



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 18, 2024 – 10:35 AM EDT

PDB ID : 4JI4
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 : 3.69 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

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A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 1.20.1
EDS : 2.37.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.37.1

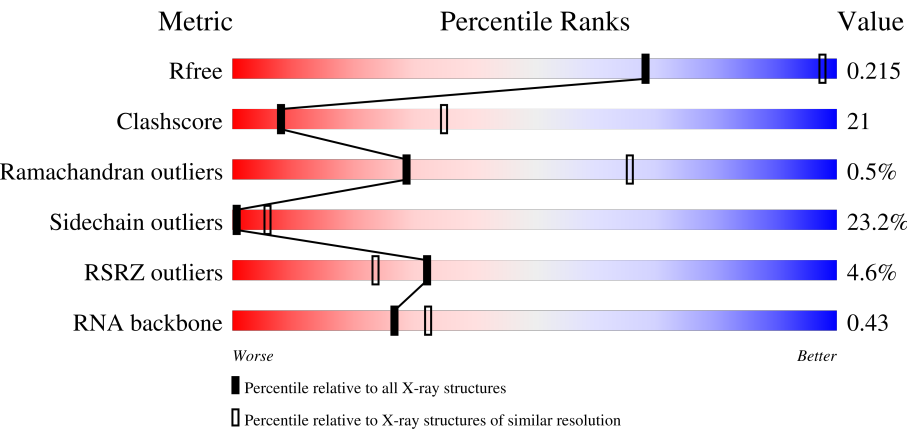
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.69 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	130704	1049 (3.88-3.52)
Clashscore	141614	1027 (3.86-3.54)
Ramachandran outliers	138981	1069 (3.88-3.52)
Sidechain outliers	138945	1065 (3.88-3.52)
RSRZ outliers	127900	1578 (3.90-3.50)
RNA backbone	3102	1027 (4.40-3.00)

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

Mol	Chain	Length	Quality of chain
1	A	1522	<div><div>3%</div><div>19%43%31%7%</div></div>
2	B	256	<div><div>39%40%12%9%</div></div>
3	C	239	<div><div>9%</div><div>36%40%10%14%</div></div>
4	D	209	<div><div>4%</div><div>45%45%9%</div></div>

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

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	PSU	A	1540	-	-	-	X
1	5MC	A	967	-	-	X	-
12	0TD	L	92	-	-	X	-
22	MG	A	1625	-	-	-	X
22	MG	A	1632	-	-	-	X
22	MG	A	1683	-	-	-	X
22	MG	A	1702	-	-	-	X
22	MG	A	1735	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	MG	A	1742	-	-	-	X
22	MG	A	1743	-	-	-	X
22	MG	A	1745	-	-	-	X
22	MG	A	1747	-	-	-	X
22	MG	A	1759	-	-	-	X
22	MG	A	1762	-	-	-	X
22	MG	A	1764	-	-	-	X
22	MG	A	1769	-	-	-	X
22	MG	A	1771	-	-	-	X
22	MG	A	1772	-	-	-	X
22	MG	A	1784	-	-	-	X
22	MG	A	1797	-	-	-	X
22	MG	A	1806	-	-	-	X
22	MG	A	1810	-	-	-	X
22	MG	A	1815	-	-	-	X
22	MG	A	1820	-	-	-	X
22	MG	A	1824	-	-	-	X
22	MG	A	1829	-	-	-	X
22	MG	A	1831	-	-	-	X
22	MG	A	1834	-	-	-	X
22	MG	A	1844	-	-	-	X
22	MG	A	1857	-	-	-	X
22	MG	A	1858	-	-	-	X
22	MG	A	1861	-	-	-	X
22	MG	H	201	-	-	-	X

2 Entry composition

There are 24 unique types of molecules in this entry. The entry contains 52281 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1512	Total	C	N	O	P	0	6	0
			32644	14540	6038	10548	1518			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1490	U	C	CONFLICT	GB M26923.1
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	A	262	Total	Mg	0	0
			262	262		
22	B	1	Total	Mg	0	0
			1	1		
22	C	1	Total	Mg	0	0
			1	1		
22	D	3	Total	Mg	0	0
			3	3		
22	E	1	Total	Mg	0	0
			1	1		
22	F	1	Total	Mg	0	0
			1	1		
22	H	1	Total	Mg	0	0
			1	1		
22	I	1	Total	Mg	0	0
			1	1		
22	J	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	P	1	Total 1	Mg 1	0	0
22	Q	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

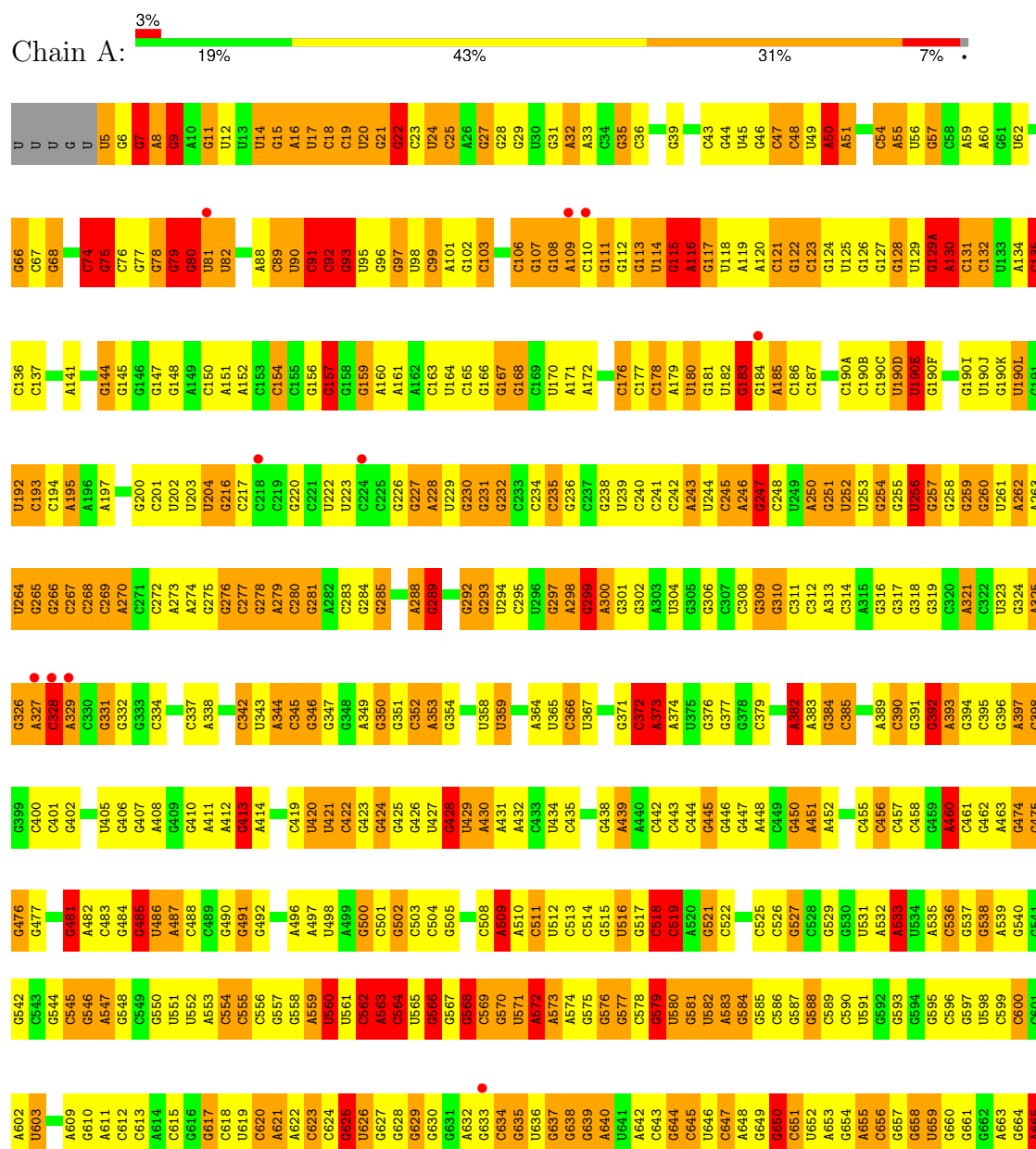
- Molecule 24 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
24	A	261	Total 261	O 261	0	0
24	C	1	Total 1	O 1	0	0
24	D	1	Total 1	O 1	0	0
24	E	6	Total 6	O 6	0	0
24	Q	2	Total 2	O 2	0	0
24	T	1	Total 1	O 1	0	0

