3'	9.32	130.01	109.50
1	A	1528	U	C2'-C3'-O3'	8.97	129.23	109.50

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	181	G	C3'
1	A	243	A	C3'
1	A	559	A	C3'
1	A	1528	U	C3'
3	X	37	T6A	C14

5 of 60 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	107	G	Sidechain
1	A	108	G	Sidechain
1	A	39	G	Sidechain
1	A	77	G	Sidechain
1	A	84	U	Sidechain

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within

the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	32380	0	16346	1337	0
2	W	64	0	35	4	0
3	X	239	0	127	7	0
4	B	1900	0	1951	305	0
5	C	1612	0	1677	245	0
6	D	1703	0	1764	150	0
7	E	1146	0	1207	140	0
8	F	843	0	857	102	0
9	G	1257	0	1296	131	0
10	H	1116	0	1177	112	0
11	I	1011	0	1043	153	0
12	J	792	0	835	127	0
13	K	885	0	904	71	0
14	L	970	0	1057	130	0
15	M	997	0	1072	155	0
16	N	492	0	530	67	0
17	O	734	0	771	78	0
18	P	700	0	720	81	0
19	Q	857	0	930	125	0
20	R	597	0	668	100	0
21	S	647	0	673	83	0
22	T	762	0	856	87	0
23	V	208	0	221	19	0
24	A	42	0	45	2	0
25	A	104	0	0	0	0
25	J	1	0	0	0	0
25	X	2	0	0	0	0
26	D	1	0	0	0	0
26	N	1	0	0	1	0
All	All	52063	0	36762	3496	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 39.

The worst 5 of 3496 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:1489:G:H2'	1:A:1490:C:H5''	1.26	1.10
6:D:36:ARG:H	6:D:37:PRO:HD3	1.13	1.08
5:C:179:ARG:HG2	5:C:180:ALA:H	0.98	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:26:LYS:HD3	5:C:26:LYS:H	1.14	1.06
4:B:132:LYS:HA	4:B:135:GLN:HB3	1.36	1.05

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	B	232/256 (91%)	129 (56%)	80 (34%)	23 (10%)	0	3
5	C	204/239 (85%)	123 (60%)	48 (24%)	33 (16%)	0	1
6	D	206/209 (99%)	151 (73%)	38 (18%)	17 (8%)	1	5
7	E	148/162 (91%)	120 (81%)	18 (12%)	10 (7%)	1	8
8	F	99/101 (98%)	68 (69%)	24 (24%)	7 (7%)	1	7
9	G	153/156 (98%)	99 (65%)	41 (27%)	13 (8%)	1	5
10	H	136/138 (99%)	106 (78%)	25 (18%)	5 (4%)	3	19
11	I	125/128 (98%)	85 (68%)	27 (22%)	13 (10%)	0	3
12	J	96/105 (91%)	57 (59%)	23 (24%)	16 (17%)	0	1
13	K	117/129 (91%)	85 (73%)	26 (22%)	6 (5%)	2	13
14	L	122/135 (90%)	85 (70%)	24 (20%)	13 (11%)	0	3
15	M	123/126 (98%)	75 (61%)	30 (24%)	18 (15%)	0	1
16	N	58/61 (95%)	34 (59%)	16 (28%)	8 (14%)	0	1
17	O	86/89 (97%)	54 (63%)	28 (33%)	4 (5%)	2	14
18	P	81/88 (92%)	59 (73%)	16 (20%)	6 (7%)	1	7
19	Q	102/105 (97%)	75 (74%)	17 (17%)	10 (10%)	0	3
20	R	71/88 (81%)	50 (70%)	16 (22%)	5 (7%)	1	7
21	S	78/93 (84%)	56 (72%)	14 (18%)	8 (10%)	0	3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
22	T	97/106 (92%)	56 (58%)	30 (31%)	11 (11%)	0	2
23	V	22/27 (82%)	18 (82%)	2 (9%)	2 (9%)	1	4
All	All	2356/2541 (93%)	1585 (67%)	543 (23%)	228 (10%)	0	4

