



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 03:57 PM GMT

PDB ID : 4DR4
Title : Crystal structure of the *Thermus thermophilus* (HB8) 30S ribosomal subunit with codon, cognate transfer RNA anticodon stem-loop and multiple copies of paromomycin molecules bound
Authors : Demirci, H.; Murphy IV, F.; Murphy, E.; Gregory, S.T.; Dahlberg, A.E.; Jogl, G.
Deposited on : 2012-02-16
Resolution : 3.97 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

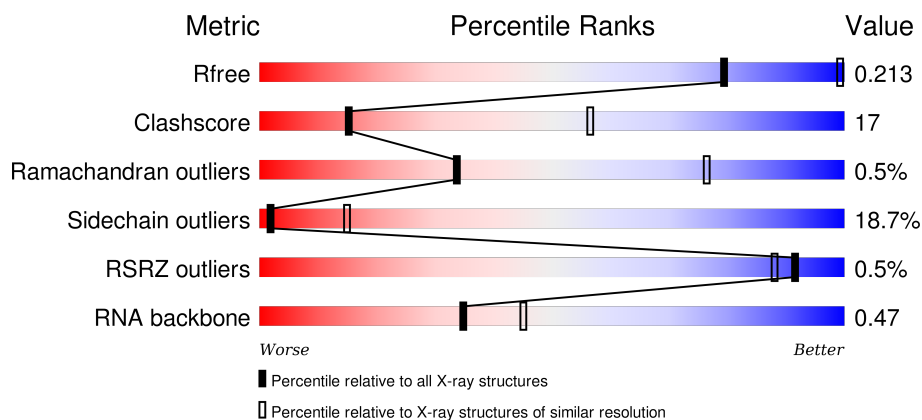
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

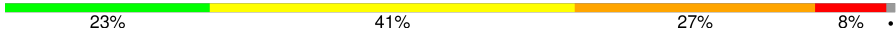



The reported resolution of this entry is 3.97 Å.

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}	91344	1011 (4.38-3.54)
Clashscore	102246	1025 (4.32-3.60)
Ramachandran outliers	100387	1008 (4.34-3.58)
Sidechain outliers	100360	1027 (4.36-3.56)
RSRZ outliers	91569	1015 (4.38-3.54)
RNA backbone	2183	1079 (5.04-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1522	
2	B	256	
3	C	239	
4	D	209	

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Mol	Chain	Length	Quality of chain
5	E	162	
6	F	101	
7	G	156	
8	H	138	
9	I	128	
10	J	105	
11	K	129	
12	L	135	
13	M	126	
14	N	61	
15	O	89	
16	P	88	
17	Q	105	
18	R	88	
19	S	93	
20	T	106	
21	U	27	
22	V	3	
23	W	15	

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
24	PAR	A	1608	-	-	-	X
24	PAR	A	1610	-	-	-	X
24	PAR	A	1611	-	-	-	X
24	PAR	A	1612	-	-	-	X
24	PAR	A	1613	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	PAR	A	1614	-	-	-	X
24	PAR	A	1615	-	-	-	X
24	PAR	A	1616	-	-	-	X
24	PAR	A	1617	-	-	-	X
24	PAR	A	1618	-	-	-	X
25	MG	A	1619	-	-	-	X
25	MG	A	1651	-	-	-	X
25	MG	A	1694	-	-	-	X
25	MG	A	1740	-	-	-	X
25	MG	A	1794	-	-	-	X
25	MG	A	1803	-	-	-	X
25	MG	A	1818	-	-	-	X
25	MG	A	1823	-	-	-	X
25	MG	A	1832	-	-	-	X
25	MG	A	1853	-	-	-	X
25	MG	A	1862	-	-	-	X
25	MG	A	1867	-	-	-	X
25	MG	A	1883	-	-	-	X
25	MG	A	1888	-	-	-	X
25	MG	A	1890	-	-	-	X
25	MG	A	1912	-	-	-	X
25	MG	A	1914	-	-	-	X
25	MG	A	1918	-	-	-	X
25	MG	A	1934	-	-	-	X
25	MG	A	1935	-	-	-	X
25	MG	N	102	-	-	-	X
26	ZN	D	301	-	-	-	X

2 Entry composition

There are 27 unique types of molecules in this entry. The entry contains 53651 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1512	Total	C	N	O	P	0	0	0
			32504	14477	6011	10505	1511			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1534	C	A	CONFLICT	GB M26923.1
A	1535	A	C	CONFLICT	GB M26923.1

- Molecule 2 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	236	Total	C	N	O	S	0	0	1
			1896	1211	337	343	5			

- Molecule 3 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	207	Total	C	N	O	S	0	0	1
			1613	1016	315	281	1			

- Molecule 4 is a protein called 30S ribosomal protein S4.

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

- Molecule 5 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	151	Total	C	N	O	S	0	0	1
			1147	724	218	201	4			

- Molecule 6 is a protein called 30S ribosomal protein S6.

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

- Molecule 7 is a protein called 30S ribosomal protein S7.

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

- Molecule 8 is a protein called 30S ribosomal protein S8.

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

- Molecule 9 is a protein called 30S ribosomal protein S9.

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

- Molecule 10 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	99	Total	C	N	O	S	0	0	1
			793	498	157	137	1			

- Molecule 11 is a protein called 30S ribosomal protein S11.

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

- Molecule 12 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	125	Total	C	N	O	S	0	0	1
			973	612	196	163	2			

- Molecule 13 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	118	Total	C	N	O	S	0	0	0
			937	579	193	163	2			

- Molecule 14 is a protein called 30S ribosomal protein S14.

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

- Molecule 15 is a protein called 30S ribosomal protein S15.

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

- Molecule 16 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	P	84	Total	C	N	O	S	0	0	1
			701	443	140	117	1			

- Molecule 17 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Q	100	Total	C	N	O	S	0	0	0
			834	534	156	142	2			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	96	GLN	GLU	CONFLICT	UNP Q5SHP7

- Molecule 18 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	R	73	Total	C	N	O		0	0	0
			598	381	118	99				

- Molecule 19 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	S	81	Total	C	N	O	S	0	0	1
			648	414	120	112	2			

- Molecule 20 is a protein called 30S ribosomal protein S20.

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	U	25	Total	C	N	O	0	0	1
			209	128	51	30			

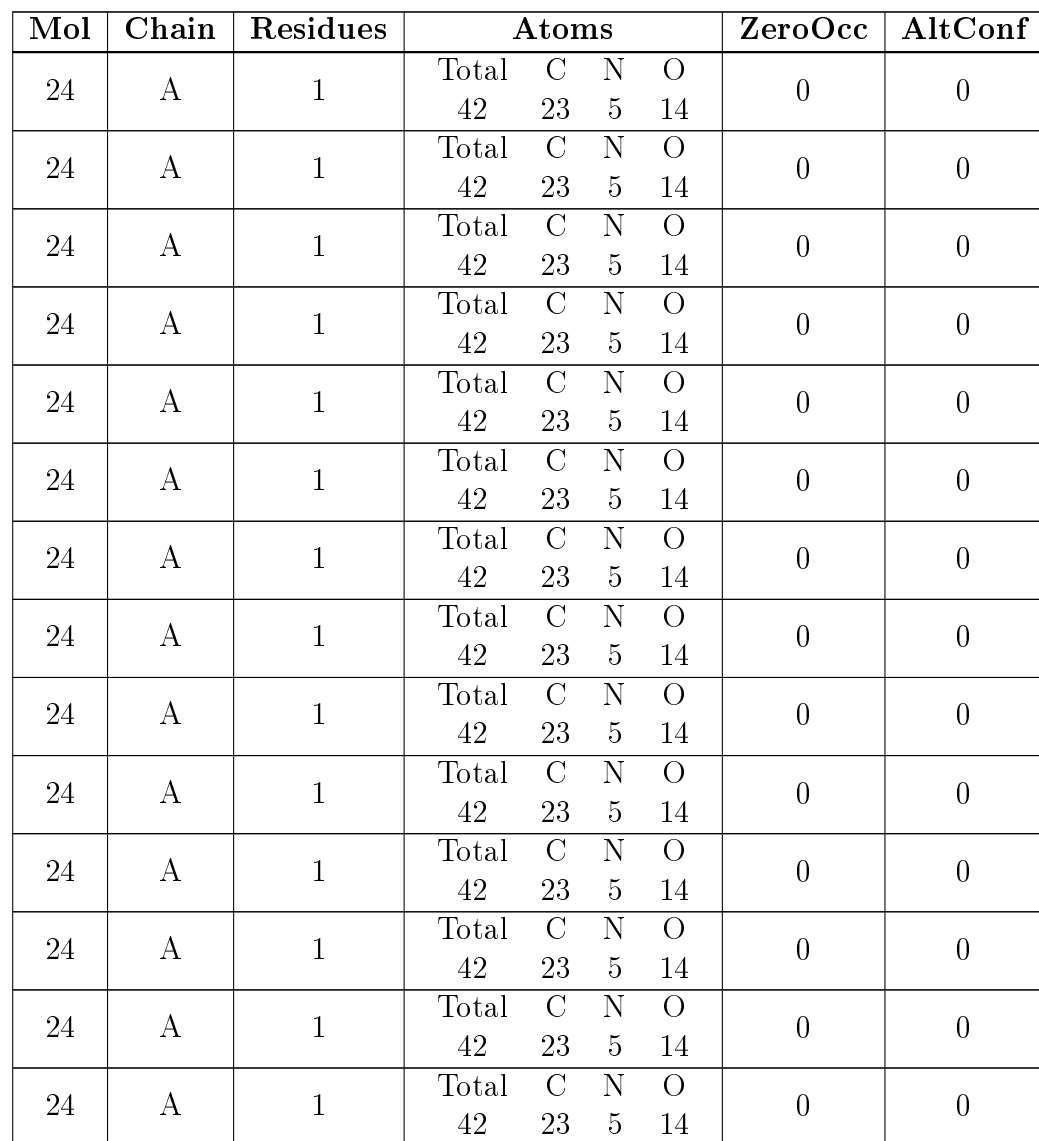
- Molecule 22 is a RNA chain called 5'-R(*UP*UP*U)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	V	3	Total	C	N	O	P	0	0	0
			57	27	6	22	2			

- Molecule 23 is a RNA chain called 5'-R(*GP*GP*GP*AP*UP*UP*GP*AP*AP*AP*AP*UP*CP*CP*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	W	15	Total	C	N	O	P	0	0	0
			319	144	60	101	14			

- Molecule 24 is PAROMOMYCIN (three-letter code: PAR) (formula: C₂₃H₄₅N₅O₁₄).



