



wwPDB X-ray Structure Validation Summary Report ⓘ

May 14, 2020 – 04:57 am BST

PDB ID : 4JI2
Title : Crystal Structure of 30S ribosomal subunit from *Thermus thermophilus*
Authors : Demirci, H.; Wang, L.; Murphy IV, F.; Murphy, E.; Carr, J.; Blanchard, S.;
Jogl, G.; Dahlberg, A.E.; Gregory, S.T.
Deposited on : 2013-03-05
Resolution : 3.64 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 : 2.11
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) : 2.11

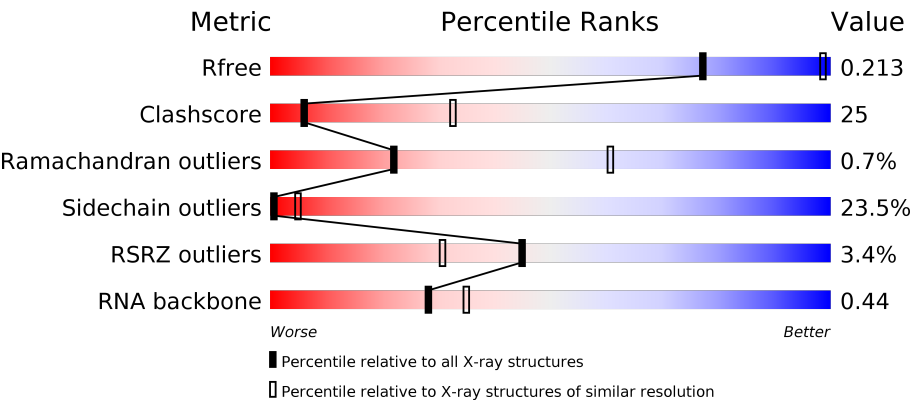
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.64 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.





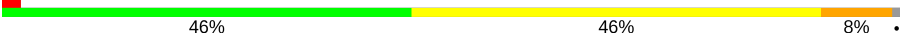
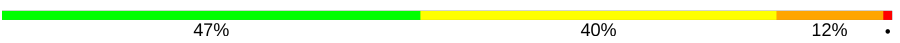


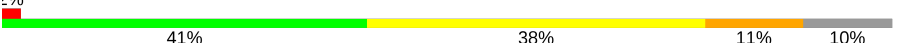
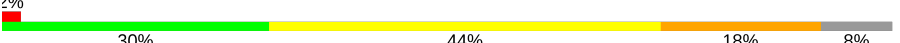
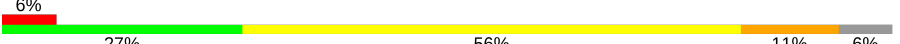

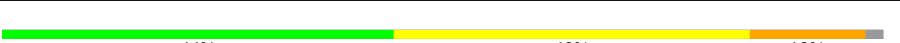
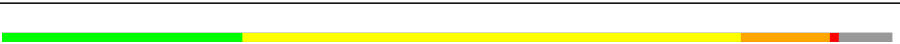
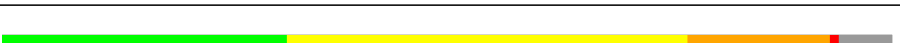
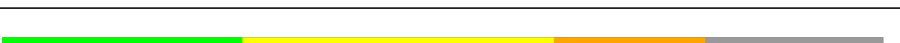

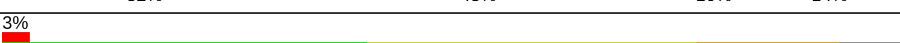
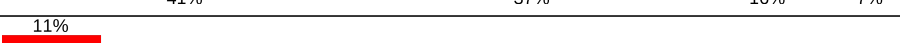
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	130704	1341 (3.78-3.50)
Clashscore	141614	1439 (3.78-3.50)
Ramachandran outliers	138981	1391 (3.78-3.50)
Sidechain outliers	138945	1391 (3.78-3.50)
RSRZ outliers	127900	1242 (3.78-3.50)
RNA backbone	3102	1019 (4.26-3.00)

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>2%</div><div>16%41%33%9%</div></div>
2	B	256	<div><div>%</div><div>37%40%13%9%</div></div>
3	C	239	<div><div>6%</div><div>27%44%14%14%</div></div>
4	D	209	<div><div>2%</div><div>35%49%14%</div></div>

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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	

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
1	PSU	A	1540	-	-	-	X
1	5MC	A	967	-	-	X	-
22	MG	A	1601	-	-	-	X
22	MG	A	1683	-	-	-	X
22	MG	A	1704	-	-	-	X
22	MG	A	1715	-	-	-	X
22	MG	A	1720	-	-	-	X
22	MG	A	1735	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	MG	A	1749	-	-	-	X
22	MG	A	1751	-	-	-	X
22	MG	A	1766	-	-	-	X
22	MG	A	1769	-	-	-	X
22	MG	A	1770	-	-	-	X
22	MG	A	1777	-	-	-	X
22	MG	A	1780	-	-	-	X
22	MG	A	1781	-	-	-	X
22	MG	A	1782	-	-	-	X
22	MG	A	1794	-	-	-	X
22	MG	A	1796	-	-	-	X
22	MG	A	1826	-	-	-	X
22	MG	A	1830	-	-	-	X
22	MG	A	1835	-	-	-	X
22	MG	A	1838	-	-	-	X
22	MG	A	1839	-	-	-	X
22	MG	A	1842	-	-	-	X
22	MG	A	1845	-	-	-	X
22	MG	A	1847	-	-	-	X
22	MG	A	1853	-	-	-	X
22	MG	A	1857	-	-	-	X
22	MG	A	1858	-	-	-	X
22	MG	A	1866	-	-	-	X
22	MG	C	301	-	-	-	X
22	MG	H	201	-	-	-	X
22	MG	P	102	-	-	-	X

2 Entry composition

There are 24 unique types of molecules in this entry. The entry contains 52307 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	6	0
			32644	14540	6039	10547	1518			

There are 2 discrepancies between the modelled and reference sequences:

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

- Molecule 2 is a protein called RIBOSOMAL PROTEIN S2.

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

- Molecule 3 is a protein called RIBOSOMAL PROTEIN S3.

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

- Molecule 4 is a protein called 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 RIBOSOMAL PROTEIN S5.

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

- Molecule 6 is a protein called 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 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 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 RIBOSOMAL PROTEIN S9.

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

- Molecule 10 is a protein called RIBOSOMAL PROTEIN S10.

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

- Molecule 11 is a protein called RIBOSOMAL PROTEIN S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	116	Total	C	N	O	S	0	0	0
			864	537	164	160	3			

- Molecule 12 is a protein called RIBOSOMAL PROTEIN S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	124	Total	C	N	O	S	0	0	0
			977	617	196	163	1			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	94	TRP	PRO	CONFLICT	UNP F6DEQ7

- Molecule 13 is a protein called 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 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 RIBOSOMAL PROTEIN S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	O	87	Total	C	N	O	S	0	0	0
			729	457	146	124	2			

- Molecule 16 is a protein called RIBOSOMAL PROTEIN S16.

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

- Molecule 17 is a protein called RIBOSOMAL PROTEIN S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Q	99	Total	C	N	O	S	0	0	0
			823	528	151	142	2			

- Molecule 18 is a protein called RIBOSOMAL PROTEIN S18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	R	70	Total	C	N	O		0	0	0
			574	367	112	95				

- Molecule 19 is a protein called RIBOSOMAL PROTEIN S19.

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

- Molecule 20 is a protein called 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 RIBOSOMAL PROTEIN THX.

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	P	2	Total	Mg	0	0
			2	2		
22	J	1	Total	Mg	0	0
			1	1		
22	Q	1	Total	Mg	0	0
			1	1		
22	D	3	Total	Mg	0	0
			3	3		
22	E	1	Total	Mg	0	0
			1	1		
22	H	1	Total	Mg	0	0
			1	1		
22	B	3	Total	Mg	0	0
			3	3		
22	I	1	Total	Mg	0	0
			1	1		
22	C	2	Total	Mg	0	0
			2	2		
22	A	276	Total	Mg	0	0
			276	276		
22	N	1	Total	Mg	0	0
			1	1		
22	F	1	Total	Mg	0	0
			1	1		

- Molecule 23 is ZINC ION (three-letter code: ZN) (formula: Zn).

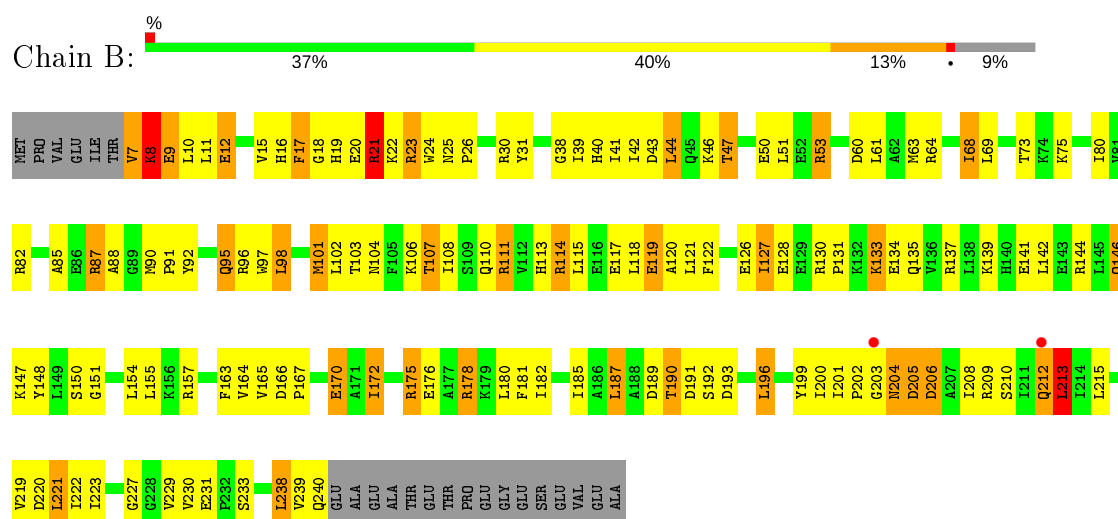
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
23	D	1	Total	Zn	0	0
			1	1		
23	N	1	Total	Zn	0	0
			1	1		

- Molecule 24 is water.