5 of 228 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	B	13	ALA
4	B	15	VAL
4	B	16	HIS
4	B	21	ARG
4	B	24	TRP

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	B	202/220 (92%)	181 (90%)	21 (10%)	7	25
5	C	160/188 (85%)	145 (91%)	15 (9%)	8	30
6	D	180/181 (99%)	164 (91%)	16 (9%)	9	32
7	E	115/123 (94%)	96 (84%)	19 (16%)	2	10
8	F	90/90 (100%)	83 (92%)	7 (8%)	12	38
9	G	126/127 (99%)	115 (91%)	11 (9%)	10	34
10	H	119/119 (100%)	107 (90%)	12 (10%)	7	27
11	I	98/99 (99%)	87 (89%)	11 (11%)	6	23
12	J	87/92 (95%)	85 (98%)	2 (2%)	50	73
13	K	90/99 (91%)	79 (88%)	11 (12%)	5	20
14	L	104/111 (94%)	100 (96%)	4 (4%)	33	62
15	M	100/101 (99%)	88 (88%)	12 (12%)	5	20
16	N	49/50 (98%)	47 (96%)	2 (4%)	30	60
17	O	79/80 (99%)	76 (96%)	3 (4%)	33	62

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	P	72/74 (97%)	66 (92%)	6 (8%)	11	36
19	Q	96/97 (99%)	90 (94%)	6 (6%)	18	47
20	R	64/77 (83%)	59 (92%)	5 (8%)	12	38
21	S	71/80 (89%)	63 (89%)	8 (11%)	6	22
22	T	75/82 (92%)	67 (89%)	8 (11%)	6	25
23	V	19/22 (86%)	18 (95%)	1 (5%)	22	53
All	All	1996/2112 (94%)	1816 (91%)	180 (9%)	9	32

5 of 180 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
9	G	45	ASP
10	H	134	ILE
21	S	34	TRP
9	G	124	LEU
10	H	51	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 59 such sidechains are listed below:

Mol	Chain	Res	Type
8	F	32	ASN
11	I	23	ASN
21	S	23	ASN
8	F	57	GLN
8	F	100	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1506/1522 (98%)	240 (15%)	62 (4%)
2	W	2/3 (66%)	1 (50%)	0
3	X	9/11 (81%)	0	0
All	All	1517/1536 (98%)	241 (15%)	62 (4%)

5 of 241 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	8	A

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

5 of 62 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	701	C
1	A	965	A
1	A	1498	U
1	A	812	C
1	A	992	U

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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$
3	T6A	X	37	3	24,34,35	1.34	3 (12%)	24,49,52	3.90	7 (29%)
3	MNU	X	34	3,2	17,24,25	1.01	1 (5%)	19,34,37	3.73	3 (15%)

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
3	T6A	X	37	3	1/1/9/11	4/15/41/42	0/3/3/3
3	MNU	X	34	3,2	-	3/7/28/29	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	X	34	MNU	C4-N3	3.05	1.38	1.33
3	X	37	T6A	O14-C14	-3.02	1.34	1.43
3	X	37	T6A	C12-N11	-2.92	1.40	1.46
3	X	37	T6A	C15-C14	-2.78	1.43	1.51

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	X	34	MNU	C4-N3-C2	14.13	127.07	115.14
3	X	37	T6A	O14-C14-C15	11.99	145.26	109.74
3	X	37	T6A	C12-N11-C10	9.28	132.66	122.75
3	X	34	MNU	C5-C4-N3	-7.35	114.48	125.25
3	X	37	T6A	O14-C14-C12	-6.97	95.20	109.14

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	X	37	T6A	C14

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	X	37	T6A	C13-C12-C14-O14
3	X	34	MNU	C2'-C1'-N1-C6
3	X	37	T6A	N11-C12-C14-O14
3	X	37	T6A	C13-C12-N11-C10
3	X	34	MNU	C4-C5-C7-N8

