



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 05:52 PM GMT

PDB ID : 4JI6
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 : 3.55 Å(reported)

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

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

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

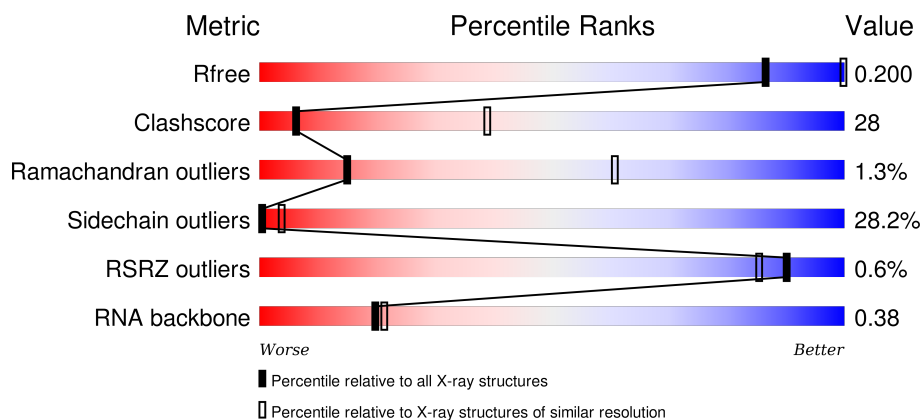
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.55 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.



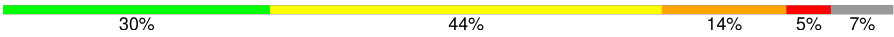
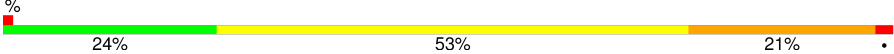

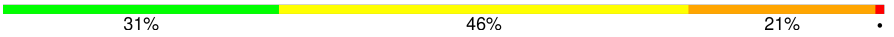

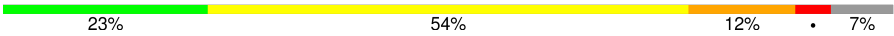
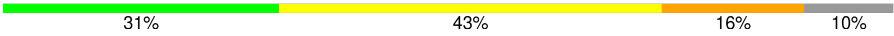

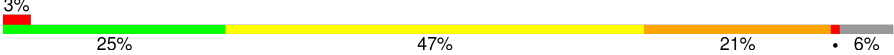
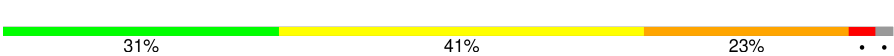
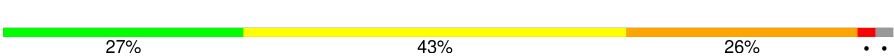
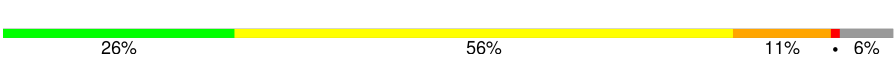
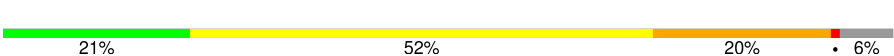
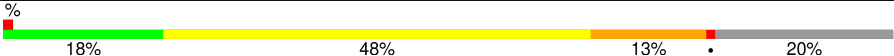
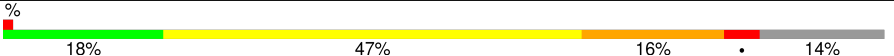
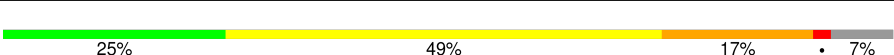
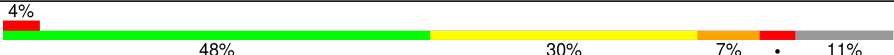
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1240 (3.72-3.40)
Clashscore	102246	1057 (3.70-3.42)
Ramachandran outliers	100387	1017 (3.70-3.42)
Sidechain outliers	100360	1017 (3.70-3.42)
RSRZ outliers	91569	1247 (3.72-3.40)
RNA backbone	2183	1057 (4.30-2.80)

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

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

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

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
22	MG	A	1614	-	-	-	X
22	MG	A	1628	-	-	-	X
22	MG	A	1657	-	-	-	X
22	MG	A	1665	-	-	-	X
22	MG	A	1666	-	-	-	X
22	MG	A	1676	-	-	-	X
22	MG	A	1686	-	-	-	X
22	MG	A	1687	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	MG	A	1691	-	-	-	X
22	MG	A	1692	-	-	-	X
22	MG	A	1704	-	-	-	X
22	MG	A	1711	-	-	-	X
22	MG	A	1715	-	-	-	X
22	MG	A	1721	-	-	-	X
22	MG	A	1722	-	-	-	X
22	MG	A	1724	-	-	-	X
22	MG	A	1746	-	-	-	X
22	MG	A	1767	-	-	-	X
22	MG	A	1806	-	-	-	X
22	MG	A	1815	-	-	-	X
22	MG	A	1865	-	-	-	X
22	MG	A	1892	-	-	-	X
22	MG	A	1893	-	-	-	X
22	MG	A	1921	-	-	-	X
22	MG	A	1926	-	-	-	X
22	MG	A	1931	-	-	-	X
22	MG	A	1971	-	-	-	X
22	MG	A	1975	-	-	-	X
22	MG	N	102	-	-	-	X

2 Entry composition

There are 24 unique types of molecules in this entry. The entry contains 53444 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	1514	Total	C	N	O	P	0	6	0
			32687	14559	6046	10562	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 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
			973	613	195	163	2			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	94	LEU	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	1	Total	Mg	0	0
			1	1		
22	G	1	Total	Mg	0	0
			1	1		
22	Q	2	Total	Mg	0	0
			2	2		
22	D	4	Total	Mg	0	0
			4	4		
22	K	1	Total	Mg	0	0
			1	1		
22	E	1	Total	Mg	0	0
			1	1		
22	H	1	Total	Mg	0	0
			1	1		
22	B	2	Total	Mg	0	0
			2	2		
22	I	2	Total	Mg	0	0
			2	2		
22	C	3	Total	Mg	0	0
			3	3		
22	A	377	Total	Mg	0	0
			377	377		
22	N	2	Total	Mg	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	O	1	Total 1	Mg 1	0	0
22	L	1	Total 1	Mg 1	0	0
22	S	1	Total 1	Mg 1	0	0
22	F	1	Total 1	Mg 1	0	0

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

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

- Molecule 24 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
24	A	1199	Total 1199	O 1199	0	0
24	C	6	Total 6	O 6	0	0
24	D	11	Total 11	O 11	0	0
24	E	7	Total 7	O 7	0	0
24	F	6	Total 6	O 6	0	0
24	G	6	Total 6	O 6	0	0
24	H	7	Total 7	O 7	0	0
24	I	1	Total 1	O 1	0	0
24	L	9	Total 9	O 9	0	0
24	M	2	Total 2	O 2	0	0
24	N	1	Total 1	O 1	0	0

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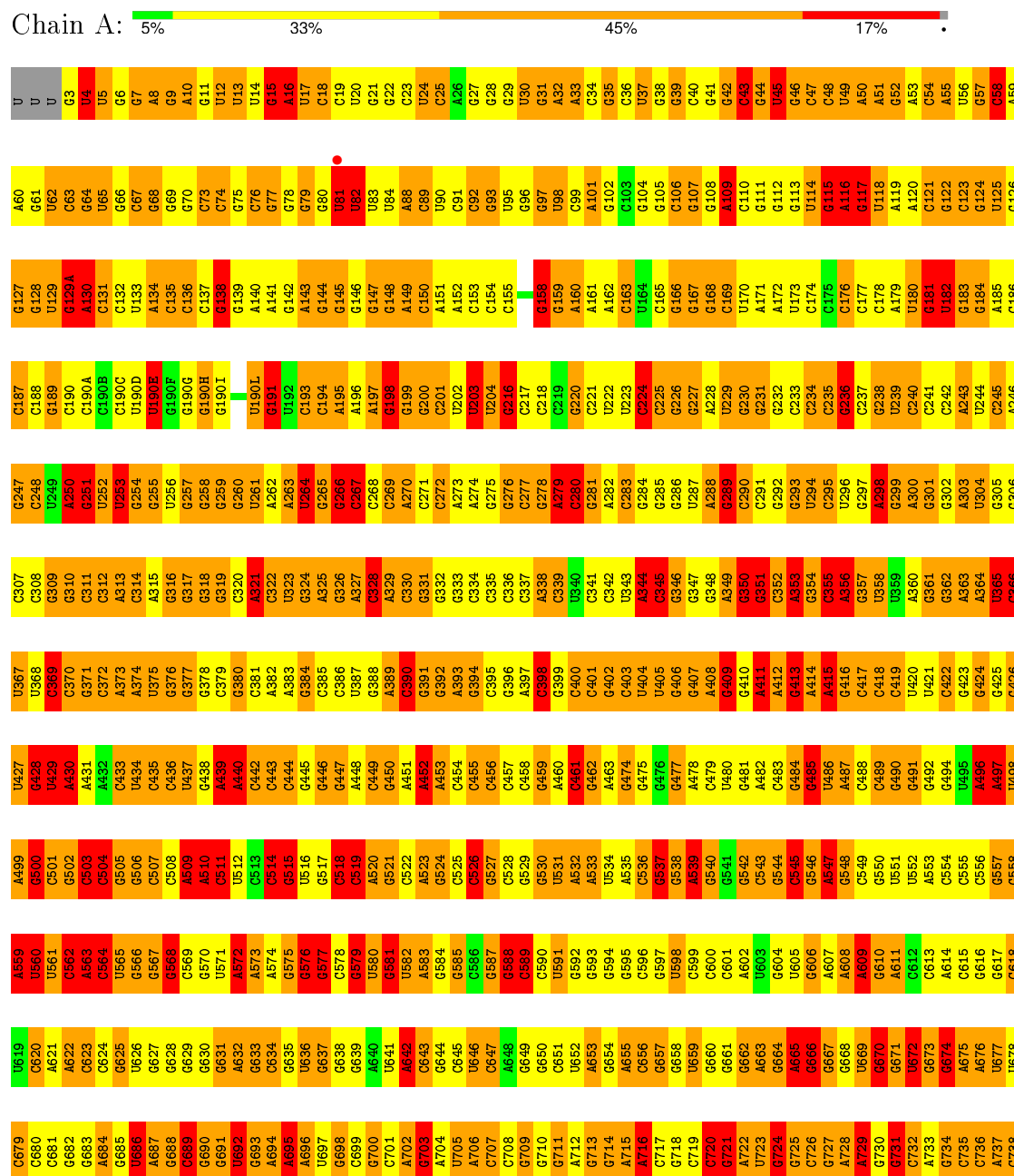
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
24	O	1	Total	O	0	0
			1	1		
24	P	3	Total	O	0	0
			3	3		
24	Q	6	Total	O	0	0
			6	6		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: 16S rRNA