3 Residue-property plots [i](#)

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

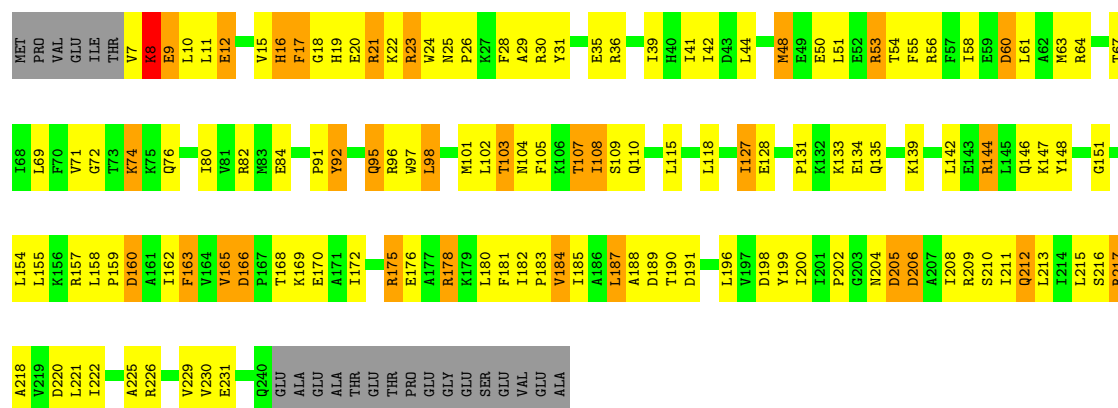
• Molecule 1: 16S rRNA



G1487	G1488	G1489	U1490	G1491	A1492	A1493	G1494	U1495	G1496	G1497	U1498	A1499	A1500	C1501	A1502	A1503	G1504	G1505	U1506	A1507	G1508	C1509	U1510	G1511	U1512	A1513	C1514	C1515	G1516	G1517	A1518	A1519	G1520	U1521	U1522	G1523	C1524	G1525	G1526	C1527	U1528	G1529	A1530	U1532	C1533	C	A	C	U	C	G1539	U1540	U1541	U1542	C1543	U1544			
A1360	G1361	G1361A	C1362	U1363	A1364	G1365	C1366	C1367	G1368	C1369	G1370	G1371	U1372	G1373	A1374	U1375	U1376	A1377	C1378	G1379	U1380	C1381	C1382	C1383	G1384	G1385	U1386	C1389	U1390	U1391	G1392	U1393	C1393	A1394	C1395	C1396	G1397	C1398	C1399	C1400	U1401	C1402	C1403	C1404	G1405	U1406	C1407	A1408	C1409	G1410	C1411	C1412	A1413	U1414	G1415	A1483	G1417	U1485	
C1420	G1421	G1422	G1423	C1424	U1425	C1426	U1427	A1428	G1429	C1430	C1431	G1432	A1433	A1434	U1435	U1436	C1437	G1438	G1441	G1442	G1443	A1444	G1447	C1448	C1449	U1450	A1451	C1452	G1453	G1454	C1455	C1459	C1459	A1460	G1461	G1462	C1463	G1464	C1465	C1466		G1469	G1470	G1471	U1472	A1473	C1474	A1475	C1476	C1477	C1478	C1479	G1480	U1481	U1482	C1543	U1544		
U1235	A1236	C1237	A1238	G1239	U1240	G1241	C1242	A1243	C1244	A1245	C1246		C1249	C1250	A1251	A1252	G1253	C1254	G1255	A1256	U1257	G1258	C1259		C1261	C1262	C1263	C1264	G1265	G1266	C1267	A1268	C1269	C1270	G1271	G1272		C1277	U1278	A1279	U1280	U1281	C1282	G1283	C1284	A1285	A1286	A1287	A1288	A1289	G1290	G1291	U1292	C1293	G1294	G1295	C1296	C1297	
G1174	G1175	G1176	G1177	A1178	A1179	A1180	G1181	A1182	A1183	G1184	G1185	G1186		C1189	G1190	A1191	C1192	G1193	U1194	C1195	U1196	G1197	G1198	U1199	C1200	A1201	C1202	C1203	A1204	U1205	G1206	G1207	C1208	C1209	C1210	U1211	U1212	A1213	C1214	G1215	G1216	C1217	C1218	U1219	G1220	G1221	C1222	C1223	G1224	A1225	C1226	A1227	C1228	A1229	C1230	G1231	U1232	C1233	C1234
G1104	A1105	G1106	C1107	G1108	C1109	A1110	A1111	C1112	G1113	C1114		G1117	G1124	U1125	U1126	G1127	C1128	C1129	A1130	G1131	C1132	G1133	G1134	U1135	U1136	C1137	G1138	G1139	C1140	C1141	G1142	G1143	G1144	C1145	A1146	C1147	U1148	C1149	U1150	A1151	A1152	C1153	G1154	A1157	C1158	U1159	G1160		C1163	G1164		A1167	A1168	A1169	G1171	C1172			
U920	U921	G922	A923	C924	G925	G926	G927	G928	G929	C930	C931	U932	C933	C934	A935	C936	A937	C938	C939	G940	G941	C942	U943	G944	G945	A946	G947	C948	A949	U950	U951	U952	G953	G954	U955	A958	A959	U960	U961	C962	G963	A964	A965	G966	C967	A968	A969	C970	A908	A909	C912	A913	A914	A915	G916	A917	A918	C980	
U981	U982	A983	C984	C985	A986	C990	U991	U992	G993	A994	C995	U1000	A1001	G1002	G1003	U1003A	A1004	A1005	C1006	C1007	C1008	G1009	G1010	U1010	U1011	U1012	A1016	G1017	C1018	C1019	G1020	G1021	G1022	G1023	G1024	U1025	G1026	C1027	C1028	C1030B	G1030C	A1031	G1032	G1033	G1034	A1035	U1036	C1037	C1038	C1039	U1040	A1041	G1042	C1043					
A1044	C1045	A1046	G1047	U1048	U1049	G1050	C1051	U1052	G1053	C1054	A1055	U1056	G1057	C1058	C1059	C1060	G1061	U1062	C1063	G1064	U1065	C1066	G1067	G1068	C1069	U1070	C1071	G1072	U1073	G1074	C1075	C1076	G1077	U1078	G1079	A1080	G1081	U1082	U1083	G1084	U1085	U1086	G1087	G1088	G1089	U1090	U1091	A1092	G1093	U1094	U1095	C1096	C1097	C1098	G1099	C1100	A1101	A1102	C1103
G666	G667	G668	U669	G670	G671	U672	G673	G674	A675	U676	U677	U678	C679	C680	C681	G682	G683	A684	G685	G686	A687	U688	C689	A690	G691	U692	G693	A694	A695	A696	U697	G698	C701	A702	G703	A704	U705	A706	C707	C708	G709	G713	G714	A715	A716	A717	C718	G719	C720	A721	A722	C723	G724	G725	C726	G727	U728		
A729	G730	G731	A732	A733	G734	C735	C736	A737	C738	C739	U740	G741	C744	C745	A746	C747	C748	C749	G750	U751	G752	A753	C754	G755	C756	U757	G758	A759	G760	G761	C762	G763	G764	A765	A766	A767	A768	G769	C770	C771	U772	G773	G774	G775	G776	A777	C778	C779	A780	A781	A782	C783	C784	G785	G786	A787	U788		
G791	A792	U793	A794	C795	G796	G797	G798	G799		A802	C803	U804	C805	C806	A807	C808	C809	C810	C811	C812	U813	A814	A815	A816	C817	G818	C819	U820	G821	C822	C823	C824	G825	C826	U827	A828	C829	G830	G831	C832	U833	C834	U835	G836	G837	G838	U839	C840	U841	C848	C849	U850	C851	C852	C853	G854	G855	C856	C857
G858	A859	A860	C861	C862	U863	A864	A865	C866	C867	C868	C869	U870	U871	A872	A873	C874	C875	C876	C877	C881	C882	C883	C884	C885	C886	C887	C888	C889	C890	C891	C892	C893	C894	C895	C896	C897	C898	C899	A900	A901	G902	G903		G906	A907	A908	A909		C912	A913	A914	A915	G916	A917	A918	C919	A919		

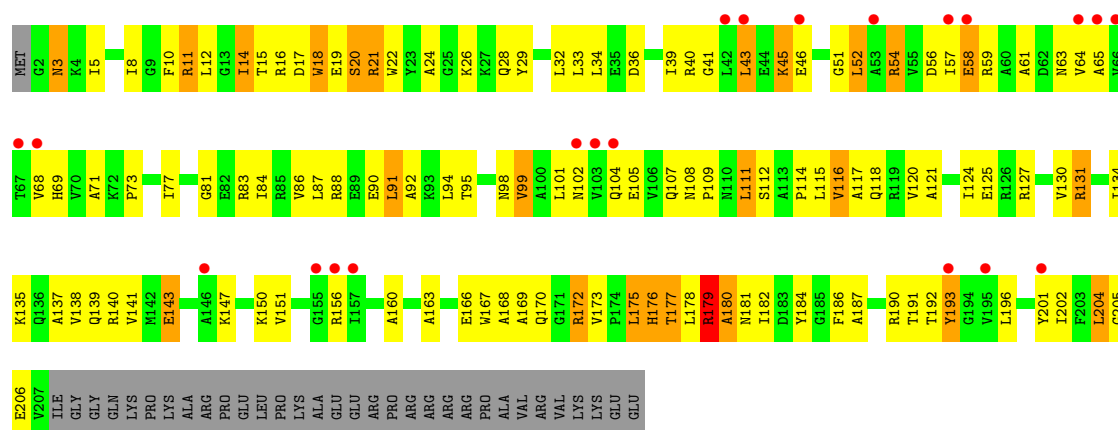
● Molecule 2: RIBOSOMAL PROTEIN S2

Chain B: 