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	X	37	T6A	2	0
3	X	34	MNU	3	0

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 110 ligands modelled in this entry, 109 are monoatomic - leaving 1 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	PAR	A	1545	-	45,45,45	1.75	11 (24%)	64,67,67	1.21	5 (7%)

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	PAR	A	1545	-	-	4/18/94/94	0/4/4/4

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	1545	PAR	C64-C54	4.62	1.58	1.52
24	A	1545	PAR	O54-C14	4.06	1.52	1.41
24	A	1545	PAR	C31-C21	3.66	1.58	1.53
24	A	1545	PAR	O51-C11	2.97	1.49	1.41
24	A	1545	PAR	O33-C14	2.86	1.49	1.41

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	1545	PAR	O52-C13-C23	4.21	116.68	107.96
24	A	1545	PAR	O54-C54-C64	3.48	112.49	106.01
24	A	1545	PAR	O52-C13-O43	-3.27	107.89	111.43
24	A	1545	PAR	C14-O54-C54	3.13	119.83	113.69
24	A	1545	PAR	O33-C14-C24	2.97	113.33	108.22

There are no chirality outliers.

All (4) torsion outliers are listed below:

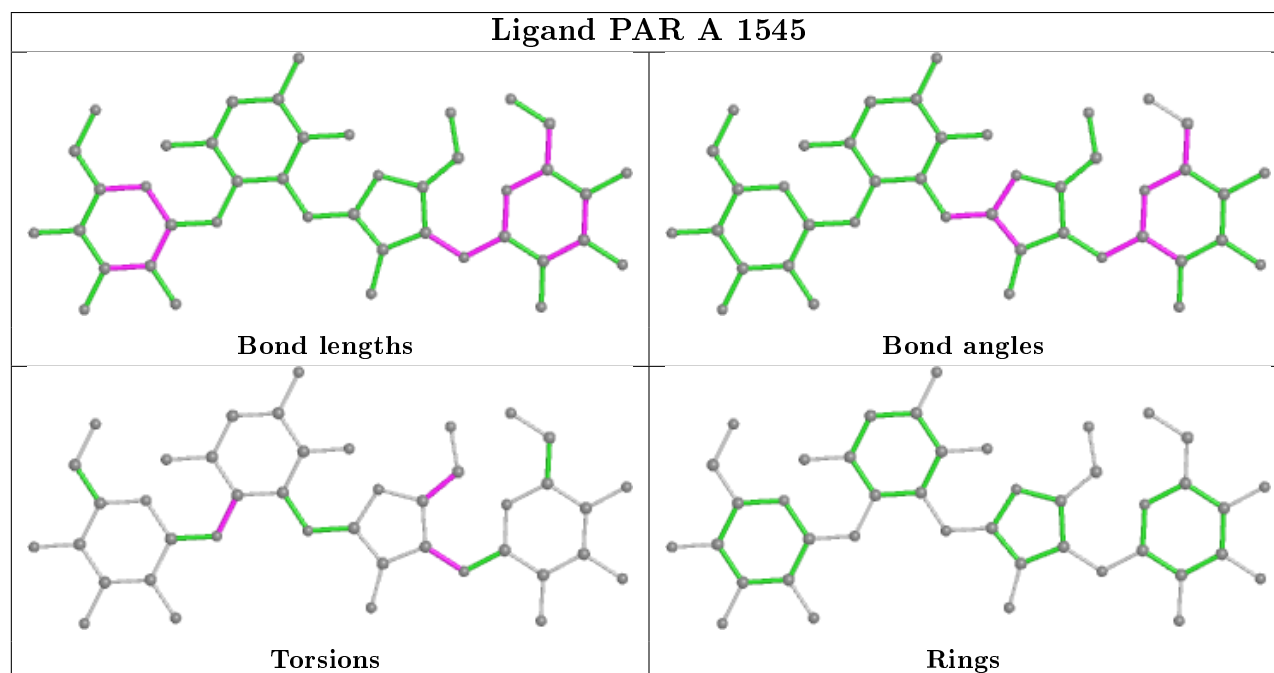
Mol	Chain	Res	Type	Atoms
24	A	1545	PAR	O43-C43-C53-O53
24	A	1545	PAR	C52-C42-O11-C11
24	A	1545	PAR	C23-C33-O33-C14
24	A	1545	PAR	C33-C43-C53-O53