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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
24	A	1	Total	C	N	O	0	0
			42	23	5	14		
24	A	1	Total	C	N	O	0	0
			42	23	5	14		
24	A	1	Total	C	N	O	0	0
			42	23	5	14		
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	P	3	Total	Mg	0	0
			3	3		
25	Q	1	Total	Mg	0	0
			1	1		
25	D	2	Total	Mg	0	0
			2	2		
25	E	4	Total	Mg	0	0
			4	4		
25	H	1	Total	Mg	0	0
			1	1		
25	V	1	Total	Mg	0	0
			1	1		
25	A	339	Total	Mg	0	8
			345	345		
25	T	1	Total	Mg	0	0
			1	1		
25	N	1	Total	Mg	0	0
			1	1		
25	O	1	Total	Mg	0	0
			1	1		
25	L	1	Total	Mg	0	0
			1	1		
25	S	2	Total	Mg	0	0
			2	2		

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

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

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

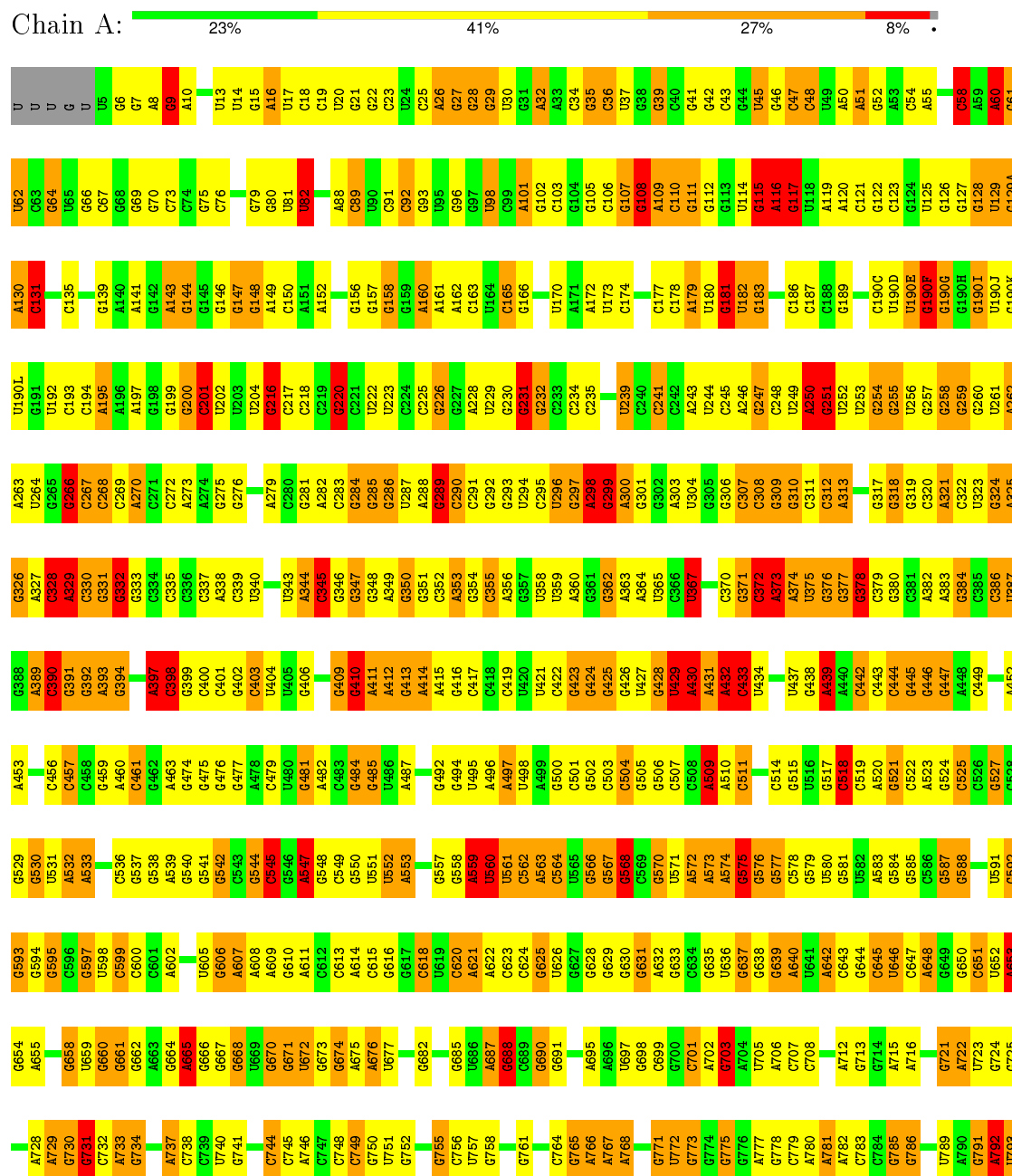
- Molecule 27 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
27	A	480	Total 480	O 480	0	0
27	C	1	Total 1	O 1	0	0
27	D	2	Total 2	O 2	0	0
27	E	5	Total 5	O 5	0	0
27	K	1	Total 1	O 1	0	0
27	L	2	Total 2	O 2	0	0
27	N	2	Total 2	O 2	0	0
27	O	4	Total 4	O 4	0	0
27	V	1	Total 1	O 1	0	0

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.

• Molecule 1: 16S rRNA

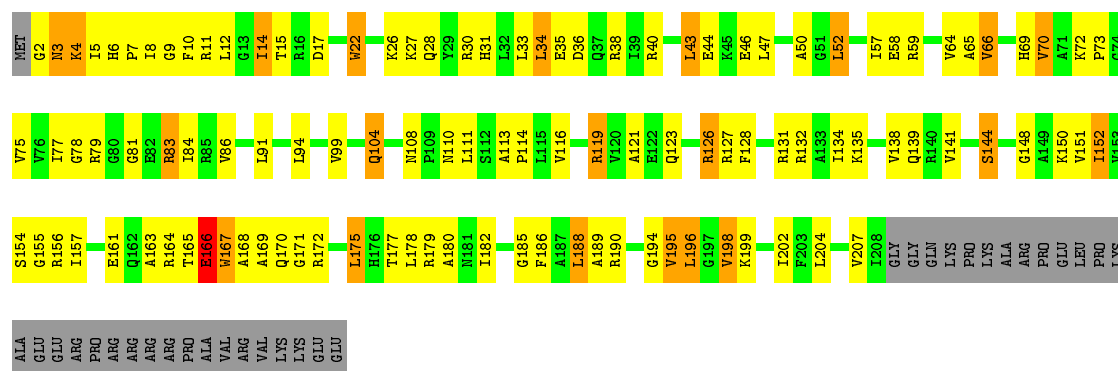


A171	A174	R176	A177	A178	F181	V184	L187	A188	T190	D191	S192	L196	V197	D198	V199	I200	I201	P202	D205	I208	R209	S210	I211	Q212	L213	V136	R137	S216	R217	L142	E143	R220	L221	I222	Q224	V230	S235	A237	L238	V239	Q240	E241	ALA	GLU	ALA	THR																																																																																																																																
U436	C1437	G1438	C1439	C1440	C1441	G1442	G1443	A1444	G1445	G1446	G1447	A1451	C1452	G1453	G1454	G1455	G1456	G1457	G1458	G1459	G1460	G1461	G1462	C1463	G1464	C1465	C1466	G1467	A1468	G1469	G1470	G1471	G1475	G1476	G1479	C1480	U1481	G1487	G1488	G1489	G1490	G1491	U1492	A1493	G1494	U1495	A1500	C1501	A1502	A1503	G1504	G1505	U1506	A1507	G1508	C1509																																																																																																																						
U1510	G1511	U1512	U1513	C1514	C1515	G1516	G1517	A1518	G1519	G1520	G1521	U1522	G1523	C1524	G1525	G1526	C1527	U1528	G1529	A1531	U1532	C1533	C	A	C	U	C	G1539	U1540	U1541	U1542	C1543	U1544	G1440	G1441	G1442	G1443	G1444	G1445	G1446	G1447	G1448	G1449	G1450	G1451	G1452	G1453	G1454	G1455	G1456	G1457	G1458	G1459	G1460	G1461	G1462	G1463	G1464	G1465	G1466	G1467	G1468	G1469	G1470	G1471	G1475	G1476	G1479	C1480	U1481	G1487	G1488	G1489	G1490	G1491	U1492	A1493	G1494	U1495	A1500	C1501	A1502	A1503	G1504	G1505	U1506	A1507	G1508	C1509																																																																																					
G1371	U1372	G1373	U1374	U1375	U1376	G1377	G1378	G1379	G1380	U1381	G1382	G1386	G1387	G1388	G1389	U1390	U1391	G1392	U1393	A1394	C1395	G1396	G1397	A1398	G1399	C1400	G1401	G1402	G1403	G1404	G1405	G1410	G1411	G1412	G1413	G1414	G1415	G1416	G1417	G1418	G1419	G1420	G1421	G1422	G1423	G1424	U1425	G1426	U1427	A1428	G1429	G1430	G1431	G1432	G1433	G1434	G1435	G1436	G1437	G1438	G1439	G1440	G1441	G1442	G1443	G1444	G1445	G1446	G1447	G1448	G1449	G1450	G1451	G1452	G1453	G1454	G1455	G1456	G1457	G1458	G1459	G1460	G1461	G1462	G1463	G1464	G1465	G1466	G1467	G1468	G1469	G1470	G1471	G1475	G1476	G1479	C1480	U1481	G1487	G1488	G1489	G1490	G1491	U1492	A1493	G1494	U1495	A1500	C1501	A1502	A1503	G1504	G1505	U1506	A1507	G1508	C1509																																																									
G1309	G1312	U1313	C1314	U1315	G1316	G1317	A1318	C1319	C1320	G1321	G1322	G1323	C1326	G1327	C1328	U1329	U1330	G1331	A1332	C1333	C1334	G1335	C1336	G1337	G1338	C1339	A1340	U1341	G1342	G1343	U1344	G1345	G1346	G1347	U1348	G1349	A1350	U1351	C1352	G1353	G1356	A1357	U1358	C1359	A1360	G1361	C1361A	C1362	A1363	U1364	G1365	C1366	C1367	C1368	C1369	G1370	G1371	U1372	G1373	U1374	U1375	U1376	G1377	G1378	G1379	G1380	U1381	G1382	G1386	G1387	G1388	G1389	U1390	U1391	G1392	U1393	A1394	C1395	G1396	G1397	A1398	G1399	C1400	G1401	G1402	G1403	G1404	G1405	G1410	G1411	G1412	G1413	G1414	G1415	G1416	G1417	G1418	G1419	G1420	G1421	G1422	G1423	G1424	U1425	G1426	U1427	A1428	G1429	G1430	G1431	G1432	G1433	G1434	G1435	G1436	G1437	G1438	G1439	G1440	G1441	G1442	G1443	G1444	G1445	G1446	G1447	G1448	G1449	G1450	G1451	G1452	G1453	G1454	G1455	G1456	G1457	G1458	G1459	G1460	G1461	G1462	G1463	G1464	G1465	G1466	G1467	G1468	G1469	G1470	G1471	G1475	G1476	G1479	C1480	U1481	G1487	G1488	G1489	G1490	G1491	U1492	A1493	G1494	U1495	A1500	C1501	A1502	A1503	G1504	G1505	U1506	A1507	G1508	C1509
C1246	U1247	A1248	C1249	A1250	C1251	A1252	G1253	C1254	G1255	A1256	U1257	G1258	G1259	C1260	A1261	C1262	C1263	A1264	G1265	G1266	C1267	C1268	A1269	C1270	G1271	G1272	G1276	C1277	U1278	A1279	C1280	C1281	C1282	C1283	C1284	A1285	A1286	A1287	C1288	A1289	C1290	G1291	U1292	G1293	C1294	G1295	G1296	C1297	C1298	A1299	C1300	A1301	U1302	C1303	G1304	G1305	U1308	C1246	U1247	A1248	C1249	A1250	C1251	A1252	G1253	C1254	G1255	A1256	U1257	G1258	G1259	C1260	A1261	C1262	C1263	A1264	G1265	G1266	C1267	C1268	A1269	C1270	G1271	G1272	G1276	C1277	U1278	A1279	C1280	C1281	C1282	C1283	C1284	A1285	A1286	A1287	C1288	A1289	C1290	G1291	U1292	G1293	C1294	G1295	G1296	C1297	C1298	A1299	C1300	A1301	U1302	C1303	G1304	G1305	U1308																																																											
G1185	G1186	G1187	A1188	C1189	G1190	A1191	C1192	C1195	G1196	G1197	G1198	U1199	G1200	A1201	C1202	C1203	A1204	U1205	G1206	G1207	C1208	C1209	C1210	U1211	C1212	A1213	C1214	G1215	G1216	C1217	C1218	U1219	C1220	C1221	G1222	C1223	G1224	A1225	C1226	A1227	C1228	A1229	C1230	G1231	U1232	G1233	C1234	U1235	A1236	G1237	C1238	A1239	U1301	U1302	C1303	G1304	G1305	U1308	C1185	G1186	G1187	A1188	C1189	G1190	A1191	C1192	C1195	G1196	G1197	G1198	U1199	G1200	A1201	C1202	C1203	A1204	U1205	G1206	G1207	C1208	C1209	C1210	U1211	C1212	A1213	C1214	G1215	G1216	C1217	C1218	U1219	C1220	C1221	G1222	C1223	G1224	A1225	C1226	A1227	C1228	A1229	C1230	G1231	U1232	G1233	C1234	U1235	A1236	G1237	C1238	A1239	U1301	U1302	C1303	G1304	G1305	U1308																																																									
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A935	C936	U937	A938	C939	G940	G941	G942	U943	A944	G945	A946	C947	C948	A949	U950	G951	U952	G953	G954	U955	C956	G957	U958	U959	G960	U961	C962	G963	A964	G965	G966	C967	A968	A969	C970	G971	C972	G973	A974	A975	G976	A977	C978	C979	U980	U981	G982	A983	C984	A985	A986	G987	C988	C989	G990	U991	U992	C993	A994	A935	C936	U937	A938	C939	G940	G941	G942	U943	A944	G945	A946	C947	C948	A949	U950	G951	U952	G953	G954	U955	C956	G957	U958	U959	G960	U961	C962	G963	A964	G965	G966	C967	A968	A969	C970	G971	C972	G973	A974	A975	G976	A977	C978	C979	U980	U981	G982	A983	C984	A985	A986	G987	C988	C989	G990	U991	U992	C993	A994																																																							
G869	U870	U871	A872	A873	G874	C875	G876	G881	C882	C883	U884	G885	G886	G887	G888	A892	C893	G894	G895	G896	U897	A901	G902	G903	C904	U905	G906	A907	A908	A909	C910	U911	C912	A913	A914	G915	G916	G917	U918	A919	U920	U921	G922	A923	C924	G925	G926	C927	G928	G929	C930	C931	G932	G933	C934	G869	U870	U871	A872	A873	G874	C875	G876	G881	C882	C883	U884	G885	G886	G887	G888	A892	C893	G894	G895	G896	U897	A901	G902	G903	C904	U905	G906	A907	A908	A909	C910	U911	C912	A913	A914	G915	G916	G917	U918	A919	U920	U921	G922	A923	C924	G925	G926	C927	G928	G929	C930	C931	G932	G933	C934																																																															
A794	C795	C796	C797	G798	G800	U801	A802	G803	U804	C805	C806	A807	G808	G809	C810	C811	C812	U813	A814	A815	A816	C817	G818	A819	U820	G821	G825	A828	G829	G830	U833	C834	U835	G836	G837	U838	G839	U841	C848	C849	U850	G851	C852	G853	G854	G855	C856	C857	G858	C859	A860	G867	C868	A794	C795	C796	C797	G798	G800	U801	A802	G803	U804	C805	C806	A807	G808	G809	C810	C811	C812	U813	A814	A815	A816	C817	G818	A819	U820	G821	G825	A																																																																																												

