



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 3, 2025 – 10:27 PM EST

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.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The 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)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

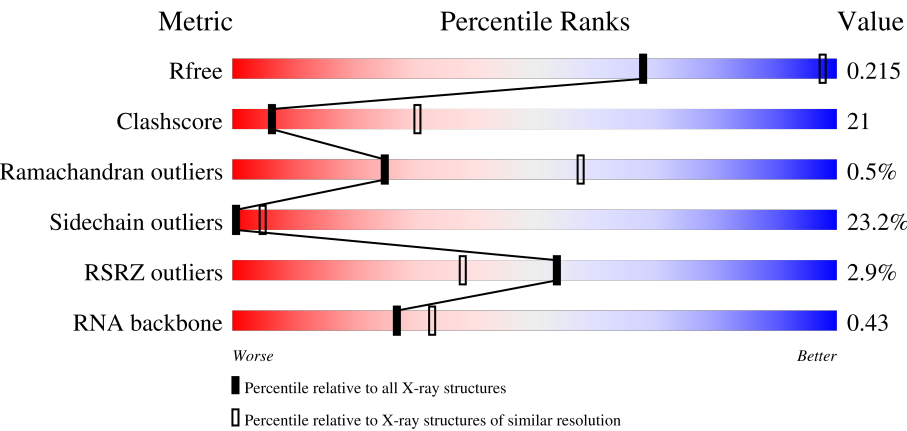
1 Overall quality at a glance i

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.




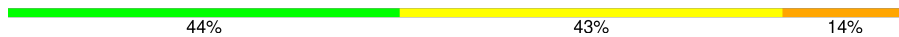
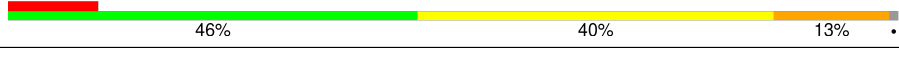
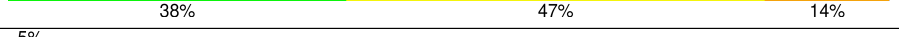
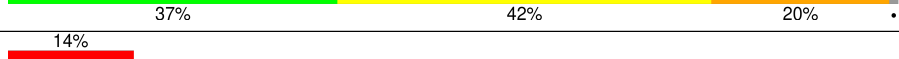
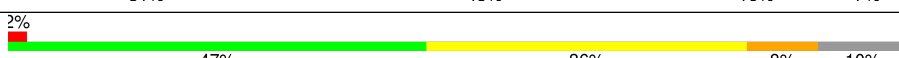

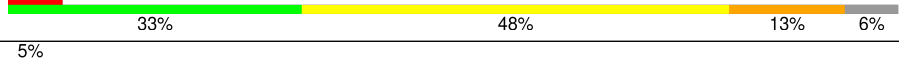
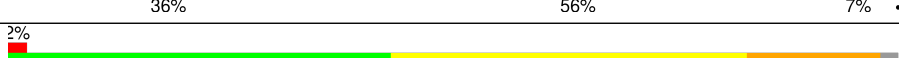
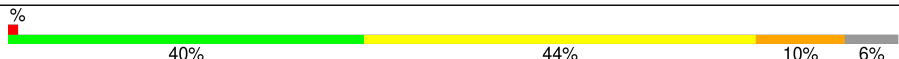
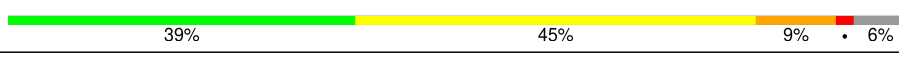
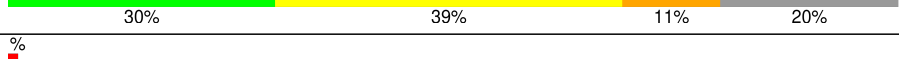
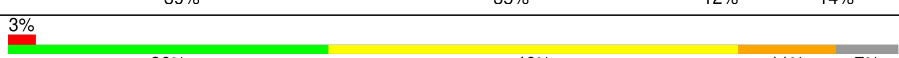



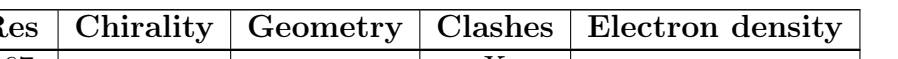
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	164625	1017 (3.80-3.60)
Clashscore	180529	1074 (3.80-3.60)
Ramachandran outliers	177936	1055 (3.80-3.60)
Sidechain outliers	177891	1052 (3.80-3.60)
RSRZ outliers	164620	1017 (3.80-3.60)
RNA backbone	3690	1122 (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>2%</div><div>19%43%31%7%</div></div>
2	B	256	<div><div>%</div><div>39%40%12%9%</div></div>
3	C	239	<div><div>5%</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	5MC	A	967	-	-	X	-
12	0TD	L	92	-	-	X	-
22	MG	A	1632	-	-	-	X
22	MG	A	1822	-	-	-	X
22	MG	A	1855	-	-	-	X
22	MG	A	1861	-	-	-	X

2 Entry composition [i](#)

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

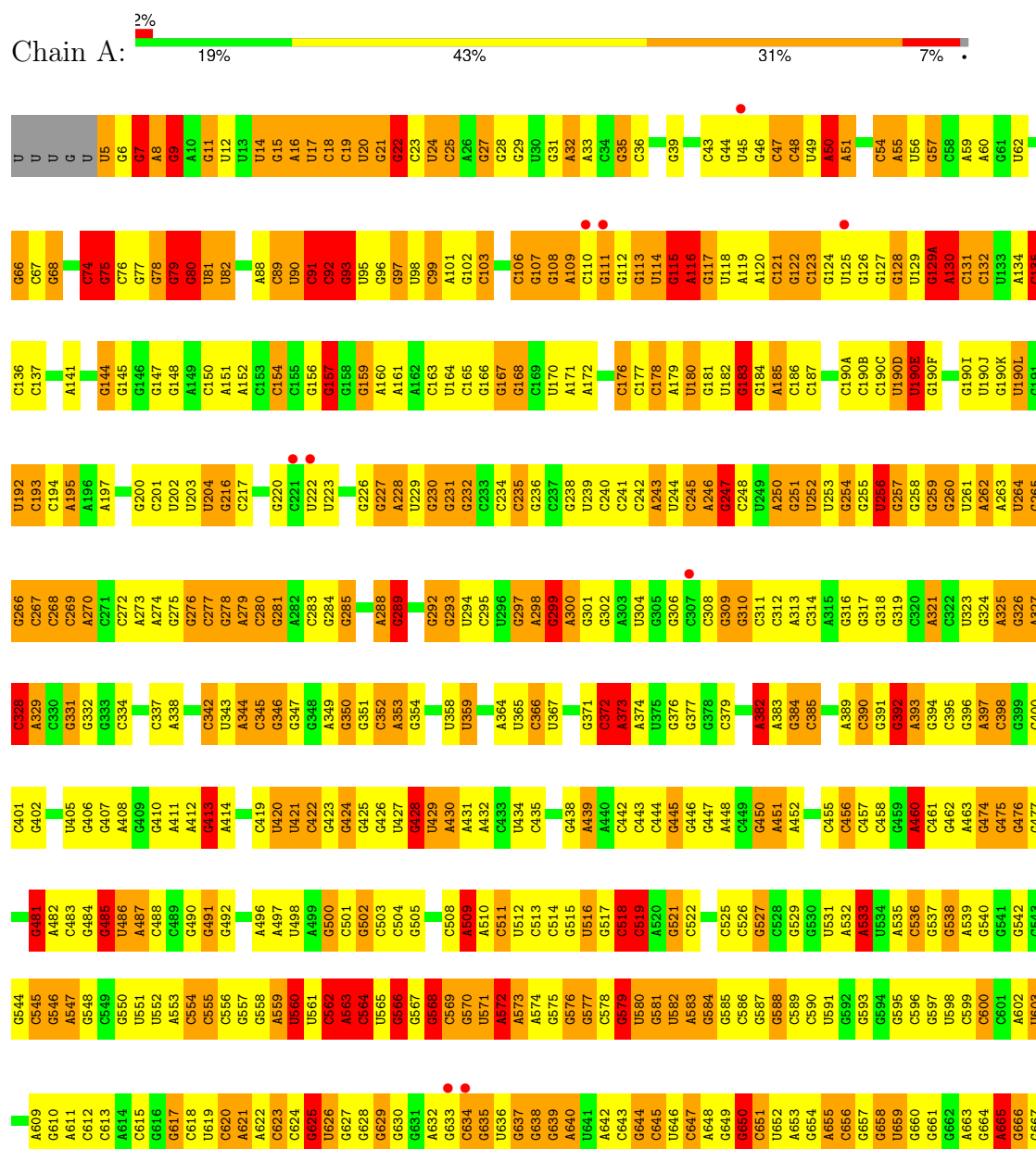
- Molecule 24 is water.