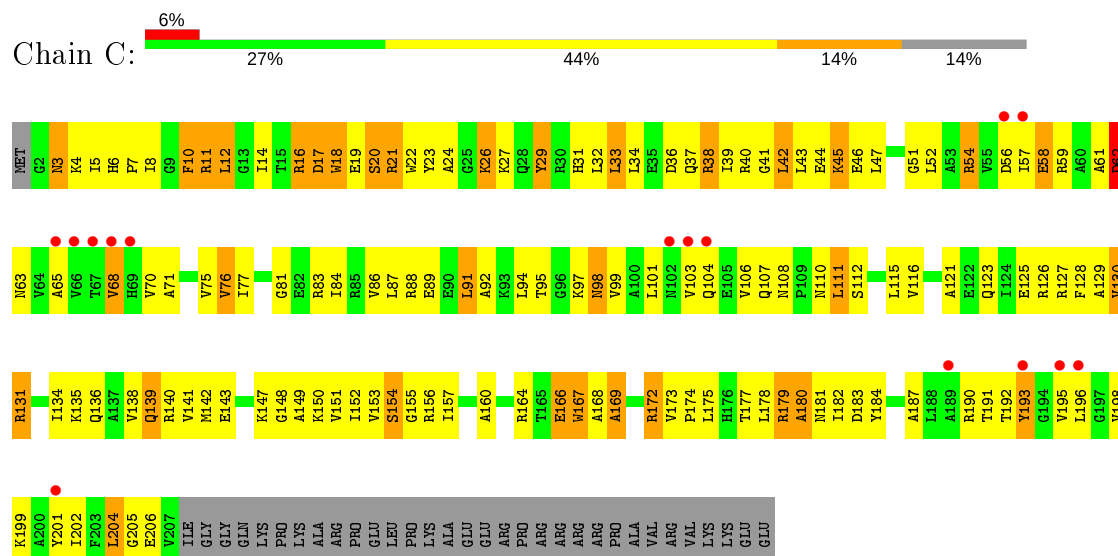
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
24	A	266	Total	O	0	0
			266	266		
24	E	3	Total	O	0	0
			3	3		
24	K	1	Total	O	0	0
			1	1		
24	L	1	Total	O	0	0
			1	1		
24	Q	2	Total	O	0	0
			2	2		
24	T	2	Total	O	0	0
			2	2		

U1532	C1397	G1338	G1276	G1214	G1149	U1078	U1020	U960	G998	C832	G770	C707
C1533	A1398	A1339	C1277	G1215	U1150	G1079	G1021	U961	C899	U833	G771	C708
C	C1399	A1340	U1278	G1216	A1151	A1080	G1022	G982	A900	U834	G772	
A	U1341	A1279	A1279	G1217	A1152	G1081	G1023	G983	A901	U835	G773	A712
C	G1401	G1342	A1280	G1218	C1153	G1084	G1024	A984	G902	G836	G774	G713
U	C1402	G1343	U1281	U1219	G1157	U1085	U1025	A965	G903	G837		G714
C	C1403	C1344	C1282	G1220	A1158	U1086	G1026	G966	C904	U838	A715	
C1539	C1404	U1345	G1283	G1221	C1159	U1087	C1027	G967		U839	A716	A716
	C1405	A1346	C1284	G1222	U1159	U1088	C1028	G968	A907	U840	C717	C717
	G1406	G1347	C1223	G1223	G1160	U1090	G1030A	A969	A908	U841	G718	G718
U1541	U1407	C1348	A1287	G1224	C1161	U1091	G1030B	A970	A909	U842	G719	G719
U1542	C1407	A1349	A1288	G1224	C1162	A1092	C1030C	G971	C910	U843	G720	G720
U1543	A1408	C1350	A1289	C1225	C1163	A1093	G1030C	G972	C911	U844	G721	G721
U1544	U1484	A1350	A1290	A1226	G1164	G1094	A1030D	G973	C912	U845	G722	A722
	U1545	U1351	G1291	A1227		U1095	G1031	A974	A913	G851	C784	
	G1411	C1352	G1292	C1228	A1167	U1096	G1032	A975	A914	G852	G785	U723
	C1412	G1353	U1292	A1229	U1168	C1097	G1033	A976	A915	G853	G786	U724
	A1413	C1354	G1293	U1232	A1169	U1098	G1034	A977	G916	G854	A787	G725
	U1414	G1355	G1294	G1233	A1171	U1099	A1035	A978	G917	G855	U788	G726
	G1415	G1356	G1295	G1234	G1172	C1100	G1036	G979	A918	C856	U789	G727
	G1416	A1357	C1296	C1235	C1173	A1101	C1037	G980	A919	C857	A790	A728
	G1417	C1358	C1297	A1236	G1174	A1102	C1038	G981	U920	C858	G791	A729
	A1418	A1359	G1298	G1237	G1175	A1103		U982	A860	A859	A792	G730
	G1419	C1360	A1299	C1237	G1176	G1104	A1041	G983	A861	C862	A794	C732
	C1420	G1361	U1301	A1239	A1177		G1042	A984	G863	C863	A795	A733
	U1421	C1362	U1302	U1240	G1178		G1043	C985	C924	U863	C796	G734
	G1422	A1363	C1303	G1241	A1179	C1108	A1044	A986	G925	A864	C797	C735
	C1423	U1364	G1304	C1242	A1180	A1110	C1045		G926	A865	G798	C736
	U1424	G1365	C1305	C1243	G1181	A1111	A1046		G927	C866	A737	A737
	C1425	C1366	A1306	G1244	G1182	C1112	G1047	G989	G928	G867	C738	C738
	U1426	C1367	U1307	A1245	A1183	C1113	G1048	G990	G929	C868	C739	
	U1427	G1368	U1308	C1246	G1184		U1049	U991	C930	C869	U740	
	C1431	C1369	G1309	C1249	G1185	G1117	G1050	U992	C931	U870	U804	
	G1432	G1370	G1310	A1250	G1186	C1118	U1051	G993	C932	U871	C805	G741
	A1433	C1371	G1311	G1251	G1187	C1119	U1052	A994	G933	U872	C806	G742
	U1434	U1372	G1312	A1252	A1188	A1123	G1053	A995	G934	A873	A807	U743
	G1435	G1373	U1313	A1252	C1189	G1124	A1054	A996	C935	C874	C808	C744
	U1436	A1374	C1314	G1253	G1190	U1125	A1055	G998	A936	C875	G809	C745
	C1437	U1375	U1315	G1254	A1191	U1126	U1056	G999	C936	C876	C810	A746
	G1438	U1376	G1316	G1255	C1192	U1127	U1057	U1000	A937	C877	C811	C747
	C1439	A1377	C1317	A1256	G1193	C1128	G1058	U1001	A938	C878	C812	C748
	C1440	G1378	A1318	U1257	U1194	C1129	C1059	G1002	G939	G879	U813	C749
	G1441	C1379	A1319	G1258	G1195	A1130	G1060	G1003	G940	C880	U814	G750
	G1442	U1380	C1320	C1259	U1196	G1131	G1061	U1003A	G941	C881	A815	U751
	U1443	U1381	G1321	C1260	G1197	C1132	U1062	A1004	G942	C882	A816	G752
	C1444	C1382	A1322	A1261	U1198		G1063	A1005	U943	C883	C817	A753
	G1445	G1383	G1323	C1262	G1199	U1135	G1064	C1006	G944	C884	G818	C754
	U1446	C1384	C1324	C1263	U1200	G1136	U1065	A946	G945	C885	G819	G755
	A1451	G1385	A1324	G1264	C1201	C1137	U1066	C1007	A947	G886	U820	C756
	C1452	G1386	G1327	G1265	G1202	G1138	A1067	G1008	G948	C887	G821	U757
	G1453	C1387	C1328	G1266	C1203	G1139	G1068	G1009	C949	C888	C822	G758
	U1454	G1388	A1329	G1267	A1204	C1140	C1069	G1010	A950	C889	C823	A759
	A1460	C1389	U1330	C1268	U1205	C1141	U1070	U1011	U951	A899	G824	G760
	G1461	U1390	A1269	G1270	G1206	C1142	C1071	G1012	G952	G890	C825	C761
	U1462	C1391	A1332	C1271	G1207	G1143	U1072	G1013	U953	U891	G826	C762
	C1463	G1392	G1333	G1271	C1208	G1144	U1073	A1014	G954	C892	U827	
	C1464	U1393	G1334	G1272	U1211	C1145	G1074	A1015	U955	C893	U828	G765
	U1465	A1394	G1273	G1274	A1146	C1147	C1075	A1016	U956	G894	A829	A766
	C1466	C1395	C1335	G1274	U1212	C1148	C1076	G1017	U957	G895	G830	A767
	G1469	U1396	C1336	A1275	A1213	U1148	G1077	C1019	A959	C896	U831	G769

