



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 03:58 PM GMT

PDB ID : 4DR7  
Title : Crystal structure of the *Thermus thermophilus* (HB8) 30S ribosomal subunit with codon, crystallographically disordered near-cognate transfer RNA anticodon stem-loop mismatched at the second codon position, and streptomycin bound  
Authors : Demirci, H.; Murphy IV, F.; Murphy, E.; Gregory, S.T.; Dahlberg, A.E.; Jogl, G.  
Deposited on : 2012-02-16  
Resolution : 3.75 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](mailto: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.

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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



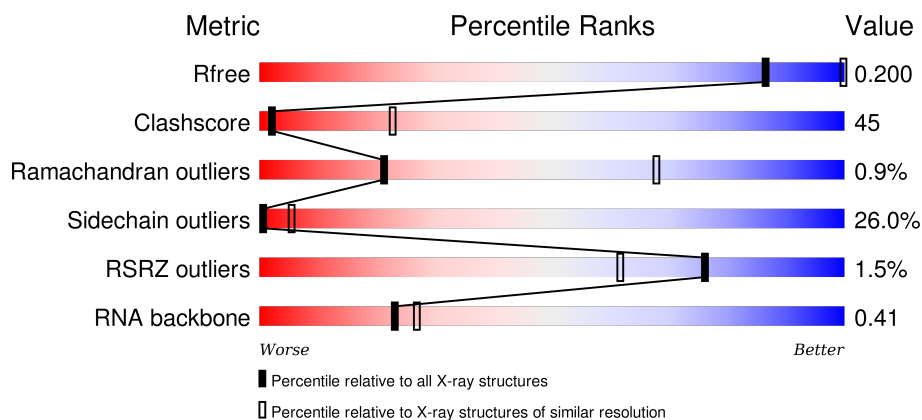
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.75 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	1268 (4.02-3.50)
Clashscore	102246	1407 (4.02-3.50)
Ramachandran outliers	100387	1346 (4.02-3.50)
Sidechain outliers	100360	1342 (4.02-3.50)
RSRZ outliers	91569	1276 (4.02-3.50)
RNA backbone	2183	1069 (4.70-2.80)

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  $\geq 3$ , 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	<div> <div>13%</div> <div>43%</div> <div>34%</div> <div>10%</div> <div>•</div> </div>
2	B	256	<div> <div>26%</div> <div>49%</div> <div>17%</div> <div>8%</div> </div>
3	C	239	<div> <div>22%</div> <div>50%</div> <div>15%</div> <div>13%</div> </div>
4	D	209	<div> <div>29%</div> <div>52%</div> <div>18%</div> <div>•</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	
22	V	4	
23	W	11	
24	a	8	
25	b	3	

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	2MG	A	1207	-	-	X	-
1	5MC	A	1407	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	UR3	A	1498	-	-	X	-
1	MA6	A	1518[A]	-	-	X	-
1	MA6	A	1518[B]	-	-	X	-
1	MA6	A	1519[A]	-	-	X	-
1	MA6	A	1519[B]	-	-	X	-
26	MG	A	1621	-	-	-	X
26	MG	A	1637	-	-	-	X
26	MG	A	1655	-	-	-	X
26	MG	A	1656	-	-	-	X
26	MG	A	1659	-	-	-	X
26	MG	A	1665	-	-	-	X
26	MG	A	1670	-	-	-	X
26	MG	A	1701	-	-	-	X
26	MG	A	1708	-	-	-	X
26	MG	A	1709	-	-	-	X
26	MG	A	1715	-	-	-	X
26	MG	A	1721	-	-	-	X
26	MG	A	1723	-	-	-	X
26	MG	A	1728	-	-	-	X
26	MG	A	1732	-	-	-	X
26	MG	A	1733	-	-	-	X
26	MG	A	1740	-	-	-	X
26	MG	A	1741	-	-	-	X
26	MG	A	1743	-	-	-	X
26	MG	A	1759	-	-	-	X
26	MG	A	1761	-	-	-	X
26	MG	A	1763	-	-	-	X
26	MG	A	1764	-	-	-	X
26	MG	A	1768	-	-	-	X
26	MG	A	1784	-	-	-	X
26	MG	A	1804	-	-	-	X
26	MG	A	1812	-	-	-	X
26	MG	A	1834	-	-	-	X
26	MG	A	1869	-	-	-	X
26	MG	A	1870	-	-	-	X
26	MG	A	1888	-	-	-	X
26	MG	A	1900	-	-	-	X
26	MG	A	1904	-	-	-	X
26	MG	E	201	-	-	-	X
26	MG	E	204	-	-	-	X
26	MG	N	102	-	-	-	X
26	MG	Q	201	-	-	-	X



## 2 Entry composition

There are 29 unique types of molecules in this entry. The entry contains 53659 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	1513	Total	C	N	O	P	0	8	0
			32707	14570	6056	10561	1520			

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	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	117	Total	C	N	O	S	0	0	0
			873	543	166	161	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	71	Total	C	N	O		0	0	0
			585	373	116	96				

- 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\*UP\*U)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	V	4	Total	C	N	O	P	0	0	0
			77	36	8	30	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	W	11	Total	C	N	O	P	0	0	0
			235	106	45	74	10			

- Molecule 24 is a RNA chain called 5'-R(P\*UP\*GP\*GP\*AP\*AP\*AP\*GP\*(PSU))-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	a	8	Total	C	N	O	P	0	0	0
			175	78	34	55	8			

- Molecule 25 is a RNA chain called 5'-R(P\*UP\*UP\*U)-3'.

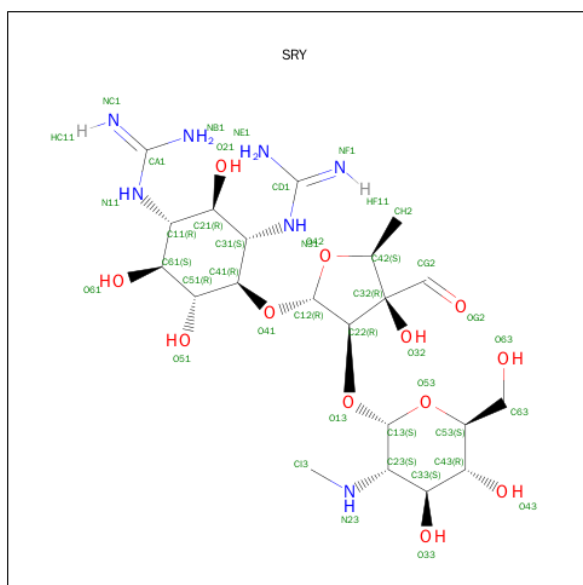
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	b	3	Total	C	N	O	P	0	0	0
			60	27	6	24	3			

- Molecule 26 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	P	3	Total Mg 3 3	0	0
26	G	1	Total Mg 1 1	0	0
26	J	1	Total Mg 1 1	0	0
26	Q	1	Total Mg 1 1	0	0
26	D	3	Total Mg 3 3	0	0
26	E	4	Total Mg 4 4	0	0
26	H	1	Total Mg 1 1	0	0
26	A	326	Total Mg 326 326	0	0
26	N	1	Total Mg 1 1	0	0
26	S	2	Total Mg 2 2	0	0
26	F	1	Total Mg 1 1	0	0

- Molecule 27 is STREPTOMYCIN (three-letter code: SRY) (formula:  $C_{21}H_{39}N_7O_{12}$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	A	1	Total C N O 40 21 7 12	0	0



- Molecule 28 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 29 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
29	A	866	Total	O	0	0
			866	866		
29	C	1	Total	O	0	0
			1	1		
29	D	7	Total	O	0	0
			7	7		
29	E	5	Total	O	0	0
			5	5		
29	L	1	Total	O	0	0
			1	1		
29	N	1	Total	O	0	0
			1	1		
29	P	1	Total	O	0	0
			1	1		
29	Q	2	Total	O	0	0
			2	2		
29	T	3	Total	O	0	0
			3	3		
29	U	4	Total	O	0	0
			4	4		
29	W	1	Total	O	0	0
			1	1		