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

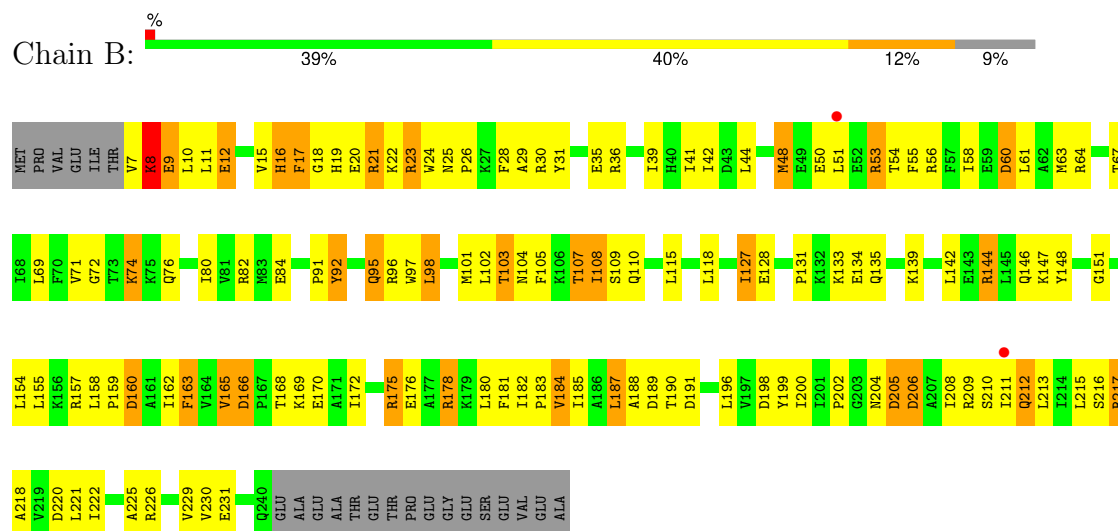
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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