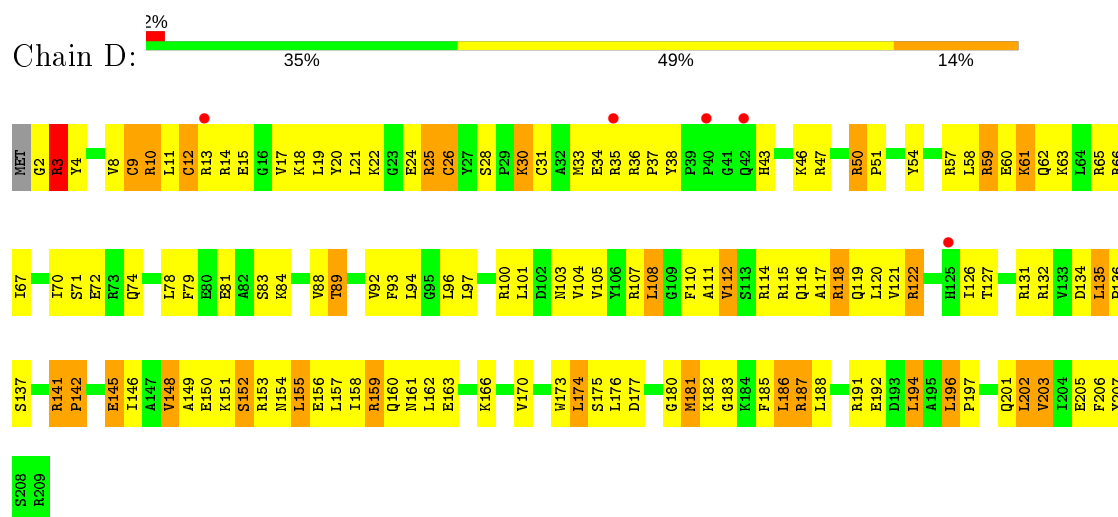
• Molecule 2: RIBOSOMAL PROTEIN S2



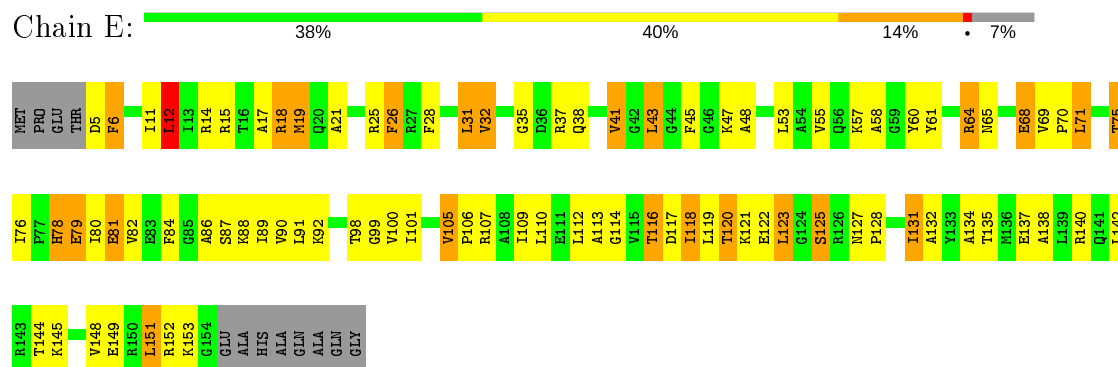
• Molecule 3: RIBOSOMAL PROTEIN S3



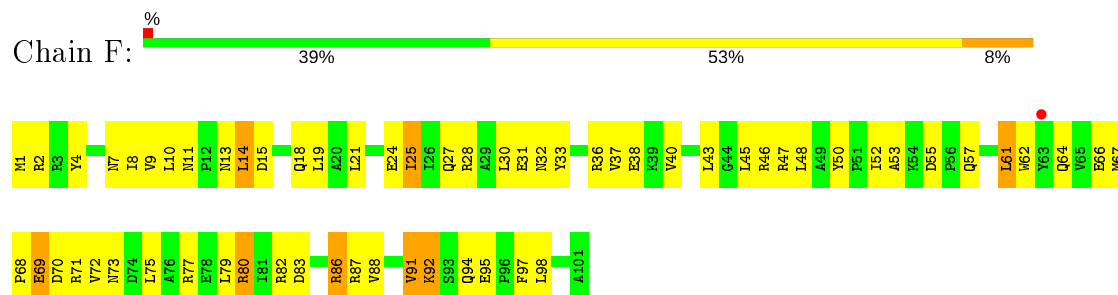
• Molecule 4: RIBOSOMAL PROTEIN S4



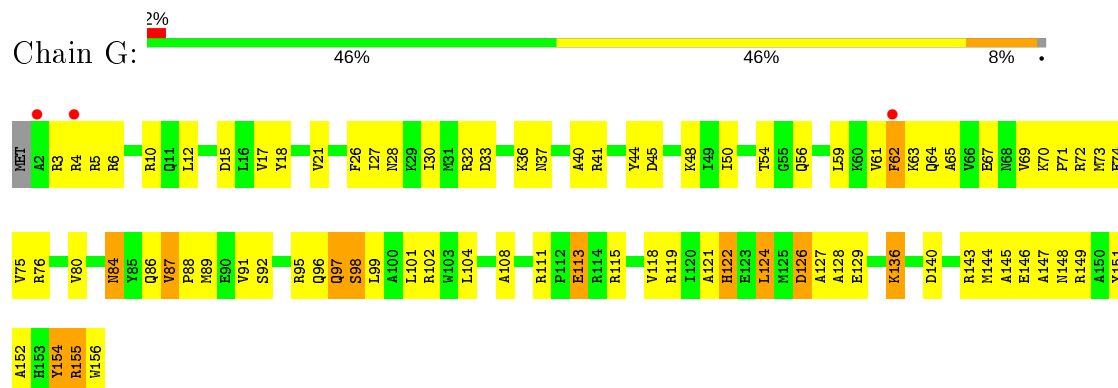
• Molecule 5: RIBOSOMAL PROTEIN S5



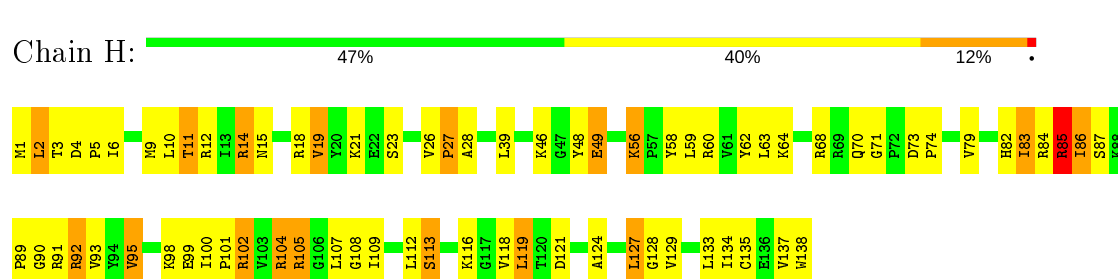
• Molecule 6: RIBOSOMAL PROTEIN S6

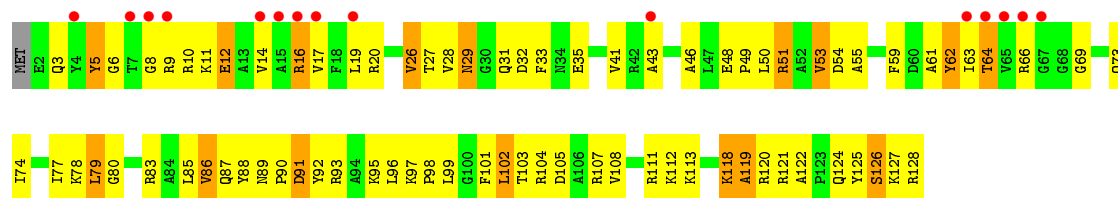


• Molecule 7: RIBOSOMAL PROTEIN S7

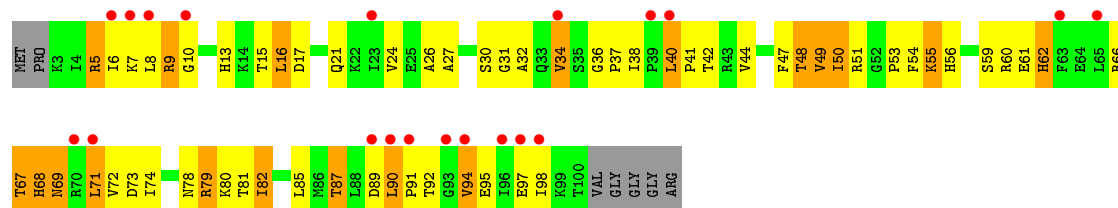


• Molecule 8: RIBOSOMAL PROTEIN S8

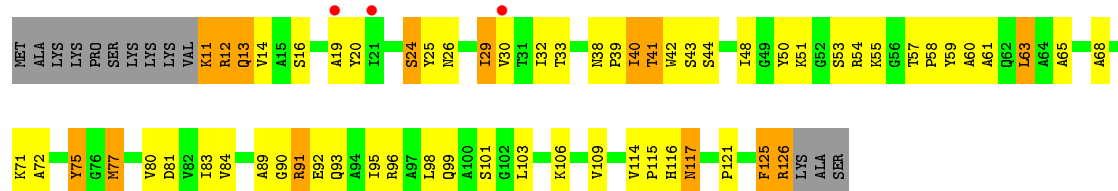
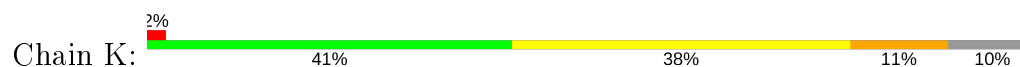