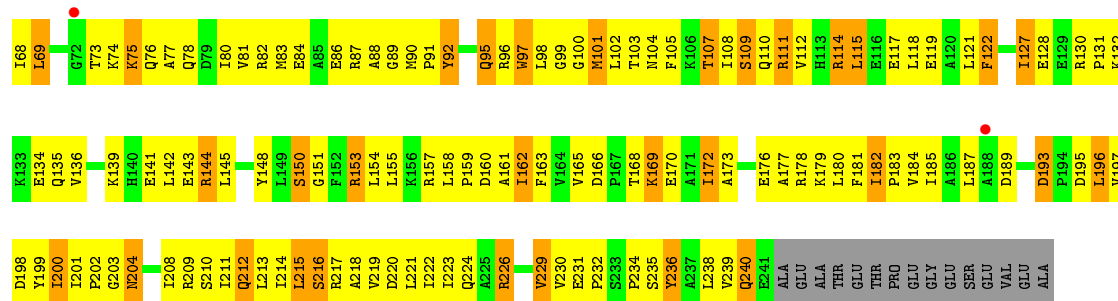
U1510	G1442	A1375	G1316	A1250	G1189	U1125	G1064	G1008	A949	G888	C822	G760
U1511	G1443	U1376	C1317	A1251	G1190	U1126	U1065	G1009	U950	A889	G823	G761
U1512	A1446	A1377	A1318	A1252	G1191	G1127	A1066	G1010	G951	A890	G824	C762
A1513	G1447	C1378	A1319	G1253	G1192	C1128	A1067	G1011	U952	U891	G825	G763
C1514	C1448	G1379	C1320	G1254	G1193	A1129	G1068	U1012	G953	A892	C826	G764
C1515	C1449	U1380	C1321	G1255	U1194	A1130	G1069	G1013	G954	C893	U827	G765
C1516	U1450	U1381	G1322	A1256	G1195	U1070	U1070	A1014	U955	C894	A828	A766
G1517	A1451	C1382	G1323	U1257	U1196	C1132	C1072	A1015	U956	G895	A829	A767
A1518	C1452	C1383	A1324	U1258	G1197	G1133	G1071	A1016	U957	C896	G830	A768
A1519	G1385	G1386	C1325	C1259	G1198	U1134	U1073	G1017	A958	C897	U831	G769
G1520	G1453	G1386	C1326	C1259	U1199	U1135	G1074	C1018	A959	G898	C832	C770
G1521	G1455	G1387	C1327	C1263	G1200	U1136	C1075	C1019	U960	C899	U833	G771
G1522	G1456	C1388	C1328	C1264	A1201	C1137	C1076	U1020	U961	A900	C834	G774
G1523	A1460	C1389	A1329	C1267	G1202	G1138	G1077	G1021	C962	A901	U835	G774
C1524	C1465	U1390	U1330	C1267	C1203	U1078	U1078	G1022	G963	G902	G836	A777
G1525	U1466	U1391	G1331	A1268	A1204	G1107	G1079	G1023	A964	G903	G837	A777
G1526	G1466	G1392	A1332	A1269	U1205	A1080	A1080	G1024	A965	C904	U838	G778
C1527	G1467	U1393	A1333	C1270	G1206	G1142	U1085	U1025	G966	U905	U839	C779
U1528	A1468	A1394	G1334	G1271	G1207	G1143	G1082	G1026	C967	U906	C840	A780
G1529	G1469	C1395	C1335	G1272	C1208	G1144	U1083	C1027	A968	A907	U841	A781
G1530	G1470	A1396	C1336	G1273	C1209	C1145	G1084	G1028	A969	A908	C848	A782
U1531	G1471	C1397	G1337	C1274	C1210	A1146	U1085	C1029	C970	A909	C849	C783
U1532	G1472	A1398	G1338	C1282	U1211	C1147	U1086	C1030	G971	C910	U850	C784
C1533	A1473	C1399	A1339	G1276	U1212	U1148	G1087	G1030A	C972	U911	G851	G785
C1534	G1474	C1400	A1340	U1277	U1213	C1149	G1088	C1030B	G973	C912	G852	G786
A1535	G1475	G1401	U1341	A1278	C1214	U1150	G1089	G1030C	A974	A913	G853	A787
C1536	G1476	C1402	C1342	U1281	G1215	A1151	U1090	A1030D	A975	U788	G854	U789
U1537	C1477	C1403	G1343	U1281	A1152	A1152	U1091	G1031	G976	G855	C856	U790
C1538	G1478	C1404	C1344	C1282	C1153	C1153	A1092	G1032	A977	C857	C857	G791
C1539	C1479	G1405	U1345	G1283	C1218	C1153	A1093	G1033	A978	A918	G858	A792
U1540	G1480	U1406	A1346	C1284	G1220	G1157	G1094	G1034	C979	A919	G859	U793
PSU	U1481	C1407	G1347	A1286	G1221	C1158	U1095	A1035	C980	U920	A860	A794
U	G1482	A1408	U1348	A1287	G1222	U1159	C1096	G1036	U981	U921	G861	C795
C	A1483	A1409	A1349	A1288	C1223	G1160	C1097	C1037	U982	G922	C862	C796
U	C1484	G1410	A1350	A1289	G1224	C1161	C1098	C1038	A983	A923	U863	C797
C1539	U1485	C1411	U1351	G1290	A1225	C1162	G1099	C1039	C984	C924	U864	G798
U1540	G1486	C1412	C1352	G1291	G1226	C1163	C1100	U1040	C985	G925	A864	G799
I39	G1487	A1413	G1353	U1292	A1227	G1164	A1101	A1041	A986	G926	A865	G800
H40	G1488	U1414	C1354	U1293	C1228	C1165	A1102	G1042	G987	G927	C866	G801
I41	G1489	G1415	G1355	G1294	A1229	C1166	C1103	C1043	G988	G928	C867	U801
D43	C1490	G1416	G1356	G1295	G1230	A1167	G1104	A1044	C989	C930	C868	A802
L44	G1491	G1417	A1357	G1296	G1231	A1168	C1045	C1045	U991	C931	U870	U804
K45	A1492	A1418	U1358	C1297	U1232	A1169	G1046	A1046	U992	C932	C805	C806
K46	A1493	G1419	C1359	C1298	G1233	G1171	G1108	G1047	U993	G933	A872	A807
T47	G1494	C1420	A1360	A1299	C1234	C1172	C1109	G1048	G993	C934	A873	C808
M48	U1495	U1301	C1361	U1300	U1235	G1173	A1110	U1049	A994	A935	G874	C809
R53	G1497	U1302	C1362	U1301	C1237	G1174	C1111	C1051	A996	C936	C875	G810
R56	U1498	C1425	A1363	G1303	A1238	C1175	C1113	U1052	U997	A937	G876	C811
F57	A1499	C1426	U1364	G1304	A1239	C1114	C1114	G1053	G998	A938	C877	C812
D60	A1500	C1426	G1365	G1305	U1240	C1115	C1115	C1054	C999	G939	G878	C813
L61	C1501	A1433	C1366	U1307	G1241	C1116	C1116	A1055	U1000	C940	C879	U813
A62	A1502	A1434	C1367	U1307	G1242	G1181	G1117	U1056	A1001	G941	C880	A814
M63	G1503	G1435	G1368	C1369	C1243	G1182	C1118	G1057	G1002	G942	G881	A815
M63	G1504	U1436	C1369	C1370	A1244	A1183	C1119	G1058	G1003	U943	C882	A816
M64	G1505	C1437	G1370	G1311	G1184	A1184	G1120	C1059	G1003A	G944	C883	C817
G65	U1506	G1438	G1371	G1312	C1246	G1185	U1121	C1060	A1004	G945	U884	G818
G66	A1507	C1439	U1372	U1313	C1247	G1186	U1122	G1061	A1005	A946	G885	A819
G1508	C1440	G1373	C1314	U1314	U1248	G1187	A1123	U1062	C1006	G947	G886	U820
C1509	G1441	A1374	A1374	U1315	C1249	A1188	G1124	C1063	C1007	G948	G887	G821

• Molecule 2: 30S ribosomal protein S2

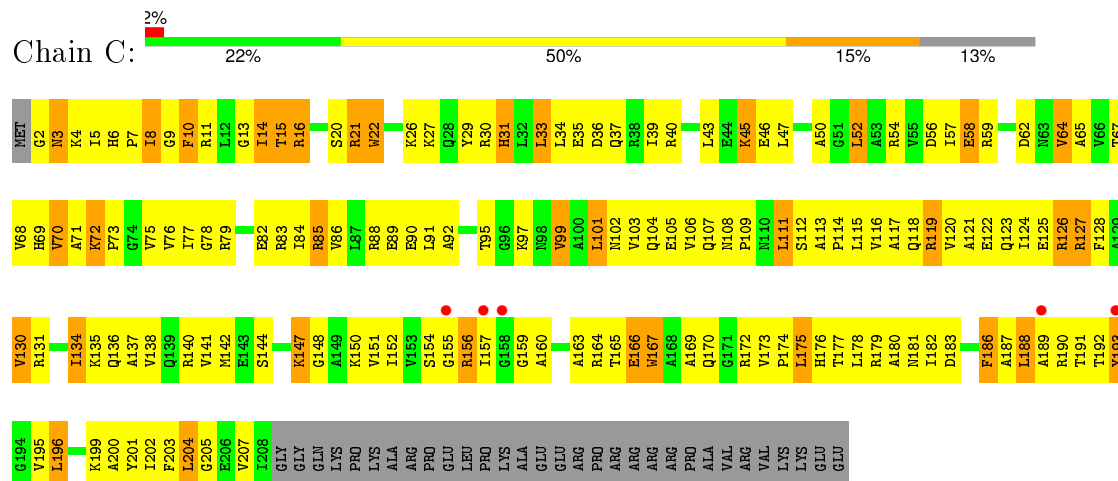


MET	G14	A13	G13	A12	G11	U11	G10	G10	A9	G8	C8	G7
PRO	G14	U13	C13	A12	G11	U11	U10	G10	U9	A8	G7	G7
VAL	A14	A13	A13	A12	G11	G11	A10	G10	G9	A8	G7	C7
GLU	G14	C13	A13	G12	G11	C11	A10	G10	U9	U8	G7	G7
ILE	C14	G13	C13	G12	G11	A11	G10	U10	G9	A8	C7	G7
T6												
V7												
E9												
L10												
L11												
	G14	A13	G13	A12	G11	U11	G10	G10	A9	G8	C8	G7
	H15	H16	F17	G18	H19	H19						
	E20											
	R21	R21	R22	R22	R23	R23	R24	R25	R26	R26		
	P28	P28	F27	F27	F28	F28	A29	A29	A29	A29		
	K29	K29	K30	K30	R30	R30	R30	R30	R30	R30		
	Y31	Y31	Y32	Y32	Y33	Y33	Y33	Y33	Y33	Y33		
	A34	A34	A35	A35	A35	A35	A35	A35	A35	A35		
	R36	R36										
	I39	H40	I41	I41	I42	I42	I42	I42	I42	I42		