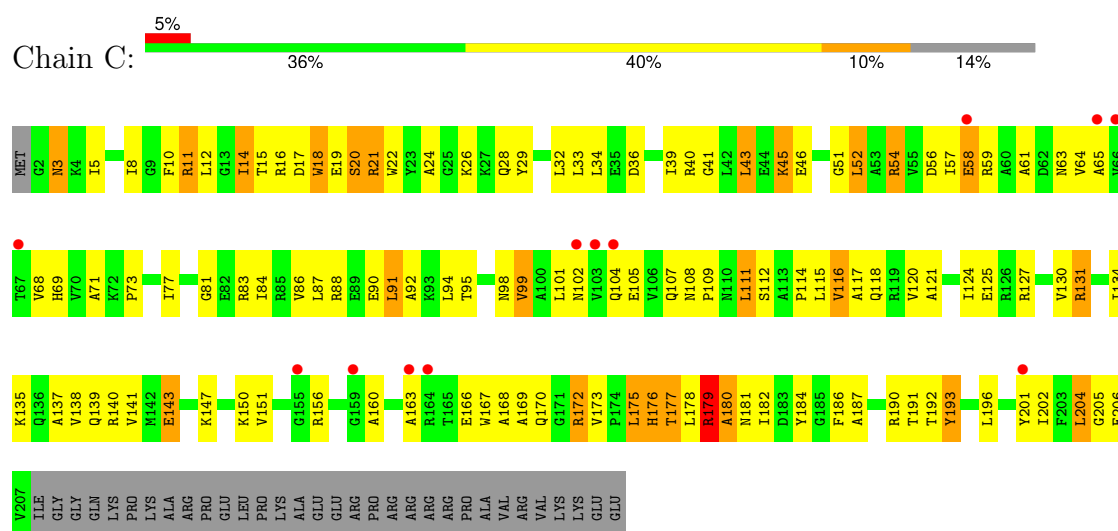


U1490	G1423	A1363	G1178	G1108	G1048	A983	G922	A860	U783	G668
G1491	C1424	U1364	A1179	C1109	U1049	C984	A923	G861	A794	U669
A1492	U1425	G1365	A1180	A1110	G1050	C985	C924	G861	C732	G670
A1493	C1426	G1366	G1181	A1111	C1051	A986	G925	U863	A733	G671
G1494	U1427	C1367	A1182	C1112	U1052	U991	G926	A864	G734	U672
U1495	A1428	U1368	A1183	G1113	G1053	U992	G927	A865	C735	G673
C1496	C1429	U1369	A1184	C1114	C1054	U993	G928	C966	C736	G674
G1497	C1430	G1370	G1185	G1117	A1055	G994	G929	C967	A737	A675
U1498	C1431	G1371	G1186	G1117	U1056	A994	C930	C968	C738	A676
A1499	U1372	G1372	G1187	G1124	G1057	U1000	C931	C969	C739	U677
A1500	A1373	U1373	G1188	U1125	G1058	A1001	C932	U870	U740	U678
A1501	A1374	C1374	C1189	U1126	C1059	G1002	G933	U871	C805	C679
A1502	A1375	U1375	A1191	U1127	G1060	G1003	C934	A872	C744	C680
A1503	U1376	G1376	C1192	G1128	G1061	U1003A	A835	A873	C745	C681
G1504	A1377	C1377	G1193	C1129	U1062	C1004	C936	G874	A746	G682
G1505	G1378	A1378	U1194	U1130	C1063	A1005	A937	C875	C747	G683
U1506	G1379	U1379	U1195	A1130	G1064	U1006	A938	G876	C748	A684
A1507	C1380	C1380	U1196	G1131	U1065	C1007	G939	C877	C749	G685
G1508	U1381	C1381	G1197	C1132	C1066	U1007	C940	G878	U750	U686
C1509	C1382	G1382	G1198	G1133	A1067	C1008	G941	C879	U751	A687
U1510	G1383	A1383	U1199	U1134	U1073	U1009	C942	C880	G752	G688
U1511	C1384	U1384	A1200	U1135	C1069	G1010	U943	G881	A753	C689
U1512	G1385	C1385	C1201	U1136	U1070	G1011	U944	C882	C754	G690
A1513	G1386	G1386	C1202	C1137	C1071	U1012	G945	C883	G691	G691
C1514	C1387	C1387	C1203	G1138	G1072	A1015	A946	U884	C755	U692
C1515	A1388	C1388	A1204	C1139	U1073	A1016	G947	G885	U756	G693
G1516	U1389	U1389	U1205	U1140	U1074	A1017	C948	G886	U757	A694
G1517	C1390	U1390	G1206	C1141	C1075	G1017	A949	G887	A759	A695
A1518	U1391	C1391	C1207	G1142	C1076	C1018	U950	G888	G760	C696
A1519	G1392	A1392	G1208	G1143	C1077	G1019	G951	A889	G761	U697
C1520	C1393	G1393	C1209	G1144	U1078	U1020	U952	G890	C762	G698
A1521	U1394	C1394	G1210	C1145	G1079	G1021	G953	U891	G763	
U1522	C1395	C1395	U1211	U1146	A1080	G1022	G954	A892	G764	C701
G1523	A1396	G1396	C1212	A1147	U1081	G1023	U955	C893	A765	A702
C1524	C1397	G1397	A1213	U1148	G1082	G1024	G894	C894	A766	G703
G1525	A1398	U1398	C1214	C1149	U1083	U1025	A958	G895	A767	A704
G1526	C1399	C1399	G1215	U1150	U1084	G1026	A959	C896	A768	U705
C1527	U1340	U1340	G1216	A1151	U1085	C1027	U960	C897	G769	A706
U1528	C1341	C1341	C1217	A1152	U1086	U1028	U961	G898	C770	C707
G1529	G1401	C1342	C1218	C1153	U1087	C1030B	C962	C899	C771	G709
G1530	C1402	G1343	U1219	G1154	G1088	U1030C	G963	A900	U772	
A1531	C1403	C1344	C1220	C1155	G1089	G1031	A964	A901	G773	
U1532	C1404	U1345	G1221	A1157	U1090	A1030D	A965	G902	G774	G713
C1533	G1405	C1346	G1222	C1158	U1091	G1032	G966	G903	G775	G714
C	U1406	G1347	C1223	U1159	A1092	G1033	C867	G906	G776	A715
A	A1407	U1348	G1224	G1160	A1093	G1034	A968	A907	A777	A716
C	C1408	A1349	A1225	C1163	G1094	A1035	A969	A908	G778	C717
U	U1409	U1350	C1226	G1164	U1095	A1036	C970	A909	C779	G718
C	C1410	C1351	A1227	C1167	C1096	C1037	G971	A909	A780	C719
U1539	C1411	G1352	C1228	A1167	C1097	C1038	C972	C912	A781	G720
U1540	C1412	C1353	A1229	A1168	C1098	C1039	G973	C913	A782	G721
U1541	U1413	G1354	C1230	A1169	G1099	C1040	A974	A913	C783	A722
U1542	G1414	G1355	G1231	A1170	C1100	U1041	A975	A914	C784	U723
C1543	G1415	C1356	U1232	G1171	A1101	A1042	G976	A915	G785	G724
U1544	C1416	A1357	U1233	C1172	A1102	C1043	A977	G916	G786	G725
	G1417	U1358	G1234	C1173	C1103	A1044	A978	G917	U787	G726
	A1418	C1359	C1235	G1174	G1104	C1045	C979	A918	U788	G727
	C1419	C1286	U1236	G1175	A1105	A1046	C980	A919	C791	A728
	G1420	A1299	A1237	A1176	A1106	U1047	U981	U920	A792	A729
	G1300	U1301	C1237	G1177	C1107		U982			G730