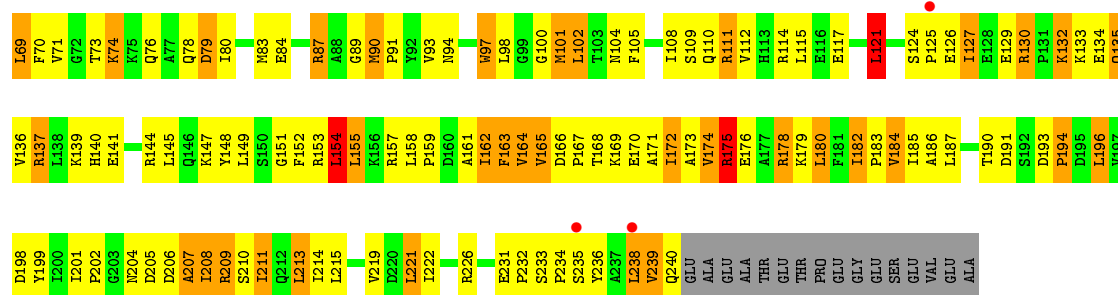


U1532	C1533	U1471	U406	G1347	A1287	A1235	G1164	C1103	U1040	C985	G925	A865	G799	G739
C1533	C1533	G1474	C1407	U1348	A1286	C1226	C1165	G1104	A1041	A986	G926	C866	G800	U740
A	A	A1475	A1408	A1349	A1289	A1227	G1166	A1106	G1042	A987	G927	C867	U801	G741
C	C	G1476	G1410	G1350	G1290	G1228	A1167	G1106	C1043	G988	G928	C868	A802	G742
U	U	G1477	G1411	G1352	G1292	A1229	A1168	C1107	A1044	C989	G929	C869	G803	U743
C	C	G1478	G1412	G1353	G1293	G1231	G1171	G1109	G1045	C990	G930	U870	U804	G744
U1413	U1413	C1479	C1413	C1354	G1294	U1232	C1172	C1110	A1046	U991	G931	U871	C805	G745
G1480	G1414	G1481	G1415	G1355	G1295	G1233	G1173	A1111	U1049	U992	G932	A872	C806	A746
G1482	G1416	G1483	G1417	G1356	C1296	C1234	G1174	A994	G1050	A994	G933	A873	A807	A747
A1483	A1417	U1484	U1418	U1357	G1297	U1235	G1175	C1113	C1051	C995	G934	G874	C808	C748
G1484	G1418	C1485	C1418	C1358	G1298	A1236	A1176	C1114	U1052	A996	G935	C875	C809	C749
U1485	U1419	G1486	G1420	G1359	A1299	C1237	G1177	C1115	G1053	U997	G936	C876	C810	G750
G1487	G1421	G1488	G1422	G1362	G1300	A1238	G1178	C1116	C1054	G998	G937	C877	C811	U751
G1488	G1422	G1489	G1423	G1363	U1301	A1239	A1179	C1117	A1055	C999	G938	G878	C812	G752
G1489	G1423	U1490	U1424	U1364	G1302	U1240	A1180	C1118	U1056	C980	G939	U813	U813	A753
C1490	C1425	G1491	G1426	G1365	G1303	G1241	G1181	C1119	G1057	A1001	G941	C881	A815	G755
U1492	U1427	G1493	G1428	G1366	G1304	C1242	G1182	G1120	G1058	G882	G942	C882	A816	C756
G1494	A1428	U1495	U1429	G1367	G1305	C1243	G1183	U1121	C1059	C883	G943	C817	A817	U757
U1496	G1430	G1497	G1431	G1370	G1311	C1249	C1188	U1122	G1060	U884	G944	G818	G818	G758
G1497	G1432	U1498	G1433	G1371	G1312	A1250	G1189	C1128	G1061	A759	G945	A819	A819	G759
A1499	G1433	G1499	A1433	G1372	U1313	A1251	A1191	C1129	G1062	U885	G946	U820	U820	G760
A1500	A1434	G1500	A1434	G1373	U1314	A1252	C1192	A1130	U1063	G886	G947	G821	G821	G761
C1501	G1435	A1501	G1435	A1374	U1315	G1253	G1193	U1012	C1069	A828	G948	C823	C823	G762
A1502	U1436	A1502	U1436	A1375	G1316	C1254	U1194	G1013	G1013	A828	G949	C824	C824	G763
A1503	U1437	A1503	U1437	U1376	G1317	G1255	U1195	A1014	G1071	A829	G950	G825	G825	G764
A1504	G1438	A1504	G1438	U1377	A1318	A1256	U1196	A1015	G1072	A830	G951	G836	G836	G775
G1505	G1439	G1505	G1439	C1378	A1319	U1257	G1197	A1016	U1073	U831	G952	G837	G837	G776
U1506	C1440	U1506	C1440	U1380	C1320	G1258	G1198	G1017	G1074	A988	U952	G838	G838	G777
A1507	G1441	U1507	G1441	U1381	C1321	C1259	G1199	C1018	C1075	A989	U953	U839	U839	G778
G1508	G1442	A1508	G1442	C1382	G1323	A1261	C1200	C1019	G1076	U960	U954	C834	C834	G779
C1509	G1443	C1509	G1443	C1383	A1324	C1262	G1202	U1020	G1077	A901	U961	U835	U835	G775
G1510	A1446	G1510	A1446	C1384	G1325	G1265	G1142	G1021	U1078	G902	C962	G836	G836	G776
U1512	G1447	U1512	G1447	G1385	C1326	G1266	G1143	G1022	G1079	G903	G963	G837	G837	G777
A1513	C1448	A1513	C1448	G1386	G1327	G1266	G1144	G1023	A1080	G904	A964	G838	G838	G778
C1514	G1449	C1514	G1449	G1387	C1328	G1266	C1145	G1024	G1079	U905	G965	U839	U839	G779
U1515	U1450	U1515	U1450	G1388	A1329	A1269	G1206	U1025	G1084	G906	G966	C840	C840	A780
A1516	A1451	A1516	A1451	C1389	U1330	C1270	A1146	G1026	U1085	A907	C967	U841	U841	A781
G1517	C1452	G1517	C1452	U1390	G1331	C1271	C1147	C1027	U1086	A908	A968	C848	C848	A782
A1518	G1453	A1518	G1453	U1391	A1332	G1272	U1148	G1028	G1087	A909	C970	U850	U850	G783
G1519	G1454	G1519	G1454	G1392	A1333	G1273	U1150	C1029	G1088	G910	C971	G851	G851	G785
A1520	C1455	A1520	C1455	U1393	G1334	G1274	A1151	C1030	G1089	U911	C972	G852	G852	G786
G1521	A1456	G1521	A1456	A1394	C1335	A1275	A1152	G1030A	U1090	G912	G973	G853	G853	A787
U1522	C1457	U1522	C1457	C1395	G1336	G1276	C1153	G1030C	A1092	A974	A974	G854	G854	U788
G1523	G1461	G1523	G1461	A1396	G1337	C1277	G1154	A1030D	A1093	A915	A975	G855	G855	U789
C1524	G1462	C1524	G1462	C1397	A1338	U1278	G1155	G1031	G1094	G916	G976	C856	C856	A790
G1525	C1463	G1525	C1463	A1398	G1339	A1279	C1156	G1032	U1095	A977	A977	G857	G857	A791
C1526	G1464	C1526	G1464	C1399	A1340	A1280	A1157	G1033	C1096	A918	A978	G858	G858	A792
G1527	C1465	G1527	C1465	G1400	U1341	U1281	C1158	G1034	C1097	C979	C979	A859	A859	U793
U1528	G1466	U1528	G1466	C1401	C1342	C1282	U1159	A1035	C1098	U920	C980	A860	A860	A794
G1529	G1467	G1529	G1467	C1402	G1343	G1283	G1160	G1036	G1099	U921	U921	G861	G861	C795
U1530	A1468	U1530	A1468	C1403	C1344	A1284	C1161	C1037	C1100	U922	U922	G862	G862	C796
A1531	G1470	A1531	G1470	G1405	A1346	A1286	C1163	C1039	A1102	C984	C984	U863	U863	C797
														G798