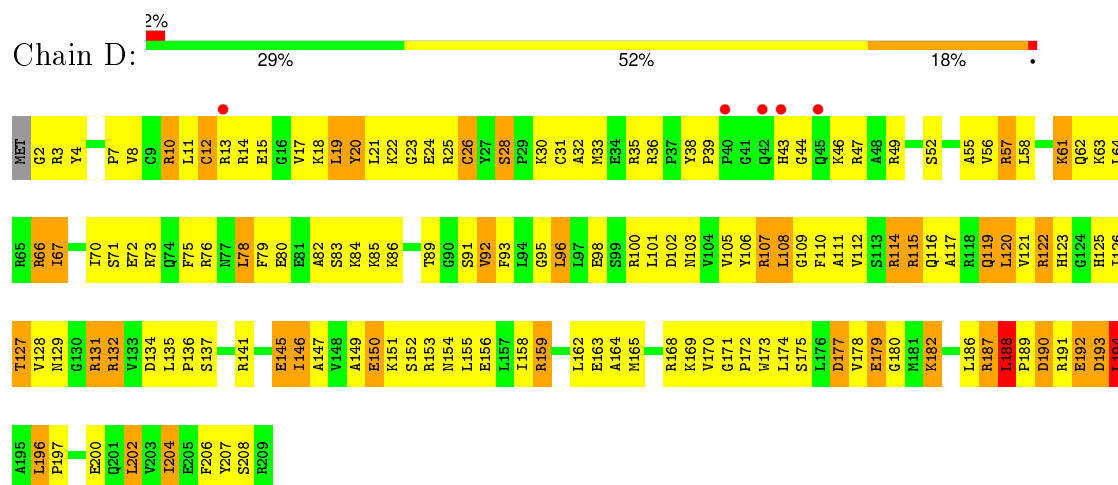




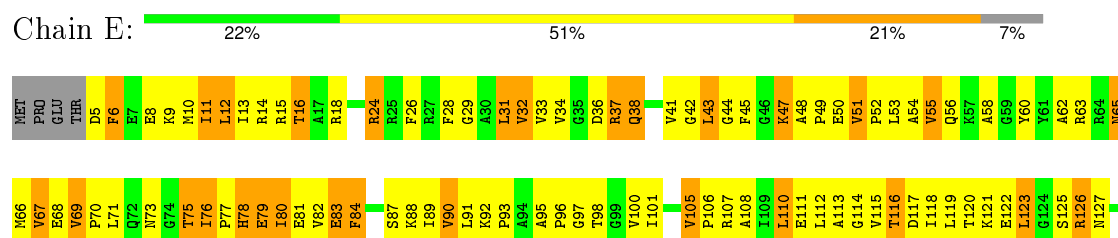
• Molecule 3: 30S ribosomal protein S3



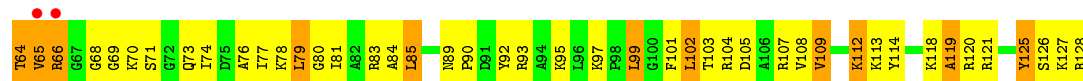
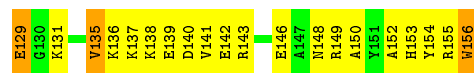
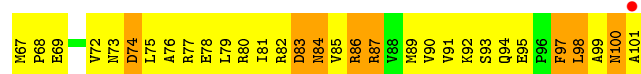
• Molecule 4: 30S ribosomal protein S4



• Molecule 5: 30S ribosomal protein S5

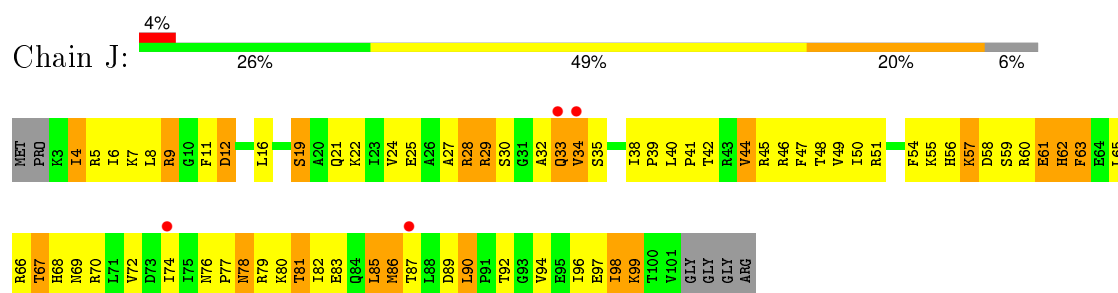




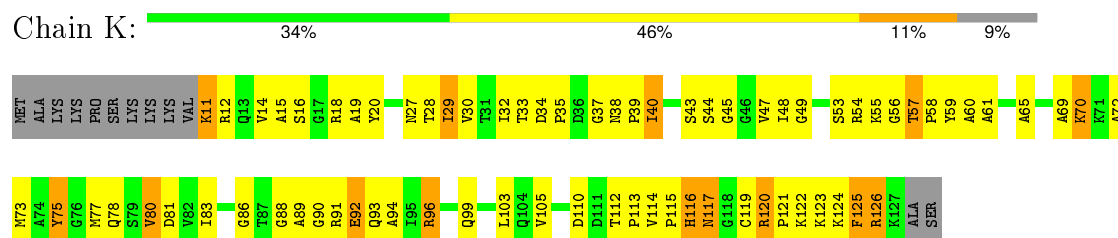


- Molecule 10: 30S ribosomal protein S10

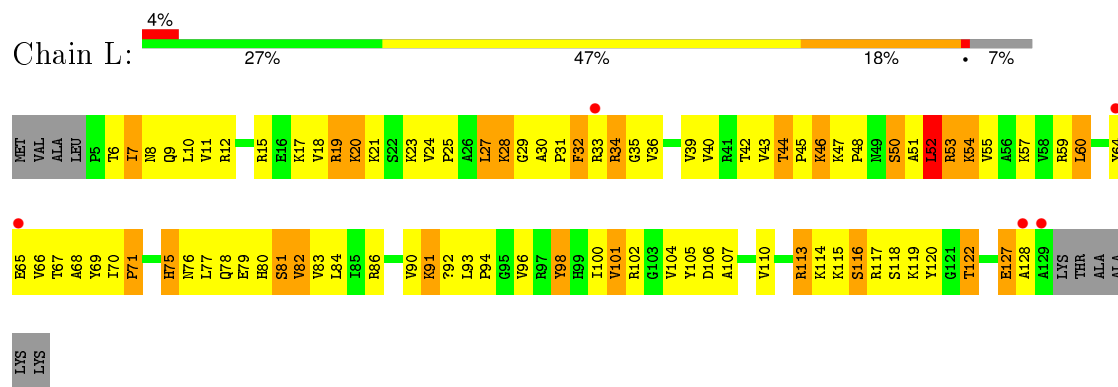




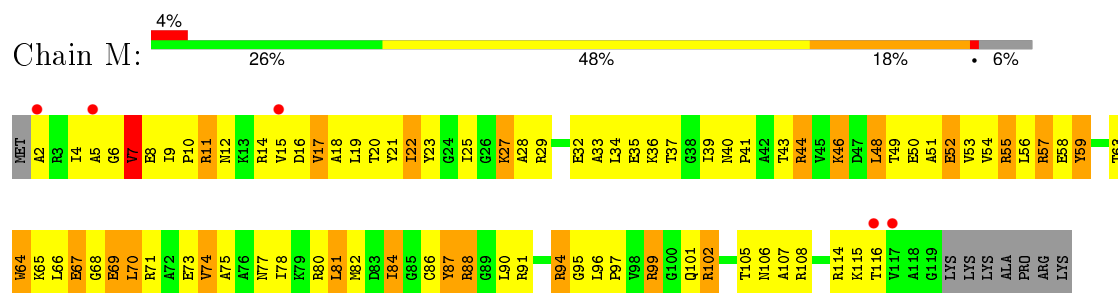
- Molecule 11: 30S ribosomal protein S11



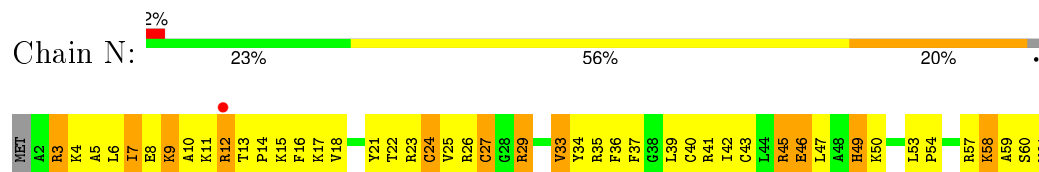
- Molecule 12: 30S ribosomal protein S12



- Molecule 13: 30S ribosomal protein S13



- Molecule 14: 30S ribosomal protein S14

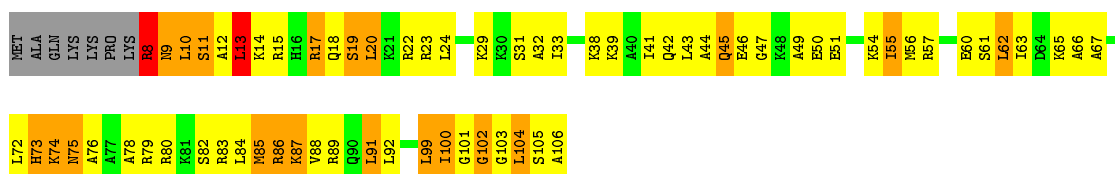


- Molecule 15: 30S ribosomal protein S15

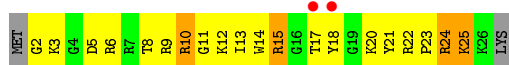








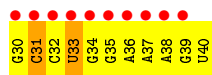
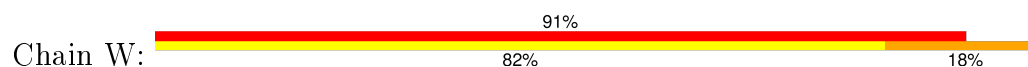
- Molecule 21: 30S ribosomal protein THX



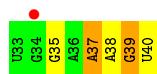
- Molecule 22: 5'-R(\*UP\*UP\*UP\*U)-3'



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



- Molecule 24: 5'-R(P\*UP\*GP\*GP\*AP\*AP\*AP\*GP\*(PSU))-3'



- Molecule 25: 5'-R(P\*UP\*UP\*U)-3'





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	402.49 Å   402.49 Å   174.79 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	48.91 – 3.75 49.65 – 3.75	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.91-3.75) 100.0 (49.65-3.75)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.41 (at 3.77 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_978)	Depositor
R, $R_{free}$	0.148 , 0.201 0.151 , 0.200	Depositor DCC
$R_{free}$ test set	7304 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	130.7	Xtriage
Anisotropy	0.226	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.25 , 102.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 146049 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	53659	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	146.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.65% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup> Intensities estimated from amplitudes.