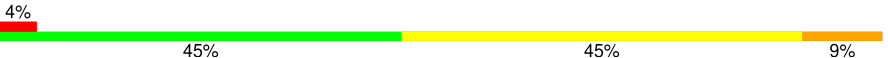


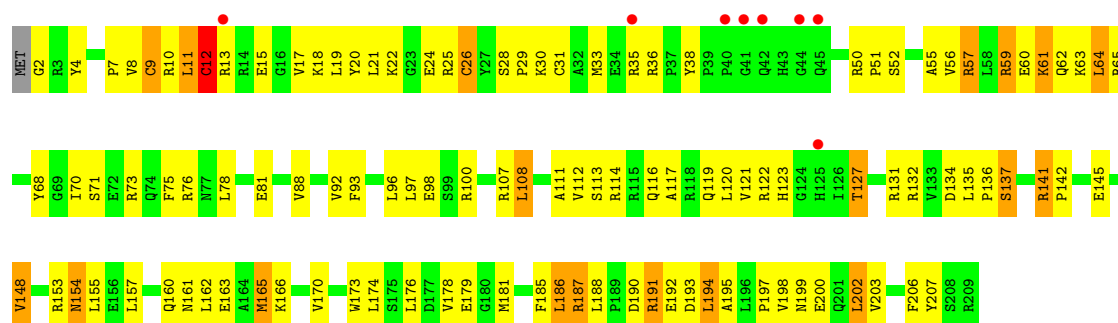
• Molecule 3: RIBOSOMAL PROTEIN S3

Chain C: 



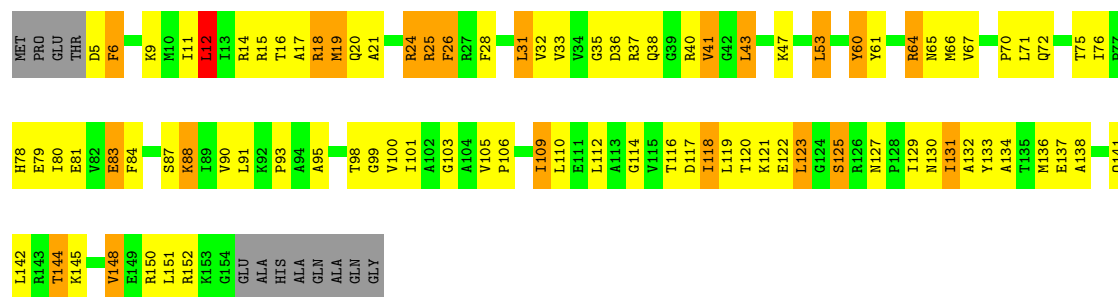
• Molecule 4: RIBOSOMAL PROTEIN S4

Chain D: 



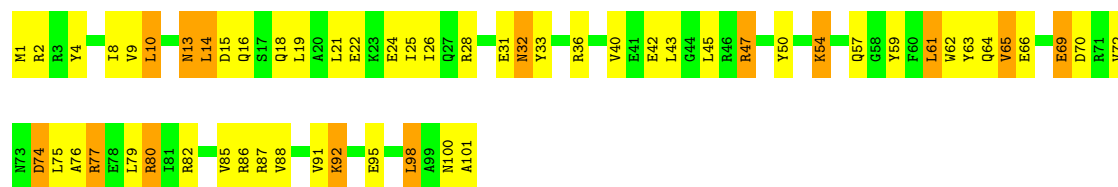
• Molecule 5: RIBOSOMAL PROTEIN S5

Chain E: 



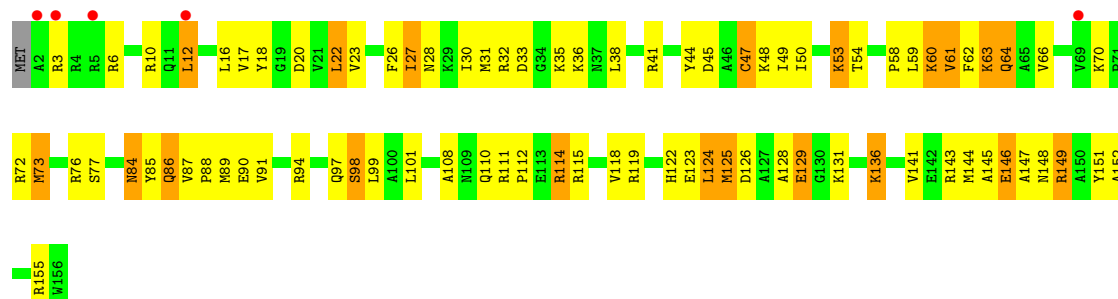
• Molecule 6: RIBOSOMAL PROTEIN S6

Chain F: 44% 43% 14%



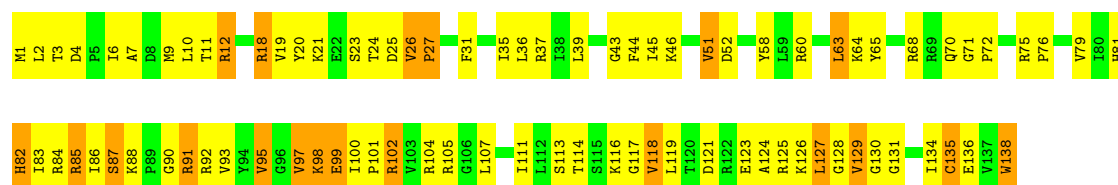
• Molecule 7: RIBOSOMAL PROTEIN S7

Chain G: 3% 46% 40% 13%



• Molecule 8: RIBOSOMAL PROTEIN S8

Chain H: 38% 47% 14%



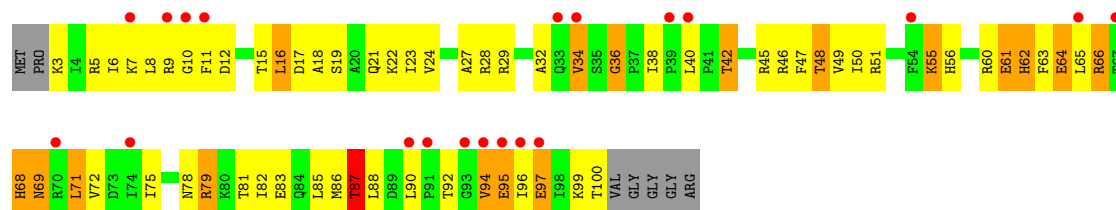
• Molecule 9: RIBOSOMAL PROTEIN S9

Chain I: 13% 37% 42% 20%

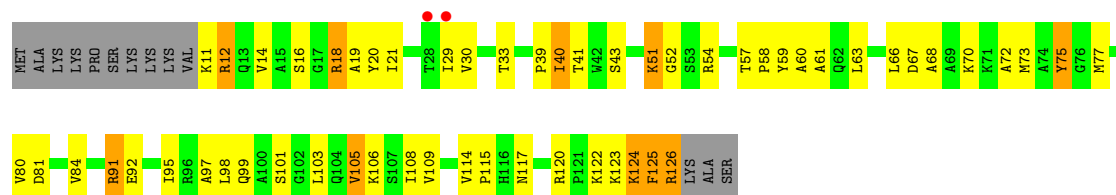




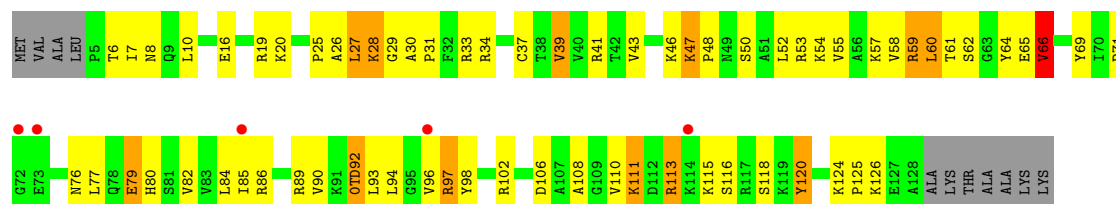
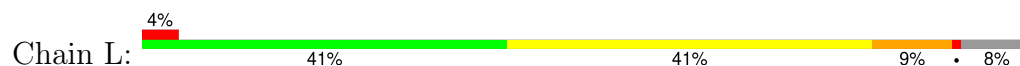
• Molecule 10: RIBOSOMAL PROTEIN S10