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	A	1545	PAR	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1507/1522 (99%)	2.20	794 (52%) 0 0	30, 65, 160, 200	0
2	W	3/3 (100%)	2.48	3 (100%) 0 0	56, 56, 63, 72	0
3	X	9/11 (81%)	1.94	3 (33%) 0 0	64, 101, 157, 157	0
4	B	234/256 (91%)	0.64	17 (7%) 15 14	37, 100, 173, 200	0
5	C	206/239 (86%)	0.70	18 (8%) 10 10	44, 93, 169, 200	0
6	D	208/209 (99%)	0.71	19 (9%) 9 10	33, 71, 149, 200	0
7	E	150/162 (92%)	0.71	6 (4%) 38 35	27, 63, 122, 200	0
8	F	101/101 (100%)	0.69	8 (7%) 12 12	48, 103, 154, 174	0
9	G	155/156 (99%)	0.63	7 (4%) 33 31	41, 81, 152, 200	0
10	H	138/138 (100%)	0.73	6 (4%) 35 33	20, 54, 113, 174	0
11	I	127/128 (99%)	0.81	14 (11%) 5 5	35, 90, 149, 178	0
12	J	98/105 (93%)	1.22	24 (24%) 0 0	44, 117, 186, 200	0
13	K	119/129 (92%)	0.82	12 (10%) 7 7	30, 67, 138, 187	0
14	L	124/135 (91%)	0.95	13 (10%) 6 6	31, 64, 139, 175	0
15	M	125/126 (99%)	1.23	19 (15%) 2 2	44, 85, 169, 200	0
16	N	60/61 (98%)	1.02	9 (15%) 2 2	42, 82, 139, 179	0
17	O	88/89 (98%)	0.85	9 (10%) 6 7	23, 76, 142, 192	0
18	P	83/88 (94%)	0.95	8 (9%) 8 8	27, 52, 96, 173	0
19	Q	104/105 (99%)	1.29	12 (11%) 4 4	22, 61, 146, 200	0
20	R	73/88 (82%)	0.74	2 (2%) 54 51	40, 79, 175, 188	0
21	S	80/93 (86%)	1.00	16 (20%) 1 1	62, 111, 162, 193	0
22	T	99/106 (93%)	0.84	9 (9%) 9 10	32, 58, 136, 168	0
23	V	24/27 (88%)	1.04	3 (12%) 3 3	41, 69, 118, 136	0
All	All	3915/4077 (96%)	1.37	1031 (26%) 0 0	20, 73, 159, 200	0

The worst 5 of 1031 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
19	Q	103	GLY	13.3
19	Q	104	LYS	12.9
15	M	120	LYS	11.3
1	A	202	U	11.2
19	Q	105	ALA	10.6