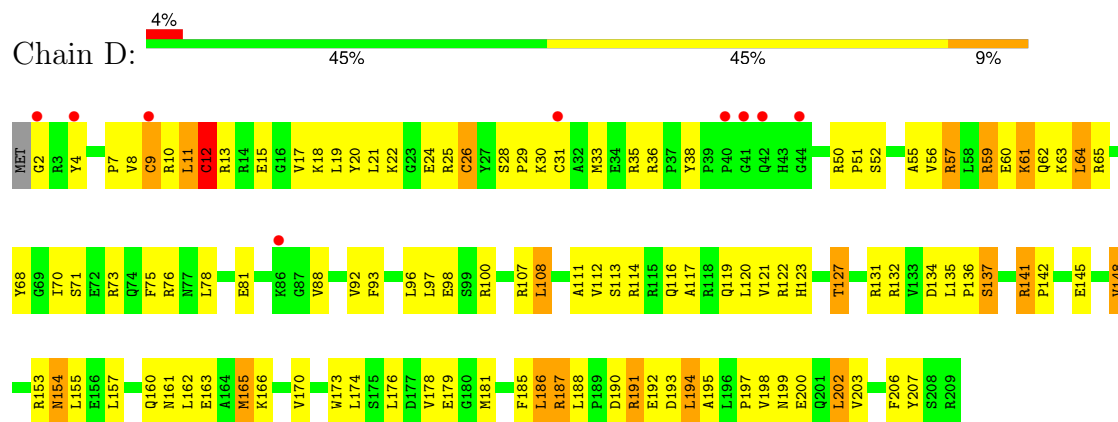
● Molecule 2: RIBOSOMAL PROTEIN S2



- Molecule 3: RIBOSOMAL PROTEIN S3

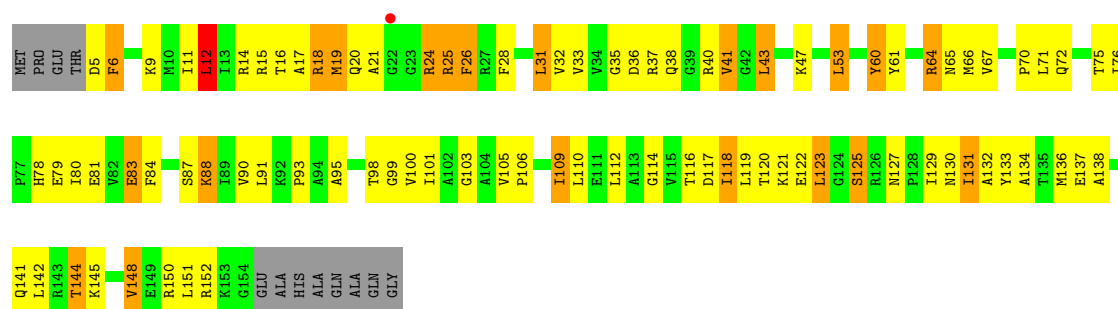


- Molecule 4: RIBOSOMAL PROTEIN S4



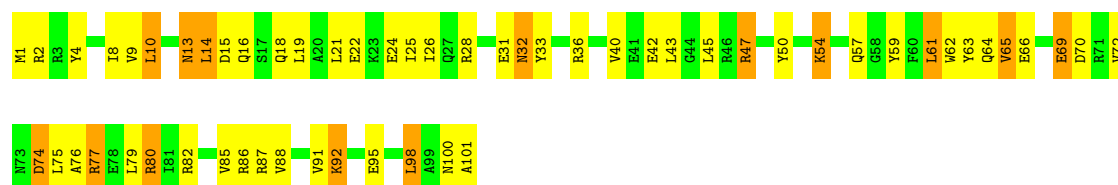
- Molecule 5: RIBOSOMAL PROTEIN S5





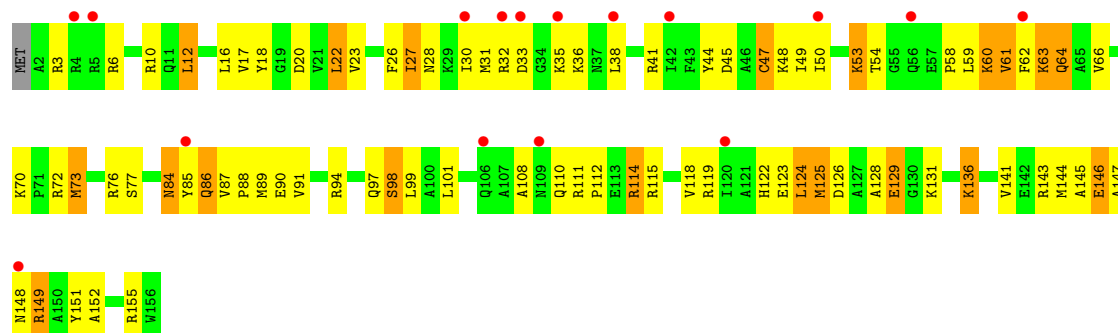
• Molecule 6: RIBOSOMAL PROTEIN S6

Chain F: 44% 43% 14%



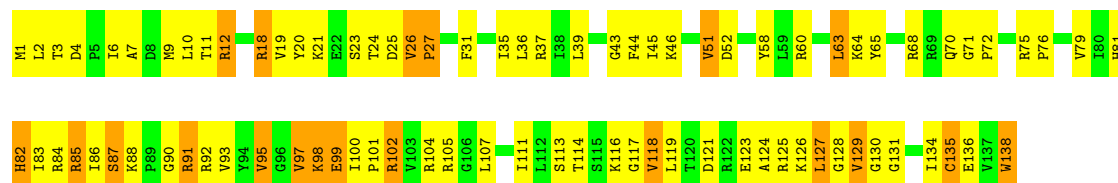
• Molecule 7: RIBOSOMAL PROTEIN S7

Chain G: 10% 46% 40% 13%



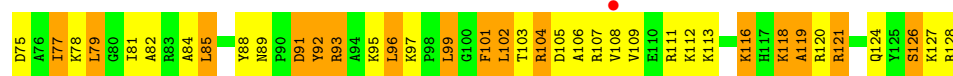
• Molecule 8: RIBOSOMAL PROTEIN S8

Chain H: 38% 47% 14%

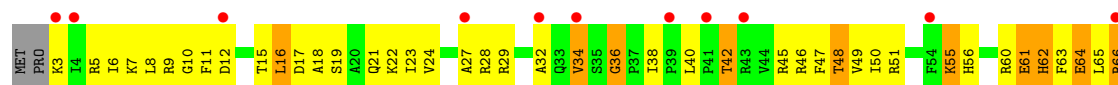


• Molecule 9: RIBOSOMAL PROTEIN S9

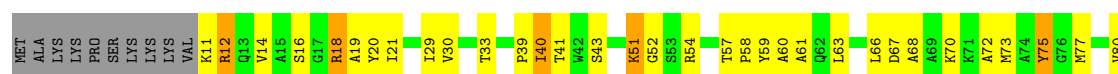
Chain I: 5% 37% 42% 20%



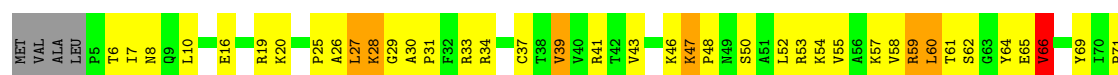
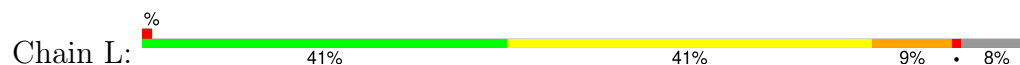
• Molecule 10: RIBOSOMAL PROTEIN S10



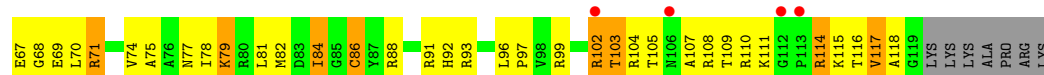
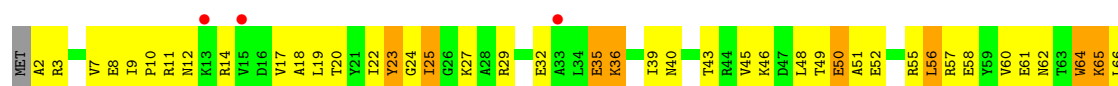
• Molecule 11: RIBOSOMAL PROTEIN S11