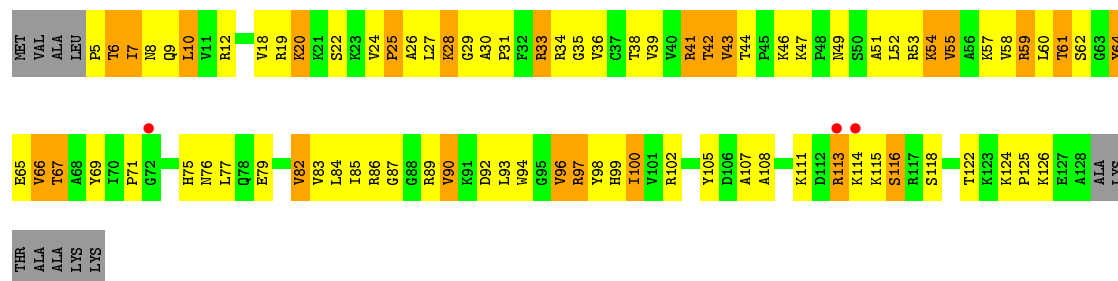
• Molecule 10: RIBOSOMAL PROTEIN S10



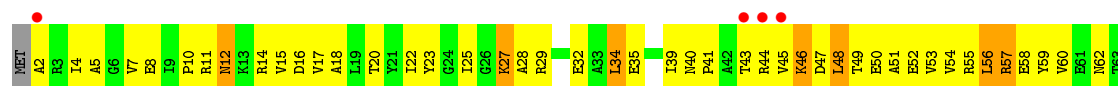
• Molecule 11: RIBOSOMAL PROTEIN S11

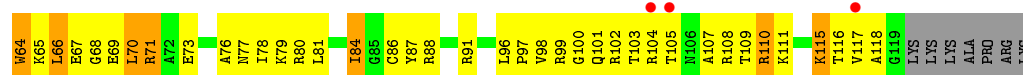


• Molecule 12: RIBOSOMAL PROTEIN S12



• Molecule 13: RIBOSOMAL PROTEIN S13

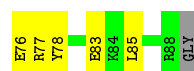
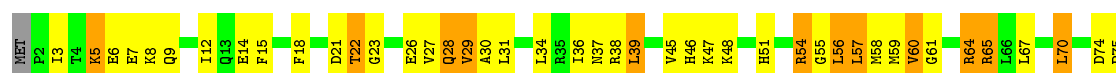




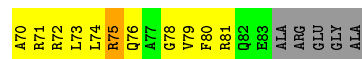
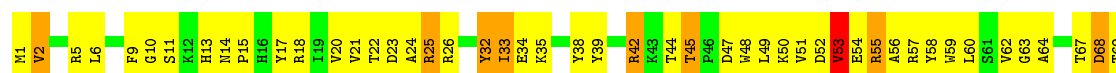
• Molecule 14: RIBOSOMAL PROTEIN S14



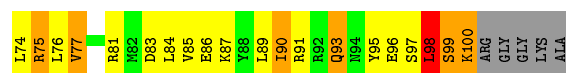
• Molecule 15: RIBOSOMAL PROTEIN S15



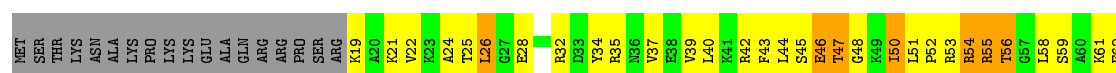
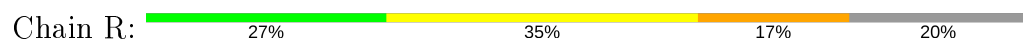
• Molecule 16: RIBOSOMAL PROTEIN S16



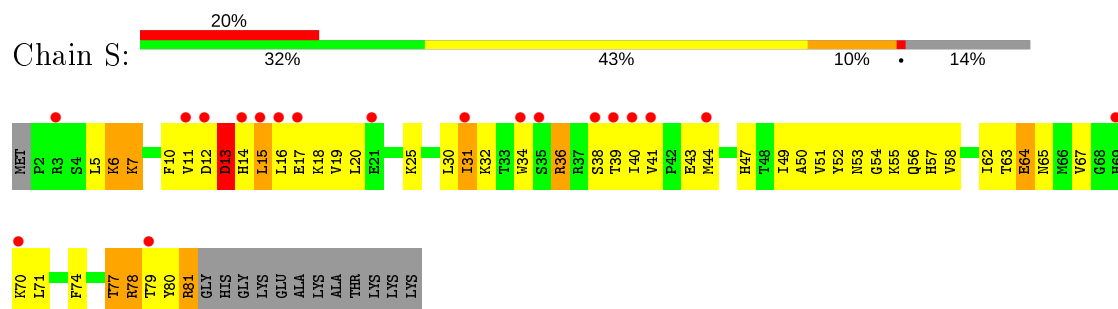
• Molecule 17: RIBOSOMAL PROTEIN S17



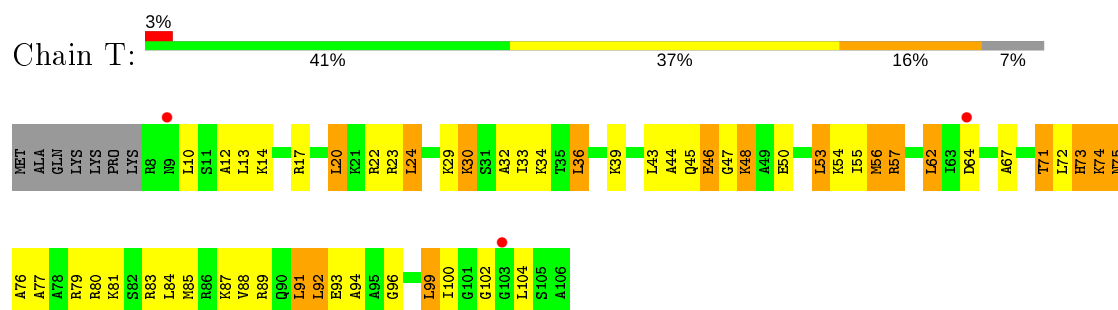
• Molecule 18: RIBOSOMAL PROTEIN S18



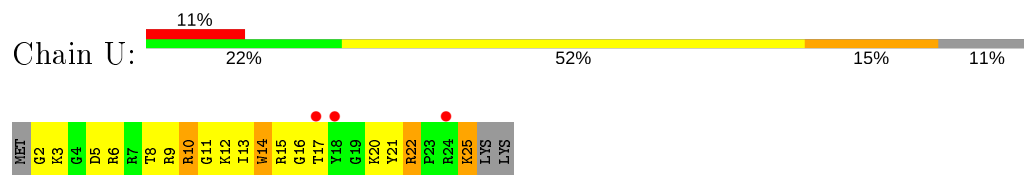
● Molecule 19: RIBOSOMAL PROTEIN S19



● Molecule 20: RIBOSOMAL PROTEIN S20



● Molecule 21: 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	402.45Å 402.45Å 174.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.34 – 3.64 49.57 – 3.64	Depositor EDS
% Data completeness (in resolution range)	98.9 (48.34-3.64) 98.9 (49.57-3.64)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.00 (at 3.67Å)	Xtriage
Refinement program	PHENIX dev_1119	Depositor
R, R_{free}	0.155 , 0.211 0.158 , 0.213	Depositor DCC
R_{free} test set	7893 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	120.3	Xtriage
Anisotropy	0.253	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 134.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	52307	wwPDB-VP
Average B, all atoms (Å ²)	153.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.70% 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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MA6, MG, 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	1.21	178/36139 (0.5%)	2.00	1849/56396 (3.3%)
2	B	0.71	0/1935	0.91	3/2609 (0.1%)
3	C	0.58	1/1636 (0.1%)	0.84	1/2205 (0.0%)
4	D	0.75	1/1733 (0.1%)	0.89	3/2318 (0.1%)
5	E	0.99	0/1162	1.13	2/1564 (0.1%)
6	F	0.61	0/856	0.81	0/1154
7	G	0.58	0/1276	0.78	0/1709
8	H	1.07	2/1136 (0.2%)	1.15	2/1527 (0.1%)
9	I	0.57	0/1029	0.79	0/1379
10	J	0.53	0/805	0.83	1/1082 (0.1%)
11	K	0.69	0/879	0.92	1/1187 (0.1%)
12	L	0.79	0/994	0.98	0/1331
13	M	0.64	0/947	0.87	0/1270
14	N	0.55	0/501	0.77	0/664
15	O	0.79	0/740	0.96	0/987
16	P	0.84	0/716	1.01	3/963 (0.3%)
17	Q	1.02	1/836 (0.1%)	1.14	2/1117 (0.2%)
18	R	0.75	0/579	0.98	1/768 (0.1%)
19	S	0.52	0/661	0.80	0/890
20	T	0.73	0/765	0.99	2/1007 (0.2%)
21	U	0.64	0/212	0.76	0/277
All	All	1.07	183/55537 (0.3%)	1.74	1870/82404 (2.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	2
3	C	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
4	D	0	1
7	G	0	1
8	H	0	2
10	J	0	2
12	L	0	2
13	M	0	1
18	R	0	1
19	S	0	1
20	T	0	2
All	All	0	18

The worst 5 of 183 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	279	A	N9-C4	-13.71	1.29	1.37
1	A	279	A	N3-C4	-13.61	1.26	1.34
1	A	279	A	N7-C5	-11.36	1.32	1.39
1	A	817	C	N1-C6	-10.06	1.31	1.37
1	A	793	U	C2-N3	9.46	1.44	1.37

The worst 5 of 1870 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	266	G	C6-C5-N7	-17.70	119.78	130.40
1	A	735	C	C6-N1-C2	16.27	126.81	120.30
1	A	117	G	N1-C6-O6	15.58	129.25	119.90
1	A	1516[A]	G	C8-N9-C4	-14.80	100.48	106.40
1	A	1516[B]	G	C8-N9-C4	-14.80	100.48	106.40

There are no chirality outliers.