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	T6A	X	37	32/33	0.89	0.34	76,80,80,80	0
3	MNU	X	34	23/24	0.90	0.37	56,96,115,115	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
25	MG	A	210	1/1	0.41	0.53	23,23,23,23	1
25	MG	A	1575	1/1	0.43	1.13	23,23,23,23	1
25	MG	A	1607	1/1	0.45	0.69	23,23,23,23	1
25	MG	A	1621	1/1	0.48	0.33	23,23,23,23	1
25	MG	A	493	1/1	0.57	1.21	23,23,23,23	1
25	MG	A	1596	1/1	0.58	1.50	23,23,23,23	1
25	MG	A	87	1/1	0.58	0.33	23,23,23,23	1
25	MG	A	1622	1/1	0.62	0.51	23,23,23,23	1
25	MG	A	1611	1/1	0.64	0.31	23,23,23,23	1
25	MG	A	211	1/1	0.67	0.34	23,23,23,23	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
25	MG	A	1627	1/1	0.67	0.28	23,23,23,23	1
25	MG	A	1595	1/1	0.69	1.31	23,23,23,23	1
25	MG	A	1619	1/1	0.74	0.23	23,23,23,23	1
25	MG	A	1620	1/1	0.74	0.29	23,23,23,23	1
25	MG	A	1616	1/1	0.74	0.30	23,23,23,23	1
25	MG	A	1566	1/1	0.76	0.53	23,23,23,23	1
25	MG	A	1632	1/1	0.76	0.26	23,23,23,23	1
25	MG	A	1634	1/1	0.76	0.43	23,23,23,23	1
25	MG	A	71	1/1	0.78	0.34	23,23,23,23	1
25	MG	A	441	1/1	0.78	0.22	23,23,23,23	1
25	MG	A	1562	1/1	0.79	0.77	23,23,23,23	1
25	MG	A	1615	1/1	0.79	0.27	23,23,23,23	1
25	MG	A	1633	1/1	0.79	0.34	23,23,23,23	1
25	MG	A	1580	1/1	0.80	0.31	23,23,23,23	1
25	MG	A	1561	1/1	0.80	0.28	23,23,23,23	1
25	MG	A	470	1/1	0.80	0.42	23,23,23,23	1
25	MG	A	1585	1/1	0.82	0.39	23,23,23,23	1
25	MG	A	1558	1/1	0.83	0.18	23,23,23,23	0
25	MG	A	1592	1/1	0.84	0.23	23,23,23,23	0
25	MG	A	1559	1/1	0.84	0.33	23,23,23,23	0
25	MG	A	1605	1/1	0.85	0.44	23,23,23,23	1
25	MG	A	1604	1/1	0.85	0.36	23,23,23,23	1
25	MG	A	1613	1/1	0.85	0.40	23,23,23,23	1
25	MG	A	1564	1/1	0.85	0.28	23,23,23,23	0
25	MG	A	1628	1/1	0.85	0.30	23,23,23,23	1
25	MG	A	1550	1/1	0.86	0.30	23,23,23,23	1
25	MG	A	1597	1/1	0.86	0.30	23,23,23,23	1
25	MG	A	471	1/1	0.86	0.29	23,23,23,23	1
25	MG	A	1548	1/1	0.88	0.32	23,23,23,23	1
25	MG	A	1612	1/1	0.88	0.28	23,23,23,23	1
25	MG	A	1560	1/1	0.88	0.26	23,23,23,23	0
25	MG	A	467	1/1	0.89	0.92	23,23,23,23	1
25	MG	A	466	1/1	0.89	0.42	23,23,23,23	1
25	MG	A	1554	1/1	0.90	0.31	23,23,23,23	1
25	MG	A	1549	1/1	0.90	0.41	23,23,23,23	1
25	MG	A	1569	1/1	0.90	0.23	23,23,23,23	1
25	MG	A	1581	1/1	0.90	0.46	23,23,23,23	1
25	MG	A	469	1/1	0.91	0.24	23,23,23,23	1
25	MG	A	1610	1/1	0.91	0.53	23,23,23,23	1
25	MG	A	1582	1/1	0.91	0.11	23,23,23,23	0
25	MG	A	1635	1/1	0.91	0.42	23,23,23,23	1
25	MG	A	1630	1/1	0.91	0.26	23,23,23,23	1