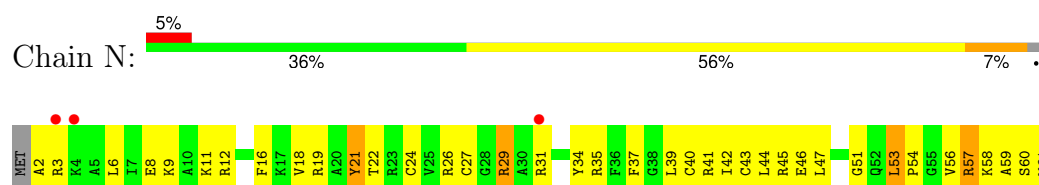
• Molecule 12: RIBOSOMAL PROTEIN S12



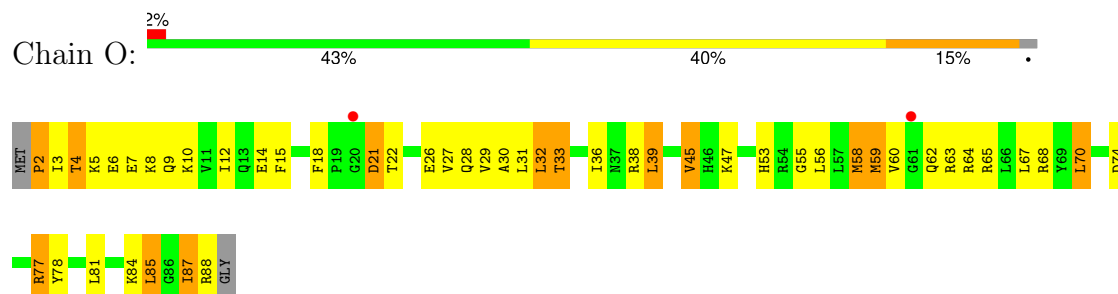
• Molecule 13: RIBOSOMAL PROTEIN S13



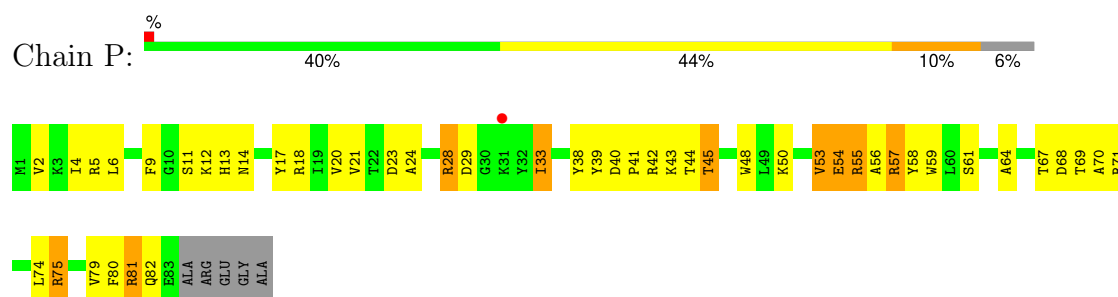
• Molecule 14: RIBOSOMAL PROTEIN S14



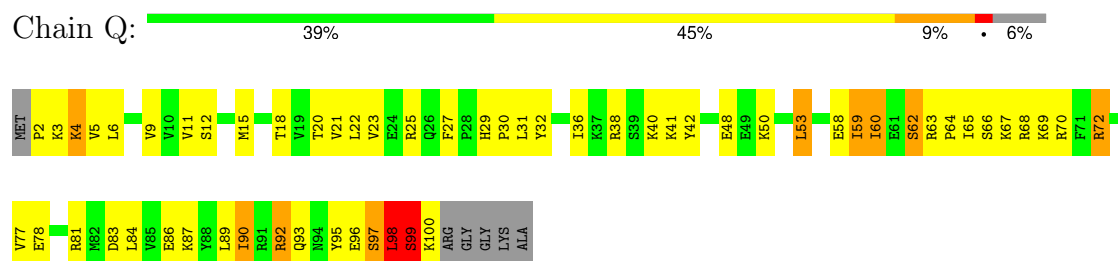
• Molecule 15: RIBOSOMAL PROTEIN S15



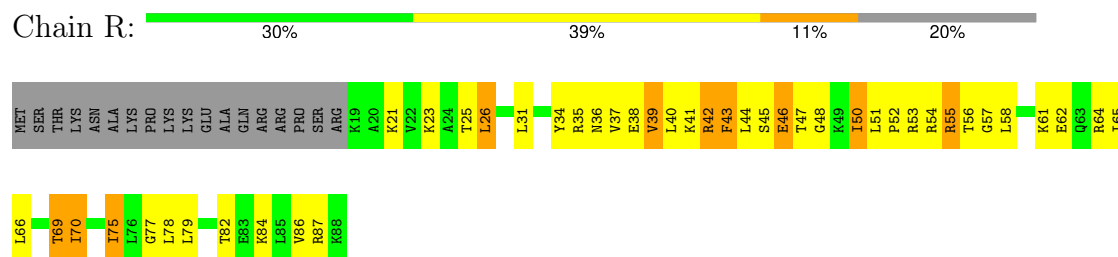
• Molecule 16: RIBOSOMAL PROTEIN S16



• Molecule 17: RIBOSOMAL PROTEIN S17

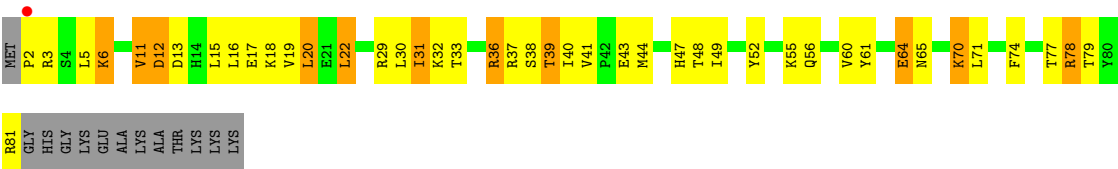


• Molecule 18: RIBOSOMAL PROTEIN S18

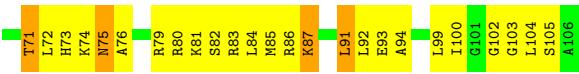


• Molecule 19: RIBOSOMAL PROTEIN S19





• 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 48.30 – 3.69	Depositor EDS
% Data completeness (in resolution range)	98.5 (48.30-3.69) 98.4 (48.30-3.69)	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	7540 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)	0.29 , 189.1	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	0.95	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: ZN, 7MG, 2MG, MA6, 5MC, 0TD, UR3, M2G, PSU, 4OC, MG

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%)	10	40
3	C	204/239 (85%)	179 (88%)	24 (12%)	1 (0%)	25	57
4	D	206/209 (99%)	190 (92%)	16 (8%)	0	100	100
5	E	148/162 (91%)	139 (94%)	8 (5%)	1 (1%)	19	51
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%)	16	49
10	J	96/105 (91%)	78 (81%)	17 (18%)	1 (1%)	13	44
11	K	114/129 (88%)	101 (89%)	13 (11%)	0	100	100
12	L	121/135 (90%)	109 (90%)	11 (9%)	1 (1%)	16	49
13	M	116/126 (92%)	102 (88%)	12 (10%)	2 (2%)	7	36

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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%)	11	41
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%)	10	40
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%)	25	57

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	5
3	C	160/188 (85%)	121 (76%)	39 (24%)	0	4
4	D	180/181 (99%)	146 (81%)	34 (19%)	1	8
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	6
8	H	119/119 (100%)	90 (76%)	29 (24%)	0	4
9	I	98/99 (99%)	68 (69%)	30 (31%)	0	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	J	87/92 (95%)	67 (77%)	20 (23%)	0	5
11	K	88/99 (89%)	67 (76%)	21 (24%)	0	4
12	L	103/110 (94%)	84 (82%)	19 (18%)	1	8
13	M	94/101 (93%)	73 (78%)	21 (22%)	1	5
14	N	49/50 (98%)	42 (86%)	7 (14%)	2	16
15	O	79/80 (99%)	62 (78%)	17 (22%)	1	6
16	P	72/74 (97%)	59 (82%)	13 (18%)	1	9
17	Q	94/97 (97%)	74 (79%)	20 (21%)	1	6
18	R	61/77 (79%)	48 (79%)	13 (21%)	1	6
19	S	71/80 (89%)	56 (79%)	15 (21%)	1	6
20	T	76/82 (93%)	55 (72%)	21 (28%)	0	2
21	U	19/22 (86%)	13 (68%)	6 (32%)	0	1
All	All	1983/2111 (94%)	1522 (77%)	461 (23%)	0	5