GLU
THR
PRO
GLU
GLY
GLY
SER
GLU
VAL
GLU
ALA

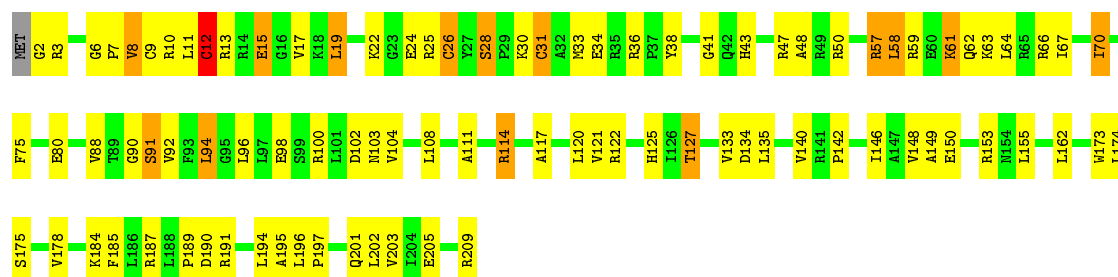
• Molecule 3: 30S ribosomal protein S3

Chain C: 40% 38% 9% 13%



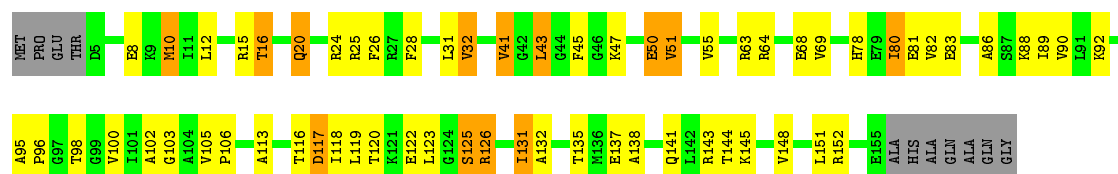
• Molecule 4: 30S ribosomal protein S4

Chain D: 56% 37% 7%



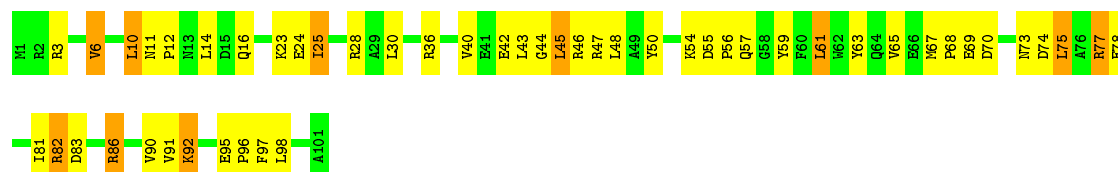
• Molecule 5: 30S ribosomal protein S5

Chain E: 54% 31% 8% 7%

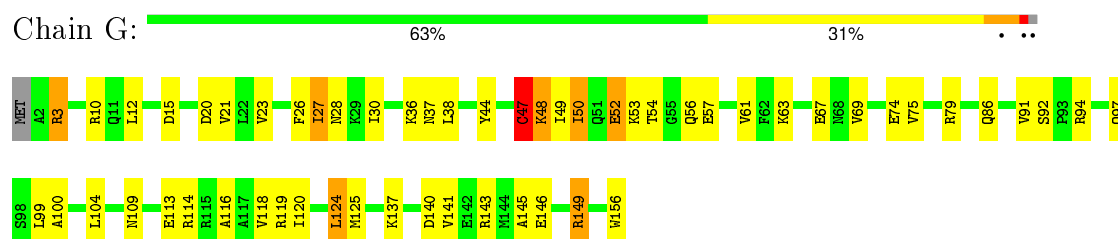


• Molecule 6: 30S ribosomal protein S6

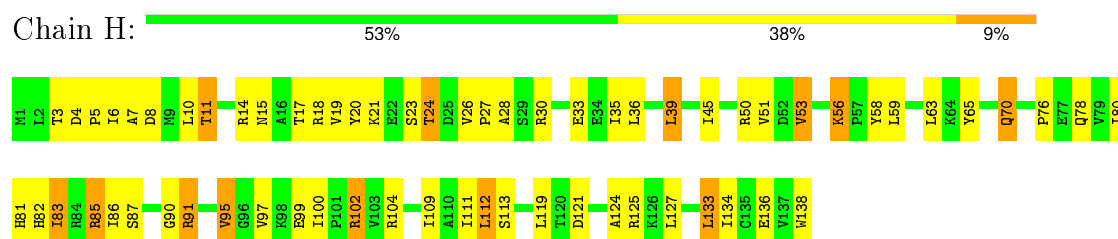
Chain F: 50% 40% 10%



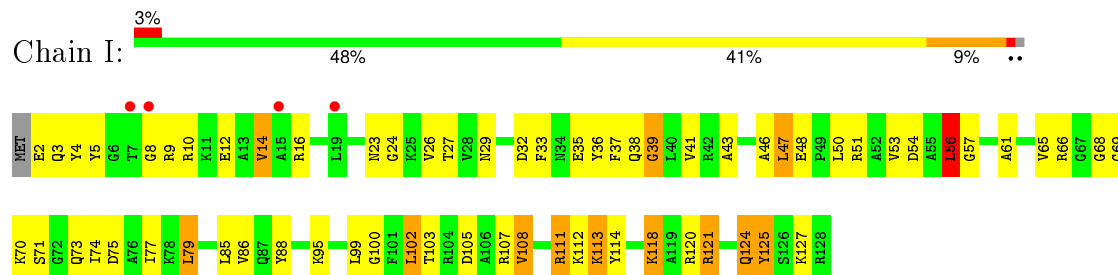
- Molecule 7: 30S ribosomal protein S7



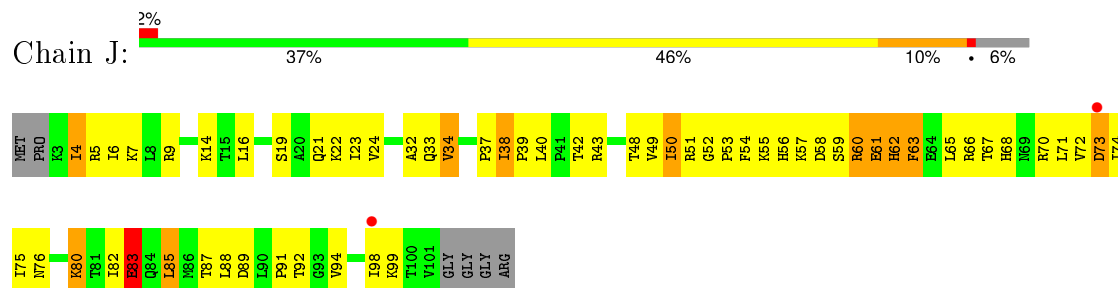
- Molecule 8: 30S ribosomal protein S8



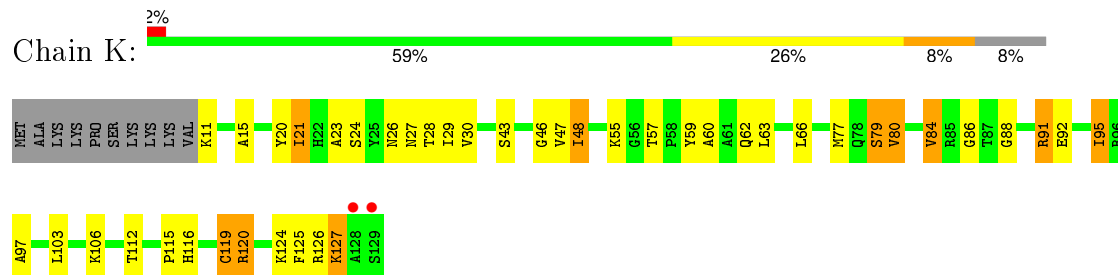
- Molecule 9: 30S ribosomal protein S9



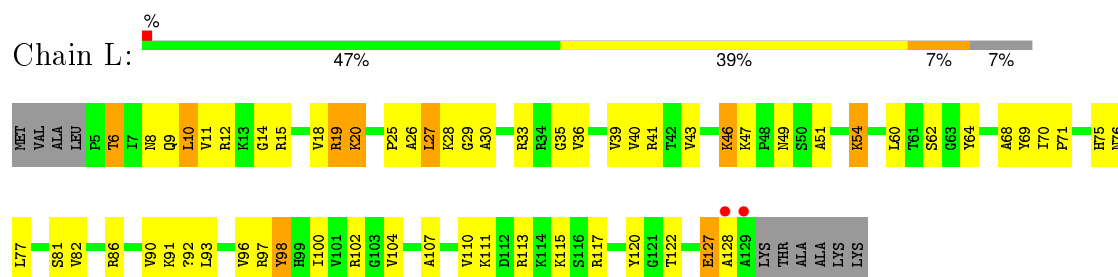
- Molecule 10: 30S ribosomal protein S10



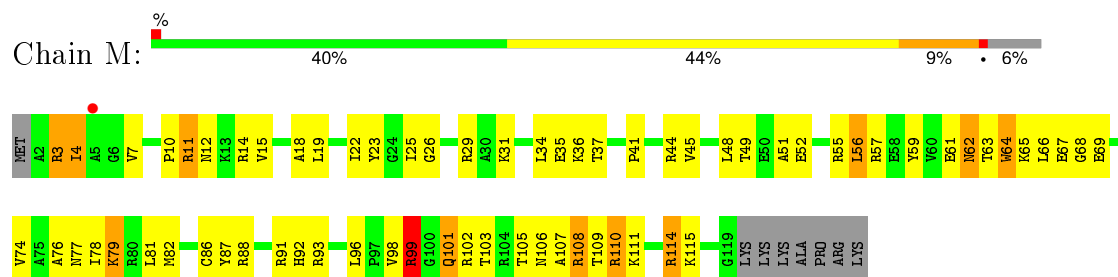
- Molecule 11: 30S ribosomal protein S11