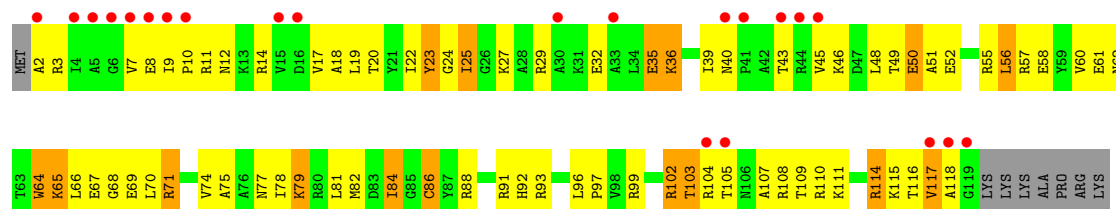
• Molecule 11: RIBOSOMAL PROTEIN S11



• Molecule 12: RIBOSOMAL PROTEIN S12

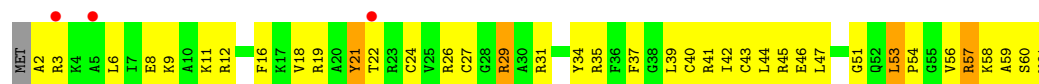


• Molecule 13: RIBOSOMAL PROTEIN S13

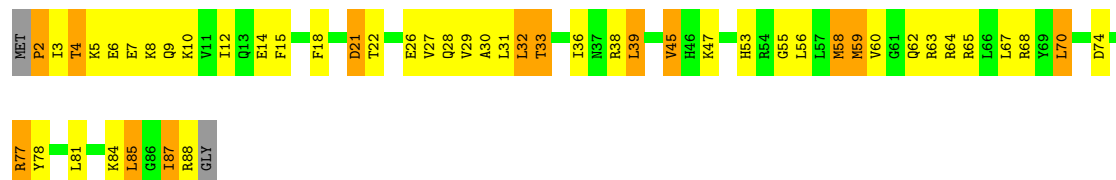


• Molecule 14: RIBOSOMAL PROTEIN S14

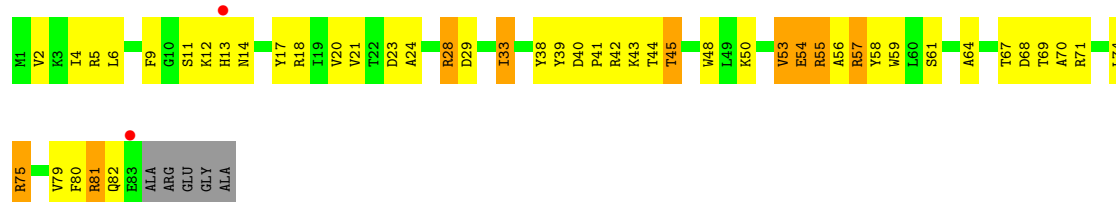




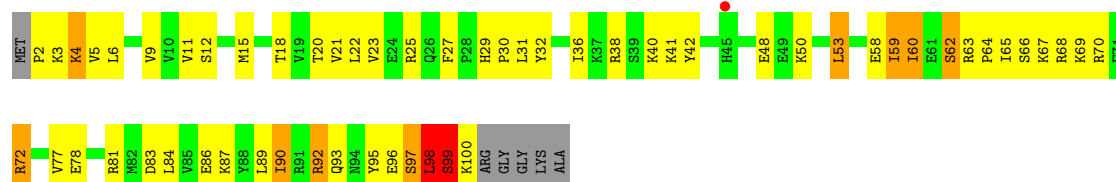
• Molecule 15: RIBOSOMAL PROTEIN S15



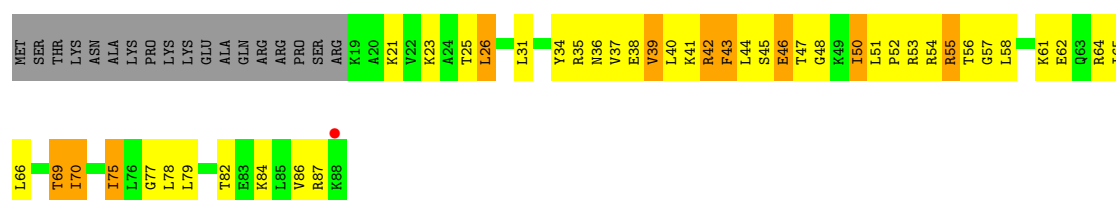
• Molecule 16: RIBOSOMAL PROTEIN S16



• Molecule 17: RIBOSOMAL PROTEIN S17

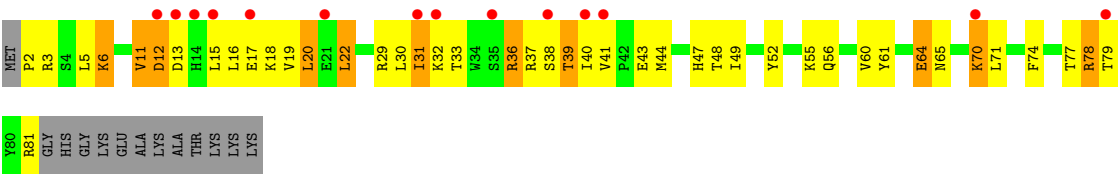


• Molecule 18: RIBOSOMAL PROTEIN S18

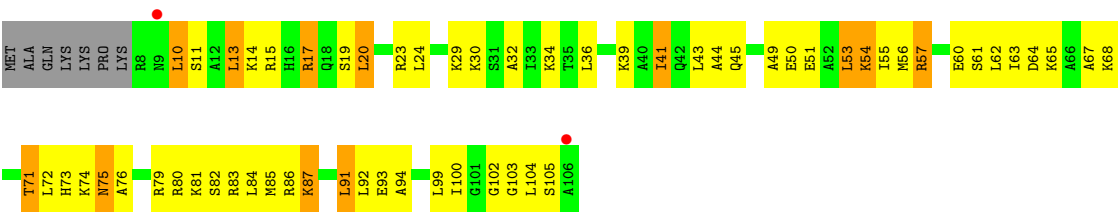


• Molecule 19: RIBOSOMAL PROTEIN S19





• Molecule 20: RIBOSOMAL PROTEIN S20



• Molecule 21: RIBOSOMAL PROTEIN THX



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	402.08Å 402.08Å 174.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.30 – 3.69 49.60 – 3.69	Depositor EDS
% Data completeness (in resolution range)	98.5 (48.30-3.69) 98.5 (49.60-3.69)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.87 (at 3.67Å)	Xtriage
Refinement program	PHENIX dev_1119	Depositor
R, R_{free}	0.156 , 0.214 0.159 , 0.215	Depositor DCC
R_{free} test set	7541 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	140.3	Xtriage
Anisotropy	0.183	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 175.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	52281	wwPDB-VP
Average B, all atoms (Å ²)	183.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.54% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	1.17	188/36139 (0.5%)	1.92	1603/56396 (2.8%)
2	B	0.72	0/1935	0.88	2/2609 (0.1%)
3	C	0.54	0/1636	0.76	2/2205 (0.1%)
4	D	0.71	1/1733 (0.1%)	0.88	1/2318 (0.0%)
5	E	0.92	0/1162	1.07	1/1564 (0.1%)
6	F	0.63	0/856	0.77	0/1154
7	G	0.57	0/1276	0.77	1/1709 (0.1%)
8	H	1.05	1/1136 (0.1%)	1.11	2/1527 (0.1%)
9	I	0.53	0/1029	0.77	0/1379
10	J	0.55	0/805	0.78	0/1082
11	K	0.71	0/879	0.88	0/1187
12	L	0.72	0/977	0.99	2/1305 (0.2%)
13	M	0.60	0/947	0.81	0/1270
14	N	0.48	0/501	0.75	0/664
15	O	0.77	0/740	0.92	1/987 (0.1%)
16	P	0.84	0/716	0.95	0/963
17	Q	0.93	0/836	1.10	2/1117 (0.2%)
18	R	0.77	1/579 (0.2%)	0.94	1/768 (0.1%)
19	S	0.46	0/661	0.76	1/890 (0.1%)
20	T	0.67	0/765	0.94	1/1007 (0.1%)
21	U	0.57	0/212	0.79	0/277
All	All	1.03	191/55520 (0.3%)	1.66	1620/82378 (2.0%)

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

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

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Mol	Chain	#Chirality outliers	#Planarity outliers
4	D	0	2
7	G	0	1
8	H	0	2
10	J	0	4
12	L	0	1
15	O	0	1
20	T	0	2
All	All	0	17

The worst 5 of 191 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	817	C	N1-C6	-13.12	1.29	1.37
1	A	279	A	N9-C4	-11.47	1.30	1.37
1	A	279	A	N3-C4	-11.02	1.28	1.34
1	A	822	C	N1-C6	-10.98	1.30	1.37
1	A	279	A	N7-C5	-9.71	1.33	1.39

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	858	G	N1-C6-O6	25.57	135.24	119.90
1	A	858	G	C6-C5-N7	-18.08	119.55	130.40
1	A	266	G	C6-C5-N7	-17.84	119.70	130.40
1	A	869	G	N1-C6-O6	17.27	130.26	119.90
1	A	869	G	C4-C5-N7	16.36	117.34	110.80

There are no chirality outliers.