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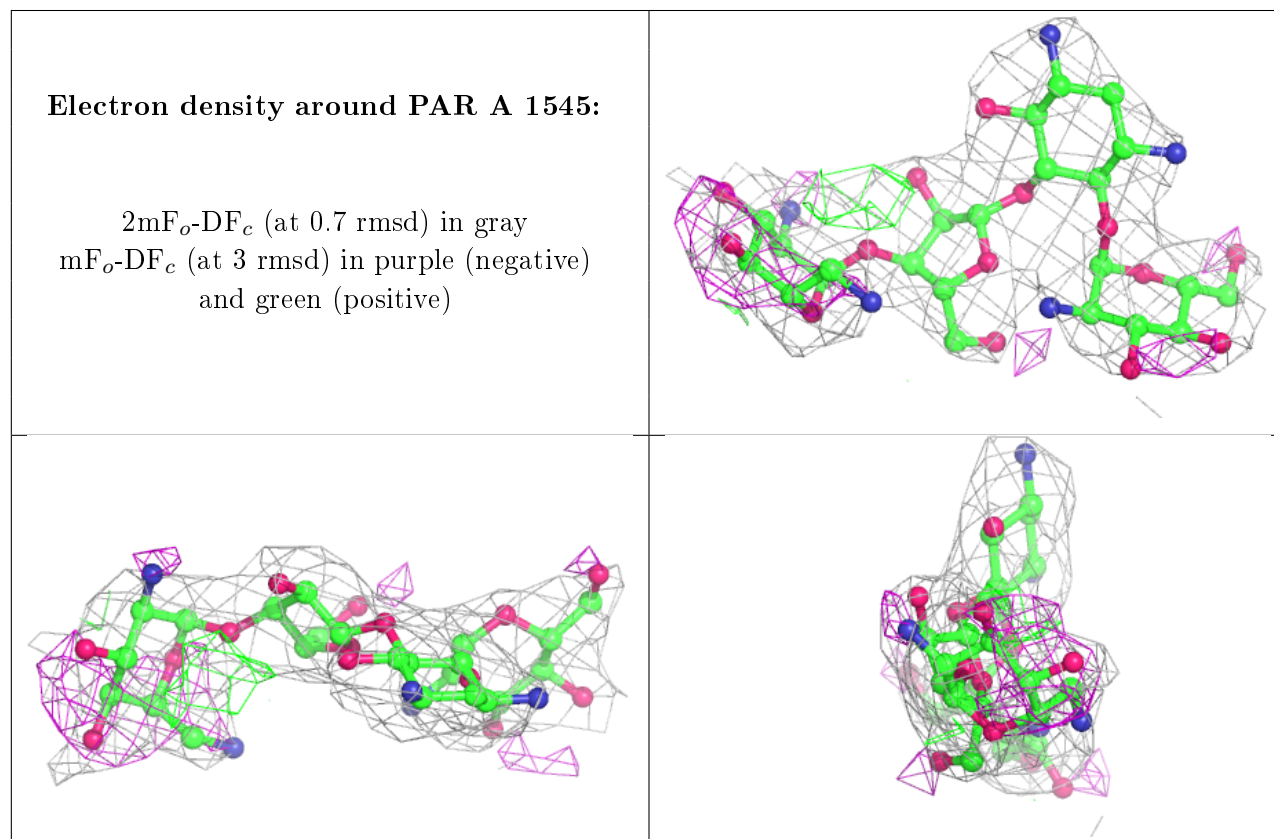
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
25	MG	A	1631	1/1	0.91	0.14	23,23,23,23	1
25	MG	A	1593	1/1	0.91	0.33	23,23,23,23	1
25	MG	A	1556	1/1	0.91	0.24	23,23,23,23	0
25	MG	A	1609	1/1	0.92	0.27	23,23,23,23	0
24	PAR	A	1545	42/42	0.92	0.39	25,25,25,25	0
25	MG	A	1571	1/1	0.92	0.15	23,23,23,23	0
25	MG	A	1606	1/1	0.92	0.50	23,23,23,23	1
25	MG	A	473	1/1	0.92	0.36	23,23,23,23	1
25	MG	A	1629	1/1	0.92	0.23	23,23,23,23	0
25	MG	A	1573	1/1	0.92	0.23	23,23,23,23	0
25	MG	A	1608	1/1	0.92	0.29	23,23,23,23	1
25	MG	A	1600	1/1	0.92	0.38	23,23,23,23	1
25	MG	A	1578	1/1	0.93	0.21	23,23,23,23	0
25	MG	A	1624	1/1	0.93	0.20	23,23,23,23	1
25	MG	A	1565	1/1	0.93	0.27	23,23,23,23	0
25	MG	A	1598	1/1	0.93	0.40	23,23,23,23	0
25	MG	A	1602	1/1	0.93	0.19	23,23,23,23	0
25	MG	A	214	1/1	0.93	0.37	23,23,23,23	1
25	MG	A	1599	1/1	0.93	0.26	23,23,23,23	1
25	MG	A	1603	1/1	0.94	0.30	23,23,23,23	1
25	MG	A	1568	1/1	0.94	0.16	23,23,23,23	0
25	MG	A	1589	1/1	0.94	0.33	23,23,23,23	0
25	MG	A	1577	1/1	0.94	0.15	23,23,23,23	0
25	MG	A	1563	1/1	0.94	0.47	23,23,23,23	1
25	MG	A	1601	1/1	0.94	0.67	23,23,23,23	1
25	MG	A	1583	1/1	0.94	0.16	23,23,23,23	0
25	MG	A	1552	1/1	0.94	0.21	23,23,23,23	0
25	MG	X	502	1/1	0.94	0.31	23,23,23,23	1
25	MG	A	1570	1/1	0.95	0.20	23,23,23,23	0