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	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
1	PSU	A	516	1	18,21,22	1.19	1 (5%)	21,30,33	1.79	4 (19%)
1	7MG	A	527	22,1	23,26,27	3.75	7 (30%)	27,39,42	2.28	10 (37%)
1	M2G	A	966	1	20,27,28	1.33	2 (10%)	19,40,43	1.47	2 (10%)
1	MA6	A	1518[B]	1	19,26,27	1.31	3 (15%)	18,38,41	0.74	0
1	MA6	A	1519[A]	1	19,26,27	1.22	2 (10%)	18,38,41	0.67	0
1	PSU	A	1540	1	18,21,22	1.16	1 (5%)	21,30,33	1.86	5 (23%)
1	MA6	A	1518[A]	1	19,26,27	1.12	2 (10%)	18,38,41	0.68	0
1	PSU	A	1541	1	18,21,22	1.11	1 (5%)	21,30,33	1.89	4 (19%)
1	4OC	A	1402	1	20,23,24	1.78	5 (25%)	25,32,35	0.76	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	2MG	A	1207	1	18,26,27	1.72	4 (22%)	16,38,41	1.45	3 (18%)
1	5MC	A	1404	1	19,22,23	1.54	3 (15%)	26,32,35	1.52	4 (15%)
1	5MC	A	1407	1	19,22,23	1.64	4 (21%)	26,32,35	1.24	2 (7%)
1	UR3	A	1498	1	19,22,23	1.05	2 (10%)	26,32,35	1.40	4 (15%)
1	5MC	A	967	1	19,22,23	1.33	2 (10%)	26,32,35	1.02	2 (7%)
12	0TD	L	92	12	8,9,10	1.16	0	6,11,13	3.02	4 (66%)

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

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

5.5 Carbohydrates

There are no oligosaccharides 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%)	-0.48	29 (1%) 66 47	62, 162, 316, 389	4 (0%)
2	B	234/256 (91%)	-0.52	2 (0%) 81 64	133, 184, 270, 282	0
3	C	206/239 (86%)	-0.01	12 (5%) 30 23	206, 252, 287, 299	0
4	D	208/209 (99%)	-0.19	9 (4%) 40 30	111, 168, 217, 268	0
5	E	150/162 (92%)	-0.50	1 (0%) 84 68	94, 134, 188, 231	0
6	F	101/101 (100%)	-0.80	0 100 100	133, 181, 218, 291	0
7	G	155/156 (99%)	0.12	16 (10%) 13 13	158, 220, 277, 309	0
8	H	138/138 (100%)	-0.66	0 100 100	95, 124, 178, 206	0
9	I	127/128 (99%)	-0.16	6 (4%) 37 28	171, 232, 283, 313	0
10	J	98/105 (93%)	0.56	15 (15%) 6 9	209, 279, 336, 389	0
11	K	116/129 (89%)	-0.50	2 (1%) 69 50	115, 162, 201, 226	0
12	L	123/135 (91%)	-0.45	1 (0%) 82 66	107, 168, 206, 263	0
13	M	118/126 (93%)	0.02	7 (5%) 29 23	154, 195, 252, 307	0
14	N	60/61 (98%)	0.22	3 (5%) 35 26	202, 244, 301, 320	0
15	O	87/89 (97%)	-0.11	2 (2%) 61 43	118, 158, 219, 250	0
16	P	83/88 (94%)	-0.26	1 (1%) 76 57	111, 173, 212, 270	0
17	Q	99/105 (94%)	-0.54	0 100 100	103, 137, 184, 194	0
18	R	70/88 (79%)	-0.71	0 100 100	118, 173, 224, 263	0
19	S	80/93 (86%)	-0.35	1 (1%) 74 55	207, 262, 310, 335	0
20	T	99/106 (93%)	-0.20	3 (3%) 52 37	127, 166, 233, 261	0
21	U	24/27 (88%)	0.77	4 (16%) 5 7	150, 219, 232, 233	0
All	All	3874/4063 (95%)	-0.35	114 (2%) 54 38	62, 177, 288, 389	4 (0%)

The worst 5 of 114 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1516[A]	G	6.2
7	G	32	ARG	6.1
14	N	31	ARG	5.4
10	J	74	ILE	5.3
21	U	25	LYS	5.1

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. 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	0.83	0.23	318,324,373,375	0
1	PSU	A	516	20/21	0.87	0.11	169,189,225,229	0
1	PSU	A	1541	20/21	0.91	0.18	303,317,323,326	0
1	2MG	A	1207	24/25	0.94	0.10	239,249,316,321	0
1	7MG	A	527	24/25	0.95	0.12	142,153,170,174	0
1	5MC	A	1407	21/22	0.96	0.07	180,203,212,220	0
1	UR3	A	1498	21/22	0.96	0.12	131,139,164,169	0
1	5MC	A	1400	21/22	0.97	0.08	125,139,150,167	0
1	MA6	A	1518[A]	24/25	0.97	0.15	133,147,161,163	24
1	MA6	A	1518[B]	24/25	0.97	0.15	132,148,153,153	24
1	4OC	A	1402	22/23	0.97	0.07	130,142,160,168	0
1	M2G	A	966	25/26	0.97	0.09	168,177,186,189	0
1	5MC	A	967	21/22	0.98	0.07	154,169,181,182	0
1	5MC	A	1404	21/22	0.98	0.07	132,144,188,193	0
1	MA6	A	1519[A]	24/25	0.99	0.09	118,127,134,135	24
1	MA6	A	1519[B]	24/25	0.99	0.09	123,131,165,167	24
12	0TD	L	92	10/11	0.99	0.10	161,185,287,345	0