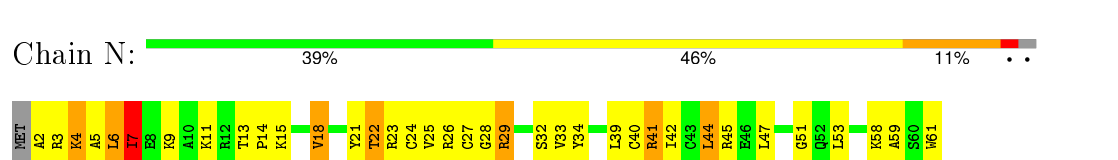
- Molecule 12: 30S ribosomal protein S12



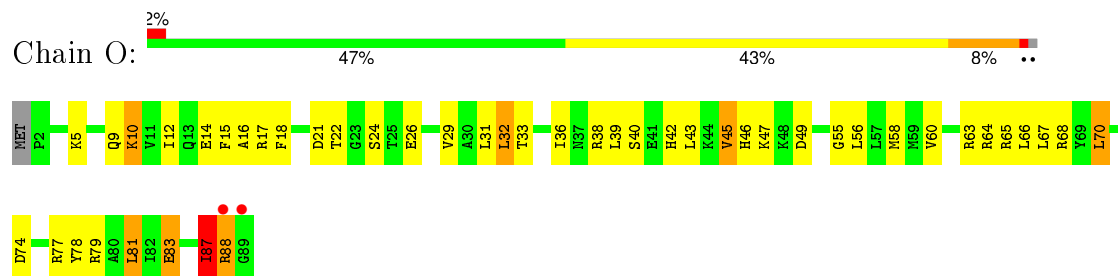
- Molecule 13: 30S ribosomal protein S13



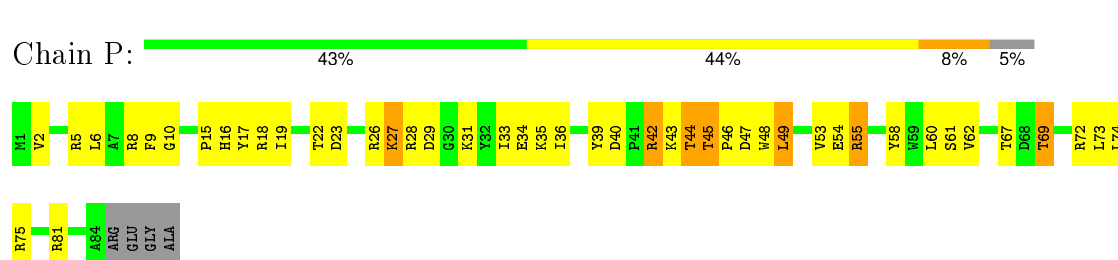
- Molecule 14: 30S ribosomal protein S14



- Molecule 15: 30S ribosomal protein S15

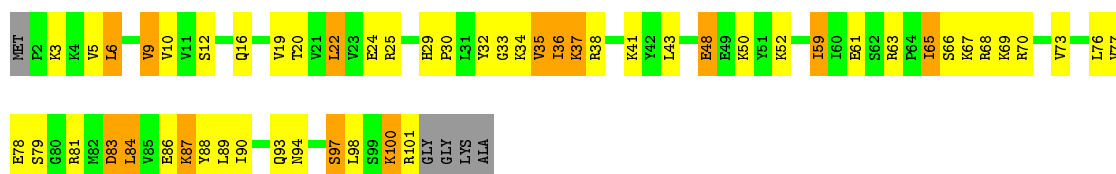


- Molecule 16: 30S ribosomal protein S16

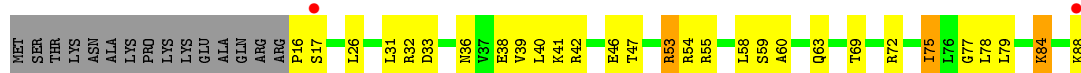


- Molecule 17: 30S ribosomal protein S17

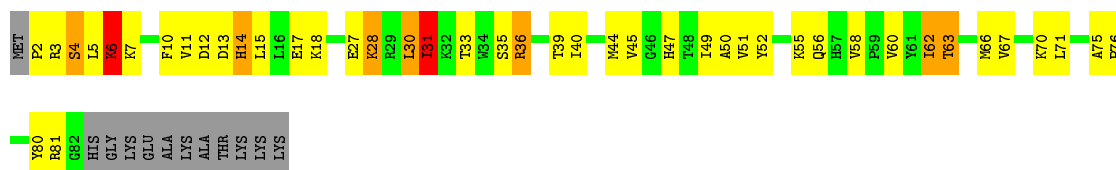




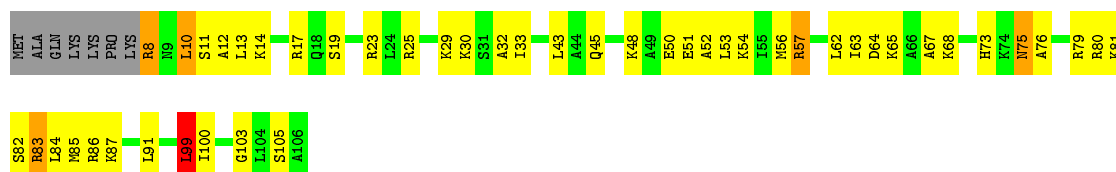
- Molecule 18: 30S ribosomal protein S18



- Molecule 19: 30S ribosomal protein S19



- Molecule 20: 30S ribosomal protein S20



- Molecule 21: 30S ribosomal protein THX



- Molecule 22: 5'-R(*UP*UP*U)-3'



- Molecule 23: 5'-R(*GP*GP*GP*AP*UP*UP*GP*AP*AP*AP*AP*UP*CP*CP*C)-3'



G28	G29	G30	A31	U32	U33	G34	A35	A36	A37	A38	U39	C40	C41	C42
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4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	400.95Å 400.95Å 176.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.73 – 3.97 49.73 – 3.97	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.73-3.97) 99.6 (49.73-3.97)	Depositor EDS
R_{merge}	0.25	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.94 (at 4.00Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_978)	Depositor
R, R_{free}	0.153 , 0.212 0.159 , 0.213	Depositor DCC
R_{free} test set	6190 reflections (5.28%)	DCC
Wilson B-factor (Å ²)	100.0	Xtriage
Anisotropy	0.167	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 94.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 123790 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	53651	wwPDB-VP
Average B, all atoms (Å ²)	101.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.58% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MA6, MG, 0TD, PAR, 2MG, 5MC, UR3, 4OC, M2G, 7MG, PSU

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	1.11	67/36037 (0.2%)	1.84	1584/56239 (2.8%)
2	B	0.68	0/1931	0.86	3/2607 (0.1%)
3	C	0.71	1/1637 (0.1%)	0.86	1/2207 (0.0%)
4	D	0.74	2/1733 (0.1%)	0.92	4/2318 (0.2%)
5	E	0.79	0/1163	1.02	1/1566 (0.1%)
6	F	0.66	0/856	0.85	0/1154
7	G	0.68	1/1276 (0.1%)	0.84	1/1709 (0.1%)
8	H	0.77	0/1136	0.96	0/1527
9	I	0.68	0/1029	0.94	2/1379 (0.1%)
10	J	0.73	0/806	0.92	1/1084 (0.1%)
11	K	0.66	0/900	0.87	0/1213
12	L	0.90	1/978 (0.1%)	1.05	3/1308 (0.2%)
13	M	0.72	0/947	0.88	1/1270 (0.1%)
14	N	0.79	0/501	0.98	1/664 (0.2%)
15	O	0.67	0/745	0.88	0/992
16	P	0.82	0/717	0.95	0/965
17	Q	0.86	0/847	1.06	3/1131 (0.3%)
18	R	0.71	0/604	0.91	1/801 (0.1%)
19	S	0.62	0/662	0.84	0/892
20	T	0.77	0/765	1.04	1/1007 (0.1%)
21	U	0.70	0/213	0.82	0/279
22	V	1.12	0/62	2.13	6/94 (6.4%)
23	W	1.00	0/357	1.41	7/555 (1.3%)
All	All	0.99	72/55902 (0.1%)	1.60	1620/82961 (2.0%)

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
2	B	0	2
3	C	0	1
4	D	0	1
8	H	0	1
12	L	0	1
13	M	0	1
14	N	0	1
17	Q	0	1
19	S	0	1
All	All	0	10

The worst 5 of 72 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1227	A	N9-C4	-8.38	1.32	1.37
1	A	116	A	N9-C4	-8.37	1.32	1.37
1	A	372	C	N3-C4	8.23	1.39	1.33
1	A	372	C	C2-O2	7.65	1.31	1.24
1	A	622	A	N9-C4	-7.50	1.33	1.37

The worst 5 of 1620 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1054	C	C4-C5-C6	-15.67	109.57	117.40
1	A	1054	C	C5-C6-N1	14.40	128.20	121.00
1	A	1054	C	N1-C2-N3	-13.92	109.46	119.20
1	A	1054	C	C2-N3-C4	13.81	126.80	119.90
1	A	1331	G	C5-N7-C8	13.48	111.04	104.30

There are no chirality outliers.

5 of 10 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	14	GLY	Peptide
2	B	89	GLY	Peptide
3	C	166	GLU	Peptide
4	D	195	ALA	Peptide
8	H	90	GLY	Peptide

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	32504	0	16432	801	0
2	B	1896	0	1936	77	0
3	C	1613	0	1677	81	0
4	D	1703	0	1763	78	0
5	E	1147	0	1207	41	0
6	F	843	0	857	32	0
7	G	1257	0	1296	41	0
8	H	1116	0	1177	58	0
9	I	1010	0	1037	49	0
10	J	793	0	835	57	0
11	K	885	0	904	30	0
12	L	973	0	1058	39	0
13	M	937	0	995	46	0
14	N	492	0	529	35	0
15	O	734	0	771	34	0
16	P	701	0	720	39	0
17	Q	834	0	906	43	0
18	R	598	0	670	25	0
19	S	648	0	673	30	0
20	T	763	0	861	28	0
21	U	209	0	221	10	0
22	V	57	0	32	3	0
23	W	319	0	164	9	0
24	A	756	0	810	61	0
25	A	345	0	0	0	0
25	D	2	0	0	0	0
25	E	4	0	0	0	0
25	H	1	0	0	0	0
25	L	1	0	0	0	0
25	N	1	0	0	0	0
25	O	1	0	0	0	0
25	P	3	0	0	0	0
25	Q	1	0	0	0	0
25	S	2	0	0	0	0
25	T	1	0	0	0	0
25	V	1	0	0	0	0
26	D	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	N	1	0	0	0	0
27	A	480	0	0	7	0
27	C	1	0	0	0	0
27	D	2	0	0	0	0
27	E	5	0	0	0	0
27	K	1	0	0	0	0
27	L	2	0	0	0	0
27	N	2	0	0	1	0
27	O	4	0	0	0	0
27	V	1	0	0	0	0
All	All	53651	0	37531	1549	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 17.