5 of 18 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	20	GLU	Peptide
2	B	8	LYS	Peptide
3	C	166	GLU	Peptide
3	C	3	ASN	Peptide
3	C	89	GLU	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	32644	0	16503	1058	0
2	B	1900	0	1950	123	0
3	C	1612	0	1676	115	0
4	D	1703	0	1763	132	0
5	E	1146	0	1207	66	0
6	F	843	0	857	38	0
7	G	1257	0	1296	78	0
8	H	1116	0	1177	70	0
9	I	1010	0	1037	78	0
10	J	792	0	835	59	0
11	K	864	0	881	51	0
12	L	977	0	1060	78	0
13	M	937	0	995	72	0
14	N	492	0	529	37	0
15	O	729	0	768	38	0
16	P	700	0	720	45	0
17	Q	823	0	891	59	0
18	R	574	0	644	50	0
19	S	647	0	673	42	0
20	T	763	0	861	44	0
21	U	208	0	221	22	0
22	A	276	0	0	0	0
22	B	3	0	0	0	0
22	C	2	0	0	0	0
22	D	3	0	0	0	0
22	E	1	0	0	0	0
22	F	1	0	0	0	0
22	H	1	0	0	0	0
22	I	1	0	0	0	0
22	J	1	0	0	0	0
22	N	1	0	0	0	0
22	P	2	0	0	0	0
22	Q	1	0	0	0	0
23	D	1	0	0	0	0
23	N	1	0	0	0	0
24	A	266	0	0	7	0
24	E	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	K	1	0	0	0	0
24	L	1	0	0	0	0
24	Q	2	0	0	0	0
24	T	2	0	0	1	0
All	All	52307	0	36544	2147	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 25.

The worst 5 of 2147 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)
6:F:14:LEU:HD13	6:F:18:GLN:HB3	1.36	1.05
4:D:3:ARG:HH11	4:D:71:SER:H	1.13	0.94
1:A:1240:U:OP1	7:G:119:ARG:NH2	2.01	0.93
1:A:1399:C:H4'	1:A:1400:5MC:H5''	1.51	0.93
1:A:992:U:H3	1:A:1044:A:H62	1.09	0.92

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	232/256 (91%)	211 (91%)	18 (8%)	3 (1%)	12	48
3	C	204/239 (85%)	170 (83%)	32 (16%)	2 (1%)	15	54
4	D	206/209 (99%)	189 (92%)	17 (8%)	0	100	100
5	E	148/162 (91%)	135 (91%)	12 (8%)	1 (1%)	22	61
6	F	99/101 (98%)	90 (91%)	9 (9%)	0	100	100
7	G	153/156 (98%)	138 (90%)	15 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	H	136/138 (99%)	126 (93%)	10 (7%)	0	100	100
9	I	125/128 (98%)	112 (90%)	12 (10%)	1 (1%)	19	58
10	J	96/105 (91%)	79 (82%)	16 (17%)	1 (1%)	15	54
11	K	114/129 (88%)	100 (88%)	14 (12%)	0	100	100
12	L	122/135 (90%)	109 (89%)	12 (10%)	1 (1%)	19	58
13	M	116/126 (92%)	104 (90%)	9 (8%)	3 (3%)	5	34
14	N	58/61 (95%)	47 (81%)	11 (19%)	0	100	100
15	O	85/89 (96%)	71 (84%)	14 (16%)	0	100	100
16	P	81/88 (92%)	73 (90%)	7 (9%)	1 (1%)	13	50
17	Q	97/105 (92%)	89 (92%)	8 (8%)	0	100	100
18	R	68/88 (77%)	58 (85%)	10 (15%)	0	100	100
19	S	78/93 (84%)	68 (87%)	8 (10%)	2 (3%)	5	34
20	T	97/106 (92%)	88 (91%)	7 (7%)	2 (2%)	7	39
21	U	22/27 (82%)	20 (91%)	2 (9%)	0	100	100
All	All	2337/2541 (92%)	2077 (89%)	243 (10%)	17 (1%)	22	61

5 of 17 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	21	ARG
9	I	119	ALA
12	L	28	LYS
3	C	180	ALA
19	S	31	ILE

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	202/220 (92%)	148 (73%)	54 (27%)	0	3
3	C	160/188 (85%)	113 (71%)	47 (29%)	0	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	D	180/181 (99%)	139 (77%)	41 (23%)	1	5
5	E	115/123 (94%)	80 (70%)	35 (30%)	0	2
6	F	90/90 (100%)	68 (76%)	22 (24%)	0	4
7	G	126/127 (99%)	104 (82%)	22 (18%)	2	12
8	H	119/119 (100%)	95 (80%)	24 (20%)	1	8
9	I	98/99 (99%)	77 (79%)	21 (21%)	1	6
10	J	87/92 (95%)	65 (75%)	22 (25%)	0	4
11	K	88/99 (89%)	72 (82%)	16 (18%)	1	10
12	L	104/111 (94%)	74 (71%)	30 (29%)	0	2
13	M	94/101 (93%)	71 (76%)	23 (24%)	0	4
14	N	49/50 (98%)	42 (86%)	7 (14%)	3	21
15	O	79/80 (99%)	62 (78%)	17 (22%)	1	6
16	P	72/74 (97%)	57 (79%)	15 (21%)	1	7
17	Q	94/97 (97%)	74 (79%)	20 (21%)	1	7
18	R	61/77 (79%)	46 (75%)	15 (25%)	0	4
19	S	71/80 (89%)	57 (80%)	14 (20%)	1	8
20	T	76/82 (93%)	59 (78%)	17 (22%)	1	6
21	U	19/22 (86%)	14 (74%)	5 (26%)	0	4
All	All	1984/2112 (94%)	1517 (76%)	467 (24%)	1	5

5 of 467 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	G	87	VAL
9	I	102	LEU
19	S	6	LYS
7	G	126	ASP
8	H	98	LYS

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

Mol	Chain	Res	Type
7	G	148	ASN
9	I	73	GLN
11	K	116	HIS

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Mol	Chain	Res	Type
5	E	65	ASN
9	I	124	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1504/1522 (98%)	377 (25%)	59 (3%)

5 of 377 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	6	G
1	A	7	G
1	A	8	A
1	A	9	G
1	A	32	A

5 of 59 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	792	A
1	A	991	U
1	A	1347	G
1	A	812	C
1	A	840	C

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

16 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	MA6	A	1519[B]	1	19,26,27	1.31	4 (21%)	18,38,41	0.55	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	4OC	A	1402	1	16,23,24	1.01	0	17,32,35	0.93	1 (5%)
1	5MC	A	1404	1	15,22,23	1.79	2 (13%)	19,32,35	1.43	3 (15%)
1	PSU	A	516	1	17,21,22	0.99	1 (5%)	20,30,33	2.94	7 (35%)
1	5MC	A	1400	1	15,22,23	0.88	0	19,32,35	1.52	3 (15%)
1	MA6	A	1519[A]	1	19,26,27	0.86	1 (5%)	18,38,41	0.75	1 (5%)
1	M2G	A	966	1	20,27,28	1.32	2 (10%)	22,40,43	2.28	2 (9%)
1	MA6	A	1518[B]	1	19,26,27	1.32	3 (15%)	18,38,41	1.12	2 (11%)
1	5MC	A	967	1	15,22,23	0.86	0	19,32,35	1.32	2 (10%)
1	MA6	A	1518[A]	1	19,26,27	1.08	2 (10%)	18,38,41	0.73	0
1	PSU	A	1540	1	17,21,22	1.01	1 (5%)	20,30,33	3.03	5 (25%)
1	UR3	A	1498	1,22	14,22,23	1.35	2 (14%)	15,32,35	1.43	2 (13%)
1	5MC	A	1407	1	15,22,23	1.54	3 (20%)	19,32,35	1.22	1 (5%)
1	7MG	A	527	1,22	22,26,27	2.17	7 (31%)	28,39,42	1.55	8 (28%)
1	2MG	A	1207	1	19,26,27	2.79	5 (26%)	21,38,41	2.01	3 (14%)
1	PSU	A	1541	1	17,21,22	0.96	2 (11%)	20,30,33	3.12	6 (30%)

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	MA6	A	1519[B]	1	-	3/7/29/30	0/3/3/3
1	4OC	A	1402	1	-	4/9/29/30	0/2/2/2
1	5MC	A	1404	1	-	1/5/25/26	0/2/2/2
1	PSU	A	516	1	-	0/7/25/26	0/2/2/2
1	5MC	A	1400	1	-	2/5/25/26	0/2/2/2
1	MA6	A	1519[A]	1	-	5/7/29/30	0/3/3/3
1	M2G	A	966	1	-	6/7/29/30	0/3/3/3
1	MA6	A	1518[B]	1	-	2/7/29/30	0/3/3/3
1	5MC	A	967	1	-	3/5/25/26	0/2/2/2
1	MA6	A	1518[A]	1	-	0/7/29/30	0/3/3/3
1	PSU	A	1540	1	-	2/7/25/26	0/2/2/2
1	UR3	A	1498	1,22	-	2/5/25/26	0/2/2/2
1	5MC	A	1407	1	-	0/5/25/26	0/2/2/2
1	7MG	A	527	1,22	-	2/7/37/38	0/3/3/3
1	2MG	A	1207	1	-	4/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	A	1541	1	-	0/7/25/26	0/2/2/2

The worst 5 of 35 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1207	2MG	C2-N2	8.85	1.41	1.34
1	A	1207	2MG	C6-N1	6.67	1.44	1.33
1	A	1404	5MC	C5-C4	5.89	1.50	1.41
1	A	527	7MG	C2-N2	4.50	1.42	1.33
1	A	527	7MG	C4-N3	4.48	1.40	1.34

The worst 5 of 46 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1540	PSU	N1-C2-N3	-10.54	120.05	128.43
1	A	1541	PSU	N1-C2-N3	-10.51	120.08	128.43
1	A	516	PSU	N1-C2-N3	-9.57	120.82	128.43
1	A	966	M2G	C5-C6-N1	-8.12	112.33	123.43
1	A	1207	2MG	C5-C6-N1	-7.20	113.58	123.43

There are no chirality outliers.