6.3 Carbohydrates [i](#)

There are no monosaccharides 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. 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	1802	1/1	0.41	0.35	180,180,180,180	0
22	MG	A	1747	1/1	0.47	0.37	132,132,132,132	0
22	MG	A	1742	1/1	0.51	0.35	152,152,152,152	0
22	MG	A	1789	1/1	0.57	0.33	157,157,157,157	0
22	MG	A	1843	1/1	0.57	0.39	132,132,132,132	0
22	MG	B	301	1/1	0.58	0.19	132,132,132,132	0
22	MG	A	1702	1/1	0.64	0.34	166,166,166,166	0
22	MG	A	1838	1/1	0.67	0.26	150,150,150,150	0
22	MG	A	1827	1/1	0.68	0.27	151,151,151,151	0
22	MG	A	1857	1/1	0.68	0.29	128,128,128,128	0
22	MG	A	1808	1/1	0.68	0.23	164,164,164,164	0
22	MG	A	1850	1/1	0.69	0.08	450,450,450,450	0
22	MG	A	1667	1/1	0.70	0.23	157,157,157,157	0
22	MG	Q	201	1/1	0.70	0.20	142,142,142,142	0
22	MG	A	1683	1/1	0.71	0.36	118,118,118,118	0
22	MG	A	1807	1/1	0.71	0.21	141,141,141,141	0
22	MG	A	1795	1/1	0.72	0.21	182,182,182,182	0
22	MG	A	1855	1/1	0.74	0.42	143,143,143,143	0
22	MG	A	1731	1/1	0.74	0.28	145,145,145,145	0
22	MG	A	1797	1/1	0.75	0.18	146,146,146,146	0
22	MG	A	1815	1/1	0.75	0.24	124,124,124,124	0
22	MG	A	1816	1/1	0.75	0.21	181,181,181,181	0
22	MG	A	1822	1/1	0.75	0.42	148,148,148,148	0
22	MG	A	1675	1/1	0.75	0.28	143,143,143,143	0
22	MG	A	1624	1/1	0.75	0.26	134,134,134,134	0
22	MG	A	1847	1/1	0.76	0.14	145,145,145,145	0
22	MG	A	1861	1/1	0.76	0.61	178,178,178,178	0
22	MG	A	1641	1/1	0.76	0.20	130,130,130,130	0
22	MG	A	1829	1/1	0.76	0.36	156,156,156,156	0
22	MG	A	1673	1/1	0.77	0.16	211,211,211,211	0
22	MG	A	1831	1/1	0.78	0.29	160,160,160,160	0
22	MG	A	1632	1/1	0.78	0.46	131,131,131,131	0
22	MG	A	1678	1/1	0.78	0.16	350,350,350,350	0
22	MG	D	304	1/1	0.78	0.35	147,147,147,147	0
22	MG	A	1856	1/1	0.78	0.25	143,143,143,143	0
22	MG	A	1796	1/1	0.79	0.24	121,121,121,121	0
22	MG	A	1704	1/1	0.79	0.13	211,211,211,211	0
22	MG	A	1849	1/1	0.80	0.15	550,550,550,550	0
22	MG	A	1746	1/1	0.80	0.34	111,111,111,111	0
22	MG	A	1605	1/1	0.80	0.36	103,103,103,103	0
22	MG	A	1743	1/1	0.81	0.21	147,147,147,147	0
22	MG	A	1791	1/1	0.81	0.05	294,294,294,294	0
22	MG	A	1834	1/1	0.81	0.15	138,138,138,138	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
22	MG	A	1771	1/1	0.82	0.15	127,127,127,127	0
22	MG	A	1689	1/1	0.82	0.78	214,214,214,214	0
22	MG	A	1739	1/1	0.82	0.15	139,139,139,139	0
22	MG	A	1729	1/1	0.82	0.15	119,119,119,119	0
22	MG	A	1785	1/1	0.83	0.10	184,184,184,184	0
22	MG	A	1759	1/1	0.83	0.11	126,126,126,126	0
22	MG	A	1769	1/1	0.83	0.23	151,151,151,151	0
22	MG	A	1662	1/1	0.83	0.32	108,108,108,108	0
22	MG	A	1811	1/1	0.83	0.34	156,156,156,156	0
22	MG	A	1781	1/1	0.83	0.23	158,158,158,158	0
22	MG	A	1854	1/1	0.84	0.37	149,149,149,149	0
22	MG	A	1833	1/1	0.84	0.15	182,182,182,182	0
22	MG	A	1688	1/1	0.84	0.12	164,164,164,164	0
22	MG	A	1826	1/1	0.84	0.19	121,121,121,121	0
22	MG	A	1770	1/1	0.84	0.24	103,103,103,103	0
22	MG	A	1682	1/1	0.84	0.12	180,180,180,180	0
22	MG	A	1734	1/1	0.84	0.23	139,139,139,139	0
22	MG	A	1832	1/1	0.84	0.33	149,149,149,149	0
22	MG	A	1858	1/1	0.85	0.32	147,147,147,147	0
22	MG	A	1859	1/1	0.85	0.11	147,147,147,147	0
22	MG	A	1844	1/1	0.85	0.19	132,132,132,132	0
22	MG	A	1862	1/1	0.85	0.23	161,161,161,161	0
22	MG	A	1836	1/1	0.85	0.58	143,143,143,143	0
22	MG	A	1776	1/1	0.85	0.21	139,139,139,139	0
22	MG	A	1735	1/1	0.85	0.23	93,93,93,93	0
22	MG	A	1800	1/1	0.86	0.19	158,158,158,158	0
22	MG	A	1818	1/1	0.86	0.33	109,109,109,109	0
22	MG	A	1812	1/1	0.86	0.08	417,417,417,417	0
22	MG	A	1798	1/1	0.86	0.08	163,163,163,163	0
22	MG	A	1813	1/1	0.87	0.18	520,520,520,520	0
22	MG	A	1686	1/1	0.87	0.08	241,241,241,241	0
22	MG	J	201	1/1	0.87	0.18	128,128,128,128	0
22	MG	A	1810	1/1	0.87	0.29	143,143,143,143	0
22	MG	A	1835	1/1	0.88	0.29	139,139,139,139	0
22	MG	A	1730	1/1	0.88	0.29	138,138,138,138	0
22	MG	A	1792	1/1	0.88	0.12	313,313,313,313	0
22	MG	A	1841	1/1	0.88	0.19	147,147,147,147	0
22	MG	A	1752	1/1	0.88	0.23	142,142,142,142	0
22	MG	A	1727	1/1	0.88	0.19	106,106,106,106	0
22	MG	A	1774	1/1	0.88	0.25	157,157,157,157	0
22	MG	A	1732	1/1	0.89	0.18	94,94,94,94	0
22	MG	A	1690	1/1	0.89	0.08	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	1764	1/1	0.89	0.16	137,137,137,137	0
22	MG	A	1661	1/1	0.89	0.40	120,120,120,120	0
22	MG	A	1630	1/1	0.89	0.39	124,124,124,124	0
22	MG	A	1665	1/1	0.89	0.26	111,111,111,111	0
22	MG	A	1618	1/1	0.89	0.44	141,141,141,141	0
22	MG	A	1612	1/1	0.89	0.09	178,178,178,178	0
22	MG	A	1643	1/1	0.89	0.15	102,102,102,102	0
22	MG	A	1782	1/1	0.89	0.17	159,159,159,159	0
22	MG	A	1824	1/1	0.89	0.26	139,139,139,139	0
22	MG	A	1803	1/1	0.89	0.39	115,115,115,115	0
22	MG	A	1806	1/1	0.89	0.13	127,127,127,127	0
22	MG	A	1809	1/1	0.90	0.17	114,114,114,114	0
22	MG	A	1820	1/1	0.90	0.36	144,144,144,144	0
22	MG	A	1860	1/1	0.90	0.38	133,133,133,133	0
22	MG	A	1711	1/1	0.90	0.10	185,185,185,185	0
22	MG	A	1778	1/1	0.90	0.15	127,127,127,127	0