The worst 5 of 1549 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)
11:K:15:ALA:HA	11:K:77:MET:HA	1.47	0.97
1:A:1053:G:HO2'	1:A:1199:U:H5	0.97	0.92
1:A:737:A:H1'	6:F:73:ASN:HD21	1.34	0.91
19:S:33:THR:HG22	19:S:35:SER:H	1.38	0.88
1:A:975:A:H4'	1:A:976:G:H5''	1.57	0.87

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	
2	B	234/256 (91%)	204 (87%)	30 (13%)	0	100	100
3	C	205/239 (86%)	184 (90%)	20 (10%)	1 (0%)	34	76

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	D	206/209 (99%)	195 (95%)	11 (5%)	0	100	100
5	E	149/162 (92%)	144 (97%)	5 (3%)	0	100	100
6	F	99/101 (98%)	97 (98%)	2 (2%)	0	100	100
7	G	153/156 (98%)	141 (92%)	12 (8%)	0	100	100
8	H	136/138 (99%)	132 (97%)	4 (3%)	0	100	100
9	I	125/128 (98%)	110 (88%)	14 (11%)	1 (1%)	24	69
10	J	97/105 (92%)	80 (82%)	14 (14%)	3 (3%)	5	44
11	K	117/129 (91%)	105 (90%)	11 (9%)	1 (1%)	21	66
12	L	122/135 (90%)	111 (91%)	10 (8%)	1 (1%)	24	69
13	M	116/126 (92%)	104 (90%)	12 (10%)	0	100	100
14	N	58/61 (95%)	53 (91%)	5 (9%)	0	100	100
15	O	86/89 (97%)	76 (88%)	9 (10%)	1 (1%)	16	62
16	P	82/88 (93%)	77 (94%)	5 (6%)	0	100	100
17	Q	98/105 (93%)	93 (95%)	5 (5%)	0	100	100
18	R	71/88 (81%)	65 (92%)	6 (8%)	0	100	100
19	S	79/93 (85%)	70 (89%)	7 (9%)	2 (2%)	7	48
20	T	97/106 (92%)	82 (84%)	14 (14%)	1 (1%)	19	65
21	U	23/27 (85%)	22 (96%)	1 (4%)	0	100	100
All	All	2353/2541 (93%)	2145 (91%)	197 (8%)	11 (0%)	34	76

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
12	L	28	LYS
19	S	31	ILE
20	T	99	LEU
9	I	38	GLN
19	S	6	LYS

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	
2	B	201/220 (91%)	176 (88%)	25 (12%)	6	32
3	C	160/188 (85%)	121 (76%)	39 (24%)	1	7
4	D	180/181 (99%)	159 (88%)	21 (12%)	7	35
5	E	115/123 (94%)	91 (79%)	24 (21%)	1	11
6	F	90/90 (100%)	66 (73%)	24 (27%)	0	5
7	G	126/127 (99%)	105 (83%)	21 (17%)	3	20
8	H	119/119 (100%)	94 (79%)	25 (21%)	1	11
9	I	98/99 (99%)	75 (76%)	23 (24%)	1	8
10	J	87/92 (95%)	69 (79%)	18 (21%)	1	11
11	K	90/99 (91%)	78 (87%)	12 (13%)	5	30
12	L	103/110 (94%)	86 (84%)	17 (16%)	3	21
13	M	94/101 (93%)	75 (80%)	19 (20%)	1	12
14	N	49/50 (98%)	39 (80%)	10 (20%)	1	12
15	O	79/80 (99%)	63 (80%)	16 (20%)	1	12
16	P	72/74 (97%)	60 (83%)	12 (17%)	3	20
17	Q	95/97 (98%)	75 (79%)	20 (21%)	1	11
18	R	64/77 (83%)	56 (88%)	8 (12%)	6	32
19	S	71/80 (89%)	53 (75%)	18 (25%)	1	7
20	T	76/82 (93%)	60 (79%)	16 (21%)	1	11
21	U	19/22 (86%)	16 (84%)	3 (16%)	3	23
All	All	1988/2111 (94%)	1617 (81%)	371 (19%)	2	15

5 of 371 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	H	53	VAL
10	J	33	GLN
19	S	18	LYS
8	H	91	ARG
9	I	66	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
6	F	73	ASN
6	F	94	GLN
17	Q	16	GLN
3	C	108	ASN
9	I	73	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1507/1522 (99%)	318 (21%)	46 (3%)
22	V	2/3 (66%)	1 (50%)	0
23	W	14/15 (93%)	4 (28%)	0
All	All	1523/1540 (98%)	323 (21%)	46 (3%)

5 of 323 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	9	G
1	A	32	A
1	A	39	G
1	A	48	C
1	A	51	A

5 of 46 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	812	C
1	A	1065	U
1	A	1397	C
1	A	913	A
1	A	965	A

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

15 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
1	2MG	A	1207	1	17,26,27	2.30	4 (23%)	21,38,41	2.75	4 (19%)
1	5MC	A	1400	1	13,22,23	1.18	1 (7%)	15,32,35	1.04	1 (6%)
1	4OC	A	1402	1	13,23,24	0.82	0	18,32,35	0.82	1 (5%)
1	5MC	A	1404	1	13,22,23	1.02	1 (7%)	15,32,35	0.72	0
1	5MC	A	1407	1	13,22,23	1.10	1 (7%)	15,32,35	1.28	3 (20%)
1	UR3	A	1498	1	12,22,23	0.85	0	16,32,35	1.28	1 (6%)
1	MA6	A	1518	1	16,26,27	0.86	1 (6%)	18,38,41	1.48	5 (27%)
1	MA6	A	1519	1	16,26,27	1.29	3 (18%)	18,38,41	1.35	3 (16%)
1	PSU	A	1540	1	13,21,22	1.27	2 (15%)	18,30,33	3.92	5 (27%)
1	PSU	A	1541	1	13,21,22	1.18	2 (15%)	18,30,33	3.73	7 (38%)
1	PSU	A	516	1	13,21,22	1.41	2 (15%)	18,30,33	4.69	4 (22%)
1	7MG	A	527	1,25	19,26,27	2.91	7 (36%)	24,39,42	1.71	6 (25%)
1	M2G	A	966	1	17,27,28	1.25	1 (5%)	22,40,43	2.46	4 (18%)
1	5MC	A	967	1	13,22,23	0.79	0	15,32,35	0.79	1 (6%)
12	0TD	L	92	12	4,9,10	0.99	0	4,11,13	3.34	3 (75%)

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
1	2MG	A	1207	1	-	0/5/27/28	0/3/3/3
1	5MC	A	1400	1	-	0/3/25/26	0/2/2/2
1	4OC	A	1402	1	-	0/7/29/30	0/2/2/2
1	5MC	A	1404	1	-	0/3/25/26	0/2/2/2
1	5MC	A	1407	1	-	0/3/25/26	0/2/2/2
1	UR3	A	1498	1	-	0/3/25/26	0/2/2/2
1	MA6	A	1518	1	-	0/7/29/30	0/3/3/3
1	MA6	A	1519	1	-	0/7/29/30	0/3/3/3
1	PSU	A	1540	1	-	0/7/25/26	0/2/2/2
1	PSU	A	1541	1	-	0/7/25/26	0/2/2/2
1	PSU	A	516	1	-	0/7/25/26	0/2/2/2
1	7MG	A	527	1,25	-	0/7/37/38	0/3/3/3
1	M2G	A	966	1	-	0/7/29/30	0/3/3/3
1	5MC	A	967	1	-	0/3/25/26	0/2/2/2
12	0TD	L	92	12	-	0/2/12/14	0/0/0/0

The worst 5 of 25 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	527	7MG	C8-N9	-7.94	1.33	1.45
1	A	527	7MG	CM7-N7	-3.68	1.39	1.46
1	A	527	7MG	C8-N7	-2.54	1.31	1.43
1	A	1407	5MC	C4-N3	-2.39	1.31	1.35
1	A	527	7MG	O6-C6	-2.36	1.19	1.24

The worst 5 of 48 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	516	PSU	N1-C2-N3	-17.40	117.23	128.33
1	A	1540	PSU	N1-C2-N3	-13.66	119.62	128.33
1	A	1541	PSU	N1-C2-N3	-13.39	119.79	128.33
1	A	1207	2MG	C5-C6-N1	-10.69	108.97	123.59
1	A	966	M2G	C5-C6-N1	-9.64	110.41	123.59

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1207	2MG	1	0
1	A	1400	5MC	1	0
1	A	1402	4OC	5	0
1	A	1404	5MC	2	0
1	A	1498	UR3	4	0
1	A	1518	MA6	2	0
1	A	527	7MG	1	0
1	A	966	M2G	3	0
1	A	967	5MC	2	0
12	L	92	0TD	2	0

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 383 ligands modelled in this entry, 365 are monoatomic - leaving 18 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	1601	-	45,45,45	1.39	6 (13%)	59,67,67	1.57	11 (18%)
24	PAR	A	1602	-	45,45,45	1.60	7 (15%)	59,67,67	1.71	12 (20%)
24	PAR	A	1603	-	45,45,45	1.41	8 (17%)	59,67,67	1.68	12 (20%)
24	PAR	A	1604	-	45,45,45	1.30	7 (15%)	59,67,67	1.56	11 (18%)
24	PAR	A	1605	-	45,45,45	1.30	8 (17%)	59,67,67	1.48	9 (15%)
24	PAR	A	1606	-	45,45,45	1.44	7 (15%)	59,67,67	1.66	12 (20%)
24	PAR	A	1607	-	45,45,45	1.68	9 (20%)	59,67,67	1.65	11 (18%)
24	PAR	A	1608	25	45,45,45	1.27	6 (13%)	59,67,67	1.60	12 (20%)
24	PAR	A	1609	-	45,45,45	1.76	14 (31%)	59,67,67	1.68	11 (18%)
24	PAR	A	1610	-	45,45,45	1.73	14 (31%)	59,67,67	1.71	12 (20%)
24	PAR	A	1611	-	45,45,45	1.59	6 (13%)	59,67,67	1.62	11 (18%)
24	PAR	A	1612	-	45,45,45	1.54	7 (15%)	59,67,67	1.60	10 (16%)
24	PAR	A	1613	-	45,45,45	1.66	8 (17%)	59,67,67	1.60	9 (15%)
24	PAR	A	1614	-	45,45,45	1.69	12 (26%)	59,67,67	1.59	10 (16%)
24	PAR	A	1615	-	45,45,45	2.06	11 (24%)	59,67,67	1.67	12 (20%)
24	PAR	A	1616	-	45,45,45	1.98	11 (24%)	59,67,67	1.62	12 (20%)
24	PAR	A	1617	25	45,45,45	2.07	13 (28%)	59,67,67	1.63	10 (16%)
24	PAR	A	1618	-	45,45,45	2.25	17 (37%)	59,67,67	1.61	10 (16%)

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	1601	-	-	0/18/94/94	0/4/4/4
24	PAR	A	1602	-	-	1/18/94/94	1/4/4/4
24	PAR	A	1603	-	-	0/18/94/94	0/4/4/4
24	PAR	A	1604	-	-	0/18/94/94	0/4/4/4
24	PAR	A	1605	-	-	0/18/94/94	0/4/4/4
24	PAR	A	1606	-	-	0/18/94/94	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	PAR	A	1607	-	-	0/18/94/94	0/4/4/4
24	PAR	A	1608	25	-	0/18/94/94	0/4/4/4
24	PAR	A	1609	-	-	1/18/94/94	0/4/4/4
24	PAR	A	1610	-	-	1/18/94/94	1/4/4/4
24	PAR	A	1611	-	-	0/18/94/94	0/4/4/4
24	PAR	A	1612	-	-	1/18/94/94	1/4/4/4
24	PAR	A	1613	-	-	2/18/94/94	0/4/4/4
24	PAR	A	1614	-	-	0/18/94/94	1/4/4/4
24	PAR	A	1615	-	-	1/18/94/94	0/4/4/4
24	PAR	A	1616	-	-	0/18/94/94	1/4/4/4
24	PAR	A	1617	25	-	0/18/94/94	0/4/4/4
24	PAR	A	1618	-	-	1/18/94/94	1/4/4/4

The worst 5 of 171 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	1604	PAR	C62-C12	-2.06	1.49	1.53
24	A	1602	PAR	C44-C34	-2.04	1.47	1.52
24	A	1610	PAR	C13-C23	2.00	1.55	1.52
24	A	1615	PAR	C41-C51	2.02	1.57	1.53
24	A	1603	PAR	C41-C51	2.02	1.57	1.53

The worst 5 of 197 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	1602	PAR	C34-C24-N24	-4.09	103.27	110.86
24	A	1603	PAR	C34-C24-N24	-3.70	104.00	110.86
24	A	1610	PAR	C34-C24-N24	-3.69	104.01	110.86
24	A	1612	PAR	C34-C24-N24	-3.49	104.39	110.86
24	A	1605	PAR	C34-C24-N24	-3.38	104.60	110.86

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	A	1618	PAR	C33-O33-C14-C24
24	A	1613	PAR	C42-O11-C11-C21
24	A	1615	PAR	C33-O33-C14-C24
24	A	1612	PAR	C42-O11-C11-C21
24	A	1602	PAR	C33-O33-C14-C24

5 of 6 ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	A	1616	PAR	C12-C22-C32-C42-C52-C62
24	A	1602	PAR	C14-C24-C34-C44-C54-O54
24	A	1618	PAR	C12-C22-C32-C42-C52-C62
24	A	1614	PAR	C12-C22-C32-C42-C52-C62
24	A	1610	PAR	C14-C24-C34-C44-C54-O54