● Molecule 2: RIBOSOMAL PROTEIN S2

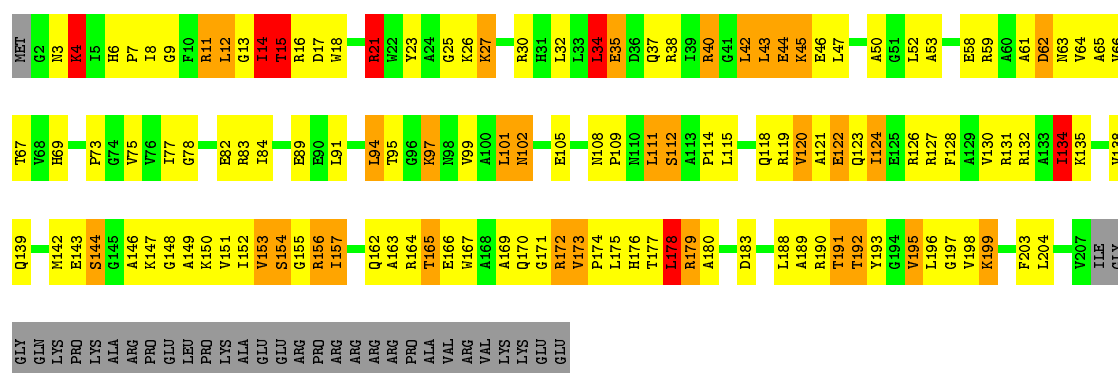


MET	P80	VAL	GLU	ILE	THR	V7	K3	E9	L10	L11	E12	V15	H16	F17	G18	H19	E20	R21	K22	R23	W24	N25	P26	R30	Y31	I32	Y33	A34	E35	R36	N37	G38	I39	H40	I41	I42	D43	L44	Q45	K46	T47	M48	E49	E50	L51	E52	R53	T54	I58	E59	D60	L61	R64	I68
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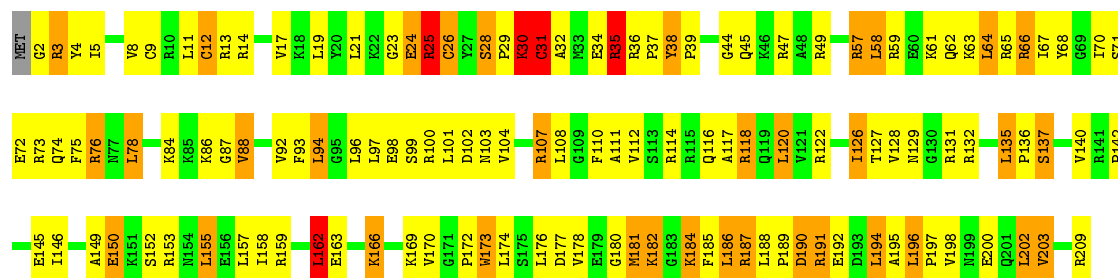
• Molecule 3: RIBOSOMAL PROTEIN S3

Chain C: 31% 38% 13% 14%



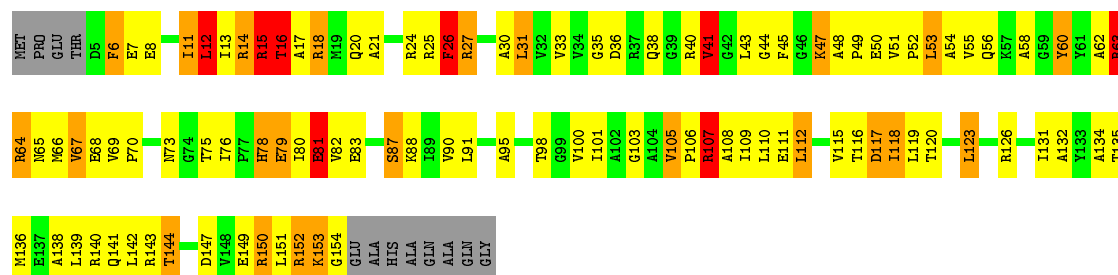
• Molecule 4: RIBOSOMAL PROTEIN S4

Chain D: 37% 44% 17%

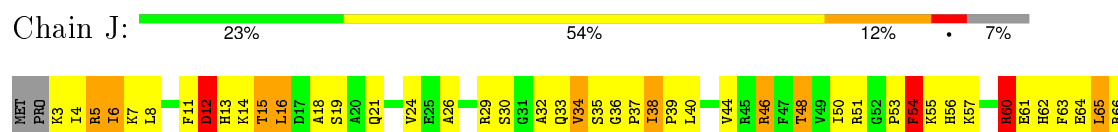


• Molecule 5: RIBOSOMAL PROTEIN S5

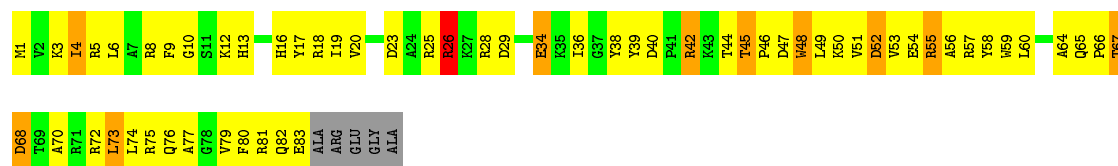
Chain E: 30% 44% 14% 5% 7%



• Molecule 6: RIBOSOMAL PROTEIN S6

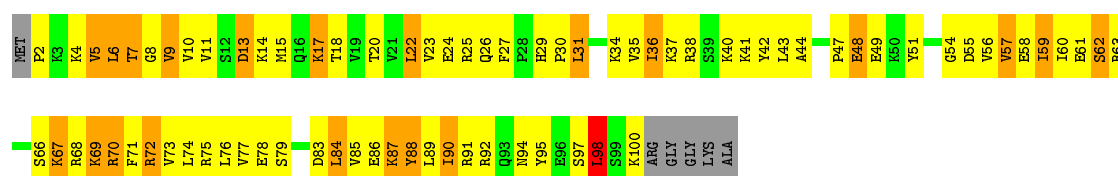


Chain P: 




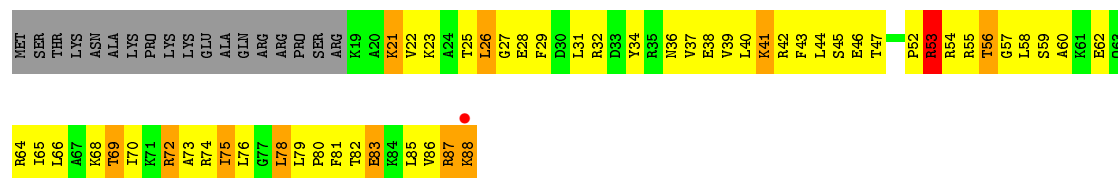
• Molecule 17: RIBOSOMAL PROTEIN S17

Chain Q: 

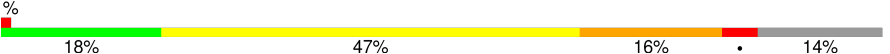


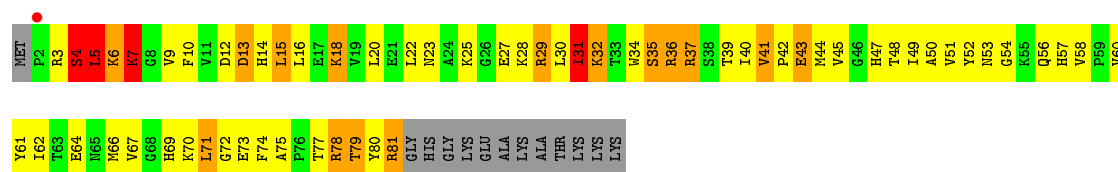
• Molecule 18: RIBOSOMAL PROTEIN S18

Chain R: 



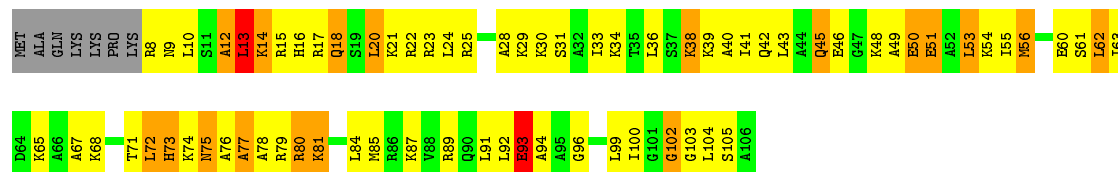
• Molecule 19: RIBOSOMAL PROTEIN S19

Chain S: 



• Molecule 20: RIBOSOMAL PROTEIN S20

Chain T: 



• Molecule 21: RIBOSOMAL PROTEIN THX

Chain U: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	401.94Å 401.94Å 217.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.55 50.08 – 3.55	Depositor EDS
% Data completeness (in resolution range)	98.3 (50.00-3.55) 98.3 (50.08-3.55)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.04 (at 3.57Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1119)	Depositor
R, R_{free}	0.151 , 0.201 0.155 , 0.200	Depositor DCC
R_{free} test set	10475 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	127.6	Xtriage
Anisotropy	0.355	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 153.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	1 of 209634 reflections (0.000%)	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	53444	wwPDB-VP
Average B, all atoms (Å ²)	142.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.44% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MA6, 0TD, 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	1.77	785/36187 (2.2%)	2.98	5484/56471 (9.7%)
2	B	1.18	8/1935 (0.4%)	1.33	19/2609 (0.7%)
3	C	1.17	2/1636 (0.1%)	1.29	11/2205 (0.5%)
4	D	1.32	6/1733 (0.3%)	1.44	19/2318 (0.8%)
5	E	1.38	3/1162 (0.3%)	1.59	15/1564 (1.0%)
6	F	1.19	2/856 (0.2%)	1.40	12/1154 (1.0%)
7	G	0.98	1/1276 (0.1%)	1.13	4/1709 (0.2%)
8	H	1.23	2/1136 (0.2%)	1.38	8/1527 (0.5%)
9	I	0.94	0/1029	1.12	3/1379 (0.2%)
10	J	1.07	0/805	1.35	5/1082 (0.5%)
11	K	1.02	0/879	1.24	6/1187 (0.5%)
12	L	1.48	7/977 (0.7%)	1.59	17/1305 (1.3%)
13	M	0.88	1/947 (0.1%)	1.10	0/1270
14	N	1.02	1/501 (0.2%)	1.41	8/664 (1.2%)
15	O	1.07	0/740	1.30	7/987 (0.7%)
16	P	1.17	1/716 (0.1%)	1.30	3/963 (0.3%)
17	Q	1.35	2/836 (0.2%)	1.45	7/1117 (0.6%)
18	R	1.09	0/579	1.29	2/768 (0.3%)
19	S	0.89	0/661	1.28	7/890 (0.8%)
20	T	1.13	0/765	1.40	9/1007 (0.9%)
21	U	0.98	2/212 (0.9%)	0.97	0/277
All	All	1.58	823/55568 (1.5%)	2.58	5646/82453 (6.8%)