<sup>2</sup> Theoretical 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, M2G, MA6, 0TD, MG, 2MG, 5MC, UR3, 4OC, SRY, 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	135/36234 (0.4%)	1.90	1769/56547 (3.1%)
2	B	0.74	0/1931	0.93	2/2607 (0.1%)
3	C	0.62	0/1637	0.83	0/2207
4	D	0.73	1/1733 (0.1%)	0.93	4/2318 (0.2%)
5	E	1.04	1/1163 (0.1%)	1.17	3/1566 (0.2%)
6	F	0.65	0/856	0.86	0/1154
7	G	0.68	0/1276	0.87	0/1709
8	H	1.11	2/1136 (0.2%)	1.18	4/1527 (0.3%)
9	I	0.65	0/1029	0.88	2/1379 (0.1%)
10	J	0.71	1/806 (0.1%)	0.95	2/1084 (0.2%)
11	K	0.76	0/888	0.97	0/1198
12	L	0.90	0/978	1.08	3/1308 (0.2%)
13	M	0.68	0/947	0.94	0/1270
14	N	0.68	0/501	0.85	1/664 (0.2%)
15	O	0.86	0/745	1.02	3/992 (0.3%)
16	P	0.93	0/717	1.08	3/965 (0.3%)
17	Q	1.08	1/847 (0.1%)	1.25	4/1131 (0.4%)
18	R	0.76	0/590	1.00	1/782 (0.1%)
19	S	0.57	0/662	0.77	0/892
20	T	0.87	0/765	1.18	4/1007 (0.4%)
21	U	0.69	0/213	0.87	0/279
22	V	0.53	0/84	0.98	0/128
23	W	0.62	0/241	0.92	0/375
24	a	0.85	0/174	1.89	10/270 (3.7%)
25	b	0.76	0/65	1.31	2/98 (2.0%)
All	All	1.08	141/56218 (0.3%)	1.66	1817/83457 (2.2%)

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



Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	3
3	C	0	2
4	D	0	1
8	H	0	2
9	I	0	1
10	J	0	2
12	L	0	2
16	P	0	1
19	S	0	1
20	T	0	2
21	U	0	1
All	All	0	18

The worst 5 of 141 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	828	A	N9-C4	-10.24	1.31	1.37
1	A	1513	A	N9-C4	-9.49	1.32	1.37
1	A	266	G	N7-C5	-9.34	1.33	1.39
1	A	573	A	N7-C5	-9.28	1.33	1.39
8	H	135	CYS	CB-SG	-9.04	1.66	1.82

The worst 5 of 1817 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	266	G	C6-C5-N7	-19.86	118.48	130.40
1	A	366	C	N1-C2-O2	17.84	129.60	118.90
1	A	117	G	N1-C6-O6	15.21	129.03	119.90
1	A	1200	C	C2-N1-C1'	15.12	135.43	118.80
1	A	573	A	C8-N9-C4	-15.02	99.79	105.80

There are no chirality outliers.

5 of 18 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	14	GLY	Peptide
2	B	75	LYS	Peptide
2	B	89	GLY	Peptide
3	C	166	GLU	Peptide
3	C	2	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	32707	0	16542	1874	1
2	B	1896	0	1936	217	0
3	C	1613	0	1677	201	0
4	D	1703	0	1763	203	0
5	E	1147	0	1207	135	1
6	F	843	0	857	87	0
7	G	1257	0	1296	146	0
8	H	1116	0	1177	118	0
9	I	1010	0	1037	144	0
10	J	793	0	835	125	0
11	K	873	0	894	76	0
12	L	973	0	1058	109	0
13	M	937	0	995	134	0
14	N	492	0	529	85	0
15	O	734	0	771	101	0
16	P	701	0	720	73	0
17	Q	834	0	906	115	0
18	R	585	0	657	80	0
19	S	648	0	673	83	0
20	T	763	0	861	101	0
21	U	209	0	221	43	0
22	V	77	0	42	1	0
23	W	235	0	121	34	0
24	a	175	0	87	0	0
25	b	60	0	31	0	0
26	A	326	0	0	0	0
26	D	3	0	0	0	0
26	E	4	0	0	0	0
26	F	1	0	0	0	0
26	G	1	0	0	0	0
26	H	1	0	0	0	0
26	J	1	0	0	0	0
26	N	1	0	0	0	0
26	P	3	0	0	0	0
26	Q	1	0	0	0	0
26	S	2	0	0	0	0
27	A	40	0	38	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	D	1	0	0	0	0
28	N	1	0	0	0	0
29	A	866	0	0	97	0
29	C	1	0	0	0	0
29	D	7	0	0	1	0
29	E	5	0	0	0	0
29	L	1	0	0	0	0
29	N	1	0	0	0	0
29	P	1	0	0	0	0
29	Q	2	0	0	0	0
29	T	3	0	0	0	0
29	U	4	0	0	0	0
29	W	1	0	0	0	0
All	All	53659	0	36931	3978	2

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 45.

The worst 5 of 3978 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:451:A:O2'	29:A:2729:HOH:O	1.59	1.20
12:L:70:ILE:HG21	12:L:75:HIS:HD2	1.13	1.14
15:O:88:ARG:HE	15:O:88:ARG:HA	1.10	1.12
1:A:266:G:H5'	1:A:266:G:C8	1.83	1.12
21:U:10:ARG:CB	21:U:10:ARG:HH11	1.62	1.12

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:U:O2	1:A:1400:5MC:N4[3_545]	2.15	0.05
5:E:73:ASN:N	5:E:149:GLU:OE1[7_555]	2.18	0.02



## 5.3 Torsion angles

### 5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	234/256 (91%)	197 (84%)	34 (14%)	3 (1%)	15	61
3	C	205/239 (86%)	169 (82%)	35 (17%)	1 (0%)	34	77
4	D	206/209 (99%)	180 (87%)	25 (12%)	1 (0%)	34	77
5	E	149/162 (92%)	137 (92%)	11 (7%)	1 (1%)	26	72
6	F	99/101 (98%)	93 (94%)	6 (6%)	0	100	100
7	G	153/156 (98%)	132 (86%)	21 (14%)	0	100	100
8	H	136/138 (99%)	128 (94%)	7 (5%)	1 (1%)	26	72
9	I	125/128 (98%)	107 (86%)	17 (14%)	1 (1%)	24	70
10	J	97/105 (92%)	77 (79%)	17 (18%)	3 (3%)	5	45
11	K	115/129 (89%)	98 (85%)	17 (15%)	0	100	100
12	L	122/135 (90%)	110 (90%)	8 (7%)	4 (3%)	5	44
13	M	116/126 (92%)	99 (85%)	16 (14%)	1 (1%)	21	68
14	N	58/61 (95%)	50 (86%)	8 (14%)	0	100	100
15	O	86/89 (97%)	72 (84%)	14 (16%)	0	100	100
16	P	82/88 (93%)	74 (90%)	7 (8%)	1 (1%)	16	63
17	Q	98/105 (93%)	93 (95%)	5 (5%)	0	100	100
18	R	69/88 (78%)	60 (87%)	9 (13%)	0	100	100
19	S	79/93 (85%)	68 (86%)	9 (11%)	2 (2%)	7	49
20	T	97/106 (92%)	80 (82%)	16 (16%)	1 (1%)	19	66
21	U	23/27 (85%)	22 (96%)	1 (4%)	0	100	100
All	All	2349/2541 (92%)	2046 (87%)	283 (12%)	20 (1%)	21	68

5 of 20 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	15	THR

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Mol	Chain	Res	Type
9	I	119	ALA
12	L	28	LYS
16	P	83	GLU
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	201/220 (91%)	151 (75%)	50 (25%)	1	6
3	C	160/188 (85%)	119 (74%)	41 (26%)	0	6
4	D	180/181 (99%)	134 (74%)	46 (26%)	0	6
5	E	115/123 (94%)	75 (65%)	40 (35%)	0	2
6	F	90/90 (100%)	60 (67%)	30 (33%)	0	2
7	G	126/127 (99%)	92 (73%)	34 (27%)	0	5
8	H	119/119 (100%)	83 (70%)	36 (30%)	0	4
9	I	98/99 (99%)	75 (76%)	23 (24%)	1	7
10	J	87/92 (95%)	70 (80%)	17 (20%)	2	13
11	K	89/99 (90%)	72 (81%)	17 (19%)	2	13
12	L	103/110 (94%)	80 (78%)	23 (22%)	1	9
13	M	94/101 (93%)	64 (68%)	30 (32%)	0	3
14	N	49/50 (98%)	35 (71%)	14 (29%)	0	4
15	O	79/80 (99%)	60 (76%)	19 (24%)	1	7
16	P	72/74 (97%)	54 (75%)	18 (25%)	1	6
17	Q	95/97 (98%)	74 (78%)	21 (22%)	1	9
18	R	62/77 (80%)	48 (77%)	14 (23%)	1	8
19	S	71/80 (89%)	55 (78%)	16 (22%)	1	9
20	T	76/82 (93%)	51 (67%)	25 (33%)	0	3
21	U	19/22 (86%)	16 (84%)	3 (16%)	3	23

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1985/2111 (94%)	1468 (74%)	517 (26%)	<b>0</b> <b>5</b>

5 of 517 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	G	120	ILE
9	I	63	ILE
19	S	15	LEU
7	G	156	TRP
8	H	95	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
9	I	73	GLN
12	L	75	HIS
19	S	23	ASN
7	G	37	ASN
16	P	16	HIS