17 monomers are involved in 61 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	A	1601	PAR	2	0
24	A	1602	PAR	4	0
24	A	1603	PAR	7	0
24	A	1604	PAR	3	0
24	A	1605	PAR	4	0
24	A	1606	PAR	1	0
24	A	1608	PAR	5	0
24	A	1609	PAR	1	0
24	A	1610	PAR	6	0
24	A	1611	PAR	5	0
24	A	1612	PAR	4	0
24	A	1613	PAR	7	0
24	A	1614	PAR	1	0
24	A	1615	PAR	3	0
24	A	1616	PAR	5	0
24	A	1617	PAR	1	0
24	A	1618	PAR	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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	1498/1522 (98%)	-0.40	3 (0%) 95 94	49, 88, 175, 339	0
2	B	236/256 (92%)	-0.33	0 100 100	70, 114, 159, 187	0
3	C	207/239 (86%)	-0.34	0 100 100	80, 108, 146, 160	0
4	D	208/209 (99%)	-0.48	0 100 100	56, 92, 128, 166	0
5	E	151/162 (93%)	-0.41	0 100 100	47, 73, 107, 151	0
6	F	101/101 (100%)	-0.44	0 100 100	68, 108, 134, 160	0
7	G	155/156 (99%)	-0.55	0 100 100	66, 106, 162, 193	0
8	H	138/138 (100%)	-0.58	0 100 100	47, 74, 104, 132	0
9	I	127/128 (99%)	0.02	4 (3%) 52 40	69, 112, 142, 158	0
10	J	99/105 (94%)	-0.04	2 (2%) 68 57	75, 127, 185, 199	0
11	K	119/129 (92%)	-0.30	2 (1%) 73 62	54, 94, 132, 210	0
12	L	124/135 (91%)	-0.20	2 (1%) 74 63	55, 80, 124, 185	0
13	M	118/126 (93%)	0.03	1 (0%) 87 82	78, 108, 137, 149	0
14	N	60/61 (98%)	-0.48	0 100 100	75, 99, 139, 181	0
15	O	88/89 (98%)	-0.28	2 (2%) 64 52	56, 90, 123, 172	0
16	P	84/88 (95%)	-0.40	0 100 100	58, 77, 107, 151	0
17	Q	100/105 (95%)	-0.06	0 100 100	63, 81, 120, 155	0
18	R	73/88 (82%)	0.06	2 (2%) 58 46	68, 100, 153, 221	0
19	S	81/93 (87%)	-0.31	0 100 100	89, 124, 151, 179	0
20	T	99/106 (93%)	-0.16	0 100 100	65, 85, 130, 168	0
21	U	25/27 (92%)	0.09	0 100 100	87, 113, 132, 139	0
22	V	3/3 (100%)	0.40	0 100 100	99, 99, 103, 105	0
23	W	15/15 (100%)	0.64	0 100 100	127, 144, 218, 227	0
All	All	3909/4081 (95%)	-0.33	18 (0%) 91 88	47, 96, 156, 339	0

The worst 5 of 18 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
12	L	129	ALA	6.7
1	A	1539	C	4.3
11	K	128	ALA	3.3
15	O	89	GLY	3.2
1	A	1129	C	3.2

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

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
1	5MC	A	1407	21/22	0.98	0.13	-	61,67,72,74	0
1	MA6	A	1519	24/25	0.96	0.27	-	55,57,64,67	0
1	M2G	A	966	25/26	0.96	0.16	-	66,100,115,127	0
1	PSU	A	1541	20/21	0.85	0.54	-	228,249,272,273	0
1	7MG	A	527	24/25	0.96	0.19	-	63,69,82,84	0
1	PSU	A	516	20/21	0.95	0.23	-	83,94,105,108	0
1	PSU	A	1540	20/21	0.80	0.73	-	210,258,270,270	0
12	0TD	L	92	10/11	0.97	0.40	-	55,83,98,428	0
1	5MC	A	967	21/22	0.98	0.14	-	59,75,118,121	0
1	UR3	A	1498	21/22	0.98	0.20	-	63,71,81,88	0
1	2MG	A	1207	24/25	0.95	0.12	-	91,106,114,118	0
1	5MC	A	1400	21/22	0.97	0.18	-	44,73,95,101	0
1	MA6	A	1518	24/25	0.98	0.20	-	58,69,75,78	0
1	4OC	A	1402	22/23	0.96	0.20	-	57,63,67,91	0
1	5MC	A	1404	21/22	0.98	0.14	-	55,64,71,72	0

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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. LLDF column lists the quality of electron