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	5

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Mol	Chain	#Chirality outliers	#Planarity outliers
4	D	0	5
6	F	0	1
7	G	0	2
8	H	0	2
9	I	0	1
10	J	0	2
11	K	0	1
12	L	0	5
13	M	0	1
14	N	0	2
16	P	0	1
17	Q	0	1
18	R	0	1
19	S	0	2
20	T	0	2
All	All	0	36

The worst 5 of 823 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	975	A	N9-C4	-14.45	1.29	1.37
1	A	1493	A	N9-C4	13.90	1.46	1.37
4	D	12	CYS	CB-SG	13.89	2.05	1.82
1	A	768	A	N3-C4	-12.61	1.27	1.34
1	A	108	G	N1-C2	11.64	1.47	1.37

The worst 5 of 5646 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1528	U	O5'-P-OP2	-27.91	77.21	110.70
1	A	279	A	N1-C6-N6	24.78	133.47	118.60
1	A	975	A	C2-N3-C4	-23.57	98.82	110.60
1	A	117	G	C5-C6-N1	-23.41	99.80	111.50
1	A	279	A	C5-N7-C8	-21.45	93.17	103.90

There are no chirality outliers.

5 of 36 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	8	LYS	Peptide
2	B	89	GLY	Peptide

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Mol	Chain	Res	Type	Group
3	C	154	SER	Peptide
3	C	166	GLU	Peptide
3	C	3	ASN	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	32687	0	16508	1072	0
2	B	1900	0	1951	144	0
3	C	1612	0	1677	118	0
4	D	1703	0	1763	124	0
5	E	1146	0	1207	94	0
6	F	843	0	857	77	0
7	G	1257	0	1296	101	0
8	H	1116	0	1177	90	0
9	I	1010	0	1037	84	0
10	J	792	0	835	75	0
11	K	864	0	881	66	0
12	L	973	0	1062	83	0
13	M	937	0	995	88	0
14	N	492	0	529	48	0
15	O	729	0	768	66	0
16	P	700	0	720	54	0
17	Q	823	0	891	68	0
18	R	574	0	644	58	1
19	S	647	0	673	83	0
20	T	763	0	861	54	0
21	U	208	0	221	12	0
22	A	377	0	0	0	0
22	B	2	0	0	0	0
22	C	3	0	0	0	0
22	D	4	0	0	0	0
22	E	1	0	0	0	0
22	F	1	0	0	0	0
22	G	1	0	0	0	0
22	H	1	0	0	0	0
22	I	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	K	1	0	0	0	0
22	L	1	0	0	0	0
22	N	2	0	0	0	0
22	O	1	0	0	0	0
22	P	1	0	0	0	0
22	Q	2	0	0	0	0
22	S	1	0	0	0	0
23	D	1	0	0	0	0
23	N	1	0	0	0	0
24	A	1199	0	0	56	0
24	C	6	0	0	0	0
24	D	11	0	0	0	0
24	E	7	0	0	0	0
24	F	6	0	0	1	0
24	G	6	0	0	0	0
24	H	7	0	0	1	0
24	I	1	0	0	0	0
24	L	9	0	0	1	0
24	M	2	0	0	1	0
24	N	1	0	0	0	0
24	O	1	0	0	0	0
24	P	3	0	0	0	0
24	Q	6	0	0	2	0
All	All	53444	0	36553	2457	1

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 28.

The worst 5 of 2457 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)
4:D:12:CYS:SG	4:D:12:CYS:CB	2.05	1.44
11:K:120:ARG:HB3	11:K:120:ARG:HH11	1.22	1.02
1:A:966:M2G:HM13	1:A:967:5MC:H1'	1.37	1.01
15:O:70:LEU:HB3	15:O:78:TYR:HB2	1.44	0.99
4:D:187:ARG:HH22	4:D:188:LEU:HD12	1.31	0.96

All (1) 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)
18:R:25:THR:OG1	18:R:25:THR:OG1[8_555]	2.07	0.13

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%)	194 (84%)	32 (14%)	6 (3%)	7	46
3	C	204/239 (85%)	170 (83%)	32 (16%)	2 (1%)	19	66
4	D	206/209 (99%)	186 (90%)	19 (9%)	1 (0%)	34	77
5	E	148/162 (91%)	137 (93%)	8 (5%)	3 (2%)	9	53
6	F	99/101 (98%)	87 (88%)	11 (11%)	1 (1%)	19	66
7	G	153/156 (98%)	135 (88%)	18 (12%)	0	100	100
8	H	136/138 (99%)	123 (90%)	13 (10%)	0	100	100
9	I	125/128 (98%)	105 (84%)	19 (15%)	1 (1%)	24	69
10	J	96/105 (91%)	77 (80%)	14 (15%)	5 (5%)	2	27
11	K	114/129 (88%)	97 (85%)	16 (14%)	1 (1%)	21	67
12	L	121/135 (90%)	101 (84%)	16 (13%)	4 (3%)	5	41
13	M	116/126 (92%)	94 (81%)	20 (17%)	2 (2%)	11	56
14	N	58/61 (95%)	49 (84%)	9 (16%)	0	100	100
15	O	85/89 (96%)	74 (87%)	11 (13%)	0	100	100
16	P	81/88 (92%)	75 (93%)	6 (7%)	0	100	100
17	Q	97/105 (92%)	90 (93%)	7 (7%)	0	100	100
18	R	68/88 (77%)	62 (91%)	5 (7%)	1 (2%)	13	58
19	S	78/93 (84%)	72 (92%)	5 (6%)	1 (1%)	15	61
20	T	97/106 (92%)	75 (77%)	20 (21%)	2 (2%)	9	52
21	U	22/27 (82%)	20 (91%)	2 (9%)	0	100	100
All	All	2336/2541 (92%)	2023 (87%)	283 (12%)	30 (1%)	15	61

5 of 30 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	21	ARG
10	J	35	SER
12	L	28	LYS
2	B	9	GLU
2	B	11	LEU

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%)	144 (71%)	58 (29%)	0	4
3	C	160/188 (85%)	108 (68%)	52 (32%)	0	2
4	D	180/181 (99%)	135 (75%)	45 (25%)	1	6
5	E	115/123 (94%)	81 (70%)	34 (30%)	0	3
6	F	90/90 (100%)	75 (83%)	15 (17%)	3	18
7	G	126/127 (99%)	94 (75%)	32 (25%)	1	5
8	H	119/119 (100%)	83 (70%)	36 (30%)	0	3
9	I	98/99 (99%)	71 (72%)	27 (28%)	0	4
10	J	87/92 (95%)	64 (74%)	23 (26%)	0	5
11	K	88/99 (89%)	66 (75%)	22 (25%)	1	6
12	L	103/110 (94%)	68 (66%)	35 (34%)	0	2
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%)	50 (63%)	29 (37%)	0	1
16	P	72/74 (97%)	58 (81%)	14 (19%)	2	12
17	Q	94/97 (97%)	67 (71%)	27 (29%)	0	4
18	R	61/77 (79%)	43 (70%)	18 (30%)	0	3
19	S	71/80 (89%)	51 (72%)	20 (28%)	0	4
20	T	76/82 (93%)	53 (70%)	23 (30%)	0	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	U	19/22 (86%)	14 (74%)	5 (26%)	0	5
All	All	1983/2111 (94%)	1424 (72%)	559 (28%)	0	4

5 of 559 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	H	62	TYR
10	J	69	ASN
19	S	13	ASP
8	H	87	SER
9	I	62	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
8	H	15	ASN
19	S	47	HIS
17	Q	94	ASN
5	E	65	ASN
9	I	29	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1505/1522 (98%)	418 (27%)	46 (3%)

5 of 418 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	4	U
1	A	9	G
1	A	12	U
1	A	15	G
1	A	16	A

5 of 46 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	758	G

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Mol	Chain	Res	Type
1	A	890	G
1	A	1493	A
1	A	780	A
1	A	817	C

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

17 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	1,22	17,26,27	1.07	1 (5%)	21,38,41	2.42	7 (33%)
1	5MC	A	1400	1	13,22,23	4.47	4 (30%)	15,32,35	2.54	4 (26%)
1	4OC	A	1402	1	13,23,24	1.78	1 (7%)	18,32,35	0.72	0
1	5MC	A	1404	1	13,22,23	1.35	3 (23%)	15,32,35	0.95	1 (6%)
1	5MC	A	1407	1	13,22,23	1.28	1 (7%)	15,32,35	1.30	3 (20%)
1	UR3	A	1498	1	12,22,23	2.28	4 (33%)	16,32,35	1.58	4 (25%)
1	MA6	A	1518[A]	1	16,26,27	1.13	2 (12%)	18,38,41	0.93	2 (11%)
1	MA6	A	1518[B]	1	16,26,27	1.33	2 (12%)	18,38,41	1.07	2 (11%)
1	MA6	A	1519[A]	1	16,26,27	1.50	3 (18%)	18,38,41	1.43	4 (22%)
1	MA6	A	1519[B]	1	16,26,27	1.69	5 (31%)	18,38,41	1.00	2 (11%)
1	PSU	A	1540	1	13,21,22	1.06	1 (7%)	18,30,33	3.78	5 (27%)
1	PSU	A	1541	1	13,21,22	1.15	2 (15%)	18,30,33	4.24	5 (27%)
1	PSU	A	516	1,22	13,21,22	1.25	2 (15%)	18,30,33	5.32	5 (27%)
1	7MG	A	527	1	19,26,27	2.05	6 (31%)	24,39,42	2.41	7 (29%)
1	M2G	A	966	1	17,27,28	1.36	4 (23%)	22,40,43	2.58	4 (18%)
1	5MC	A	967	1	13,22,23	1.29	1 (7%)	15,32,35	1.08	1 (6%)
12	0TD	L	92	12	4,9,10	1.16	0	4,11,13	4.78	2 (50%)