5 of 17 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	71	VAL	Peptide
2	B	8	LYS	Peptide
3	C	166	GLU	Peptide
3	C	179	ARG	Peptide
4	D	29	PRO	Peptide

5.2 Too-close contacts [i](#)

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

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	32644	0	16503	885	0
2	B	1900	0	1951	115	0
3	C	1612	0	1677	94	0
4	D	1703	0	1763	88	0
5	E	1146	0	1207	65	0
6	F	843	0	857	43	0
7	G	1257	0	1296	67	0
8	H	1116	0	1177	73	0
9	I	1010	0	1037	81	0
10	J	792	0	835	54	0
11	K	864	0	881	34	0
12	L	973	0	1062	62	0
13	M	937	0	995	62	0
14	N	492	0	529	40	0
15	O	729	0	768	38	0
16	P	700	0	720	38	0
17	Q	823	0	891	54	0
18	R	574	0	644	44	0
19	S	647	0	673	42	0
20	T	763	0	861	44	0
21	U	208	0	221	11	0
22	A	262	0	0	0	0
22	B	1	0	0	0	0
22	C	1	0	0	0	0
22	D	3	0	0	0	0
22	E	1	0	0	0	0
22	F	1	0	0	0	0
22	H	1	0	0	0	0
22	I	1	0	0	0	0
22	J	1	0	0	0	0
22	P	1	0	0	0	0
22	Q	1	0	0	0	0
23	D	1	0	0	0	0
23	N	1	0	0	0	0
24	A	261	0	0	11	0
24	C	1	0	0	1	0
24	D	1	0	0	0	0
24	E	6	0	0	0	0
24	Q	2	0	0	0	0
24	T	1	0	0	1	0
All	All	52281	0	36548	1858	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 21.

The worst 5 of 1858 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)
16:P:9:PHE:HD1	16:P:18:ARG:HG3	1.23	0.99
4:D:63:LYS:NZ	4:D:197:PRO:O	1.97	0.95
1:A:671:G:H4'	6:F:77:ARG:HE	1.32	0.95
1:A:1195:C:H3'	1:A:1196:U:H5''	1.49	0.94
8:H:95:VAL:HG12	8:H:99:GLU:HB2	1.51	0.93

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	232/256 (91%)	206 (89%)	23 (10%)	3 (1%)	12	47
3	C	204/239 (85%)	179 (88%)	24 (12%)	1 (0%)	29	66
4	D	206/209 (99%)	190 (92%)	16 (8%)	0	100	100
5	E	148/162 (91%)	139 (94%)	8 (5%)	1 (1%)	22	59
6	F	99/101 (98%)	95 (96%)	4 (4%)	0	100	100
7	G	153/156 (98%)	137 (90%)	16 (10%)	0	100	100
8	H	136/138 (99%)	131 (96%)	5 (4%)	0	100	100
9	I	125/128 (98%)	113 (90%)	11 (9%)	1 (1%)	19	56
10	J	96/105 (91%)	78 (81%)	17 (18%)	1 (1%)	15	51
11	K	114/129 (88%)	101 (89%)	13 (11%)	0	100	100
12	L	121/135 (90%)	109 (90%)	11 (9%)	1 (1%)	19	56
13	M	116/126 (92%)	102 (88%)	12 (10%)	2 (2%)	9	42

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	N	58/61 (95%)	48 (83%)	10 (17%)	0	100	100
15	O	85/89 (96%)	74 (87%)	10 (12%)	1 (1%)	13	48
16	P	81/88 (92%)	72 (89%)	9 (11%)	0	100	100
17	Q	97/105 (92%)	89 (92%)	8 (8%)	0	100	100
18	R	68/88 (77%)	58 (85%)	10 (15%)	0	100	100
19	S	78/93 (84%)	71 (91%)	6 (8%)	1 (1%)	12	47
20	T	97/106 (92%)	83 (86%)	14 (14%)	0	100	100
21	U	22/27 (82%)	21 (96%)	1 (4%)	0	100	100
All	All	2336/2541 (92%)	2096 (90%)	228 (10%)	12 (0%)	29	66

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	21	ARG
12	L	28	LYS
19	S	31	ILE
2	B	95	GLN
9	I	119	ALA

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%)	157 (78%)	45 (22%)	1	6
3	C	160/188 (85%)	121 (76%)	39 (24%)	0	5
4	D	180/181 (99%)	146 (81%)	34 (19%)	1	9
5	E	115/123 (94%)	77 (67%)	38 (33%)	0	1
6	F	90/90 (100%)	64 (71%)	26 (29%)	0	2
7	G	126/127 (99%)	99 (79%)	27 (21%)	1	7
8	H	119/119 (100%)	90 (76%)	29 (24%)	0	5
9	I	98/99 (99%)	68 (69%)	30 (31%)	0	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	J	87/92 (95%)	67 (77%)	20 (23%)	1	6
11	K	88/99 (89%)	67 (76%)	21 (24%)	0	5
12	L	103/110 (94%)	84 (82%)	19 (18%)	1	10
13	M	94/101 (93%)	73 (78%)	21 (22%)	1	6
14	N	49/50 (98%)	42 (86%)	7 (14%)	3	19
15	O	79/80 (99%)	62 (78%)	17 (22%)	1	7
16	P	72/74 (97%)	59 (82%)	13 (18%)	1	11
17	Q	94/97 (97%)	74 (79%)	20 (21%)	1	7
18	R	61/77 (79%)	48 (79%)	13 (21%)	1	7
19	S	71/80 (89%)	56 (79%)	15 (21%)	1	7
20	T	76/82 (93%)	55 (72%)	21 (28%)	0	3
21	U	19/22 (86%)	13 (68%)	6 (32%)	0	1
All	All	1983/2111 (94%)	1522 (77%)	461 (23%)	1	6

5 of 461 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	H	118	VAL
20	T	43	LEU
10	J	96	ILE
20	T	19	SER
17	Q	89	LEU

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

Mol	Chain	Res	Type
19	S	47	HIS
13	M	77	ASN
6	F	7	ASN
5	E	127	ASN
9	I	73	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1504/1522 (98%)	379 (25%)	43 (2%)

5 of 379 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	6	G
1	A	7	G
1	A	8	A
1	A	9	G
1	A	22	G

5 of 43 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	1065	U
1	A	1257	U
1	A	1139	G
1	A	1196	U
1	A	1300	G

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

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	5MC	A	1407	1	19,22,23	1.64	4 (21%)	26,32,35	1.24	2 (7%)
1	5MC	A	967	1	19,22,23	1.33	2 (10%)	26,32,35	1.02	2 (7%)
1	4OC	A	1402	1	20,23,24	1.78	5 (25%)	25,32,35	0.76	0
1	7MG	A	527	22,1	23,26,27	3.75	7 (30%)	27,39,42	2.28	10 (37%)
1	UR3	A	1498	1	19,22,23	1.05	2 (10%)	26,32,35	1.40	4 (15%)
12	0TD	L	92	12	8,9,10	1.16	0	6,11,13	3.02	4 (66%)
1	PSU	A	516	1	18,21,22	1.19	1 (5%)	21,30,33	1.79	4 (19%)
1	MA6	A	1518[A]	1	19,26,27	1.12	2 (10%)	18,38,41	0.68	0
1	M2G	A	966	1	20,27,28	1.33	2 (10%)	19,40,43	1.47	2 (10%)
1	5MC	A	1400	1	19,22,23	1.44	5 (26%)	26,32,35	1.12	1 (3%)
1	MA6	A	1519[B]	1	19,26,27	1.64	5 (26%)	18,38,41	0.71	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	PSU	A	1541	1	18,21,22	1.11	1 (5%)	21,30,33	1.89	4 (19%)
1	2MG	A	1207	1	18,26,27	1.72	4 (22%)	16,38,41	1.45	3 (18%)
1	MA6	A	1519[A]	1	19,26,27	1.22	2 (10%)	18,38,41	0.67	0
1	5MC	A	1404	1	19,22,23	1.54	3 (15%)	26,32,35	1.52	4 (15%)
1	PSU	A	1540	1	18,21,22	1.16	1 (5%)	21,30,33	1.86	5 (23%)
1	MA6	A	1518[B]	1	19,26,27	1.31	3 (15%)	18,38,41	0.74	0

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	5MC	A	1407	1	-	0/7/25/26	0/2/2/2
1	5MC	A	967	1	-	4/7/25/26	0/2/2/2
1	4OC	A	1402	1	-	4/9/29/30	0/2/2/2
1	7MG	A	527	22,1	-	2/7/37/38	0/3/3/3
1	UR3	A	1498	1	-	2/7/25/26	0/2/2/2
12	0TD	L	92	12	-	3/7/12/14	-
1	PSU	A	516	1	-	0/7/25/26	0/2/2/2
1	MA6	A	1518[A]	1	-	2/7/29/30	0/3/3/3
1	M2G	A	966	1	-	2/7/29/30	0/3/3/3
1	5MC	A	1400	1	-	2/7/25/26	0/2/2/2
1	MA6	A	1519[B]	1	-	5/7/29/30	0/3/3/3
1	PSU	A	1541	1	-	1/7/25/26	0/2/2/2
1	2MG	A	1207	1	-	4/5/27/28	0/3/3/3
1	MA6	A	1519[A]	1	-	3/7/29/30	0/3/3/3
1	5MC	A	1404	1	-	0/7/25/26	0/2/2/2
1	PSU	A	1540	1	-	2/7/25/26	0/2/2/2
1	MA6	A	1518[B]	1	-	3/7/29/30	0/3/3/3

The worst 5 of 49 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	527	7MG	C8-N9	-15.91	1.35	1.45
1	A	1407	5MC	C5-C4	5.48	1.48	1.44
1	A	1404	5MC	C5-C4	5.15	1.48	1.44
1	A	1207	2MG	C6-N1	4.63	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	967	5MC	C5-C4	-4.41	1.40	1.44

The worst 5 of 45 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	527	7MG	C5-C6-N1	5.76	121.07	110.94
1	A	1540	PSU	C4-N3-C2	-4.86	119.68	126.37
1	A	1541	PSU	N1-C2-N3	4.86	120.29	115.17
1	A	1541	PSU	C4-N3-C2	-4.64	119.99	126.37
1	A	1540	PSU	N1-C2-N3	4.50	119.91	115.17

There are no chirality outliers.