density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
25	MG	N	102	1/1	0.84	0.57	26.02	82,82,82,82	0
25	MG	A	1914	1/1	0.90	0.75	19.16	44,44,44,44	0
25	MG	A	1867	1/1	0.92	0.57	17.64	29,29,29,29	0
24	PAR	A	1618	42/42	0.79	0.37	15.47	166,166,166,166	0
25	MG	A	1912	1/1	0.91	0.34	14.32	51,51,51,51	0
25	MG	A	1888	1/1	0.71	0.66	13.55	71,71,71,71	0
25	MG	A	1619	1/1	0.96	0.34	10.83	69,69,69,69	0
25	MG	A	1803	1/1	0.69	0.36	10.31	71,71,71,71	0
25	MG	A	1823	1/1	0.98	0.36	9.59	57,57,57,57	0
25	MG	A	1853	1/1	0.49	0.54	9.11	44,44,44,44	0
24	PAR	A	1614	42/42	0.84	0.29	8.11	174,174,174,174	0
25	MG	A	1832	1/1	0.56	0.41	7.12	77,77,77,77	0
25	MG	A	1890	1/1	0.88	0.53	7.06	59,59,59,59	0
25	MG	A	1818	1/1	0.86	0.21	6.45	36,36,36,36	0
24	PAR	A	1611	42/42	0.91	0.30	6.43	131,131,131,131	0
25	MG	A	1794	1/1	0.80	0.34	6.37	61,61,61,61	0
25	MG	A	1883	1/1	0.74	0.37	5.84	62,62,62,62	0
25	MG	A	1694	1/1	0.92	0.26	5.27	108,108,108,108	0
25	MG	A	1934	1/1	0.85	0.25	5.04	69,69,69,69	0
24	PAR	A	1615	42/42	0.81	0.32	5.03	149,149,149,149	0
24	PAR	A	1616	42/42	0.76	0.28	4.51	216,216,216,216	0
24	PAR	A	1608	42/42	0.89	0.25	4.14	81,81,81,81	42
25	MG	A	1918	1/1	0.87	0.25	3.95	39,39,39,39	0
24	PAR	A	1613	42/42	0.92	0.24	3.94	120,120,120,120	0
24	PAR	A	1610	42/42	0.88	0.38	3.69	144,144,144,144	0
24	PAR	A	1617	42/42	0.87	0.30	3.61	189,189,189,189	0
25	MG	A	1862	1/1	0.90	0.27	3.34	38,38,38,38	0
25	MG	A	1935	1/1	0.83	0.32	3.27	57,57,57,57	0
24	PAR	A	1612	42/42	0.90	0.22	2.99	131,131,131,131	0
25	MG	A	1651	1/1	0.96	0.20	2.60	48,48,48,48	0
25	MG	A	1740	1/1	0.98	0.17	2.58	113,113,113,113	0
26	ZN	D	301	1/1	0.98	0.30	2.03	141,141,141,141	0
24	PAR	A	1604	42/42	0.95	0.24	1.98	64,64,64,64	0
25	MG	A	1657	1/1	0.92	0.22	1.96	101,101,101,101	0
25	MG	A	1682	1/1	0.86	0.16	1.72	104,104,104,104	0
25	MG	S	101	1/1	0.97	0.28	1.72	22,22,22,22	0
24	PAR	A	1609	42/42	0.89	0.34	1.50	121,121,121,121	42
25	MG	A	1802	1/1	0.96	0.26	1.46	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
24	PAR	A	1606	42/42	0.93	0.21	1.39	113,113,113,113	0
25	MG	A	1915	1/1	0.96	0.22	1.37	59,59,59,59	0
25	MG	A	1635	1/1	0.88	0.26	1.18	45,45,45,45	0
25	MG	A	1649	1/1	0.91	0.19	0.93	47,47,47,47	0
24	PAR	A	1601	42/42	0.96	0.17	0.90	64,64,64,64	0
25	MG	A	1858	1/1	0.88	0.16	0.90	37,37,37,37	0
24	PAR	A	1605	42/42	0.90	0.23	0.89	94,94,94,94	42
25	MG	A	1760	1/1	0.94	0.18	0.87	44,44,44,44	0
25	MG	A	1764	1/1	0.96	0.22	0.82	65,65,65,65	0
25	MG	A	1754	1/1	0.90	0.22	0.77	67,67,67,67	0
24	PAR	A	1603	42/42	0.94	0.19	0.44	103,103,103,103	3
24	PAR	A	1607	42/42	0.92	0.23	0.33	99,99,99,99	42
25	MG	A	1673	1/1	0.94	0.17	0.21	73,73,73,73	0
25	MG	A	1879	1/1	0.96	0.17	0.02	56,56,56,56	0
25	MG	A	1678	1/1	0.97	0.20	-0.05	48,48,48,48	0
24	PAR	A	1602	42/42	0.95	0.16	-0.09	71,71,71,71	0
25	MG	A	1687	1/1	0.96	0.13	-0.11	53,53,53,53	0
25	MG	A	1759	1/1	0.82	0.16	-0.23	121,121,121,121	0
25	MG	A	1907	1/1	0.95	0.14	-0.31	53,53,53,53	0
26	ZN	N	101	1/1	0.99	0.14	-0.45	88,88,88,88	0
25	MG	A	1793	1/1	0.96	0.19	-0.55	22,22,22,22	0
25	MG	D	303	1/1	0.95	0.16	-0.87	73,73,73,73	0
25	MG	A	1844	1/1	0.85	0.17	-1.02	35,35,35,35	0
25	MG	A	1749	1/1	0.99	0.15	-1.04	72,72,72,72	0
25	MG	A	1666	1/1	0.97	0.13	-1.18	91,91,91,91	0
25	MG	A	1826	1/1	0.97	0.12	-1.25	44,44,44,44	0
25	MG	A	1661	1/1	0.95	0.10	-1.27	90,90,90,90	0
25	MG	A	1634	1/1	0.98	0.13	-1.48	42,42,42,42	0
25	MG	Q	201	1/1	0.93	0.15	-1.53	60,60,60,60	0
25	MG	A	1762	1/1	0.98	0.13	-1.60	63,63,63,63	0
25	MG	A	1910	1/1	0.96	0.10	-1.66	45,45,45,45	0
25	MG	A	1711	1/1	0.98	0.09	-1.70	64,64,64,64	0
25	MG	A	1942	1/1	0.92	0.08	-1.74	143,143,143,143	0
25	MG	A	1814	1/1	0.97	0.16	-1.85	26,26,26,26	0
25	MG	A	1646	1/1	0.96	0.12	-2.01	69,69,69,69	0
25	MG	A	1743	1/1	0.94	0.12	-2.05	71,71,71,71	0
25	MG	A	1938	1/1	0.97	0.05	-2.16	43,43,43,43	0
25	MG	A	1667	1/1	0.97	0.15	-2.35	56,56,56,56	0
25	MG	A	1774	1/1	0.89	0.08	-3.32	71,71,71,71	0
25	MG	A	1644	1/1	0.99	0.09	-3.32	40,40,40,40	0
25	MG	A	1775	1/1	0.99	0.07	-3.52	75,75,75,75	0
25	MG	A	1848	1/1	0.94	0.13	-3.74	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
25	MG	A	1658	1/1	0.98	0.08	-4.83	57,57,57,57	0
25	MG	A	1698	1/1	0.98	0.08	-5.37	56,56,56,56	0
25	MG	A	1751	1/1	0.93	0.08	-7.98	95,95,95,95	0
25	MG	A	1629	1/1	0.99	0.10	-8.18	60,60,60,60	0
25	MG	A	1874	1/1	0.98	0.37	-	13,13,13,13	0
25	MG	A	1648	1/1	0.99	0.13	-	64,64,64,64	0
25	MG	A	1880	1/1	0.81	0.28	-	60,60,60,60	0
25	MG	A	1729	1/1	0.99	0.04	-	73,73,73,73	0
25	MG	A	1840	1/1	0.87	0.34	-	22,22,22,22	0
25	MG	A	1654	1/1	0.98	0.09	-	75,75,75,75	0
25	MG	A	1913	1/1	0.89	0.37	-	49,49,49,49	0
25	MG	A	1919[A]	1/1	0.70	0.27	-	9,9,9,9	1
25	MG	A	1664	1/1	0.93	0.38	-	74,74,74,74	0
25	MG	A	1756	1/1	0.95	0.10	-	93,93,93,93	0
25	MG	A	1955	1/1	0.88	0.14	-	179,179,179,179	0
25	MG	A	1723	1/1	0.81	0.11	-	94,94,94,94	0
25	MG	A	1773	1/1	0.87	0.18	-	74,74,74,74	0
25	MG	A	1660	1/1	0.99	0.17	-	84,84,84,84	0
25	MG	A	1738	1/1	0.98	0.11	-	59,59,59,59	0
25	MG	A	1742	1/1	0.95	0.21	-	72,72,72,72	0
25	MG	A	1950	1/1	0.86	0.19	-	177,177,177,177	0
25	MG	A	1904	1/1	0.90	0.21	-	49,49,49,49	0
25	MG	A	1892	1/1	0.83	0.22	-	46,46,46,46	0
25	MG	A	1926	1/1	0.95	0.10	-	58,58,58,58	0
25	MG	A	1633	1/1	0.97	0.06	-	54,54,54,54	0
25	MG	A	1780	1/1	0.89	0.49	-	72,72,72,72	0
25	MG	A	1957	1/1	0.85	0.13	-	103,103,103,103	0
25	MG	A	1770	1/1	0.94	0.22	-	90,90,90,90	0
25	MG	A	1639	1/1	0.96	0.35	-	55,55,55,55	0
25	MG	A	1882[B]	1/1	0.74	0.60	-	0,0,0,0	1
25	MG	E	201	1/1	0.78	0.21	-	92,92,92,92	0
25	MG	A	1886	1/1	0.95	0.27	-	50,50,50,50	0
25	MG	A	1779	1/1	0.91	0.23	-	55,55,55,55	0
25	MG	A	1677	1/1	0.94	0.48	-	118,118,118,118	0
25	MG	A	1788	1/1	0.91	0.32	-	95,95,95,95	0
25	MG	A	1686	1/1	0.97	0.14	-	91,91,91,91	0
25	MG	A	1753	1/1	0.82	0.10	-	94,94,94,94	0
25	MG	E	203	1/1	0.89	0.10	-	80,80,80,80	0
25	MG	A	1632	1/1	0.99	0.10	-	65,65,65,65	0
25	MG	A	1638	1/1	0.91	0.26	-	56,56,56,56	0
25	MG	A	1778	1/1	0.86	0.39	-	59,59,59,59	0
25	MG	A	1836	1/1	0.42	0.30	-	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
25	MG	A	1768	1/1	0.86	0.16	-	103,103,103,103	0
25	MG	A	1732	1/1	0.95	0.09	-	84,84,84,84	0
25	MG	A	1791	1/1	0.89	0.26	-	30,30,30,30	0
25	MG	A	1931	1/1	0.76	0.69	-	58,58,58,58	0
25	MG	S	102	1/1	0.73	0.24	-	73,73,73,73	0
25	MG	A	1894	1/1	0.90	0.23	-	66,66,66,66	0
25	MG	A	1906	1/1	0.94	0.19	-	73,73,73,73	0
25	MG	A	1952	1/1	0.72	0.18	-	148,148,148,148	0
25	MG	A	1843	1/1	0.96	0.09	-	35,35,35,35	0
25	MG	A	1951	1/1	0.87	0.25	-	110,110,110,110	0
25	MG	A	1767	1/1	0.98	0.12	-	72,72,72,72	0
25	MG	A	1905	1/1	0.85	0.71	-	83,83,83,83	0
25	MG	A	1929	1/1	0.84	0.76	-	44,44,44,44	0
25	MG	A	1897[B]	1/1	0.86	0.53	-	0,0,0,0	1
25	MG	A	1721	1/1	0.76	0.83	-	43,43,43,43	0
25	MG	A	1769	1/1	0.85	0.16	-	114,114,114,114	0
25	MG	A	1835	1/1	0.77	0.24	-	71,71,71,71	0
25	MG	A	1709	1/1	0.95	0.08	-	94,94,94,94	0
25	MG	A	1670	1/1	0.76	0.19	-	64,64,64,64	0
25	MG	A	1869	1/1	0.52	0.88	-	59,59,59,59	0
25	MG	A	1898	1/1	0.86	0.31	-	61,61,61,61	0
25	MG	A	1676	1/1	0.91	0.27	-	75,75,75,75	0
25	MG	A	1817	1/1	0.88	0.63	-	54,54,54,54	0
25	MG	A	1855	1/1	0.91	0.16	-	24,24,24,24	0
25	MG	A	1893	1/1	0.75	0.55	-	53,53,53,53	0
25	MG	A	1700	1/1	0.84	0.38	-	26,26,26,26	0
25	MG	A	1662	1/1	0.74	0.43	-	77,77,77,77	0
25	MG	A	1838	1/1	0.97	0.56	-	50,50,50,50	0
25	MG	A	1882[A]	1/1	0.74	0.60	-	0,0,0,0	1
25	MG	A	1622	1/1	0.84	0.08	-	106,106,106,106	0
25	MG	A	1766	1/1	0.97	0.07	-	97,97,97,97	0
25	MG	A	1956	1/1	0.77	0.15	-	193,193,193,193	0
25	MG	A	1630	1/1	0.98	0.07	-	83,83,83,83	0
25	MG	A	1703	1/1	0.89	0.24	-	57,57,57,57	0
25	MG	A	1916	1/1	0.84	0.39	-	51,51,51,51	0
25	MG	A	1704	1/1	0.96	0.13	-	83,83,83,83	0
25	MG	A	1739	1/1	0.70	0.27	-	85,85,85,85	0
25	MG	A	1745	1/1	0.87	0.36	-	64,64,64,64	0
25	MG	A	1873	1/1	0.97	0.51	-	29,29,29,29	0
25	MG	P	103	1/1	0.87	0.20	-	44,44,44,44	0
25	MG	A	1798	1/1	0.71	0.17	-	70,70,70,70	0
25	MG	A	1801	1/1	0.70	0.84	-	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
25	MG	A	1679	1/1	0.93	0.18	-	47,47,47,47	0
25	MG	A	1800[A]	1/1	0.74	0.52	-	7,7,7,7	1
25	MG	A	1727	1/1	0.91	0.08	-	101,101,101,101	0
25	MG	A	1781	1/1	0.96	0.14	-	67,67,67,67	0
25	MG	A	1827	1/1	0.88	0.29	-	78,78,78,78	0
25	MG	A	1833	1/1	0.78	0.20	-	59,59,59,59	0
25	MG	A	1656	1/1	0.97	0.15	-	67,67,67,67	0
25	MG	A	1786	1/1	0.92	0.21	-	97,97,97,97	0
25	MG	A	1831	1/1	0.91	0.14	-	40,40,40,40	0
25	MG	A	1792	1/1	0.97	0.28	-	32,32,32,32	0
25	MG	A	1674	1/1	0.95	0.20	-	18,18,18,18	0
25	MG	A	1941	1/1	0.88	0.13	-	145,145,145,145	0
25	MG	A	1696	1/1	0.95	0.09	-	136,136,136,136	0
25	MG	A	1806	1/1	0.75	0.60	-	91,91,91,91	0
25	MG	A	1917	1/1	0.70	0.39	-	61,61,61,61	0
25	MG	A	1641	1/1	0.94	0.16	-	56,56,56,56	0
25	MG	A	1713	1/1	0.82	0.35	-	63,63,63,63	0
25	MG	A	1909	1/1	0.78	0.81	-	68,68,68,68	0
25	MG	H	201	1/1	0.95	0.55	-	53,53,53,53	0
25	MG	A	1695	1/1	0.96	0.17	-	94,94,94,94	0
25	MG	A	1799	1/1	0.96	0.34	-	59,59,59,59	0
25	MG	A	1868	1/1	0.69	0.41	-	68,68,68,68	0
25	MG	A	1652[A]	1/1	0.79	0.47	-	11,11,11,11	1
25	MG	A	1899	1/1	0.96	0.54	-	18,18,18,18	0