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	1,22	-	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	1541	1	-	0/7/25/26	0/2/2/2
1	PSU	A	516	1,22	-	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

The worst 5 of 42 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1400	5MC	C4-N3	-7.53	1.23	1.35
1	A	1402	4OC	C6-N1	-5.32	1.28	1.35
1	A	1498	UR3	C4-N3	-5.24	1.30	1.38
1	A	527	7MG	C8-N9	-4.85	1.38	1.45
1	A	527	7MG	C2-N1	-3.98	1.28	1.35

The worst 5 of 58 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	516	PSU	N1-C2-N3	-19.17	116.10	128.33
1	A	1541	PSU	N1-C2-N3	-15.54	118.42	128.33
1	A	1540	PSU	N1-C2-N3	-13.39	119.79	128.33
12	L	92	0TD	CSB-SB-CB	-9.01	84.54	101.54
1	A	966	M2G	C5-C6-N1	-8.84	111.50	123.59

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

15 monomers are involved in 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1207	2MG	2	0
1	A	1402	4OC	1	0
1	A	1407	5MC	1	0
1	A	1498	UR3	3	0
1	A	1518[A]	MA6	5	0
1	A	1518[B]	MA6	8	0
1	A	1519[A]	MA6	3	0
1	A	1519[B]	MA6	5	0
1	A	1540	PSU	1	0
1	A	1541	PSU	1	0
1	A	516	PSU	1	0
1	A	527	7MG	1	0
1	A	966	M2G	2	0
1	A	967	5MC	3	0
12	L	92	0TD	4	0

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 403 ligands modelled in this entry, 403 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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	1500/1522 (98%)	-0.34	7 (0%) 91 88	90, 130, 210, 340	0
2	B	234/256 (91%)	-0.34	3 (1%) 79 71	106, 148, 236, 282	0
3	C	206/239 (86%)	-0.48	0 100 100	100, 136, 182, 210	0
4	D	208/209 (99%)	-0.37	0 100 100	89, 127, 172, 212	0
5	E	150/162 (92%)	-0.41	0 100 100	80, 112, 151, 188	0
6	F	101/101 (100%)	-0.34	1 (0%) 84 77	118, 147, 181, 236	0
7	G	155/156 (99%)	-0.27	0 100 100	130, 166, 208, 238	0
8	H	138/138 (100%)	-0.46	0 100 100	95, 120, 158, 192	0
9	I	127/128 (99%)	-0.17	5 (3%) 43 35	126, 167, 207, 227	0
10	J	98/105 (93%)	-0.16	0 100 100	113, 164, 199, 261	0
11	K	116/129 (89%)	-0.23	0 100 100	106, 145, 192, 209	0
12	L	123/135 (91%)	-0.29	1 (0%) 87 81	87, 117, 145, 197	0
13	M	118/126 (93%)	-0.04	4 (3%) 49 39	129, 173, 210, 242	0
14	N	60/61 (98%)	-0.32	0 100 100	110, 139, 199, 221	0
15	O	87/89 (97%)	-0.31	0 100 100	115, 143, 171, 203	0
16	P	83/88 (94%)	-0.09	0 100 100	97, 128, 160, 186	0
17	Q	99/105 (94%)	-0.27	0 100 100	98, 124, 161, 168	0
18	R	70/88 (79%)	-0.09	1 (1%) 78 69	124, 162, 232, 270	0
19	S	80/93 (86%)	-0.24	1 (1%) 79 71	140, 175, 218, 249	0
20	T	99/106 (93%)	-0.34	0 100 100	107, 133, 184, 208	0
21	U	24/27 (88%)	0.31	1 (4%) 40 32	149, 172, 193, 207	0
All	All	3876/4063 (95%)	-0.31	24 (0%) 90 85	80, 138, 201, 340	0

The worst 5 of 24 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1030(D)	A	6.1
1	A	1030(C)	G	3.4
9	I	15	ALA	3.4
12	L	128	ALA	3.1
2	B	235	SER	3.1

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
1	5MC	A	1404	21/22	0.90	0.28	-	103,111,130,135	0
1	5MC	A	1407	21/22	0.96	0.12	-	109,123,133,135	0
1	5MC	A	967	21/22	0.97	0.15	-	121,129,135,138	0
1	4OC	A	1402	22/23	0.93	0.27	-	114,119,123,133	0
1	UR3	A	1498	21/22	0.94	0.23	-	94,108,123,134	0
1	7MG	A	527	24/25	0.96	0.18	-	105,113,130,135	0
1	MA6	A	1518[A]	24/25	0.89	0.26	-	96,104,114,119	24
1	PSU	A	516	20/21	0.96	0.12	-	114,123,141,142	0
1	M2G	A	966	25/26	0.96	0.17	-	121,130,137,138	0
1	5MC	A	1400	21/22	0.96	0.17	-	92,111,126,132	0
1	MA6	A	1519[B]	24/25	0.93	0.29	-	90,96,98,106	24
12	0TD	L	92	10/11	0.98	0.48	-	81,121,135,281	0
1	PSU	A	1540	20/21	0.80	0.40	-	244,249,261,261	0
1	MA6	A	1518[B]	24/25	0.89	0.26	-	101,105,117,119	24
1	PSU	A	1541	20/21	0.85	0.20	-	211,223,230,234	0
1	2MG	A	1207	24/25	0.97	0.09	-	115,127,139,142	0
1	MA6	A	1519[A]	24/25	0.93	0.29	-	91,97,106,109	24