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1503/1522 (98%)	377 (25%)	48 (3%)
22	V	3/4 (75%)	1 (33%)	0
23	W	10/11 (90%)	2 (20%)	0
24	a	7/8 (87%)	4 (57%)	0
25	b	2/3 (66%)	0	0
All	All	1525/1548 (98%)	384 (25%)	48 (3%)

5 of 384 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	7	G
1	A	9	G
1	A	16	A
1	A	31	G
1	A	32	A

5 of 48 RNA pucker outliers are listed below:



Mol	Chain	Res	Type
1	A	587	G
1	A	960	U
1	A	1361(A)	C
1	A	687	A
1	A	812	C

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

18 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	2.63	6 (35%)	21,38,41	2.47	2 (9%)
1	5MC	A	1400	1	13,22,23	1.55	3 (23%)	15,32,35	0.77	0
1	4OC	A	1402	1	13,23,24	1.32	2 (15%)	18,32,35	1.16	1 (5%)
1	5MC	A	1404	1	13,22,23	1.05	1 (7%)	15,32,35	1.09	2 (13%)
1	5MC	A	1407	1	13,22,23	2.02	3 (23%)	15,32,35	1.09	1 (6%)
1	UR3	A	1498	1	12,22,23	0.86	1 (8%)	16,32,35	1.33	3 (18%)
1	MA6	A	1518[A]	1	16,26,27	1.36	3 (18%)	18,38,41	1.10	2 (11%)
1	MA6	A	1518[B]	1	16,26,27	1.19	2 (12%)	18,38,41	1.14	2 (11%)
1	MA6	A	1519[A]	1	16,26,27	1.12	2 (12%)	18,38,41	1.38	4 (22%)
1	MA6	A	1519[B]	1	16,26,27	2.06	5 (31%)	18,38,41	1.15	2 (11%)
1	PSU	A	1540	1	13,21,22	1.15	1 (7%)	18,30,33	3.80	4 (22%)
1	PSU	A	516	1	13,21,22	1.47	2 (15%)	18,30,33	3.95	4 (22%)
1	7MG	A	527	1	19,26,27	2.87	5 (26%)	24,39,42	1.70	4 (16%)
1	M2G	A	966	1	17,27,28	1.38	3 (17%)	22,40,43	2.02	3 (13%)
1	5MC	A	967	1	13,22,23	0.89	0	15,32,35	0.96	1 (6%)
12	0TD	L	92	12	4,9,10	1.07	0	4,11,13	4.01	3 (75%)
23	PSU	W	40	23	13,21,22	1.10	2 (15%)	18,30,33	3.58	5 (27%)
24	PSU	a	40	24,1	13,21,22	1.77	2 (15%)	18,30,33	4.25	5 (27%)

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[A]	1	-	0/7/29/30	0/3/3/3
1	MA6	A	1518[B]	1	-	0/7/29/30	0/3/3/3
1	MA6	A	1519[A]	1	-	0/7/29/30	0/3/3/3
1	MA6	A	1519[B]	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	516	1	-	0/7/25/26	0/2/2/2
1	7MG	A	527	1	-	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
23	PSU	W	40	23	-	0/7/25/26	0/2/2/2
24	PSU	a	40	24,1	-	0/7/25/26	0/2/2/2

The worst 5 of 43 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	527	7MG	C8-N9	-9.11	1.32	1.45
1	A	527	7MG	CM7-N7	-2.81	1.41	1.46
1	A	527	7MG	C8-N7	-2.44	1.32	1.43
1	A	1402	4OC	C4-N3	-2.24	1.30	1.34
1	A	1498	UR3	C6-N1	-2.19	1.32	1.35

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	a	40	PSU	N1-C2-N3	-15.39	118.52	128.33
1	A	516	PSU	N1-C2-N3	-14.33	119.19	128.33
1	A	1540	PSU	N1-C2-N3	-14.07	119.36	128.33
23	W	40	PSU	N1-C2-N3	-12.77	120.19	128.33
1	A	1207	2MG	C5-C6-N1	-9.52	110.58	123.59

There are no chirality outliers.

There are no torsion outliers.



There are no ring outliers.

16 monomers are involved in 89 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1207	2MG	11	0
1	A	1400	5MC	5	1
1	A	1402	4OC	5	0
1	A	1404	5MC	5	0
1	A	1407	5MC	10	0
1	A	1498	UR3	8	0
1	A	1518[A]	MA6	10	0
1	A	1518[B]	MA6	9	0
1	A	1519[A]	MA6	18	0
1	A	1519[B]	MA6	11	0
1	A	516	PSU	1	0
1	A	527	7MG	1	0
1	A	966	M2G	3	0
1	A	967	5MC	4	0
12	L	92	0TD	2	0
23	W	40	PSU	5	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 347 ligands modelled in this entry, 346 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
27	SRY	A	1928	-	33,42,42	1.48	5 (15%)	36,63,63	2.60	15 (41%)

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
27	SRY	A	1928	-	-	0/16/87/87	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	A	1928	SRY	O53-C53	-3.48	1.35	1.44
27	A	1928	SRY	C11-N11	-3.32	1.41	1.47
27	A	1928	SRY	C23-N23	-3.04	1.42	1.47
27	A	1928	SRY	C21-C11	-2.31	1.48	1.53
27	A	1928	SRY	O51-C51	-2.00	1.38	1.43

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	A	1928	SRY	C43-C33-C23	-8.01	99.32	110.43
27	A	1928	SRY	C13-O13-C22	-5.30	106.79	116.30
27	A	1928	SRY	C61-C11-N11	-4.35	98.51	111.38
27	A	1928	SRY	O51-C51-C61	-3.03	103.52	110.34
27	A	1928	SRY	O53-C53-C63	-2.41	100.26	106.36

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	A	1928	SRY	14	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	1500/1522 (98%)	-0.43	2 (0%) 95 93	80, 129, 232, 327	0
2	B	236/256 (92%)	-0.15	2 (0%) 87 77	62, 153, 220, 247	0
3	C	207/239 (86%)	-0.22	5 (2%) 62 46	94, 191, 226, 244	0
4	D	208/209 (99%)	-0.22	5 (2%) 62 46	105, 149, 198, 214	0
5	E	151/162 (93%)	-0.43	0 100 100	80, 114, 166, 193	0
6	F	101/101 (100%)	-0.46	1 (0%) 84 72	110, 150, 182, 226	0
7	G	155/156 (99%)	-0.38	3 (1%) 70 54	121, 160, 223, 238	0
8	H	138/138 (100%)	-0.42	0 100 100	75, 104, 138, 155	0
9	I	127/128 (99%)	0.10	3 (2%) 62 46	125, 184, 217, 240	0
10	J	99/105 (94%)	0.16	4 (4%) 42 28	81, 203, 272, 295	0
11	K	117/129 (90%)	-0.39	0 100 100	88, 130, 160, 167	0
12	L	124/135 (91%)	0.06	5 (4%) 42 28	97, 136, 168, 247	0
13	M	118/126 (93%)	0.08	5 (4%) 40 27	127, 158, 192, 211	0
14	N	60/61 (98%)	-0.19	1 (1%) 73 58	144, 169, 210, 246	0
15	O	88/89 (98%)	0.02	2 (2%) 64 47	94, 127, 182, 225	0
16	P	84/88 (95%)	-0.21	0 100 100	96, 126, 164, 239	0
17	Q	100/105 (95%)	-0.31	0 100 100	83, 111, 150, 189	0
18	R	71/88 (80%)	-0.30	0 100 100	95, 132, 178, 229	0
19	S	81/93 (87%)	0.19	2 (2%) 61 44	84, 184, 228, 234	0
20	T	99/106 (93%)	-0.25	0 100 100	95, 126, 167, 212	0
21	U	25/27 (92%)	0.42	2 (8%) 15 9	77, 163, 192, 220	0
22	V	4/4 (100%)	3.91	4 (100%) 0 0	263, 267, 272, 275	0
23	W	10/11 (90%)	6.93	10 (100%) 0 0	234, 291, 345, 387	5 (50%)
24	a	7/8 (87%)	0.71	1 (14%) 4 3	200, 217, 290, 330	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
25	b	3/3 (100%)	1.07	0 100 100	172, 172, 206, 218	0
All	All	3913/4089 (95%)	-0.25	57 (1%) 76 62	62, 140, 222, 387	5 (0%)

The worst 5 of 57 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
23	W	32	C	12.9
23	W	31	C	8.5
23	W	33	U	8.1
1	A	1129	C	7.7
23	W	35	G	7.4