25	MG	A	1637	1/1	0.94	0.17	-	29,29,29,29	0
25	MG	A	1642	1/1	0.96	0.13	-	70,70,70,70	0
25	MG	A	1750	1/1	0.83	0.54	-	67,67,67,67	0
25	MG	A	1922	1/1	0.74	0.60	-	76,76,76,76	0
25	MG	A	1705	1/1	0.97	0.13	-	57,57,57,57	0
25	MG	A	1841	1/1	0.74	0.39	-	64,64,64,64	0
25	MG	A	1712	1/1	0.87	0.19	-	34,34,34,34	0
25	MG	A	1812	1/1	0.58	0.68	-	65,65,65,65	0
25	MG	A	1653[B]	1/1	0.87	0.60	-	11,11,11,11	1
25	MG	A	1821	1/1	0.87	0.29	-	33,33,33,33	0
25	MG	A	1924	1/1	0.86	0.39	-	54,54,54,54	0
25	MG	A	1684	1/1	0.99	0.09	-	25,25,25,25	0
25	MG	P	101	1/1	0.89	0.21	-	13,13,13,13	0
25	MG	A	1692	1/1	0.96	0.13	-	74,74,74,74	0
25	MG	A	1737	1/1	0.99	0.14	-	63,63,63,63	0
25	MG	A	1925	1/1	0.89	0.18	-	42,42,42,42	0
25	MG	E	202	1/1	0.75	0.37	-	45,45,45,45	0
25	MG	A	1860	1/1	0.97	0.24	-	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
25	MG	A	1881	1/1	0.74	0.37	-	63,63,63,63	0
25	MG	A	1693	1/1	0.83	0.26	-	96,96,96,96	0
25	MG	A	1797	1/1	0.54	0.55	-	47,47,47,47	0
25	MG	A	1620	1/1	0.94	0.07	-	70,70,70,70	0
25	MG	A	1825	1/1	0.82	0.34	-	59,59,59,59	0
25	MG	A	1627	1/1	0.97	0.10	-	30,30,30,30	0
25	MG	A	1744	1/1	0.98	0.30	-	62,62,62,62	0
25	MG	A	1901[A]	1/1	0.87	0.21	-	16,16,16,16	1
25	MG	A	1946	1/1	0.80	0.10	-	146,146,146,146	0
25	MG	V	101	1/1	0.59	0.56	-	75,75,75,75	0
25	MG	A	1640	1/1	0.94	0.12	-	59,59,59,59	0
25	MG	A	1854	1/1	0.97	0.14	-	40,40,40,40	0
25	MG	A	1631	1/1	0.99	0.09	-	75,75,75,75	0
25	MG	A	1834	1/1	0.92	0.16	-	57,57,57,57	0
25	MG	A	1675	1/1	0.74	0.38	-	74,74,74,74	0
25	MG	A	1872	1/1	0.93	0.25	-	30,30,30,30	0
25	MG	A	1933	1/1	0.95	0.11	-	82,82,82,82	0
25	MG	A	1947	1/1	0.86	0.09	-	133,133,133,133	0
25	MG	A	1708	1/1	0.99	0.07	-	55,55,55,55	0
25	MG	A	1685	1/1	0.99	0.08	-	57,57,57,57	0
25	MG	A	1936	1/1	0.88	0.30	-	68,68,68,68	0
25	MG	A	1896	1/1	0.76	0.40	-	57,57,57,57	0
25	MG	A	1908	1/1	0.89	0.54	-	66,66,66,66	0
25	MG	A	1655	1/1	0.96	0.10	-	78,78,78,78	0
25	MG	A	1747	1/1	0.93	0.21	-	108,108,108,108	0
25	MG	A	1805	1/1	0.92	0.41	-	34,34,34,34	0
25	MG	A	1746	1/1	0.84	0.39	-	146,146,146,146	0
25	MG	A	1804	1/1	0.95	0.17	-	62,62,62,62	0
25	MG	A	1626	1/1	0.95	0.06	-	100,100,100,100	0
25	MG	A	1715	1/1	0.89	0.32	-	82,82,82,82	0
25	MG	A	1659	1/1	0.94	0.25	-	87,87,87,87	0
25	MG	A	1911	1/1	0.89	0.16	-	49,49,49,49	0
25	MG	T	201	1/1	0.93	0.30	-	88,88,88,88	0
25	MG	A	1923	1/1	0.96	0.17	-	29,29,29,29	0
25	MG	A	1809	1/1	0.65	0.89	-	76,76,76,76	0
25	MG	A	1680	1/1	0.99	0.11	-	67,67,67,67	0
25	MG	A	1944	1/1	0.97	0.11	-	74,74,74,74	0
25	MG	A	1757	1/1	0.95	0.07	-	133,133,133,133	0
25	MG	A	1954	1/1	0.71	0.41	-	150,150,150,150	0
25	MG	A	1863	1/1	0.89	0.21	-	53,53,53,53	0
25	MG	A	1719	1/1	0.85	0.39	-	72,72,72,72	0
25	MG	A	1861	1/1	0.82	0.08	-	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
25	MG	A	1690	1/1	0.96	0.17	-	100,100,100,100	0
25	MG	A	1820	1/1	0.78	0.40	-	70,70,70,70	0
25	MG	A	1683	1/1	0.90	0.20	-	102,102,102,102	0
25	MG	A	1720	1/1	0.86	0.28	-	89,89,89,89	0
25	MG	A	1901[B]	1/1	0.87	0.21	-	16,16,16,16	1
25	MG	A	1672	1/1	0.95	0.17	-	56,56,56,56	0
25	MG	A	1714	1/1	0.81	0.24	-	66,66,66,66	0
25	MG	A	1717	1/1	0.86	0.12	-	110,110,110,110	0
25	MG	A	1864[B]	1/1	0.82	0.28	-	11,11,11,11	1
25	MG	A	1777	1/1	0.91	0.39	-	60,60,60,60	0
25	MG	A	1857	1/1	0.67	0.99	-	54,54,54,54	0
25	MG	A	1691	1/1	0.87	0.33	-	111,111,111,111	0
25	MG	A	1789	1/1	0.91	0.29	-	127,127,127,127	0
25	MG	A	1839	1/1	0.96	0.17	-	56,56,56,56	0
25	MG	A	1932	1/1	0.65	1.24	-	71,71,71,71	0
25	MG	A	1765	1/1	0.91	0.10	-	113,113,113,113	0
25	MG	A	1851	1/1	0.84	0.35	-	57,57,57,57	0
25	MG	A	1943	1/1	0.87	0.23	-	178,178,178,178	0
25	MG	A	1811	1/1	0.88	0.28	-	56,56,56,56	0
25	MG	A	1647	1/1	0.98	0.21	-	72,72,72,72	0
25	MG	A	1852	1/1	0.82	0.33	-	47,47,47,47	0
25	MG	A	1706	1/1	0.95	0.24	-	52,52,52,52	0
25	MG	A	1846	1/1	0.98	0.19	-	49,49,49,49	0
25	MG	A	1871	1/1	0.92	0.21	-	63,63,63,63	0
25	MG	A	1808	1/1	0.91	0.24	-	31,31,31,31	0
25	MG	A	1725	1/1	0.95	0.23	-	67,67,67,67	0
25	MG	A	1702	1/1	0.77	0.12	-	104,104,104,104	0
25	MG	A	1876	1/1	0.76	0.73	-	69,69,69,69	0
25	MG	A	1919[B]	1/1	0.70	0.27	-	9,9,9,9	1
25	MG	O	101	1/1	0.68	0.21	-	112,112,112,112	0
25	MG	A	1681	1/1	0.77	0.40	-	30,30,30,30	0
25	MG	A	1891	1/1	0.74	0.70	-	50,50,50,50	0
25	MG	A	1900	1/1	0.97	0.21	-	27,27,27,27	0
25	MG	A	1819	1/1	0.81	0.43	-	64,64,64,64	0
25	MG	A	1902	1/1	0.93	0.22	-	64,64,64,64	0
25	MG	A	1741	1/1	0.95	0.22	-	52,52,52,52	0
25	MG	A	1748	1/1	0.93	0.26	-	87,87,87,87	0
25	MG	A	1837	1/1	0.88	0.33	-	54,54,54,54	0
25	MG	A	1701	1/1	0.87	0.16	-	85,85,85,85	0
25	MG	A	1625	1/1	0.95	0.16	-	30,30,30,30	0
25	MG	A	1787	1/1	0.81	0.23	-	66,66,66,66	0
25	MG	A	1621	1/1	0.95	0.16	-	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
25	MG	A	1865	1/1	0.76	0.61	-	58,58,58,58	0
25	MG	A	1697	1/1	0.90	0.20	-	77,77,77,77	0
25	MG	A	1669	1/1	0.66	0.53	-	76,76,76,76	0
25	MG	A	1845	1/1	0.88	0.24	-	64,64,64,64	0
25	MG	A	1813	1/1	0.32	0.74	-	53,53,53,53	0
25	MG	A	1671	1/1	0.99	0.12	-	66,66,66,66	0
25	MG	A	1822	1/1	0.82	0.28	-	63,63,63,63	0
25	MG	A	1628	1/1	0.93	0.24	-	48,48,48,48	0
25	MG	A	1730	1/1	0.92	0.10	-	118,118,118,118	0
25	MG	A	1885	1/1	0.78	0.35	-	45,45,45,45	0
25	MG	A	1877	1/1	0.83	0.10	-	59,59,59,59	0
25	MG	E	204	1/1	0.77	0.20	-	70,70,70,70	0
25	MG	A	1795	1/1	0.94	0.22	-	57,57,57,57	0
25	MG	L	201	1/1	0.79	0.14	-	57,57,57,57	0
25	MG	A	1636	1/1	0.97	0.21	-	68,68,68,68	0
25	MG	A	1755	1/1	0.92	0.18	-	74,74,74,74	0
25	MG	A	1903	1/1	0.65	0.29	-	74,74,74,74	0
25	MG	A	1830	1/1	0.79	0.24	-	70,70,70,70	0
25	MG	A	1771	1/1	0.85	0.45	-	89,89,89,89	0
25	MG	A	1807	1/1	0.84	0.60	-	83,83,83,83	0
25	MG	A	1624	1/1	0.98	0.17	-	58,58,58,58	0
25	MG	A	1847	1/1	0.43	0.68	-	85,85,85,85	0
25	MG	A	1870	1/1	0.87	0.28	-	35,35,35,35	0
25	MG	A	1785	1/1	0.98	0.11	-	51,51,51,51	0
25	MG	A	1800[B]	1/1	0.74	0.52	-	7,7,7,7	1
25	MG	A	1716	1/1	0.95	0.23	-	92,92,92,92	0
25	MG	A	1940	1/1	0.79	0.50	-	82,82,82,82	0
25	MG	A	1688	1/1	0.93	0.15	-	60,60,60,60	0
25	MG	A	1920	1/1	0.95	0.54	-	50,50,50,50	0
25	MG	A	1726	1/1	0.87	0.10	-	93,93,93,93	0
25	MG	A	1949	1/1	0.81	0.28	-	228,228,228,228	0
25	MG	A	1782	1/1	0.99	0.10	-	68,68,68,68	0
25	MG	A	1699	1/1	0.85	0.20	-	79,79,79,79	0
25	MG	A	1689	1/1	0.97	0.11	-	75,75,75,75	0
25	MG	A	1731	1/1	0.93	0.10	-	121,121,121,121	0
25	MG	A	1772	1/1	0.58	0.66	-	61,61,61,61	0
25	MG	A	1824	1/1	0.87	0.35	-	64,64,64,64	0
25	MG	A	1668	1/1	0.95	0.48	-	66,66,66,66	0
25	MG	A	1815	1/1	0.79	0.44	-	45,45,45,45	0
25	MG	A	1945	1/1	0.94	0.16	-	156,156,156,156	0
25	MG	A	1816	1/1	0.76	0.79	-	53,53,53,53	0
25	MG	A	1790	1/1	0.87	0.15	-	162,162,162,162	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
25	MG	A	1850	1/1	0.89	0.22	-	71,71,71,71	0
25	MG	A	1884	1/1	0.90	0.37	-	55,55,55,55	0
25	MG	D	302	1/1	0.69	0.43	-	71,71,71,71	0
25	MG	A	1736	1/1	0.80	0.19	-	88,88,88,88	0
25	MG	A	1707	1/1	0.96	0.14	-	80,80,80,80	0
25	MG	A	1643	1/1	0.66	0.51	-	40,40,40,40	0
25	MG	A	1953	1/1	0.87	0.13	-	179,179,179,179	0
25	MG	A	1722	1/1	0.97	0.07	-	43,43,43,43	0
25	MG	A	1897[A]	1/1	0.86	0.53	-	0,0,0,0	1
25	MG	A	1783	1/1	0.74	0.76	-	41,41,41,41	0
25	MG	A	1829	1/1	0.98	0.16	-	37,37,37,37	0
25	MG	A	1927	1/1	0.86	0.18	-	62,62,62,62	0
25	MG	A	1733	1/1	0.83	0.30	-	61,61,61,61	0
25	MG	A	1663	1/1	0.98	0.08	-	36,36,36,36	0
25	MG	A	1939	1/1	0.45	0.27	-	57,57,57,57	0
25	MG	A	1735	1/1	0.92	0.34	-	67,67,67,67	0
25	MG	A	1796	1/1	0.60	0.84	-	58,58,58,58	0
25	MG	A	1728	1/1	0.91	0.11	-	103,103,103,103	0
25	MG	A	1864[A]	1/1	0.82	0.28	-	11,11,11,11	1
25	MG	A	1842	1/1	0.85	0.80	-	43,43,43,43	0
25	MG	A	1761	1/1	0.68	0.19	-	155,155,155,155	0
25	MG	A	1849	1/1	0.91	0.39	-	40,40,40,40	0
25	MG	A	1875	1/1	0.96	0.12	-	14,14,14,14	0
25	MG	A	1887	1/1	0.67	0.66	-	64,64,64,64	0
25	MG	A	1948	1/1	0.91	0.12	-	122,122,122,122	0
25	MG	A	1650	1/1	0.93	0.20	-	86,86,86,86	0
25	MG	A	1784	1/1	0.66	0.31	-	89,89,89,89	0
25	MG	A	1776	1/1	0.85	0.20	-	65,65,65,65	0
25	MG	A	1734	1/1	0.50	0.46	-	63,63,63,63	0
25	MG	A	1665	1/1	0.93	0.18	-	57,57,57,57	0
25	MG	A	1856	1/1	0.69	0.26	-	59,59,59,59	0
25	MG	A	1645	1/1	0.80	0.28	-	53,53,53,53	0
25	MG	A	1866	1/1	0.46	1.76	-	53,53,53,53	0
25	MG	A	1895	1/1	0.81	0.43	-	44,44,44,44	0
25	MG	A	1758	1/1	0.97	0.36	-	85,85,85,85	0
25	MG	A	1930	1/1	0.93	0.40	-	79,79,79,79	0
25	MG	A	1928	1/1	0.64	0.68	-	93,93,93,93	0
25	MG	A	1937	1/1	0.83	0.35	-	61,61,61,61	0
25	MG	A	1763	1/1	0.96	0.15	-	65,65,65,65	0
25	MG	A	1752	1/1	0.89	0.14	-	147,147,147,147	0
25	MG	A	1921	1/1	0.83	0.39	-	48,48,48,48	0
25	MG	A	1889	1/1	0.57	0.56	-	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
25	MG	A	1828	1/1	0.59	0.47	-	107,107,107,107	0
25	MG	A	1724	1/1	0.96	0.12	-	82,82,82,82	0
25	MG	A	1859	1/1	0.88	0.46	-	73,73,73,73	0
25	MG	A	1878	1/1	0.97	0.28	-	13,13,13,13	0
25	MG	P	102	1/1	0.84	0.25	-	51,51,51,51	0
25	MG	A	1710	1/1	0.82	0.35	-	82,82,82,82	0
25	MG	A	1810	1/1	0.44	0.77	-	71,71,71,71	0
25	MG	A	1623	1/1	0.61	0.48	-	64,64,64,64	0
25	MG	A	1718	1/1	0.76	0.96	-	80,80,80,80	0

6.5 Other polymers [i](#)

There are no such residues in this entry.