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron

density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
22	MG	A	1806	1/1	0.96	1.19	22.90	412,412,412,412	0
22	MG	A	1892	1/1	0.69	0.80	22.02	400,400,400,400	0
22	MG	A	1815	1/1	0.92	0.69	21.68	515,515,515,515	0
22	MG	A	1657	1/1	0.92	1.11	16.84	148,148,148,148	0
22	MG	A	1746	1/1	0.56	0.44	16.14	132,132,132,132	0
22	MG	A	1926	1/1	0.99	0.30	12.46	462,462,462,462	0
22	MG	A	1767	1/1	0.79	0.38	11.29	548,548,548,548	0
22	MG	A	1722	1/1	0.66	0.36	9.09	120,120,120,120	0
22	MG	A	1921	1/1	0.99	0.42	8.68	349,349,349,349	0
22	MG	A	1691	1/1	0.84	0.36	8.46	91,91,91,91	0
22	MG	N	102	1/1	0.85	0.74	8.13	116,116,116,116	0
22	MG	A	1676	1/1	0.95	0.33	7.90	93,93,93,93	0
22	MG	A	1715	1/1	0.92	0.28	6.42	125,125,125,125	0
22	MG	A	1724	1/1	0.88	0.42	6.26	93,93,93,93	0
22	MG	A	1865	1/1	0.91	0.35	5.09	474,474,474,474	0
22	MG	A	1704	1/1	0.95	0.41	4.99	97,97,97,97	0
22	MG	A	1971	1/1	0.78	0.23	4.98	116,116,116,116	0
22	MG	A	1931	1/1	0.98	0.24	4.22	232,232,232,232	0
22	MG	A	1614	1/1	0.83	0.29	4.07	120,120,120,120	0
22	MG	A	1666	1/1	0.92	0.25	3.89	81,81,81,81	0
22	MG	A	1893	1/1	0.94	0.17	3.63	406,406,406,406	0
22	MG	A	1686	1/1	0.98	0.28	3.62	225,225,225,225	0
22	MG	A	1721	1/1	0.93	0.37	3.42	97,97,97,97	0
22	MG	A	1711	1/1	0.99	0.59	3.34	106,106,106,106	0
22	MG	A	1687	1/1	0.99	0.20	2.81	99,99,99,99	0
22	MG	A	1975	1/1	0.83	0.20	2.69	108,108,108,108	0
22	MG	A	1665	1/1	0.99	0.20	2.66	158,158,158,158	0
22	MG	A	1628	1/1	0.87	0.21	2.64	203,203,203,203	0
22	MG	A	1692	1/1	0.97	0.26	2.10	95,95,95,95	0
22	MG	A	1627	1/1	0.99	0.23	1.73	98,98,98,98	0
22	MG	A	1803	1/1	0.99	0.18	1.43	129,129,129,129	0
22	MG	A	1680	1/1	0.93	0.22	1.42	116,116,116,116	0
22	MG	A	1718	1/1	0.94	0.24	1.27	87,87,87,87	0
22	MG	D	303	1/1	0.88	0.24	1.09	127,127,127,127	0
22	MG	B	301	1/1	0.92	0.33	1.04	141,141,141,141	0
22	MG	A	1647	1/1	0.83	0.17	1.00	201,201,201,201	0
22	MG	A	1699	1/1	0.92	0.23	0.85	112,112,112,112	0
22	MG	A	1843	1/1	0.97	0.22	0.82	456,456,456,456	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
22	MG	A	1834	1/1	0.92	0.16	0.64	349,349,349,349	0
22	MG	A	1883	1/1	0.96	0.15	0.38	500,500,500,500	0
23	ZN	D	301	1/1	1.00	0.31	0.32	119,119,119,119	0
22	MG	A	1641	1/1	0.99	0.17	0.08	158,158,158,158	0
22	MG	A	1961	1/1	0.87	0.19	0.04	126,126,126,126	0
22	MG	A	1710	1/1	0.75	0.14	0.03	105,105,105,105	0
22	MG	A	1629	1/1	0.96	0.19	-0.11	145,145,145,145	0
22	MG	A	1642	1/1	0.94	0.15	-0.20	96,96,96,96	0
22	MG	A	1673	1/1	0.98	0.21	-0.27	109,109,109,109	0
22	MG	A	1611	1/1	0.94	0.22	-0.27	148,148,148,148	0
23	ZN	N	101	1/1	0.99	0.18	-0.30	114,114,114,114	0
22	MG	A	1615	1/1	0.97	0.15	-0.47	98,98,98,98	0
22	MG	A	1863	1/1	0.96	0.10	-0.57	472,472,472,472	0
22	MG	A	1636	1/1	0.91	0.14	-0.77	79,79,79,79	0
22	MG	A	1678	1/1	0.98	0.16	-0.93	132,132,132,132	0
22	MG	A	1735	1/1	0.96	0.10	-0.94	87,87,87,87	0
22	MG	A	1701	1/1	0.99	0.15	-1.23	60,60,60,60	0
22	MG	A	1610	1/1	0.95	0.17	-1.33	123,123,123,123	0
22	MG	A	1743	1/1	0.99	0.23	-1.37	104,104,104,104	0
22	MG	A	1643	1/1	0.96	0.16	-1.44	126,126,126,126	0
22	MG	A	1830	1/1	0.97	0.09	-1.58	395,395,395,395	0
22	MG	A	1944	1/1	0.88	0.13	-2.12	153,153,153,153	0
22	MG	A	1605	1/1	0.99	0.13	-2.15	89,89,89,89	0
22	MG	A	1697	1/1	0.98	0.05	-2.48	87,87,87,87	0
22	MG	A	1839	1/1	0.98	0.11	-2.52	271,271,271,271	0
22	MG	B	302	1/1	0.84	0.06	-3.31	116,116,116,116	0
22	MG	A	1901	1/1	0.95	0.11	-3.49	212,212,212,212	0
22	MG	A	1632	1/1	0.99	0.07	-3.70	82,82,82,82	0
22	MG	A	1616	1/1	0.99	0.14	-4.78	88,88,88,88	0
22	MG	A	1664	1/1	0.93	0.09	-5.63	126,126,126,126	0
22	MG	A	1726	1/1	0.94	0.08	-9.37	104,104,104,104	0
22	MG	A	1941	1/1	0.97	0.24	-	132,132,132,132	0
22	MG	A	1809	1/1	0.88	0.42	-	485,485,485,485	0
22	MG	A	1656	1/1	0.94	0.26	-	166,166,166,166	0
22	MG	A	1916	1/1	0.91	1.28	-	290,290,290,290	0
22	MG	A	1651	1/1	0.68	0.86	-	131,131,131,131	0
22	MG	A	1776	1/1	0.93	0.19	-	523,523,523,523	0
22	MG	A	1951	1/1	0.52	0.52	-	131,131,131,131	0
22	MG	A	1848	1/1	0.85	1.23	-	550,550,550,550	0
22	MG	A	1875	1/1	0.78	0.32	-	447,447,447,447	0
22	MG	A	1671	1/1	0.94	0.30	-	121,121,121,121	0
22	MG	A	1874	1/1	0.89	0.25	-	437,437,437,437	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
22	MG	A	1728	1/1	0.86	0.17	-	140,140,140,140	0
22	MG	A	1797	1/1	0.91	0.23	-	431,431,431,431	0
22	MG	A	1972	1/1	0.85	0.17	-	135,135,135,135	0
22	MG	A	1935	1/1	0.76	0.40	-	102,102,102,102	0
22	MG	A	1620	1/1	0.96	0.87	-	82,82,82,82	0
22	MG	A	1919	1/1	0.80	0.41	-	401,401,401,401	0
22	MG	A	1750	1/1	0.97	0.09	-	96,96,96,96	0
22	MG	A	1617	1/1	0.92	1.04	-	107,107,107,107	0
22	MG	A	1654	1/1	0.85	0.50	-	113,113,113,113	0
22	MG	A	1626	1/1	0.97	0.10	-	169,169,169,169	0
22	MG	A	1741	1/1	0.97	0.10	-	137,137,137,137	0
22	MG	A	1959	1/1	0.81	0.42	-	133,133,133,133	0
22	MG	A	1733	1/1	0.88	0.09	-	116,116,116,116	0
22	MG	A	1713	1/1	0.98	0.26	-	107,107,107,107	0
22	MG	A	1677	1/1	0.98	0.07	-	191,191,191,191	0
22	MG	Q	201	1/1	0.71	0.44	-	99,99,99,99	0
22	MG	A	1872	1/1	0.91	0.21	-	389,389,389,389	0
22	MG	A	1974	1/1	0.83	0.33	-	137,137,137,137	0
22	MG	A	1660	1/1	0.84	0.14	-	132,132,132,132	0
22	MG	A	1818	1/1	0.74	0.25	-	478,478,478,478	0
22	MG	A	1842	1/1	0.95	0.09	-	151,151,151,151	0
22	MG	A	1716	1/1	0.96	0.49	-	132,132,132,132	0
22	MG	A	1930	1/1	0.96	0.09	-	156,156,156,156	0
22	MG	A	1922	1/1	0.74	0.39	-	446,446,446,446	0
22	MG	A	1640	1/1	0.97	0.32	-	143,143,143,143	0
22	MG	A	1925	1/1	0.99	0.12	-	262,262,262,262	0
22	MG	A	1706	1/1	0.94	0.36	-	110,110,110,110	0
22	MG	A	1734	1/1	0.96	0.65	-	91,91,91,91	0
22	MG	A	1822	1/1	0.97	0.28	-	443,443,443,443	0
22	MG	A	1789	1/1	0.83	0.09	-	529,529,529,529	0
22	MG	A	1645	1/1	0.83	0.29	-	144,144,144,144	0
22	MG	A	1679	1/1	0.99	0.18	-	107,107,107,107	0
22	MG	A	1933	1/1	0.88	0.34	-	483,483,483,483	0
22	MG	A	1790	1/1	0.85	0.42	-	504,504,504,504	0
22	MG	A	1672	1/1	0.88	0.13	-	144,144,144,144	0
22	MG	A	1738	1/1	0.94	0.21	-	114,114,114,114	0
22	MG	A	1751	1/1	0.64	0.30	-	130,130,130,130	0
22	MG	A	1852	1/1	0.97	0.26	-	480,480,480,480	0
22	MG	O	1000	1/1	0.71	0.37	-	242,242,242,242	0
22	MG	A	1754	1/1	0.76	0.41	-	170,170,170,170	0
22	MG	A	1784	1/1	0.72	0.54	-	486,486,486,486	0
22	MG	A	1787	1/1	0.97	0.24	-	430,430,430,430	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
22	MG	A	1634	1/1	0.97	0.31	-	154,154,154,154	0
22	MG	G	201	1/1	0.22	0.25	-	550,550,550,550	0
22	MG	A	1964	1/1	0.93	0.43	-	124,124,124,124	0
22	MG	A	1745	1/1	0.98	0.45	-	236,236,236,236	0
22	MG	A	1886	1/1	0.97	0.30	-	490,490,490,490	0
22	MG	A	1777	1/1	0.80	0.32	-	481,481,481,481	0
22	MG	A	1824	1/1	0.75	1.22	-	484,484,484,484	0
22	MG	A	1770	1/1	0.92	0.14	-	532,532,532,532	0
22	MG	A	1845	1/1	0.91	0.28	-	395,395,395,395	0