5 of 36 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1519[B]	MA6	C5-C6-N6-C9
1	A	1519[B]	MA6	N1-C6-N6-C9
1	A	1402	4OC	O4'-C4'-C5'-O5'
1	A	1402	4OC	C3'-C4'-C5'-O5'
1	A	1402	4OC	N3-C4-N4-CM4

There are no ring outliers.

11 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1402	4OC	4	0
1	A	1404	5MC	1	0
1	A	1400	5MC	1	0
1	A	1519[A]	MA6	5	0
1	A	966	M2G	6	0
1	A	967	5MC	7	0
1	A	1518[A]	MA6	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1540	PSU	1	0
1	A	1498	UR3	5	0
1	A	1407	5MC	2	0
1	A	1207	2MG	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 295 ligands modelled in this entry, 295 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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%)	-0.20	28 (1%) 66 52	74, 136, 280, 374	0
2	B	234/256 (91%)	-0.20	2 (0%) 84 73	104, 156, 254, 272	0
3	C	206/239 (86%)	0.01	15 (7%) 15 9	171, 215, 243, 274	0
4	D	208/209 (99%)	-0.23	5 (2%) 59 43	86, 137, 190, 243	0
5	E	150/162 (92%)	-0.36	0 100 100	70, 106, 151, 203	0
6	F	101/101 (100%)	-0.41	1 (0%) 82 71	117, 157, 185, 213	0
7	G	155/156 (99%)	-0.06	3 (1%) 66 52	136, 185, 233, 255	0
8	H	138/138 (100%)	-0.53	0 100 100	71, 98, 135, 168	0
9	I	127/128 (99%)	0.41	15 (11%) 4 3	139, 201, 245, 269	0
10	J	98/105 (93%)	0.69	20 (20%) 1 0	150, 241, 295, 344	0
11	K	116/129 (89%)	-0.14	3 (2%) 56 40	100, 131, 170, 192	0
12	L	124/135 (91%)	-0.07	3 (2%) 59 43	82, 134, 167, 216	0
13	M	118/126 (93%)	0.17	7 (5%) 22 13	125, 162, 214, 232	0
14	N	60/61 (98%)	0.10	3 (5%) 28 18	179, 215, 270, 292	0
15	O	87/89 (97%)	-0.41	0 100 100	84, 119, 159, 179	0
16	P	83/88 (94%)	-0.09	0 100 100	95, 134, 164, 208	0
17	Q	99/105 (94%)	-0.30	0 100 100	75, 110, 148, 162	0
18	R	70/88 (79%)	-0.56	0 100 100	95, 135, 187, 215	0
19	S	80/93 (86%)	0.88	19 (23%) 0 0	176, 219, 255, 273	0
20	T	99/106 (93%)	-0.18	3 (3%) 50 34	106, 136, 194, 226	0
21	U	24/27 (88%)	0.52	3 (12%) 3 3	131, 183, 201, 209	0
All	All	3875/4063 (95%)	-0.13	130 (3%) 45 31	70, 146, 250, 374	0

The worst 5 of 130 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1003(A)	G	7.6
19	S	38	SER	7.4
1	A	993	G	7.1
1	A	1006	C	7.1
3	C	66	VAL	5.3