5 of 39 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	527	7MG	O4'-C4'-C5'-O5'
1	A	527	7MG	C3'-C4'-C5'-O5'
1	A	967	5MC	O4'-C4'-C5'-O5'
1	A	967	5MC	C3'-C4'-C5'-O5'
1	A	1207	2MG	O4'-C4'-C5'-O5'

There are no ring outliers.

12 monomers are involved in 35 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1407	5MC	1	0
1	A	967	5MC	7	0
1	A	1402	4OC	4	0
1	A	1498	UR3	6	0
12	L	92	0TD	6	0
1	A	516	PSU	1	0
1	A	1518[A]	MA6	2	0
1	A	966	M2G	3	0
1	A	1400	5MC	3	0
1	A	1207	2MG	3	0
1	A	1519[A]	MA6	2	0
1	A	1404	5MC	3	0

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 276 ligands modelled in this entry, 276 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	1498/1522 (98%)	-0.13	51 (3%) 45 34	93, 162, 316, 389	0
2	B	234/256 (91%)	-0.23	0 100 100	133, 184, 270, 282	0
3	C	206/239 (86%)	0.11	21 (10%) 6 5	206, 252, 287, 299	0
4	D	208/209 (99%)	-0.13	8 (3%) 40 30	111, 168, 217, 268	0
5	E	150/162 (92%)	-0.25	0 100 100	94, 134, 188, 231	0
6	F	101/101 (100%)	-0.40	0 100 100	133, 181, 218, 291	0
7	G	155/156 (99%)	0.04	5 (3%) 47 35	158, 220, 277, 309	0
8	H	138/138 (100%)	-0.51	0 100 100	95, 124, 178, 206	0
9	I	127/128 (99%)	0.69	17 (13%) 3 3	171, 232, 283, 313	0
10	J	98/105 (93%)	0.90	20 (20%) 1 0	209, 279, 336, 389	0
11	K	116/129 (89%)	-0.06	2 (1%) 70 59	115, 162, 201, 226	0
12	L	123/135 (91%)	0.17	5 (4%) 37 27	107, 168, 206, 263	0
13	M	118/126 (93%)	0.54	22 (18%) 1 1	154, 195, 252, 307	0
14	N	60/61 (98%)	-0.02	3 (5%) 28 21	202, 244, 301, 320	0
15	O	87/89 (97%)	-0.18	0 100 100	118, 158, 219, 250	0
16	P	83/88 (94%)	0.14	2 (2%) 59 47	111, 173, 212, 270	0
17	Q	99/105 (94%)	-0.11	1 (1%) 82 73	103, 137, 184, 194	0
18	R	70/88 (79%)	-0.49	1 (1%) 75 64	118, 173, 224, 263	0
19	S	80/93 (86%)	0.61	14 (17%) 1 1	207, 262, 310, 335	0
20	T	99/106 (93%)	-0.15	2 (2%) 65 53	127, 166, 233, 261	0
21	U	24/27 (88%)	0.66	4 (16%) 1 1	150, 219, 232, 233	0
All	All	3874/4063 (95%)	-0.04	178 (4%) 32 24	93, 177, 288, 389	0

The worst 5 of 178 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
9	I	15	ALA	10.3
1	A	1018	C	8.1
1	A	1003(A)	G	8.0
1	A	1017	G	7.8
9	I	8	GLY	6.7

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	PSU	A	1540	20/21	0.53	0.95	318,324,373,375	0
1	MA6	A	1518[B]	24/25	0.88	0.31	132,148,153,153	24
1	MA6	A	1518[A]	24/25	0.88	0.31	133,147,161,163	24
1	PSU	A	1541	20/21	0.89	0.60	303,317,323,326	0
1	PSU	A	516	20/21	0.91	0.10	169,189,225,229	0
1	7MG	A	527	24/25	0.91	0.22	142,153,170,174	0
1	5MC	A	1404	21/22	0.92	0.22	132,144,188,193	0
1	4OC	A	1402	22/23	0.93	0.20	130,142,160,168	0
1	MA6	A	1519[A]	24/25	0.94	0.44	118,127,134,135	24
1	MA6	A	1519[B]	24/25	0.94	0.44	123,131,165,167	24
1	2MG	A	1207	24/25	0.95	0.15	239,249,316,321	0
1	5MC	A	1400	21/22	0.95	0.17	125,139,150,167	0
1	5MC	A	1407	21/22	0.95	0.12	180,203,212,220	0
12	0TD	L	92	10/11	0.95	0.58	161,185,287,345	0
1	M2G	A	966	25/26	0.96	0.15	168,177,186,189	0
1	5MC	A	967	21/22	0.96	0.13	154,169,181,182	0
1	UR3	A	1498	21/22	0.97	0.38	131,139,164,169	0