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	5MC	A	967	21/22	0.97	0.12	-	117,131,145,146	0
1	5MC	A	1404	21/22	0.95	0.17	-	102,129,148,149	0
1	7MG	A	527	24/25	0.97	0.17	-	91,114,123,126	0
1	M2G	A	966	25/26	0.94	0.18	-	122,137,142,145	0
1	2MG	A	1207	24/25	0.96	0.15	-	154,167,200,202	0
1	UR3	A	1498	21/22	0.95	0.25	-	111,124,183,193	0
1	MA6	A	1518[A]	24/25	0.94	0.20	-	110,122,127,131	24
1	5MC	A	1407	21/22	0.96	0.11	-	127,152,158,162	0
12	0TD	L	92	10/11	0.99	0.22	-	113,121,127,289	0
23	PSU	W	40	20/21	0.68	0.33	-	291,301,325,326	0
1	PSU	A	516	20/21	0.96	0.10	-	123,147,168,168	0
1	4OC	A	1402	22/23	0.92	0.21	-	104,119,127,142	0
1	PSU	A	1540	20/21	0.71	0.35	-	253,269,289,293	0
1	MA6	A	1519[A]	24/25	0.96	0.30	-	100,115,125,126	24
1	MA6	A	1518[B]	24/25	0.94	0.20	-	107,122,137,148	24
1	MA6	A	1519[B]	24/25	0.96	0.30	-	101,116,129,130	24
24	PSU	a	40	20/21	0.81	0.32	-	208,236,258,262	0
1	5MC	A	1400	21/22	0.95	0.17	-	103,130,148,159	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
26	MG	A	1870	1/1	0.94	0.48	51.50	406,406,406,406	0
26	MG	A	1834	1/1	0.83	0.93	45.54	412,412,412,412	1
26	MG	A	1759	1/1	0.78	0.86	33.73	86,86,86,86	0
26	MG	A	1804	1/1	0.89	0.50	22.88	447,447,447,447	0
26	MG	A	1670	1/1	0.86	0.47	15.78	234,234,234,234	0
26	MG	A	1904	1/1	0.64	0.65	15.63	97,97,97,97	0
26	MG	A	1728	1/1	0.82	0.86	14.98	114,114,114,114	0
26	MG	A	1761	1/1	0.98	0.59	12.51	105,105,105,105	0
26	MG	N	102	1/1	0.79	0.54	11.89	107,107,107,107	0
26	MG	A	1740	1/1	0.84	0.56	10.67	93,93,93,93	0
26	MG	A	1812	1/1	0.94	0.73	10.31	444,444,444,444	0
26	MG	E	201	1/1	0.94	0.34	7.43	95,95,95,95	0
26	MG	A	1659	1/1	0.94	0.30	6.60	90,90,90,90	0
26	MG	A	1655	1/1	0.89	0.30	6.09	125,125,125,125	0
26	MG	A	1743	1/1	0.79	0.35	6.08	105,105,105,105	0
26	MG	A	1665	1/1	0.63	0.67	5.79	117,117,117,117	0
26	MG	A	1869	1/1	0.91	0.27	5.22	431,431,431,431	0
26	MG	A	1784	1/1	0.85	0.28	5.05	122,122,122,122	0
26	MG	A	1888	1/1	0.93	0.32	4.30	89,89,89,89	0
26	MG	A	1656	1/1	0.98	0.22	4.12	236,236,236,236	0
26	MG	A	1637	1/1	0.95	0.28	3.53	228,228,228,228	0
26	MG	A	1721	1/1	0.96	0.26	3.42	92,92,92,92	0
26	MG	A	1900	1/1	0.84	0.33	3.39	93,93,93,93	0
26	MG	Q	201	1/1	0.90	0.47	3.35	145,145,145,145	0
26	MG	A	1621	1/1	0.92	0.16	3.23	131,131,131,131	0
26	MG	A	1709	1/1	0.93	0.21	3.12	245,245,245,245	0
26	MG	A	1764	1/1	0.98	0.44	2.99	78,78,78,78	0
26	MG	A	1715	1/1	0.96	0.22	2.89	229,229,229,229	0
26	MG	A	1701	1/1	0.97	0.22	2.68	108,108,108,108	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
26	MG	A	1708	1/1	0.96	0.22	2.42	152,152,152,152	0
26	MG	A	1741	1/1	0.95	0.16	2.26	105,105,105,105	0
26	MG	A	1733	1/1	0.98	0.19	2.25	70,70,70,70	0
26	MG	A	1768	1/1	0.94	0.35	2.25	107,107,107,107	0
26	MG	A	1723	1/1	0.84	0.26	2.23	117,117,117,117	0
26	MG	E	204	1/1	0.80	0.26	2.11	128,128,128,128	0
26	MG	A	1763	1/1	0.92	0.29	2.02	120,120,120,120	0
26	MG	A	1732	1/1	0.88	0.20	2.01	100,100,100,100	0
26	MG	A	1650	1/1	0.94	0.20	1.96	151,151,151,151	0
26	MG	A	1757	1/1	0.93	0.21	1.66	88,88,88,88	0
26	MG	A	1895	1/1	0.91	0.19	1.55	106,106,106,106	0
26	MG	A	1796	1/1	0.90	0.22	1.36	416,416,416,416	0
26	MG	A	1720	1/1	0.89	0.25	1.30	74,74,74,74	0
28	ZN	D	301	1/1	0.98	0.29	0.49	138,138,138,138	0
26	MG	A	1608	1/1	0.98	0.21	0.23	73,73,73,73	0
26	MG	A	1750	1/1	0.98	0.19	0.20	74,74,74,74	0
26	MG	A	1646	1/1	0.93	0.17	0.19	136,136,136,136	0
26	MG	D	303	1/1	0.96	0.21	0.17	104,104,104,104	0
26	MG	A	1847	1/1	0.98	0.18	0.02	441,441,441,441	0
26	MG	A	1617	1/1	0.89	0.22	-0.04	85,85,85,85	0
26	MG	A	1859	1/1	0.99	0.16	-0.05	427,427,427,427	0
26	MG	A	1919	1/1	0.91	0.18	-0.06	78,78,78,78	0
26	MG	A	1746	1/1	0.94	0.16	-0.08	104,104,104,104	0
26	MG	A	1736	1/1	0.98	0.15	-0.25	123,123,123,123	0
26	MG	A	1702	1/1	0.95	0.13	-0.32	279,279,279,279	0
28	ZN	N	101	1/1	0.97	0.16	-0.33	164,164,164,164	0
26	MG	A	1920	1/1	0.91	0.07	-0.39	138,138,138,138	0
26	MG	A	1776	1/1	0.96	0.17	-0.49	96,96,96,96	0
26	MG	A	1697	1/1	0.87	0.18	-0.54	135,135,135,135	0
26	MG	A	1693	1/1	0.97	0.10	-0.76	108,108,108,108	0
26	MG	A	1616	1/1	0.98	0.17	-0.77	63,63,63,63	0
27	SRY	A	1928	40/40	0.96	0.15	-0.83	70,100,124,130	0
26	MG	A	1775	1/1	0.97	0.12	-0.86	79,79,79,79	0
26	MG	A	1689	1/1	0.97	0.14	-0.92	126,126,126,126	0
26	MG	A	1786	1/1	0.91	0.09	-1.10	109,109,109,109	0
26	MG	A	1662	1/1	0.98	0.12	-1.38	123,123,123,123	0
26	MG	A	1713	1/1	0.99	0.11	-1.41	211,211,211,211	0
26	MG	A	1703	1/1	0.99	0.14	-1.45	97,97,97,97	0
26	MG	A	1672	1/1	0.98	0.10	-1.48	166,166,166,166	0
26	MG	A	1731	1/1	0.95	0.18	-1.74	68,68,68,68	0
26	MG	A	1623	1/1	0.99	0.13	-1.97	67,67,67,67	0
26	MG	A	1607	1/1	0.99	0.11	-2.19	154,154,154,154	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
26	MG	A	1638	1/1	0.99	0.13	-2.52	86,86,86,86	0
26	MG	A	1631	1/1	0.96	0.09	-2.75	158,158,158,158	0
26	MG	A	1643	1/1	0.95	0.08	-2.77	71,71,71,71	0
26	MG	A	1827	1/1	0.99	0.08	-2.79	251,251,251,251	0
26	MG	A	1906	1/1	0.96	0.13	-3.03	64,64,64,64	0
26	MG	A	1690	1/1	0.98	0.07	-3.28	114,114,114,114	0
26	MG	A	1611	1/1	1.00	0.10	-4.21	113,113,113,113	0
26	MG	A	1705	1/1	0.96	0.13	-4.40	74,74,74,74	0
26	MG	A	1835	1/1	0.95	0.13	-	309,309,309,309	0
26	MG	E	203	1/1	0.96	0.12	-	101,101,101,101	0
26	MG	A	1667	1/1	0.98	0.18	-	119,119,119,119	0
26	MG	G	201	1/1	0.61	0.83	-	117,117,117,117	0
26	MG	A	1640	1/1	0.93	0.22	-	172,172,172,172	0
26	MG	A	1907	1/1	0.91	0.27	-	120,120,120,120	0
26	MG	A	1632	1/1	0.78	0.34	-	248,248,248,248	0
26	MG	A	1606	1/1	0.97	0.41	-	87,87,87,87	0
26	MG	A	1716	1/1	0.98	0.24	-	132,132,132,132	0
26	MG	A	1781	1/1	0.73	0.35	-	104,104,104,104	0
26	MG	A	1845	1/1	0.91	0.31	-	410,410,410,410	0
26	MG	A	1829	1/1	0.90	0.28	-	489,489,489,489	0
26	MG	A	1921	1/1	0.68	0.39	-	84,84,84,84	0
26	MG	A	1657	1/1	0.89	0.34	-	220,220,220,220	0
26	MG	A	1603	1/1	0.97	0.13	-	277,277,277,277	0
26	MG	A	1896	1/1	0.96	0.13	-	114,114,114,114	0
26	MG	A	1649	1/1	0.83	0.33	-	84,84,84,84	0
26	MG	A	1725	1/1	0.90	0.26	-	92,92,92,92	0
26	MG	A	1682	1/1	0.87	0.07	-	242,242,242,242	0
26	MG	A	1604	1/1	0.94	0.25	-	91,91,91,91	0