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. 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
1	PSU	A	1540	20/21	0.66	0.71	296,308,331,333	0
1	PSU	A	1541	20/21	0.85	0.65	285,299,307,307	0
1	4OC	A	1402	22/23	0.92	0.23	108,116,134,137	0
1	MA6	A	1518[B]	24/25	0.93	0.22	111,120,133,136	24
1	7MG	A	527	24/25	0.93	0.22	103,120,142,145	0
1	MA6	A	1518[A]	24/25	0.93	0.22	107,118,124,124	24
1	2MG	A	1207	24/25	0.94	0.16	195,204,278,284	0
1	5MC	A	1400	21/22	0.95	0.19	103,123,130,131	0
1	5MC	A	1407	21/22	0.95	0.12	136,163,172,178	0
1	MA6	A	1519[A]	24/25	0.95	0.28	100,107,112,116	24
1	MA6	A	1519[B]	24/25	0.95	0.28	102,107,118,119	24
1	PSU	A	516	20/21	0.95	0.10	133,147,164,166	0
1	5MC	A	1404	21/22	0.96	0.16	99,108,151,155	0
1	UR3	A	1498	21/22	0.96	0.29	105,120,144,147	0
1	M2G	A	966	25/26	0.96	0.15	136,150,159,160	0
1	5MC	A	967	21/22	0.97	0.13	125,144,150,153	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. 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(\AA^2)	Q<0.9
22	MG	A	1838	1/1	0.20	0.87	121,121,121,121	0
22	MG	A	1847	1/1	0.30	0.90	127,127,127,127	0
22	MG	A	1858	1/1	0.34	0.63	125,125,125,125	0
22	MG	A	1766	1/1	0.37	1.26	100,100,100,100	0
22	MG	A	1776	1/1	0.44	0.15	110,110,110,110	0
22	MG	A	1642	1/1	0.46	0.15	88,88,88,88	0
22	MG	A	1810	1/1	0.47	0.39	102,102,102,102	0
22	MG	A	1731	1/1	0.49	0.38	107,107,107,107	0
22	MG	A	1716	1/1	0.53	0.40	137,137,137,137	0
22	MG	P	102	1/1	0.53	0.45	124,124,124,124	0
22	MG	A	1849	1/1	0.55	0.28	126,126,126,126	0
22	MG	A	1704	1/1	0.56	0.44	126,126,126,126	0
22	MG	A	1753	1/1	0.56	0.37	109,109,109,109	0
22	MG	A	1826	1/1	0.59	0.76	134,134,134,134	0
22	MG	A	1751	1/1	0.59	0.93	143,143,143,143	0
22	MG	A	1829	1/1	0.60	0.37	463,463,463,463	0
22	MG	A	1682	1/1	0.61	0.32	82,82,82,82	0
22	MG	A	1781	1/1	0.61	0.64	130,130,130,130	0
22	MG	A	1842	1/1	0.62	1.15	119,119,119,119	0
22	MG	A	1822	1/1	0.63	0.22	116,116,116,116	0
22	MG	A	1777	1/1	0.65	1.28	144,144,144,144	0
22	MG	A	1794	1/1	0.66	0.91	132,132,132,132	0
22	MG	A	1830	1/1	0.68	0.66	91,91,91,91	0
22	MG	A	1811	1/1	0.68	0.25	147,147,147,147	0
22	MG	A	1601	1/1	0.69	0.43	132,132,132,132	0
22	MG	A	1763	1/1	0.70	0.29	137,137,137,137	0
22	MG	A	1833	1/1	0.70	0.26	122,122,122,122	0
22	MG	A	1845	1/1	0.70	0.92	110,110,110,110	0
22	MG	A	1846	1/1	0.71	0.21	142,142,142,142	0
22	MG	A	1866	1/1	0.71	0.49	124,124,124,124	0
22	MG	A	1672	1/1	0.71	0.14	139,139,139,139	0
22	MG	A	1770	1/1	0.71	0.97	99,99,99,99	0
22	MG	A	1735	1/1	0.71	0.51	81,81,81,81	0
22	MG	A	1809	1/1	0.72	0.37	109,109,109,109	0
22	MG	H	201	1/1	0.72	0.64	118,118,118,118	0
22	MG	A	1782	1/1	0.72	0.55	118,118,118,118	0
22	MG	A	1749	1/1	0.72	0.41	121,121,121,121	0
22	MG	A	1839	1/1	0.73	0.58	133,133,133,133	0
22	MG	A	1625	1/1	0.73	0.31	122,122,122,122	0
22	MG	A	1796	1/1	0.74	0.56	92,92,92,92	0
22	MG	A	1853	1/1	0.74	0.41	116,116,116,116	0
22	MG	A	1665	1/1	0.75	0.31	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
22	MG	A	1769	1/1	0.75	0.41	118,118,118,118	0
22	MG	A	1660	1/1	0.75	0.14	113,113,113,113	0
22	MG	C	301	1/1	0.75	0.44	133,133,133,133	0
22	MG	A	1857	1/1	0.76	0.54	133,133,133,133	0
22	MG	A	1662	1/1	0.76	0.37	78,78,78,78	0
22	MG	A	1720	1/1	0.77	0.77	98,98,98,98	0
22	MG	A	1808	1/1	0.77	0.11	163,163,163,163	0
22	MG	A	1715	1/1	0.77	0.52	137,137,137,137	0
22	MG	A	1872	1/1	0.78	0.13	407,407,407,407	0
22	MG	A	1703	1/1	0.79	0.39	153,153,153,153	0
22	MG	A	1761	1/1	0.79	0.34	107,107,107,107	0
22	MG	A	1780	1/1	0.79	0.50	61,61,61,61	0
22	MG	A	1683	1/1	0.79	0.65	98,98,98,98	0
22	MG	A	1835	1/1	0.79	0.55	98,98,98,98	0
22	MG	A	1834	1/1	0.79	0.35	118,118,118,118	0
22	MG	A	1841	1/1	0.80	0.78	118,118,118,118	0
22	MG	Q	201	1/1	0.80	0.21	126,126,126,126	0
22	MG	A	1787	1/1	0.80	0.12	141,141,141,141	0
22	MG	A	1854	1/1	0.80	0.45	137,137,137,137	0
22	MG	A	1868	1/1	0.80	0.36	99,99,99,99	0
22	MG	A	1824	1/1	0.80	0.20	133,133,133,133	0
22	MG	A	1843	1/1	0.81	0.80	106,106,106,106	0
22	MG	A	1832	1/1	0.82	0.77	89,89,89,89	0
22	MG	A	1622	1/1	0.83	0.23	148,148,148,148	0
22	MG	A	1729	1/1	0.83	0.32	85,85,85,85	0
22	MG	A	1736	1/1	0.84	0.22	114,114,114,114	0
22	MG	A	1684	1/1	0.84	0.33	127,127,127,127	0
22	MG	A	1783	1/1	0.84	0.41	129,129,129,129	0
22	MG	A	1865	1/1	0.84	0.21	134,134,134,134	0
22	MG	A	1679	1/1	0.84	0.47	146,146,146,146	0
22	MG	A	1677	1/1	0.84	0.14	299,299,299,299	0
22	MG	A	1605	1/1	0.84	0.80	85,85,85,85	0
22	MG	A	1759	1/1	0.84	0.26	107,107,107,107	0
22	MG	A	1836	1/1	0.85	0.42	120,120,120,120	0
22	MG	A	1798	1/1	0.85	0.20	148,148,148,148	0
22	MG	A	1851	1/1	0.85	0.28	132,132,132,132	0
22	MG	A	1687	1/1	0.85	0.25	117,117,117,117	0
22	MG	A	1633	1/1	0.85	1.02	100,100,100,100	0
22	MG	A	1711	1/1	0.85	0.33	149,149,149,149	0
22	MG	A	1815	1/1	0.85	0.46	115,115,115,115	0
22	MG	A	1791	1/1	0.86	0.46	99,99,99,99	0
22	MG	A	1821	1/1	0.86	0.34	96,96,96,96	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
22	MG	A	1745	1/1	0.86	0.18	107,107,107,107	0
22	MG	A	1856	1/1	0.86	0.28	127,127,127,127	0
22	MG	P	101	1/1	0.86	0.22	115,115,115,115	0
22	MG	A	1867	1/1	0.86	0.55	118,118,118,118	0
22	MG	A	1850	1/1	0.86	0.36	125,125,125,125	0
22	MG	A	1855	1/1	0.87	0.87	128,128,128,128	0
22	MG	A	1799	1/1	0.87	0.26	84,84,84,84	0
22	MG	A	1767	1/1	0.87	0.23	107,107,107,107	0
22	MG	A	1712	1/1	0.87	0.34	149,149,149,149	0
22	MG	A	1629	1/1	0.87	0.52	121,121,121,121	0
22	MG	A	1797	1/1	0.87	0.54	116,116,116,116	0
22	MG	A	1755	1/1	0.88	0.38	122,122,122,122	0
22	MG	A	1718	1/1	0.88	0.16	92,92,92,92	0
22	MG	A	1696	1/1	0.88	0.35	128,128,128,128	0
22	MG	A	1874	1/1	0.88	0.20	431,431,431,431	0
22	MG	D	304	1/1	0.88	0.56	110,110,110,110	0
22	MG	A	1661	1/1	0.88	0.45	87,87,87,87	0
22	MG	J	201	1/1	0.88	0.34	105,105,105,105	0
22	MG	A	1674	1/1	0.88	0.46	124,124,124,124	0
22	MG	A	1754	1/1	0.88	0.10	156,156,156,156	0
22	MG	D	303	1/1	0.88	0.22	88,88,88,88	0
22	MG	A	1701	1/1	0.88	0.32	138,138,138,138	0
22	MG	A	1806	1/1	0.88	0.29	414,414,414,414	0
22	MG	A	1772	1/1	0.88	1.46	120,120,120,120	0
22	MG	A	1638	1/1	0.88	0.33	97,97,97,97	0
22	MG	A	1848	1/1	0.89	0.41	94,94,94,94	0
22	MG	A	1619	1/1	0.89	0.63	106,106,106,106	0
22	MG	A	1733	1/1	0.89	0.33	116,116,116,116	0
22	MG	A	1778	1/1	0.89	0.15	157,157,157,157	0
22	MG	A	1852	1/1	0.89	0.50	108,108,108,108	0
22	MG	A	1644	1/1	0.89	0.34	82,82,82,82	0
22	MG	C	302	1/1	0.89	0.12	129,129,129,129	0
22	MG	A	1823	1/1	0.89	0.20	146,146,146,146	0
22	MG	I	201	1/1	0.89	0.81	136,136,136,136	0
22	MG	A	1785	1/1	0.90	0.21	127,127,127,127	0
22	MG	A	1837	1/1	0.90	0.96	123,123,123,123	0
22	MG	A	1802	1/1	0.90	0.50	148,148,148,148	0
22	MG	A	1694	1/1	0.90	0.34	76,76,76,76	0
22	MG	A	1790	1/1	0.90	0.73	146,146,146,146	0
22	MG	A	1859	1/1	0.90	0.81	123,123,123,123	0
22	MG	A	1626	1/1	0.90	0.29	147,147,147,147	0
22	MG	A	1817	1/1	0.90	0.93	134,134,134,134	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
22	MG	A	1819	1/1	0.90	0.18	103,103,103,103	0
22	MG	A	1725	1/1	0.90	0.80	119,119,119,119	0
22	MG	A	1671	1/1	0.90	0.24	140,140,140,140	0
22	MG	A	1685	1/1	0.90	0.10	236,236,236,236	0
22	MG	A	1756	1/1	0.90	0.26	109,109,109,109	0
22	MG	A	1873	1/1	0.90	0.10	437,437,437,437	0
22	MG	A	1871	1/1	0.90	0.47	148,148,148,148	0
22	MG	A	1686	1/1	0.90	0.13	226,226,226,226	0
22	MG	A	1789	1/1	0.91	0.11	96,96,96,96	0
22	MG	A	1705	1/1	0.91	0.18	369,369,369,369	0
22	MG	A	1773	1/1	0.91	0.43	120,120,120,120	0