22	MG	D	304	1/1	0.94	0.12	-	470,470,470,470	0
22	MG	A	1762	1/1	0.97	0.09	-	137,137,137,137	0
22	MG	A	1652	1/1	0.98	0.17	-	95,95,95,95	0
22	MG	C	301	1/1	0.94	0.18	-	111,111,111,111	0
22	MG	A	1855	1/1	0.75	0.19	-	466,466,466,466	0
22	MG	N	103	1/1	0.93	0.06	-	333,333,333,333	0
22	MG	A	1889	1/1	0.93	0.21	-	456,456,456,456	0
22	MG	A	1820	1/1	0.74	0.39	-	448,448,448,448	0
22	MG	A	1700	1/1	0.91	0.77	-	142,142,142,142	0
22	MG	A	1914	1/1	0.85	0.41	-	439,439,439,439	0
22	MG	A	1690	1/1	0.94	0.05	-	190,190,190,190	0
22	MG	A	1653	1/1	0.95	0.08	-	228,228,228,228	0
22	MG	A	1693	1/1	0.92	0.50	-	131,131,131,131	0
22	MG	A	1955	1/1	0.79	0.12	-	132,132,132,132	0
22	MG	A	1621	1/1	0.50	0.66	-	178,178,178,178	0
22	MG	A	1851	1/1	0.90	0.22	-	481,481,481,481	0
22	MG	A	1956	1/1	0.83	0.26	-	156,156,156,156	0
22	MG	A	1828	1/1	0.84	0.56	-	467,467,467,467	0
22	MG	A	1823	1/1	0.94	0.10	-	496,496,496,496	0
22	MG	A	1674	1/1	0.88	0.19	-	189,189,189,189	0
22	MG	A	1604	1/1	0.88	0.35	-	93,93,93,93	0
22	MG	A	1917	1/1	0.67	0.65	-	456,456,456,456	0
22	MG	A	1887	1/1	0.98	0.49	-	191,191,191,191	0
22	MG	A	1891	1/1	0.88	1.05	-	496,496,496,496	0
22	MG	A	1965	1/1	0.94	0.23	-	101,101,101,101	0
22	MG	A	1912	1/1	1.00	0.17	-	46,46,46,46	0
22	MG	A	1811	1/1	0.98	0.29	-	436,436,436,436	0
22	MG	A	1736	1/1	0.81	0.63	-	118,118,118,118	0
22	MG	A	1768	1/1	0.63	0.23	-	501,501,501,501	0
22	MG	A	1759	1/1	0.89	0.41	-	496,496,496,496	0
22	MG	A	1783	1/1	0.80	0.20	-	535,535,535,535	0
22	MG	A	1744	1/1	0.85	0.06	-	237,237,237,237	0
22	MG	A	1939	1/1	0.70	0.49	-	103,103,103,103	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
22	MG	A	1832	1/1	0.91	0.22	-	312,312,312,312	0
22	MG	A	1758	1/1	0.91	0.53	-	481,481,481,481	0
22	MG	A	1897	1/1	0.94	0.49	-	428,428,428,428	0
22	MG	A	1903	1/1	0.98	0.16	-	223,223,223,223	0
22	MG	A	1847	1/1	0.93	0.48	-	453,453,453,453	0
22	MG	A	1833	1/1	0.95	0.19	-	319,319,319,319	0
22	MG	A	1607	1/1	0.96	0.14	-	121,121,121,121	0
22	MG	A	1877	1/1	0.98	0.23	-	460,460,460,460	0
22	MG	A	1766	1/1	0.74	0.28	-	549,549,549,549	0
22	MG	A	1708	1/1	0.61	0.69	-	129,129,129,129	0
22	MG	A	1771	1/1	0.94	0.37	-	519,519,519,519	0
22	MG	A	1739	1/1	0.89	0.31	-	83,83,83,83	0
22	MG	A	1749	1/1	0.96	0.05	-	122,122,122,122	0
22	MG	A	1946	1/1	0.74	0.45	-	155,155,155,155	0
22	MG	A	1633	1/1	0.92	0.39	-	101,101,101,101	0
22	MG	A	1689	1/1	0.82	0.61	-	125,125,125,125	0
22	MG	A	1960	1/1	0.56	0.27	-	136,136,136,136	0
22	MG	A	1603	1/1	0.95	0.04	-	157,157,157,157	0
22	MG	A	1819	1/1	0.96	0.57	-	360,360,360,360	0
22	MG	A	1963	1/1	0.90	0.31	-	153,153,153,153	0
22	MG	A	1850	1/1	0.95	0.26	-	233,233,233,233	0
22	MG	A	1904	1/1	0.98	0.29	-	217,217,217,217	0
22	MG	A	1829	1/1	0.90	0.42	-	507,507,507,507	0
22	MG	A	1853	1/1	0.97	0.43	-	264,264,264,264	0
22	MG	D	305	1/1	0.58	0.57	-	103,103,103,103	0
22	MG	A	1772	1/1	0.94	0.19	-	274,274,274,274	0
22	MG	A	1702	1/1	0.97	0.22	-	122,122,122,122	0
22	MG	A	1793	1/1	0.88	0.38	-	550,550,550,550	0
22	MG	A	1967	1/1	0.11	0.85	-	144,144,144,144	0
22	MG	A	1966	1/1	0.77	0.17	-	138,138,138,138	0
22	MG	A	1950	1/1	0.70	0.45	-	126,126,126,126	0
22	MG	A	1723	1/1	0.72	0.42	-	126,126,126,126	0
22	MG	A	1601	1/1	0.98	0.04	-	145,145,145,145	0
22	MG	A	1870	1/1	0.98	0.24	-	444,444,444,444	0
22	MG	A	1840	1/1	0.75	0.20	-	493,493,493,493	0
22	MG	A	1858	1/1	0.76	0.93	-	429,429,429,429	0
22	MG	A	1663	1/1	0.99	0.38	-	166,166,166,166	0
22	MG	A	1688	1/1	0.78	0.45	-	122,122,122,122	0
22	MG	A	1649	1/1	0.86	0.45	-	137,137,137,137	0
22	MG	A	1927	1/1	0.97	0.15	-	160,160,160,160	0
22	MG	A	1612	1/1	0.99	0.34	-	116,116,116,116	0
22	MG	A	1923	1/1	0.80	0.31	-	424,424,424,424	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
22	MG	A	1608	1/1	0.94	0.11	-	122,122,122,122	0
22	MG	A	1895	1/1	0.97	0.68	-	525,525,525,525	0
22	MG	A	1884	1/1	0.99	0.37	-	428,428,428,428	0
22	MG	A	1748	1/1	0.95	0.30	-	153,153,153,153	0
22	MG	A	1948	1/1	0.64	0.98	-	127,127,127,127	0
22	MG	A	1942	1/1	0.65	0.43	-	122,122,122,122	0
22	MG	A	1742	1/1	0.71	0.51	-	133,133,133,133	0
22	MG	A	1953	1/1	0.68	0.18	-	130,130,130,130	0
22	MG	A	1658	1/1	0.50	0.10	-	207,207,207,207	0
22	MG	A	1813	1/1	0.97	0.13	-	491,491,491,491	0
22	MG	A	1646	1/1	0.97	0.25	-	95,95,95,95	0
22	MG	I	201	1/1	0.73	0.31	-	137,137,137,137	0
22	MG	K	201	1/1	0.79	0.08	-	123,123,123,123	0
22	MG	A	1780	1/1	0.92	0.12	-	432,432,432,432	0
22	MG	A	1796	1/1	0.88	0.42	-	480,480,480,480	0
22	MG	A	1805	1/1	0.92	0.94	-	550,550,550,550	0
22	MG	A	1888	1/1	0.93	0.19	-	470,470,470,470	0
22	MG	A	1624	1/1	0.82	0.30	-	106,106,106,106	0
22	MG	A	1720	1/1	0.93	0.27	-	130,130,130,130	0
22	MG	A	1812	1/1	0.94	0.18	-	474,474,474,474	0
22	MG	A	1737	1/1	0.59	0.13	-	133,133,133,133	0
22	MG	A	1881	1/1	0.90	0.31	-	525,525,525,525	0
22	MG	A	1764	1/1	0.68	0.29	-	502,502,502,502	0
22	MG	A	1826	1/1	0.96	0.06	-	537,537,537,537	0
22	MG	A	1775	1/1	0.73	0.20	-	538,538,538,538	0
22	MG	A	1683	1/1	0.66	1.00	-	135,135,135,135	0
22	MG	A	1876	1/1	0.68	0.46	-	422,422,422,422	0
22	MG	A	1761	1/1	0.98	0.11	-	458,458,458,458	0
22	MG	A	1622	1/1	0.93	0.21	-	119,119,119,119	0
22	MG	A	1907	1/1	0.99	0.08	-	329,329,329,329	0
22	MG	L	201	1/1	0.92	0.45	-	468,468,468,468	0
22	MG	C	302	1/1	0.53	0.57	-	122,122,122,122	0
22	MG	A	1841	1/1	0.91	0.70	-	462,462,462,462	0
22	MG	A	1860	1/1	0.90	0.39	-	434,434,434,434	0
22	MG	A	1781	1/1	0.68	0.25	-	504,504,504,504	0
22	MG	A	1866	1/1	0.83	0.13	-	497,497,497,497	0
22	MG	A	1808	1/1	0.97	0.11	-	480,480,480,480	0
22	MG	A	1712	1/1	0.80	0.45	-	123,123,123,123	0
22	MG	A	1915	1/1	0.94	0.42	-	419,419,419,419	0
22	MG	A	1864	1/1	0.94	0.29	-	316,316,316,316	0
22	MG	A	1900	1/1	0.96	0.37	-	442,442,442,442	0
22	MG	A	1659	1/1	0.52	0.46	-	131,131,131,131	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
22	MG	A	1769	1/1	0.88	0.07	-	397,397,397,397	0
22	MG	I	202	1/1	0.74	0.20	-	146,146,146,146	0
22	MG	A	1717	1/1	0.96	0.27	-	102,102,102,102	0
22	MG	A	1707	1/1	0.78	0.38	-	100,100,100,100	0
22	MG	A	1740	1/1	0.97	0.10	-	85,85,85,85	0
22	MG	A	1630	1/1	0.93	0.34	-	146,146,146,146	0
22	MG	A	1785	1/1	0.90	0.06	-	353,353,353,353	0
22	MG	A	1976	1/1	0.76	0.14	-	133,133,133,133	0
22	MG	A	1969	1/1	0.92	0.15	-	78,78,78,78	0
22	MG	A	1644	1/1	0.83	0.58	-	141,141,141,141	0
22	MG	A	1755	1/1	0.91	0.20	-	144,144,144,144	0
22	MG	A	1890	1/1	0.94	0.47	-	425,425,425,425	0
22	MG	A	1856	1/1	0.71	0.23	-	484,484,484,484	0
22	MG	A	1827	1/1	0.90	0.42	-	500,500,500,500	0
22	MG	F	201	1/1	0.93	0.10	-	435,435,435,435	0
22	MG	A	1625	1/1	0.75	0.34	-	188,188,188,188	0
22	MG	A	1947	1/1	0.92	0.25	-	116,116,116,116	0
22	MG	A	1732	1/1	0.71	0.32	-	123,123,123,123	0
22	MG	A	1694	1/1	0.91	0.20	-	127,127,127,127	0