26	MG	A	1807	1/1	0.84	0.47	-	517,517,517,517	1
26	MG	A	1860	1/1	0.93	0.22	-	460,460,460,460	0
26	MG	A	1626	1/1	0.99	0.26	-	245,245,245,245	0
26	MG	A	1668	1/1	0.97	0.25	-	173,173,173,173	0
26	MG	A	1855	1/1	0.93	0.18	-	401,401,401,401	0
26	MG	A	1612	1/1	0.95	0.45	-	281,281,281,281	0
26	MG	A	1816	1/1	0.92	0.44	-	454,454,454,454	0
26	MG	A	1853	1/1	0.92	0.25	-	502,502,502,502	0
26	MG	A	1926	1/1	0.51	0.58	-	116,116,116,116	0
26	MG	A	1858	1/1	0.99	0.23	-	355,355,355,355	0
26	MG	A	1641	1/1	0.95	0.17	-	102,102,102,102	0
26	MG	A	1633	1/1	0.98	0.18	-	118,118,118,118	0
26	MG	A	1675	1/1	0.53	1.12	-	122,122,122,122	0
26	MG	A	1873	1/1	0.98	0.12	-	361,361,361,361	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
26	MG	A	1753	1/1	0.93	0.24	-	109,109,109,109	0
26	MG	A	1622	1/1	0.62	0.51	-	81,81,81,81	0
26	MG	H	201	1/1	0.82	0.33	-	67,67,67,67	0
26	MG	A	1609	1/1	0.92	0.07	-	157,157,157,157	0
26	MG	A	1780	1/1	0.96	0.33	-	119,119,119,119	0
26	MG	A	1910	1/1	0.10	0.29	-	120,120,120,120	0
26	MG	A	1914	1/1	0.68	1.02	-	99,99,99,99	0
26	MG	A	1771	1/1	0.96	0.57	-	102,102,102,102	0
26	MG	A	1918	1/1	0.92	0.20	-	75,75,75,75	0
26	MG	A	1848	1/1	0.93	0.21	-	407,407,407,407	0
26	MG	A	1676	1/1	0.90	0.28	-	158,158,158,158	0
26	MG	A	1801	1/1	0.95	0.20	-	464,464,464,464	0
26	MG	A	1838	1/1	0.88	0.56	-	538,538,538,538	0
26	MG	A	1688	1/1	0.91	0.41	-	186,186,186,186	0
26	MG	A	1824	1/1	0.94	0.26	-	503,503,503,503	0
26	MG	A	1788	1/1	0.90	0.10	-	285,285,285,285	0
26	MG	A	1864	1/1	0.94	0.20	-	393,393,393,393	0
26	MG	A	1878	1/1	0.89	0.20	-	346,346,346,346	0
26	MG	A	1779	1/1	0.83	0.32	-	102,102,102,102	0
26	MG	A	1830	1/1	0.97	0.27	-	480,480,480,480	0
26	MG	A	1729	1/1	0.59	0.55	-	101,101,101,101	0
26	MG	A	1791	1/1	0.96	0.19	-	283,283,283,283	0
26	MG	A	1844	1/1	0.92	0.09	-	420,420,420,420	0
26	MG	A	1739	1/1	0.91	0.17	-	78,78,78,78	0
26	MG	A	1917	1/1	0.63	0.86	-	128,128,128,128	0
26	MG	A	1880	1/1	0.76	0.49	-	508,508,508,508	0
26	MG	A	1745	1/1	0.89	0.48	-	92,92,92,92	0
26	MG	A	1644	1/1	0.87	0.37	-	127,127,127,127	0
26	MG	A	1724	1/1	0.75	0.54	-	117,117,117,117	0
26	MG	A	1911	1/1	0.99	0.12	-	100,100,100,100	0
26	MG	A	1862	1/1	0.96	0.35	-	268,268,268,268	0
26	MG	A	1680	1/1	0.95	0.23	-	214,214,214,214	0
26	MG	A	1634	1/1	0.97	0.08	-	107,107,107,107	0
26	MG	A	1679	1/1	0.81	0.18	-	369,369,369,369	0
26	MG	A	1698	1/1	0.97	0.18	-	124,124,124,124	0
26	MG	A	1666	1/1	0.98	0.08	-	149,149,149,149	0
26	MG	A	1852	1/1	0.80	0.33	-	450,450,450,450	0
26	MG	A	1794	1/1	0.42	0.27	-	518,518,518,518	0
26	MG	A	1828	1/1	0.97	0.13	-	432,432,432,432	0
26	MG	A	1923	1/1	0.78	0.77	-	86,86,86,86	0
26	MG	A	1727	1/1	0.88	0.65	-	84,84,84,84	0
26	MG	A	1822	1/1	0.95	0.12	-	293,293,293,293	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
26	MG	A	1819	1/1	0.85	0.52	-	493,493,493,493	0
26	MG	A	1793	1/1	0.76	0.27	-	483,483,483,483	0
26	MG	A	1774	1/1	0.73	0.41	-	109,109,109,109	0
26	MG	A	1890	1/1	0.90	0.18	-	112,112,112,112	0
26	MG	A	1814	1/1	0.87	0.18	-	440,440,440,440	0
26	MG	A	1803	1/1	0.98	0.20	-	345,345,345,345	0
26	MG	A	1755	1/1	0.94	0.50	-	74,74,74,74	0
26	MG	A	1815	1/1	0.91	0.23	-	506,506,506,506	0
26	MG	A	1671	1/1	0.92	0.24	-	96,96,96,96	0
26	MG	A	1636	1/1	0.84	0.41	-	88,88,88,88	0
26	MG	A	1898	1/1	0.82	0.64	-	89,89,89,89	0
26	MG	A	1887	1/1	0.79	0.55	-	102,102,102,102	0
26	MG	A	1837	1/1	0.83	0.24	-	469,469,469,469	0
26	MG	A	1823	1/1	0.93	0.11	-	422,422,422,422	0
26	MG	A	1658	1/1	0.96	0.18	-	115,115,115,115	0
26	MG	A	1885	1/1	0.96	0.08	-	84,84,84,84	0
26	MG	A	1642	1/1	0.94	0.28	-	78,78,78,78	0
26	MG	S	101	1/1	0.92	0.11	-	115,115,115,115	0
26	MG	A	1800	1/1	0.96	0.32	-	415,415,415,415	1
26	MG	A	1678	1/1	0.88	0.11	-	217,217,217,217	0
26	MG	A	1851	1/1	0.97	0.27	-	328,328,328,328	0
26	MG	A	1694	1/1	0.85	0.39	-	87,87,87,87	0
26	MG	A	1866	1/1	0.91	0.20	-	434,434,434,434	0
26	MG	A	1901	1/1	0.24	0.36	-	101,101,101,101	0
26	MG	A	1661	1/1	0.91	0.28	-	244,244,244,244	0
26	MG	A	1908	1/1	0.83	0.30	-	81,81,81,81	0
26	MG	A	1899	1/1	0.77	0.33	-	68,68,68,68	0
26	MG	A	1767	1/1	0.91	0.33	-	111,111,111,111	0
26	MG	A	1783	1/1	0.95	0.13	-	110,110,110,110	0
26	MG	A	1663	1/1	0.92	0.14	-	160,160,160,160	0
26	MG	A	1686	1/1	0.98	0.38	-	184,184,184,184	0
26	MG	A	1778	1/1	0.97	0.11	-	119,119,119,119	1
26	MG	J	201	1/1	0.94	0.42	-	109,109,109,109	0
26	MG	A	1839	1/1	0.91	0.05	-	467,467,467,467	0
26	MG	A	1712	1/1	0.94	0.20	-	170,170,170,170	0
26	MG	A	1808	1/1	0.62	0.44	-	498,498,498,498	0
26	MG	A	1639	1/1	0.88	0.19	-	87,87,87,87	0
26	MG	A	1710	1/1	0.97	0.13	-	253,253,253,253	0
26	MG	A	1630	1/1	0.96	0.26	-	158,158,158,158	0
26	MG	A	1876	1/1	0.87	0.48	-	463,463,463,463	1
26	MG	A	1700	1/1	0.80	0.37	-	302,302,302,302	0
26	MG	A	1881	1/1	0.88	0.13	-	414,414,414,414	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
26	MG	A	1696	1/1	0.96	0.32	-	263,263,263,263	0
26	MG	A	1717	1/1	0.89	0.22	-	152,152,152,152	0
26	MG	F	601	1/1	0.88	0.06	-	102,102,102,102	0
26	MG	A	1785	1/1	0.90	0.21	-	108,108,108,108	0
26	MG	A	1836	1/1	0.86	0.22	-	416,416,416,416	1
26	MG	A	1893	1/1	0.82	0.44	-	114,114,114,114	0
26	MG	A	1648	1/1	0.98	0.25	-	93,93,93,93	0
26	MG	P	101	1/1	0.80	0.32	-	58,58,58,58	0
26	MG	A	1699	1/1	0.75	0.07	-	414,414,414,414	0
26	MG	A	1818	1/1	0.98	0.09	-	189,189,189,189	0
26	MG	A	1738	1/1	1.00	0.05	-	68,68,68,68	0
26	MG	A	1748	1/1	0.91	0.14	-	110,110,110,110	0
26	MG	A	1865	1/1	0.83	0.39	-	457,457,457,457	0
26	MG	A	1897	1/1	0.84	0.43	-	114,114,114,114	0
26	MG	A	1916	1/1	0.75	0.19	-	119,119,119,119	0
26	MG	A	1654	1/1	0.98	0.09	-	161,161,161,161	0
26	MG	A	1773	1/1	0.92	0.10	-	103,103,103,103	0
26	MG	A	1787	1/1	0.96	0.24	-	496,496,496,496	0
26	MG	A	1820	1/1	0.94	0.22	-	373,373,373,373	0
26	MG	A	1894	1/1	0.79	0.21	-	94,94,94,94	0
26	MG	A	1868	1/1	0.96	0.44	-	380,380,380,380	0
26	MG	A	1737	1/1	0.88	0.69	-	89,89,89,89	0
26	MG	P	103	1/1	0.74	0.47	-	96,96,96,96	0
26	MG	A	1628	1/1	0.80	0.28	-	152,152,152,152	0
26	MG	A	1806	1/1	0.93	0.19	-	505,505,505,505	0
26	MG	A	1915	1/1	0.93	0.66	-	117,117,117,117	0
26	MG	A	1863	1/1	0.82	0.22	-	409,409,409,409	0