22	MG	A	1673	1/1	0.91	0.10	120,120,120,120	0
22	MG	A	1800	1/1	0.91	0.09	132,132,132,132	0
22	MG	A	1863	1/1	0.91	0.31	101,101,101,101	0
22	MG	A	1803	1/1	0.91	0.47	250,250,250,250	0
23	ZN	N	101	1/1	0.91	0.14	214,214,214,214	0
22	MG	A	1827	1/1	0.91	0.98	147,147,147,147	0
22	MG	E	201	1/1	0.91	0.12	121,121,121,121	0
22	MG	A	1631	1/1	0.91	0.32	109,109,109,109	0
22	MG	A	1699	1/1	0.91	0.39	97,97,97,97	0
22	MG	A	1666	1/1	0.91	0.21	123,123,123,123	0
22	MG	B	302	1/1	0.91	0.15	111,111,111,111	0
22	MG	A	1740	1/1	0.91	0.40	125,125,125,125	0
22	MG	D	302	1/1	0.92	0.19	103,103,103,103	0
22	MG	A	1639	1/1	0.92	0.31	216,216,216,216	0
22	MG	A	1814	1/1	0.92	0.56	131,131,131,131	0
22	MG	A	1743	1/1	0.92	0.19	104,104,104,104	0
22	MG	A	1774	1/1	0.92	0.51	112,112,112,112	0
22	MG	A	1739	1/1	0.92	0.49	74,74,74,74	0
22	MG	A	1758	1/1	0.92	0.28	109,109,109,109	0
22	MG	A	1689	1/1	0.92	0.76	170,170,170,170	0
22	MG	A	1678	1/1	0.92	0.44	106,106,106,106	0
22	MG	A	1765	1/1	0.92	0.76	90,90,90,90	0
22	MG	A	1784	1/1	0.92	0.20	120,120,120,120	0
22	MG	A	1768	1/1	0.92	0.13	147,147,147,147	0
22	MG	A	1700	1/1	0.92	0.17	184,184,184,184	0
22	MG	A	1738	1/1	0.92	0.54	100,100,100,100	0
22	MG	A	1864	1/1	0.92	0.43	122,122,122,122	0
22	MG	A	1786	1/1	0.92	0.18	153,153,153,153	0
22	MG	A	1748	1/1	0.92	0.32	120,120,120,120	0
22	MG	A	1667	1/1	0.92	0.27	115,115,115,115	0
22	MG	A	1752	1/1	0.92	0.50	89,89,89,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
22	MG	A	1764	1/1	0.93	0.25	101,101,101,101	0
22	MG	A	1779	1/1	0.93	0.20	129,129,129,129	0
22	MG	A	1653	1/1	0.93	0.17	113,113,113,113	0
22	MG	A	1676	1/1	0.93	0.24	113,113,113,113	0
22	MG	A	1608	1/1	0.93	0.11	143,143,143,143	0
22	MG	A	1664	1/1	0.93	0.44	101,101,101,101	0
22	MG	A	1732	1/1	0.93	0.33	136,136,136,136	0
22	MG	A	1688	1/1	0.93	0.13	144,144,144,144	0
22	MG	F	201	1/1	0.93	0.16	107,107,107,107	0
22	MG	A	1844	1/1	0.93	0.18	100,100,100,100	0
22	MG	A	1793	1/1	0.94	0.25	80,80,80,80	0
22	MG	A	1681	1/1	0.94	0.35	132,132,132,132	0
22	MG	A	1669	1/1	0.94	0.19	152,152,152,152	0
22	MG	A	1801	1/1	0.94	0.18	154,154,154,154	0
22	MG	A	1628	1/1	0.94	0.78	85,85,85,85	0
22	MG	A	1825	1/1	0.94	0.35	110,110,110,110	0
22	MG	A	1870	1/1	0.94	0.58	85,85,85,85	0
22	MG	A	1652	1/1	0.94	0.13	98,98,98,98	0
22	MG	A	1744	1/1	0.94	0.32	117,117,117,117	0
22	MG	A	1818	1/1	0.94	0.97	100,100,100,100	0
22	MG	A	1737	1/1	0.94	0.24	99,99,99,99	0
22	MG	A	1861	1/1	0.94	0.11	89,89,89,89	0
22	MG	A	1610	1/1	0.94	0.24	124,124,124,124	0
22	MG	A	1840	1/1	0.94	0.22	104,104,104,104	0
22	MG	A	1702	1/1	0.94	0.21	184,184,184,184	0
22	MG	A	1657	1/1	0.94	0.15	98,98,98,98	0
22	MG	A	1690	1/1	0.94	0.06	136,136,136,136	0
22	MG	A	1727	1/1	0.95	0.74	140,140,140,140	0
22	MG	A	1816	1/1	0.95	0.41	105,105,105,105	0
22	MG	A	1649	1/1	0.95	0.48	116,116,116,116	0
22	MG	A	1722	1/1	0.95	0.24	155,155,155,155	0
22	MG	A	1635	1/1	0.95	0.12	99,99,99,99	0
22	MG	A	1831	1/1	0.95	0.33	52,52,52,52	0
22	MG	A	1714	1/1	0.95	0.21	219,219,219,219	0
22	MG	A	1728	1/1	0.95	0.05	214,214,214,214	0
22	MG	A	1692	1/1	0.95	0.27	150,150,150,150	0
22	MG	A	1646	1/1	0.95	0.40	91,91,91,91	0
22	MG	A	1650	1/1	0.95	0.24	90,90,90,90	0
22	MG	A	1723	1/1	0.95	0.16	102,102,102,102	0
22	MG	A	1862	1/1	0.95	0.32	127,127,127,127	0
22	MG	A	1710	1/1	0.95	0.41	114,114,114,114	0
22	MG	A	1828	1/1	0.95	0.28	447,447,447,447	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
22	MG	B	301	1/1	0.95	0.20	99,99,99,99	0
22	MG	A	1792	1/1	0.96	0.13	97,97,97,97	0
22	MG	A	1675	1/1	0.96	0.21	116,116,116,116	0
22	MG	A	1659	1/1	0.96	0.12	121,121,121,121	0
22	MG	A	1624	1/1	0.96	0.25	117,117,117,117	0
22	MG	A	1697	1/1	0.96	0.33	127,127,127,127	0
22	MG	A	1647	1/1	0.96	0.44	182,182,182,182	0
22	MG	A	1645	1/1	0.96	0.06	91,91,91,91	0
22	MG	A	1643	1/1	0.96	0.15	90,90,90,90	0
22	MG	A	1869	1/1	0.96	0.19	106,106,106,106	0
22	MG	A	1612	1/1	0.96	0.12	164,164,164,164	0
22	MG	A	1603	1/1	0.96	0.23	84,84,84,84	0
22	MG	A	1805	1/1	0.96	0.12	203,203,203,203	0
22	MG	A	1648	1/1	0.96	0.14	164,164,164,164	0
22	MG	A	1726	1/1	0.96	0.41	134,134,134,134	0
22	MG	A	1742	1/1	0.96	0.31	116,116,116,116	0
22	MG	A	1741	1/1	0.96	0.17	76,76,76,76	0
22	MG	A	1807	1/1	0.96	0.12	278,278,278,278	0
22	MG	A	1795	1/1	0.96	0.52	117,117,117,117	0
22	MG	A	1875	1/1	0.96	0.07	228,228,228,228	0
22	MG	A	1813	1/1	0.96	0.19	122,122,122,122	0
22	MG	A	1707	1/1	0.97	0.07	167,167,167,167	0
22	MG	A	1820	1/1	0.97	0.06	91,91,91,91	0
22	MG	A	1621	1/1	0.97	0.31	123,123,123,123	0
22	MG	A	1730	1/1	0.97	0.26	110,110,110,110	0
22	MG	A	1654	1/1	0.97	0.10	49,49,49,49	0
22	MG	A	1747	1/1	0.97	0.07	105,105,105,105	0
22	MG	A	1771	1/1	0.97	0.67	83,83,83,83	0
22	MG	A	1734	1/1	0.97	0.26	129,129,129,129	0
22	MG	A	1804	1/1	0.97	0.11	194,194,194,194	0
22	MG	A	1615	1/1	0.97	0.12	99,99,99,99	0
22	MG	A	1706	1/1	0.98	0.36	97,97,97,97	0
22	MG	A	1616	1/1	0.98	0.18	66,66,66,66	0
22	MG	A	1876	1/1	0.98	0.24	399,399,399,399	0
22	MG	A	1724	1/1	0.98	0.37	92,92,92,92	0
22	MG	A	1860	1/1	0.98	0.56	123,123,123,123	0
22	MG	A	1695	1/1	0.98	0.11	81,81,81,81	0
22	MG	A	1614	1/1	0.98	0.18	135,135,135,135	0
22	MG	A	1691	1/1	0.98	0.38	155,155,155,155	0
22	MG	A	1656	1/1	0.98	0.14	178,178,178,178	0
22	MG	A	1668	1/1	0.98	0.12	136,136,136,136	0
22	MG	A	1604	1/1	0.98	0.12	100,100,100,100	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
22	MG	A	1609	1/1	0.98	0.18	94,94,94,94	0
22	MG	A	1680	1/1	0.98	0.29	136,136,136,136	0
23	ZN	D	301	1/1	0.98	0.28	122,122,122,122	0
22	MG	A	1670	1/1	0.98	0.10	140,140,140,140	0
22	MG	A	1658	1/1	0.98	0.18	130,130,130,130	0
22	MG	A	1618	1/1	0.98	0.35	94,94,94,94	0
22	MG	A	1713	1/1	0.98	0.32	431,431,431,431	0
22	MG	N	102	1/1	0.98	0.30	225,225,225,225	0
22	MG	A	1762	1/1	0.98	0.30	83,83,83,83	0
22	MG	A	1617	1/1	0.98	0.29	56,56,56,56	0
22	MG	A	1788	1/1	0.98	0.51	77,77,77,77	0
22	MG	A	1602	1/1	0.98	0.21	130,130,130,130	0
22	MG	A	1627	1/1	0.98	0.83	79,79,79,79	0
22	MG	A	1760	1/1	0.98	0.20	98,98,98,98	0
22	MG	A	1613	1/1	0.98	0.21	121,121,121,121	0
22	MG	A	1717	1/1	0.98	0.24	94,94,94,94	0
22	MG	A	1746	1/1	0.99	0.17	101,101,101,101	0
22	MG	A	1708	1/1	0.99	0.18	120,120,120,120	0
22	MG	A	1636	1/1	0.99	0.12	69,69,69,69	0
22	MG	A	1812	1/1	0.99	0.16	99,99,99,99	0
22	MG	A	1634	1/1	0.99	0.20	235,235,235,235	0
22	MG	A	1693	1/1	0.99	0.15	133,133,133,133	0
22	MG	A	1640	1/1	0.99	0.16	72,72,72,72	0
22	MG	A	1637	1/1	0.99	0.37	85,85,85,85	0
22	MG	A	1620	1/1	0.99	0.10	83,83,83,83	0
22	MG	A	1623	1/1	0.99	0.14	135,135,135,135	0
22	MG	A	1632	1/1	0.99	0.14	128,128,128,128	0
22	MG	B	303	1/1	0.99	0.18	184,184,184,184	0
22	MG	A	1641	1/1	0.99	0.12	99,99,99,99	0
22	MG	A	1757	1/1	0.99	0.09	80,80,80,80	0
22	MG	A	1719	1/1	0.99	0.19	139,139,139,139	0
22	MG	A	1709	1/1	0.99	0.11	140,140,140,140	0
22	MG	A	1651	1/1	0.99	0.15	61,61,61,61	0
22	MG	A	1775	1/1	0.99	0.12	121,121,121,121	0
22	MG	A	1698	1/1	0.99	0.36	182,182,182,182	0
22	MG	A	1630	1/1	0.99	0.24	83,83,83,83	0
22	MG	A	1750	1/1	0.99	0.23	123,123,123,123	0
22	MG	A	1611	1/1	0.99	0.12	92,92,92,92	0
22	MG	A	1606	1/1	0.99	0.11	96,96,96,96	0
22	MG	A	1655	1/1	0.99	0.14	131,131,131,131	0
22	MG	A	1607	1/1	0.99	0.20	91,91,91,91	0
22	MG	A	1663	1/1	1.00	0.09	127,127,127,127	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
22	MG	A	1721	1/1	1.00	0.20	46,46,46,46	0

6.5 Other polymers [i](#)

There are no such residues in this entry.