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
22	MG	A	1667	1/1	0.34	0.37	157,157,157,157	0
22	MG	A	1683	1/1	0.38	0.42	118,118,118,118	0
22	MG	A	1743	1/1	0.38	0.61	147,147,147,147	0
22	MG	A	1795	1/1	0.44	0.39	182,182,182,182	0
22	MG	H	201	1/1	0.48	0.62	167,167,167,167	0
22	MG	A	1747	1/1	0.52	0.63	132,132,132,132	0
22	MG	A	1829	1/1	0.53	0.43	156,156,156,156	0
22	MG	A	1665	1/1	0.55	0.31	111,111,111,111	0
22	MG	A	1844	1/1	0.56	0.47	132,132,132,132	0
22	MG	A	1858	1/1	0.61	0.98	147,147,147,147	0
22	MG	A	1861	1/1	0.61	1.43	178,178,178,178	0
22	MG	A	1810	1/1	0.61	1.06	143,143,143,143	0
22	MG	A	1632	1/1	0.62	0.73	131,131,131,131	0
22	MG	A	1831	1/1	0.63	1.12	160,160,160,160	0
22	MG	A	1807	1/1	0.63	0.15	141,141,141,141	0
22	MG	A	1850	1/1	0.63	0.06	450,450,450,450	0
22	MG	Q	201	1/1	0.63	0.18	142,142,142,142	0
22	MG	A	1842	1/1	0.65	0.30	152,152,152,152	0
22	MG	A	1834	1/1	0.68	0.42	138,138,138,138	0
22	MG	A	1624	1/1	0.68	0.29	134,134,134,134	0
22	MG	A	1806	1/1	0.68	0.82	127,127,127,127	0
22	MG	A	1759	1/1	0.68	0.51	126,126,126,126	0
22	MG	A	1847	1/1	0.69	0.14	145,145,145,145	0
22	MG	A	1815	1/1	0.69	0.99	124,124,124,124	0
22	MG	A	1797	1/1	0.70	0.45	146,146,146,146	0
22	MG	A	1753	1/1	0.70	0.29	136,136,136,136	0
22	MG	A	1816	1/1	0.71	0.29	181,181,181,181	0
22	MG	A	1682	1/1	0.71	0.36	180,180,180,180	0
22	MG	A	1702	1/1	0.71	0.66	166,166,166,166	0
22	MG	A	1776	1/1	0.71	0.26	139,139,139,139	0
22	MG	A	1824	1/1	0.72	0.67	139,139,139,139	0
22	MG	A	1662	1/1	0.72	0.33	108,108,108,108	0
22	MG	A	1771	1/1	0.72	0.71	127,127,127,127	0
22	MG	A	1769	1/1	0.73	0.68	151,151,151,151	0
22	MG	A	1748	1/1	0.73	0.11	177,177,177,177	0
22	MG	A	1848	1/1	0.74	0.26	527,527,527,527	0
22	MG	A	1798	1/1	0.74	0.21	163,163,163,163	0
22	MG	A	1784	1/1	0.74	0.41	175,175,175,175	0
22	MG	A	1820	1/1	0.74	0.62	144,144,144,144	0
22	MG	A	1745	1/1	0.74	0.69	169,169,169,169	0
22	MG	A	1700	1/1	0.74	0.16	204,204,204,204	0
22	MG	A	1673	1/1	0.75	0.31	211,211,211,211	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
22	MG	A	1785	1/1	0.76	0.19	184,184,184,184	0
22	MG	A	1735	1/1	0.77	0.43	93,93,93,93	0
22	MG	B	301	1/1	0.77	0.10	132,132,132,132	0
22	MG	A	1857	1/1	0.77	1.22	128,128,128,128	0
22	MG	A	1742	1/1	0.77	0.55	152,152,152,152	0
22	MG	A	1764	1/1	0.78	1.51	137,137,137,137	0
22	MG	E	201	1/1	0.78	0.19	177,177,177,177	0
22	MG	A	1772	1/1	0.79	0.47	120,120,120,120	0
22	MG	C	301	1/1	0.79	0.21	143,143,143,143	0
22	MG	A	1796	1/1	0.79	0.30	121,121,121,121	0
22	MG	A	1625	1/1	0.79	0.48	101,101,101,101	0
22	MG	A	1808	1/1	0.79	0.15	164,164,164,164	0
22	MG	A	1746	1/1	0.80	0.71	111,111,111,111	0
22	MG	A	1838	1/1	0.80	0.40	150,150,150,150	0
22	MG	A	1688	1/1	0.80	0.26	164,164,164,164	0
22	MG	A	1762	1/1	0.80	0.61	124,124,124,124	0
22	MG	A	1694	1/1	0.80	0.28	105,105,105,105	0
22	MG	A	1730	1/1	0.81	0.39	138,138,138,138	0
22	MG	A	1684	1/1	0.81	0.96	135,135,135,135	0
22	MG	A	1704	1/1	0.81	0.11	211,211,211,211	0
22	MG	A	1855	1/1	0.81	1.27	143,143,143,143	0
22	MG	A	1783	1/1	0.82	0.32	119,119,119,119	0
22	MG	A	1770	1/1	0.82	0.40	103,103,103,103	0
22	MG	A	1849	1/1	0.82	0.20	550,550,550,550	0
22	MG	A	1859	1/1	0.82	0.13	147,147,147,147	0
22	MG	A	1752	1/1	0.82	0.45	142,142,142,142	0
22	MG	A	1819	1/1	0.83	0.67	137,137,137,137	0
22	MG	A	1664	1/1	0.83	0.31	121,121,121,121	0
22	MG	A	1685	1/1	0.83	0.35	159,159,159,159	0
22	MG	A	1641	1/1	0.83	0.24	130,130,130,130	0
22	MG	A	1723	1/1	0.83	0.82	120,120,120,120	0
22	MG	A	1601	1/1	0.83	0.28	152,152,152,152	0
22	MG	A	1835	1/1	0.83	0.73	139,139,139,139	0
22	MG	A	1731	1/1	0.83	0.26	145,145,145,145	0
22	MG	A	1660	1/1	0.84	0.29	155,155,155,155	0
22	MG	A	1862	1/1	0.84	0.38	161,161,161,161	0
22	MG	A	1760	1/1	0.84	0.24	140,140,140,140	0
22	MG	A	1714	1/1	0.84	0.61	162,162,162,162	0
22	MG	A	1773	1/1	0.84	0.34	156,156,156,156	0
22	MG	A	1732	1/1	0.84	0.65	94,94,94,94	0
22	MG	A	1608	1/1	0.84	0.14	169,169,169,169	0
22	MG	A	1775	1/1	0.85	0.30	146,146,146,146	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
22	MG	A	1603	1/1	0.85	0.18	137,137,137,137	0
22	MG	A	1680	1/1	0.86	0.24	175,175,175,175	0
22	MG	A	1782	1/1	0.86	0.64	159,159,159,159	0
22	MG	A	1768	1/1	0.86	0.25	166,166,166,166	0
22	MG	A	1841	1/1	0.86	0.15	147,147,147,147	0
22	MG	D	303	1/1	0.86	0.20	137,137,137,137	0
22	MG	A	1672	1/1	0.86	0.32	146,146,146,146	0
22	MG	A	1729	1/1	0.86	0.26	119,119,119,119	0
22	MG	A	1833	1/1	0.86	0.35	182,182,182,182	0
22	MG	A	1637	1/1	0.87	0.28	116,116,116,116	0
22	MG	A	1728	1/1	0.87	0.41	138,138,138,138	0
22	MG	A	1645	1/1	0.87	0.90	141,141,141,141	0
22	MG	A	1822	1/1	0.87	0.82	148,148,148,148	0
22	MG	A	1716	1/1	0.87	0.27	118,118,118,118	0
22	MG	A	1621	1/1	0.88	0.20	149,149,149,149	0
22	MG	A	1670	1/1	0.88	0.25	199,199,199,199	0
22	MG	A	1813	1/1	0.88	0.53	520,520,520,520	0
22	MG	A	1678	1/1	0.88	0.24	350,350,350,350	0
22	MG	A	1733	1/1	0.88	0.28	147,147,147,147	0
22	MG	A	1755	1/1	0.88	0.41	150,150,150,150	0
22	MG	D	304	1/1	0.88	0.88	147,147,147,147	0
22	MG	A	1758	1/1	0.88	0.52	103,103,103,103	0
22	MG	A	1840	1/1	0.88	0.29	143,143,143,143	0
22	MG	A	1734	1/1	0.88	0.58	139,139,139,139	0
22	MG	A	1765	1/1	0.89	0.12	126,126,126,126	0
22	MG	A	1790	1/1	0.89	0.17	217,217,217,217	0
22	MG	A	1860	1/1	0.89	0.53	133,133,133,133	0
22	MG	A	1627	1/1	0.89	1.47	101,101,101,101	0
22	MG	A	1827	1/1	0.89	0.13	151,151,151,151	0
22	MG	A	1801	1/1	0.89	0.20	129,129,129,129	0
22	MG	A	1661	1/1	0.90	0.25	120,120,120,120	0
22	MG	A	1843	1/1	0.90	0.51	132,132,132,132	0
22	MG	A	1618	1/1	0.90	0.56	141,141,141,141	0
22	MG	A	1605	1/1	0.90	0.99	103,103,103,103	0
22	MG	A	1828	1/1	0.90	0.41	114,114,114,114	0
22	MG	A	1703	1/1	0.90	0.17	291,291,291,291	0
22	MG	A	1761	1/1	0.90	0.22	147,147,147,147	0
22	MG	A	1750	1/1	0.91	0.25	157,157,157,157	0
22	MG	A	1623	1/1	0.91	0.50	129,129,129,129	0
22	MG	A	1832	1/1	0.91	0.23	149,149,149,149	0
22	MG	A	1689	1/1	0.91	1.29	214,214,214,214	0
22	MG	A	1690	1/1	0.91	0.13	169,169,169,169	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
22	MG	A	1711	1/1	0.91	0.45	185,185,185,185	0
22	MG	A	1675	1/1	0.91	0.89	143,143,143,143	0
22	MG	A	1687	1/1	0.91	0.12	234,234,234,234	0
22	MG	A	1701	1/1	0.91	0.33	161,161,161,161	0
22	MG	P	101	1/1	0.91	0.26	106,106,106,106	0
22	MG	A	1793	1/1	0.91	0.24	444,444,444,444	0
22	MG	A	1787	1/1	0.92	0.08	147,147,147,147	0
22	MG	A	1692	1/1	0.92	0.25	165,165,165,165	0
22	MG	A	1749	1/1	0.92	0.30	157,157,157,157	0
22	MG	A	1853	1/1	0.92	0.95	150,150,150,150	0
22	MG	A	1818	1/1	0.92	0.53	109,109,109,109	0
22	MG	A	1856	1/1	0.92	0.65	143,143,143,143	0