26	MG	A	1912	1/1	0.75	0.55	-	104,104,104,104	0
26	MG	A	1770	1/1	0.61	0.63	-	106,106,106,106	0
26	MG	A	1902	1/1	0.83	0.35	-	119,119,119,119	0
26	MG	A	1742	1/1	0.91	0.35	-	97,97,97,97	0
26	MG	A	1685	1/1	0.97	0.50	-	126,126,126,126	0
26	MG	A	1627	1/1	1.00	0.11	-	141,141,141,141	0
26	MG	A	1674	1/1	0.96	0.08	-	260,260,260,260	0
26	MG	A	1817	1/1	0.92	0.18	-	419,419,419,419	0
26	MG	A	1872	1/1	0.96	0.25	-	359,359,359,359	0
26	MG	A	1811	1/1	0.97	1.57	-	468,468,468,468	0
26	MG	A	1809	1/1	0.79	0.24	-	494,494,494,494	0
26	MG	A	1846	1/1	0.54	0.32	-	449,449,449,449	0
26	MG	E	202	1/1	0.91	0.12	-	124,124,124,124	0
26	MG	A	1605	1/1	0.98	0.09	-	254,254,254,254	0
26	MG	A	1886	1/1	-0.01	1.21	-	121,121,121,121	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
26	MG	A	1647	1/1	0.87	0.30	-	104,104,104,104	0
26	MG	A	1619	1/1	0.98	0.12	-	64,64,64,64	0
26	MG	A	1602	1/1	0.97	0.47	-	66,66,66,66	1
26	MG	A	1782	1/1	0.90	0.59	-	87,87,87,87	0
26	MG	A	1762	1/1	0.89	0.43	-	82,82,82,82	0
26	MG	A	1645	1/1	0.97	0.40	-	227,227,227,227	0
26	MG	D	304	1/1	0.35	0.54	-	455,455,455,455	0
26	MG	A	1620	1/1	0.96	0.21	-	166,166,166,166	0
26	MG	A	1730	1/1	0.64	0.72	-	97,97,97,97	0
26	MG	A	1610	1/1	0.99	0.23	-	81,81,81,81	0
26	MG	A	1925	1/1	0.82	0.15	-	114,114,114,114	0
26	MG	P	102	1/1	0.69	0.35	-	101,101,101,101	0
26	MG	A	1913	1/1	0.78	0.79	-	108,108,108,108	0
26	MG	A	1695	1/1	0.92	0.06	-	176,176,176,176	0
26	MG	A	1922	1/1	0.95	0.34	-	110,110,110,110	0
26	MG	A	1927	1/1	0.92	0.21	-	112,112,112,112	0
26	MG	A	1760	1/1	0.76	0.60	-	88,88,88,88	0
26	MG	A	1726	1/1	0.85	0.17	-	98,98,98,98	0
26	MG	A	1677	1/1	0.98	0.23	-	235,235,235,235	0
26	MG	A	1722	1/1	0.87	0.89	-	95,95,95,95	0
26	MG	A	1772	1/1	0.89	0.12	-	93,93,93,93	0
26	MG	A	1826	1/1	0.87	0.08	-	395,395,395,395	0
26	MG	A	1810	1/1	0.91	0.37	-	474,474,474,474	0
26	MG	A	1879	1/1	0.89	0.28	-	438,438,438,438	0
26	MG	A	1850	1/1	0.93	0.07	-	236,236,236,236	0
26	MG	A	1861	1/1	0.94	0.11	-	443,443,443,443	0
26	MG	A	1765	1/1	0.91	0.16	-	104,104,104,104	0
26	MG	A	1789	1/1	0.96	0.16	-	378,378,378,378	0
26	MG	A	1849	1/1	0.96	0.31	-	471,471,471,471	0
26	MG	A	1875	1/1	0.93	0.20	-	460,460,460,460	0
26	MG	A	1735	1/1	0.96	0.12	-	106,106,106,106	0
26	MG	A	1795	1/1	0.90	1.11	-	359,359,359,359	0
26	MG	A	1874	1/1	0.96	0.09	-	467,467,467,467	0
26	MG	A	1909	1/1	0.71	0.34	-	93,93,93,93	0
26	MG	A	1704	1/1	0.98	0.15	-	104,104,104,104	0
26	MG	A	1882	1/1	0.99	0.34	-	315,315,315,315	0
26	MG	A	1749	1/1	0.97	0.14	-	84,84,84,84	0
26	MG	A	1871	1/1	0.80	0.25	-	392,392,392,392	0
26	MG	A	1618	1/1	0.83	0.39	-	130,130,130,130	0
26	MG	A	1758	1/1	0.70	0.32	-	101,101,101,101	0
26	MG	A	1651	1/1	0.98	0.17	-	110,110,110,110	0
26	MG	A	1798	1/1	0.91	0.07	-	464,464,464,464	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
26	MG	A	1857	1/1	0.93	0.33	-	308,308,308,308	0
26	MG	A	1805	1/1	0.91	0.09	-	331,331,331,331	0
26	MG	A	1714	1/1	0.93	0.24	-	108,108,108,108	0
26	MG	A	1840	1/1	0.93	0.17	-	467,467,467,467	1
26	MG	A	1683	1/1	0.91	0.05	-	154,154,154,154	0
26	MG	A	1883	1/1	0.93	0.27	-	443,443,443,443	0
26	MG	A	1625	1/1	0.99	0.06	-	113,113,113,113	0
26	MG	A	1614	1/1	0.86	0.17	-	285,285,285,285	0
26	MG	A	1856	1/1	0.90	0.06	-	478,478,478,478	0
26	MG	A	1867	1/1	0.98	0.55	-	413,413,413,413	1
26	MG	A	1747	1/1	0.97	0.15	-	115,115,115,115	0
26	MG	S	102	1/1	0.96	0.13	-	106,106,106,106	0
26	MG	A	1707	1/1	0.85	0.36	-	135,135,135,135	0
26	MG	A	1718	1/1	0.93	0.24	-	326,326,326,326	0
26	MG	A	1832	1/1	0.98	0.08	-	278,278,278,278	0
26	MG	A	1669	1/1	0.97	0.09	-	123,123,123,123	0
26	MG	A	1877	1/1	0.77	0.43	-	456,456,456,456	1
26	MG	A	1684	1/1	0.83	0.13	-	109,109,109,109	0
26	MG	A	1924	1/1	0.96	0.11	-	131,131,131,131	0
26	MG	A	1635	1/1	0.99	0.14	-	74,74,74,74	0
26	MG	A	1613	1/1	0.92	0.15	-	202,202,202,202	0
26	MG	A	1744	1/1	0.72	0.32	-	82,82,82,82	0
26	MG	A	1792	1/1	0.92	0.17	-	415,415,415,415	0
26	MG	D	302	1/1	0.81	0.38	-	104,104,104,104	0
26	MG	A	1664	1/1	0.96	0.19	-	154,154,154,154	0
26	MG	A	1691	1/1	0.95	0.21	-	186,186,186,186	0
26	MG	A	1711	1/1	0.77	0.99	-	133,133,133,133	0
26	MG	A	1624	1/1	0.43	1.10	-	147,147,147,147	0
26	MG	A	1802	1/1	0.94	0.11	-	355,355,355,355	0
26	MG	A	1905	1/1	0.90	0.20	-	105,105,105,105	0
26	MG	A	1734	1/1	0.75	0.52	-	124,124,124,124	0
26	MG	A	1889	1/1	0.88	0.22	-	95,95,95,95	0
26	MG	A	1615	1/1	0.97	0.09	-	147,147,147,147	0
26	MG	A	1673	1/1	0.90	0.93	-	91,91,91,91	0
26	MG	A	1777	1/1	0.91	0.15	-	94,94,94,94	0
26	MG	A	1681	1/1	0.94	0.03	-	256,256,256,256	0
26	MG	A	1903	1/1	0.93	0.21	-	78,78,78,78	0
26	MG	A	1843	1/1	0.98	0.68	-	357,357,357,357	0
26	MG	A	1751	1/1	0.91	0.46	-	76,76,76,76	0
26	MG	A	1825	1/1	0.94	0.20	-	436,436,436,436	0
26	MG	A	1653	1/1	0.99	0.25	-	96,96,96,96	0
26	MG	A	1752	1/1	0.93	0.22	-	91,91,91,91	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
26	MG	A	1841	1/1	0.93	0.26	-	496,496,496,496	0
26	MG	A	1797	1/1	0.87	0.16	-	502,502,502,502	0
26	MG	A	1754	1/1	0.97	0.16	-	85,85,85,85	0
26	MG	A	1813	1/1	0.76	0.65	-	471,471,471,471	0
26	MG	A	1692	1/1	0.99	0.20	-	182,182,182,182	0
26	MG	A	1884	1/1	0.82	1.04	-	119,119,119,119	0
26	MG	A	1756	1/1	0.91	0.16	-	126,126,126,126	0
26	MG	A	1706	1/1	0.95	0.13	-	190,190,190,190	0
26	MG	A	1719	1/1	0.96	0.08	-	262,262,262,262	0
26	MG	A	1660	1/1	0.89	0.23	-	224,224,224,224	0
26	MG	A	1766	1/1	0.83	0.52	-	105,105,105,105	0
26	MG	A	1842	1/1	0.92	0.50	-	488,488,488,488	0
26	MG	A	1821	1/1	0.96	0.29	-	428,428,428,428	0
26	MG	A	1892	1/1	0.54	0.38	-	92,92,92,92	0
26	MG	A	1854	1/1	0.95	0.51	-	418,418,418,418	0
26	MG	A	1769	1/1	0.67	0.54	-	127,127,127,127	0
26	MG	A	1891	1/1	0.75	0.16	-	127,127,127,127	0
26	MG	A	1833	1/1	0.98	0.12	-	335,335,335,335	0
26	MG	A	1652	1/1	0.97	0.09	-	72,72,72,72	0
26	MG	A	1687	1/1	0.97	0.14	-	106,106,106,106	0
26	MG	A	1831	1/1	0.95	0.18	-	395,395,395,395	0
26	MG	A	1799	1/1	0.90	0.22	-	426,426,426,426	0
26	MG	A	1790	1/1	0.91	0.14	-	444,444,444,444	0
26	MG	A	1629	1/1	0.90	0.26	-	223,223,223,223	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.