25	MG	A	1547	1/1	0.95	0.34	23,23,23,23	0
25	MG	A	86	1/1	0.95	0.30	23,23,23,23	1
25	MG	A	1625	1/1	0.95	0.27	23,23,23,23	1
25	MG	A	1553	1/1	0.95	0.35	23,23,23,23	0
25	MG	A	1579	1/1	0.96	0.29	23,23,23,23	1
25	MG	A	1546	1/1	0.96	0.28	23,23,23,23	0
25	MG	X	500	1/1	0.96	0.23	23,23,23,23	1
25	MG	A	1587	1/1	0.96	0.13	23,23,23,23	0
25	MG	A	1551	1/1	0.96	0.24	23,23,23,23	0
25	MG	A	1567	1/1	0.96	0.32	23,23,23,23	0
25	MG	A	1590	1/1	0.96	0.25	23,23,23,23	0
25	MG	A	1617	1/1	0.96	0.18	23,23,23,23	1
25	MG	A	1586	1/1	0.96	0.18	23,23,23,23	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
25	MG	A	1591	1/1	0.96	0.29	23,23,23,23	1
25	MG	A	1618	1/1	0.97	0.23	23,23,23,23	0
25	MG	A	1594	1/1	0.97	0.23	23,23,23,23	1
25	MG	A	1588	1/1	0.97	0.28	23,23,23,23	0
25	MG	A	1574	1/1	0.97	0.22	23,23,23,23	0
25	MG	A	1623	1/1	0.97	0.40	23,23,23,23	1
25	MG	J	449	1/1	0.97	0.33	23,23,23,23	1
25	MG	A	1626	1/1	0.97	0.19	23,23,23,23	1
25	MG	A	1557	1/1	0.97	0.22	23,23,23,23	0
25	MG	A	1555	1/1	0.97	0.27	23,23,23,23	0
25	MG	A	1576	1/1	0.98	0.26	23,23,23,23	0
25	MG	A	1614	1/1	0.98	0.21	23,23,23,23	1
25	MG	A	1572	1/1	0.98	0.16	23,23,23,23	0
26	ZN	D	306	1/1	0.99	0.33	23,23,23,23	1
25	MG	A	1584	1/1	0.99	0.15	23,23,23,23	0
26	ZN	N	307	1/1	1.00	0.24	23,23,23,23	1

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers [i](#)

There are no such residues in this entry.