22	MG	A	1804	1/1	0.90	0.16	-	318,318,318,318	0
22	MG	A	1802	1/1	0.90	0.56	-	458,458,458,458	0
22	MG	A	1757	1/1	0.79	0.48	-	550,550,550,550	0
22	MG	A	1936	1/1	0.75	0.46	-	110,110,110,110	0
22	MG	A	1885	1/1	0.87	0.14	-	534,534,534,534	0
22	MG	A	1859	1/1	0.74	0.36	-	495,495,495,495	0
22	MG	A	1831	1/1	0.85	0.36	-	486,486,486,486	0
22	MG	A	1869	1/1	0.78	0.20	-	550,550,550,550	0
22	MG	A	1662	1/1	0.98	0.06	-	110,110,110,110	0
22	MG	A	1871	1/1	0.97	0.14	-	426,426,426,426	0
22	MG	A	1779	1/1	0.91	0.19	-	411,411,411,411	0
22	MG	A	1635	1/1	0.92	0.21	-	74,74,74,74	0
22	MG	A	1857	1/1	0.36	0.39	-	487,487,487,487	0
22	MG	A	1910	1/1	0.96	0.63	-	526,526,526,526	0
22	MG	A	1685	1/1	0.94	0.14	-	141,141,141,141	0
22	MG	A	1613	1/1	0.97	0.17	-	97,97,97,97	0
22	MG	A	1799	1/1	0.88	0.47	-	550,550,550,550	0
22	MG	A	1695	1/1	0.90	0.19	-	118,118,118,118	0
22	MG	H	201	1/1	0.94	0.40	-	421,421,421,421	0
22	MG	A	1623	1/1	0.97	0.10	-	90,90,90,90	0
22	MG	A	1795	1/1	0.90	0.25	-	416,416,416,416	0
22	MG	A	1928	1/1	0.90	0.49	-	126,126,126,126	0
22	MG	A	1905	1/1	0.92	0.17	-	426,426,426,426	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
22	MG	A	1821	1/1	0.85	0.42	-	543,543,543,543	0
22	MG	A	1682	1/1	0.81	0.11	-	218,218,218,218	0
22	MG	A	1940	1/1	0.81	0.69	-	119,119,119,119	0
22	MG	A	1962	1/1	0.97	0.25	-	127,127,127,127	0
22	MG	A	1773	1/1	0.87	0.43	-	550,550,550,550	0
22	MG	A	1913	1/1	0.96	0.20	-	317,317,317,317	0
22	MG	A	1810	1/1	0.97	0.07	-	264,264,264,264	0
22	MG	A	1908	1/1	0.96	0.24	-	345,345,345,345	0
22	MG	D	302	1/1	0.74	0.18	-	92,92,92,92	0
22	MG	C	303	1/1	0.82	0.07	-	144,144,144,144	0
22	MG	A	1817	1/1	0.96	0.28	-	385,385,385,385	0
22	MG	A	1973	1/1	0.70	0.24	-	137,137,137,137	0
22	MG	A	1725	1/1	0.96	0.13	-	120,120,120,120	0
22	MG	A	1639	1/1	0.98	0.12	-	126,126,126,126	0
22	MG	A	1814	1/1	0.86	0.24	-	506,506,506,506	0
22	MG	A	1727	1/1	0.57	0.48	-	122,122,122,122	0
22	MG	A	1945	1/1	0.80	0.17	-	168,168,168,168	0
22	MG	A	1752	1/1	0.96	0.47	-	141,141,141,141	0
22	MG	A	1667	1/1	0.98	0.07	-	112,112,112,112	0
22	MG	A	1763	1/1	0.89	0.15	-	451,451,451,451	0
22	MG	E	201	1/1	0.84	0.13	-	135,135,135,135	0
22	MG	A	1631	1/1	0.95	0.29	-	99,99,99,99	0
22	MG	A	1937	1/1	0.99	0.06	-	107,107,107,107	0
22	MG	A	1882	1/1	0.87	0.29	-	501,501,501,501	0
22	MG	A	1619	1/1	0.91	0.27	-	132,132,132,132	0
22	MG	A	1730	1/1	0.83	0.32	-	118,118,118,118	0
22	MG	A	1920	1/1	0.96	0.18	-	245,245,245,245	0
22	MG	A	1854	1/1	0.99	0.12	-	126,126,126,126	0
22	MG	A	1760	1/1	0.97	0.33	-	407,407,407,407	0
22	MG	A	1719	1/1	0.72	0.98	-	121,121,121,121	0
22	MG	A	1618	1/1	0.78	0.27	-	107,107,107,107	0
22	MG	A	1765	1/1	0.84	0.32	-	482,482,482,482	0
22	MG	A	1879	1/1	0.98	0.17	-	509,509,509,509	0
22	MG	A	1709	1/1	0.79	0.31	-	112,112,112,112	0
22	MG	A	1837	1/1	0.73	0.16	-	523,523,523,523	0
22	MG	A	1918	1/1	0.89	0.26	-	422,422,422,422	0
22	MG	A	1801	1/1	0.91	0.58	-	480,480,480,480	0
22	MG	A	1878	1/1	0.76	0.29	-	498,498,498,498	0
22	MG	A	1932	1/1	0.99	0.22	-	92,92,92,92	0
22	MG	A	1794	1/1	0.99	0.08	-	393,393,393,393	0
22	MG	A	1747	1/1	0.70	0.26	-	131,131,131,131	0
22	MG	A	1637	1/1	1.00	0.12	-	124,124,124,124	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
22	MG	A	1670	1/1	0.99	0.19	-	87,87,87,87	0
22	MG	A	1703	1/1	0.92	0.30	-	125,125,125,125	0
22	MG	A	1894	1/1	0.99	0.37	-	379,379,379,379	0
22	MG	A	1924	1/1	0.91	0.09	-	322,322,322,322	0
22	MG	A	1698	1/1	0.96	0.33	-	113,113,113,113	0
22	MG	A	1705	1/1	0.98	0.20	-	135,135,135,135	0
22	MG	A	1606	1/1	0.89	0.16	-	183,183,183,183	0
22	MG	A	1696	1/1	0.89	0.30	-	127,127,127,127	0
22	MG	A	1788	1/1	0.71	0.23	-	550,550,550,550	0
22	MG	A	1957	1/1	0.90	0.37	-	105,105,105,105	0
22	MG	A	1868	1/1	0.95	0.06	-	442,442,442,442	0
22	MG	A	1838	1/1	0.92	0.42	-	388,388,388,388	0
22	MG	A	1880	1/1	0.91	0.21	-	431,431,431,431	0
22	MG	A	1792	1/1	0.68	0.42	-	530,530,530,530	0
22	MG	A	1602	1/1	0.99	0.16	-	124,124,124,124	0
22	MG	A	1684	1/1	0.81	0.52	-	121,121,121,121	0
22	MG	A	1970	1/1	0.68	0.17	-	140,140,140,140	0
22	MG	A	1816	1/1	0.90	0.44	-	449,449,449,449	0
22	MG	A	1729	1/1	0.89	0.26	-	125,125,125,125	0
22	MG	A	1929	1/1	0.80	0.77	-	111,111,111,111	0
22	MG	A	1798	1/1	0.88	0.29	-	550,550,550,550	0
22	MG	A	1899	1/1	0.92	0.24	-	550,550,550,550	0
22	MG	S	101	1/1	0.84	0.17	-	127,127,127,127	0
22	MG	A	1778	1/1	0.81	0.10	-	232,232,232,232	0
22	MG	A	1638	1/1	0.97	0.28	-	96,96,96,96	0
22	MG	A	1807	1/1	0.83	1.65	-	550,550,550,550	0
22	MG	A	1714	1/1	0.96	0.18	-	76,76,76,76	0
22	MG	A	1675	1/1	0.50	1.31	-	125,125,125,125	0
22	MG	A	1655	1/1	0.90	0.22	-	150,150,150,150	0
22	MG	A	1849	1/1	0.88	0.36	-	512,512,512,512	0
22	MG	A	1934	1/1	0.95	0.21	-	111,111,111,111	0
22	MG	A	1896	1/1	0.78	0.60	-	436,436,436,436	0
22	MG	A	1774	1/1	0.96	0.08	-	402,402,402,402	0
22	MG	A	1731	1/1	0.95	0.45	-	114,114,114,114	0
22	MG	A	1867	1/1	0.92	0.36	-	459,459,459,459	0
22	MG	A	1681	1/1	0.99	0.14	-	247,247,247,247	0
22	MG	A	1668	1/1	0.53	0.24	-	111,111,111,111	0
22	MG	Q	202	1/1	0.94	0.27	-	455,455,455,455	0
22	MG	A	1825	1/1	0.96	0.62	-	490,490,490,490	0
22	MG	A	1836	1/1	0.94	0.11	-	409,409,409,409	0
22	MG	A	1609	1/1	0.96	0.21	-	114,114,114,114	0
22	MG	A	1800	1/1	0.94	0.30	-	441,441,441,441	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
22	MG	A	1786	1/1	0.96	0.08	-	300,300,300,300	0
22	MG	A	1949	1/1	0.56	0.52	-	116,116,116,116	0
22	MG	A	1911	1/1	0.70	0.44	-	502,502,502,502	0
22	MG	A	1791	1/1	0.92	0.72	-	373,373,373,373	0
22	MG	A	1938	1/1	0.91	0.36	-	149,149,149,149	0
22	MG	A	1909	1/1	0.99	0.18	-	149,149,149,149	0
22	MG	A	1661	1/1	0.94	0.64	-	163,163,163,163	0
22	MG	A	1902	1/1	0.87	0.46	-	435,435,435,435	0
22	MG	A	1873	1/1	0.99	0.35	-	390,390,390,390	0
22	MG	A	1954	1/1	0.59	0.43	-	139,139,139,139	0
22	MG	A	1648	1/1	0.97	0.12	-	121,121,121,121	0
22	MG	A	1753	1/1	0.92	0.52	-	117,117,117,117	0
22	MG	A	1906	1/1	0.94	0.23	-	394,394,394,394	0
22	MG	A	1958	1/1	0.80	0.36	-	124,124,124,124	0
22	MG	A	1835	1/1	0.90	0.12	-	363,363,363,363	0
22	MG	A	1756	1/1	0.98	0.64	-	127,127,127,127	0
22	MG	A	1782	1/1	0.78	0.23	-	501,501,501,501	0
22	MG	A	1898	1/1	0.85	0.53	-	463,463,463,463	0
22	MG	P	101	1/1	0.62	0.39	-	111,111,111,111	0
22	MG	A	1861	1/1	0.80	0.65	-	497,497,497,497	0
22	MG	A	1952	1/1	0.97	0.26	-	93,93,93,93	0
22	MG	A	1862	1/1	0.71	0.17	-	487,487,487,487	0
22	MG	A	1650	1/1	0.97	0.17	-	129,129,129,129	0
22	MG	A	1844	1/1	0.93	0.13	-	369,369,369,369	0
22	MG	A	1669	1/1	0.99	0.18	-	137,137,137,137	0
22	MG	A	1977	1/1	0.92	0.22	-	129,129,129,129	0
22	MG	A	1846	1/1	0.99	0.15	-	484,484,484,484	0
22	MG	A	1943	1/1	0.59	0.62	-	139,139,139,139	0
22	MG	A	1968	1/1	0.82	0.86	-	127,127,127,127	0

6.5 Other polymers ⓘ

There are no such residues in this entry.