22	MG	A	1628	1/1	0.92	0.40	141,141,141,141	0
22	MG	F	201	1/1	0.92	0.13	127,127,127,127	0
22	MG	A	1676	1/1	0.92	0.20	136,136,136,136	0
22	MG	J	201	1/1	0.92	0.57	128,128,128,128	0
22	MG	A	1611	1/1	0.92	0.09	184,184,184,184	0
22	MG	A	1823	1/1	0.92	0.25	128,128,128,128	0
22	MG	A	1643	1/1	0.93	0.25	102,102,102,102	0
22	MG	A	1854	1/1	0.93	0.77	149,149,149,149	0
22	MG	A	1718	1/1	0.93	0.35	134,134,134,134	0
22	MG	A	1817	1/1	0.93	0.28	148,148,148,148	0
22	MG	A	1630	1/1	0.93	0.27	124,124,124,124	0
22	MG	A	1737	1/1	0.93	0.24	119,119,119,119	0
22	MG	A	1809	1/1	0.93	0.26	114,114,114,114	0
22	MG	A	1739	1/1	0.93	0.14	139,139,139,139	0
22	MG	A	1668	1/1	0.93	0.37	134,134,134,134	0
22	MG	A	1814	1/1	0.93	0.16	70,70,70,70	0
22	MG	A	1825	1/1	0.94	0.16	139,139,139,139	0
22	MG	A	1620	1/1	0.94	0.26	162,162,162,162	0
22	MG	A	1656	1/1	0.94	0.30	106,106,106,106	0
22	MG	A	1846	1/1	0.94	0.20	126,126,126,126	0
22	MG	A	1803	1/1	0.94	1.15	115,115,115,115	0
22	MG	A	1830	1/1	0.94	0.18	130,130,130,130	0
22	MG	A	1804	1/1	0.94	0.11	120,120,120,120	0
22	MG	A	1677	1/1	0.94	0.23	128,128,128,128	0
22	MG	A	1791	1/1	0.94	0.09	294,294,294,294	0
22	MG	A	1659	1/1	0.94	0.21	128,128,128,128	0
22	MG	A	1821	1/1	0.94	0.38	138,138,138,138	0
22	MG	A	1738	1/1	0.94	0.27	113,113,113,113	0
22	MG	A	1614	1/1	0.94	0.19	141,141,141,141	0
22	MG	A	1666	1/1	0.94	0.19	141,141,141,141	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
23	ZN	N	101	1/1	0.94	0.18	223,223,223,223	0
22	MG	A	1646	1/1	0.95	0.72	236,236,236,236	0
22	MG	A	1800	1/1	0.95	0.19	158,158,158,158	0
22	MG	A	1741	1/1	0.95	0.16	128,128,128,128	0
22	MG	A	1839	1/1	0.95	0.13	144,144,144,144	0
22	MG	A	1802	1/1	0.95	0.74	180,180,180,180	0
22	MG	A	1648	1/1	0.95	0.27	149,149,149,149	0
22	MG	A	1720	1/1	0.95	0.14	196,196,196,196	0
22	MG	A	1786	1/1	0.95	0.35	131,131,131,131	0
22	MG	A	1721	1/1	0.95	0.17	149,149,149,149	0
22	MG	D	302	1/1	0.95	0.18	137,137,137,137	0
22	MG	A	1789	1/1	0.95	0.38	157,157,157,157	0
22	MG	A	1697	1/1	0.95	0.34	133,133,133,133	0
22	MG	A	1727	1/1	0.95	0.18	106,106,106,106	0
22	MG	A	1811	1/1	0.95	1.04	156,156,156,156	0
22	MG	A	1638	1/1	0.95	0.58	189,189,189,189	0
22	MG	A	1851	1/1	0.95	0.10	366,366,366,366	0
22	MG	A	1669	1/1	0.95	0.18	149,149,149,149	0
22	MG	A	1763	1/1	0.95	0.26	111,111,111,111	0
22	MG	A	1781	1/1	0.95	0.89	158,158,158,158	0
22	MG	A	1792	1/1	0.96	0.32	313,313,313,313	0
22	MG	A	1725	1/1	0.96	0.51	156,156,156,156	0
22	MG	A	1794	1/1	0.96	0.16	278,278,278,278	0
22	MG	A	1757	1/1	0.96	0.22	103,103,103,103	0
22	MG	A	1774	1/1	0.96	0.40	157,157,157,157	0
22	MG	A	1726	1/1	0.96	0.09	349,349,349,349	0
22	MG	A	1708	1/1	0.96	0.24	155,155,155,155	0
22	MG	A	1779	1/1	0.96	0.42	112,112,112,112	0
22	MG	A	1699	1/1	0.96	0.25	124,124,124,124	0
22	MG	A	1712	1/1	0.96	0.27	324,324,324,324	0
22	MG	A	1713	1/1	0.96	0.16	229,229,229,229	0
22	MG	A	1613	1/1	0.96	0.23	153,153,153,153	0
22	MG	A	1651	1/1	0.96	0.21	113,113,113,113	0
22	MG	A	1686	1/1	0.96	0.11	241,241,241,241	0
22	MG	A	1612	1/1	0.96	0.34	178,178,178,178	0
22	MG	A	1657	1/1	0.96	0.26	146,146,146,146	0
22	MG	A	1736	1/1	0.96	0.18	99,99,99,99	0
22	MG	A	1705	1/1	0.96	0.34	319,319,319,319	0
22	MG	A	1812	1/1	0.96	0.33	417,417,417,417	0
22	MG	A	1756	1/1	0.97	0.27	112,112,112,112	0
22	MG	A	1778	1/1	0.97	0.15	127,127,127,127	0
22	MG	A	1845	1/1	0.97	0.19	113,113,113,113	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
22	MG	A	1766	1/1	0.97	0.09	126,126,126,126	0
22	MG	A	1706	1/1	0.97	0.37	105,105,105,105	0
22	MG	A	1634	1/1	0.97	0.07	161,161,161,161	0
22	MG	A	1674	1/1	0.97	0.15	136,136,136,136	0
22	MG	A	1617	1/1	0.97	0.43	175,175,175,175	0
22	MG	A	1836	1/1	0.97	0.55	143,143,143,143	0
22	MG	A	1852	1/1	0.97	0.52	530,530,530,530	0
22	MG	A	1837	1/1	0.97	0.16	87,87,87,87	0
22	MG	A	1724	1/1	0.97	0.47	169,169,169,169	0
22	MG	A	1696	1/1	0.97	0.28	160,160,160,160	0
22	MG	A	1642	1/1	0.97	0.30	98,98,98,98	0
22	MG	A	1788	1/1	0.97	0.29	151,151,151,151	0
22	MG	A	1647	1/1	0.97	0.17	175,175,175,175	0
22	MG	A	1619	1/1	0.98	0.16	106,106,106,106	0
22	MG	A	1602	1/1	0.98	0.40	168,168,168,168	0
22	MG	A	1805	1/1	0.98	0.09	119,119,119,119	0
22	MG	A	1629	1/1	0.98	0.16	131,131,131,131	0
22	MG	A	1644	1/1	0.98	0.05	111,111,111,111	0
22	MG	A	1615	1/1	0.98	0.20	81,81,81,81	0
22	MG	A	1740	1/1	0.98	0.18	119,119,119,119	0
22	MG	A	1722	1/1	0.98	0.29	122,122,122,122	0
22	MG	A	1681	1/1	0.98	0.30	167,167,167,167	0
22	MG	A	1616	1/1	0.98	0.32	85,85,85,85	0
22	MG	A	1744	1/1	0.98	0.25	127,127,127,127	0
22	MG	A	1604	1/1	0.98	0.12	123,123,123,123	0
22	MG	A	1609	1/1	0.98	0.15	120,120,120,120	0
22	MG	A	1650	1/1	0.98	0.12	104,104,104,104	0
22	MG	A	1626	1/1	0.98	1.14	105,105,105,105	0
22	MG	A	1653	1/1	0.98	0.12	76,76,76,76	0
22	MG	A	1639	1/1	0.98	0.16	82,82,82,82	0
22	MG	A	1710	1/1	0.98	0.14	94,94,94,94	0
22	MG	A	1640	1/1	0.98	0.10	186,186,186,186	0
22	MG	A	1799	1/1	0.98	0.21	125,125,125,125	0
22	MG	A	1754	1/1	0.98	0.31	137,137,137,137	0
22	MG	A	1658	1/1	0.98	0.23	156,156,156,156	0
22	MG	A	1691	1/1	0.98	0.48	155,155,155,155	0
22	MG	A	1826	1/1	0.98	0.53	121,121,121,121	0
22	MG	A	1709	1/1	0.99	0.15	169,169,169,169	0
22	MG	A	1679	1/1	0.99	0.37	124,124,124,124	0
22	MG	A	1777	1/1	0.99	0.36	111,111,111,111	0
22	MG	A	1693	1/1	0.99	0.15	160,160,160,160	0
22	MG	A	1633	1/1	0.99	0.20	198,198,198,198	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
22	MG	A	1780	1/1	0.99	0.21	143,143,143,143	0
22	MG	A	1695	1/1	0.99	0.13	113,113,113,113	0
22	MG	A	1606	1/1	0.99	0.12	107,107,107,107	0
22	MG	A	1715	1/1	0.99	0.45	112,112,112,112	0
22	MG	A	1635	1/1	0.99	0.12	99,99,99,99	0
22	MG	A	1717	1/1	0.99	0.07	157,157,157,157	0
22	MG	A	1698	1/1	0.99	0.33	186,186,186,186	0
22	MG	A	1719	1/1	0.99	0.29	514,514,514,514	0
22	MG	A	1649	1/1	0.99	0.24	150,150,150,150	0
22	MG	A	1671	1/1	0.99	0.09	170,170,170,170	0
22	MG	A	1607	1/1	0.99	0.14	105,105,105,105	0
22	MG	A	1622	1/1	0.99	0.09	106,106,106,106	0
22	MG	A	1767	1/1	0.99	0.48	130,130,130,130	0
22	MG	A	1652	1/1	0.99	0.18	132,132,132,132	0
22	MG	A	1663	1/1	0.99	0.07	162,162,162,162	0
22	MG	A	1610	1/1	0.99	0.11	112,112,112,112	0
22	MG	I	201	1/1	0.99	0.73	138,138,138,138	0
22	MG	A	1654	1/1	0.99	0.11	156,156,156,156	0
22	MG	A	1707	1/1	0.99	0.16	208,208,208,208	0
22	MG	A	1655	1/1	0.99	0.12	156,156,156,156	0
22	MG	A	1751	1/1	0.99	0.23	104,104,104,104	0
22	MG	A	1636	1/1	1.00	0.45	90,90,90,90	0
23	ZN	D	301	1/1	1.00	0.29	154,154,154,154	0
22	MG	A	1631	1/1	1.00	0.14	154,154,154,154	0

6.5 Other polymers [i](#)

There are no such residues in this entry.