22	MG	A	1715	1/1	0.90	0.07	112,112,112,112	0
22	MG	A	1677	1/1	0.90	0.18	128,128,128,128	0
22	MG	H	201	1/1	0.90	0.20	167,167,167,167	0
22	MG	A	1694	1/1	0.90	0.27	105,105,105,105	0
22	MG	A	1762	1/1	0.90	0.40	124,124,124,124	0
22	MG	A	1723	1/1	0.91	0.16	120,120,120,120	0
22	MG	A	1685	1/1	0.91	0.17	159,159,159,159	0
22	MG	A	1714	1/1	0.91	0.29	162,162,162,162	0
22	MG	A	1853	1/1	0.91	0.33	150,150,150,150	0
22	MG	A	1783	1/1	0.91	0.15	119,119,119,119	0
22	MG	A	1828	1/1	0.91	0.21	114,114,114,114	0
22	MG	A	1784	1/1	0.91	0.08	175,175,175,175	0
22	MG	A	1745	1/1	0.91	0.12	169,169,169,169	0
22	MG	A	1625	1/1	0.91	0.41	101,101,101,101	0
22	MG	A	1687	1/1	0.92	0.10	234,234,234,234	0
22	MG	A	1666	1/1	0.92	0.17	141,141,141,141	0
22	MG	A	1719	1/1	0.92	0.22	514,514,514,514	0
22	MG	A	1721	1/1	0.92	0.27	149,149,149,149	0
22	MG	A	1772	1/1	0.92	0.22	120,120,120,120	0
22	MG	A	1679	1/1	0.92	0.14	124,124,124,124	0
22	MG	A	1775	1/1	0.92	0.16	146,146,146,146	0
22	MG	A	1725	1/1	0.92	0.10	156,156,156,156	0
22	MG	A	1680	1/1	0.92	0.23	175,175,175,175	0
22	MG	A	1657	1/1	0.92	0.11	146,146,146,146	0
22	MG	A	1821	1/1	0.92	0.38	138,138,138,138	0
22	MG	A	1842	1/1	0.92	0.64	152,152,152,152	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
22	MG	D	303	1/1	0.92	0.17	137,137,137,137	0
22	MG	A	1634	1/1	0.92	0.07	161,161,161,161	0
22	MG	A	1601	1/1	0.92	0.25	152,152,152,152	0
22	MG	A	1825	1/1	0.92	0.17	139,139,139,139	0
22	MG	A	1627	1/1	0.92	0.28	101,101,101,101	0
22	MG	A	1604	1/1	0.93	0.06	123,123,123,123	0
22	MG	A	1740	1/1	0.93	0.21	119,119,119,119	0
22	MG	A	1636	1/1	0.93	0.24	90,90,90,90	0
22	MG	A	1848	1/1	0.93	0.27	527,527,527,527	0
22	MG	A	1696	1/1	0.93	0.18	160,160,160,160	0
22	MG	A	1823	1/1	0.93	0.19	128,128,128,128	0
22	MG	C	301	1/1	0.93	0.06	143,143,143,143	0
22	MG	A	1660	1/1	0.93	0.11	155,155,155,155	0
22	MG	A	1613	1/1	0.93	0.20	153,153,153,153	0
22	MG	A	1684	1/1	0.93	0.13	135,135,135,135	0
22	MG	A	1726	1/1	0.93	0.10	349,349,349,349	0
22	MG	A	1753	1/1	0.93	0.17	136,136,136,136	0
22	MG	A	1851	1/1	0.94	0.10	366,366,366,366	0
22	MG	A	1852	1/1	0.94	0.26	530,530,530,530	0
22	MG	A	1830	1/1	0.94	0.08	130,130,130,130	0
22	MG	A	1637	1/1	0.94	0.31	116,116,116,116	0
22	MG	A	1755	1/1	0.94	0.07	150,150,150,150	0
22	MG	A	1756	1/1	0.94	0.12	112,112,112,112	0
22	MG	A	1817	1/1	0.94	0.16	148,148,148,148	0
22	MG	A	1758	1/1	0.94	0.26	103,103,103,103	0
22	MG	A	1638	1/1	0.94	0.16	189,189,189,189	0
22	MG	A	1761	1/1	0.94	0.13	147,147,147,147	0
22	MG	A	1804	1/1	0.94	0.06	120,120,120,120	0
22	MG	A	1610	1/1	0.94	0.12	112,112,112,112	0
22	MG	A	1611	1/1	0.94	0.09	184,184,184,184	0
22	MG	A	1765	1/1	0.94	0.07	126,126,126,126	0
22	MG	A	1846	1/1	0.94	0.22	126,126,126,126	0
22	MG	A	1645	1/1	0.94	0.29	141,141,141,141	0
22	MG	A	1748	1/1	0.94	0.06	177,177,177,177	0
22	MG	I	201	1/1	0.94	0.20	138,138,138,138	0
22	MG	A	1749	1/1	0.94	0.19	157,157,157,157	0
22	MG	P	101	1/1	0.94	0.42	106,106,106,106	0
22	MG	A	1703	1/1	0.94	0.14	291,291,291,291	0
22	MG	A	1733	1/1	0.95	0.14	147,147,147,147	0
22	MG	A	1790	1/1	0.95	0.07	217,217,217,217	0
22	MG	A	1664	1/1	0.95	0.17	121,121,121,121	0
22	MG	A	1623	1/1	0.95	0.05	129,129,129,129	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
22	MG	A	1724	1/1	0.95	0.09	169,169,169,169	0
22	MG	A	1646	1/1	0.95	0.11	236,236,236,236	0
22	MG	A	1741	1/1	0.95	0.11	128,128,128,128	0
22	MG	A	1705	1/1	0.95	0.12	319,319,319,319	0
22	MG	A	1780	1/1	0.95	0.12	143,143,143,143	0
22	MG	A	1628	1/1	0.95	0.14	141,141,141,141	0
22	MG	A	1617	1/1	0.95	0.20	175,175,175,175	0
22	MG	A	1608	1/1	0.95	0.05	169,169,169,169	0
22	MG	A	1718	1/1	0.95	0.20	134,134,134,134	0
22	MG	A	1626	1/1	0.95	0.58	105,105,105,105	0
22	MG	A	1840	1/1	0.95	0.19	143,143,143,143	0
22	MG	A	1668	1/1	0.96	0.20	134,134,134,134	0
22	MG	A	1754	1/1	0.96	0.09	137,137,137,137	0
22	MG	A	1793	1/1	0.96	0.22	444,444,444,444	0
22	MG	A	1814	1/1	0.96	0.13	70,70,70,70	0
22	MG	A	1773	1/1	0.96	0.13	156,156,156,156	0
22	MG	A	1670	1/1	0.96	0.09	199,199,199,199	0
22	MG	A	1744	1/1	0.96	0.04	127,127,127,127	0
22	MG	A	1672	1/1	0.96	0.23	146,146,146,146	0
22	MG	A	1819	1/1	0.96	0.09	137,137,137,137	0
22	MG	A	1654	1/1	0.96	0.17	156,156,156,156	0
22	MG	A	1760	1/1	0.96	0.15	140,140,140,140	0
22	MG	A	1738	1/1	0.96	0.12	113,113,113,113	0
22	MG	A	1710	1/1	0.96	0.16	94,94,94,94	0
22	MG	D	302	1/1	0.96	0.08	137,137,137,137	0
22	MG	A	1845	1/1	0.96	0.13	113,113,113,113	0
22	MG	A	1805	1/1	0.96	0.05	119,119,119,119	0
22	MG	A	1763	1/1	0.96	0.19	111,111,111,111	0
22	MG	A	1722	1/1	0.96	0.06	122,122,122,122	0
22	MG	A	1750	1/1	0.96	0.10	157,157,157,157	0
22	MG	A	1751	1/1	0.96	0.17	104,104,104,104	0
22	MG	A	1656	1/1	0.96	0.21	106,106,106,106	0
22	MG	A	1619	1/1	0.97	0.10	106,106,106,106	0
22	MG	A	1799	1/1	0.97	0.23	125,125,125,125	0
22	MG	A	1659	1/1	0.97	0.09	128,128,128,128	0
22	MG	A	1699	1/1	0.97	0.12	124,124,124,124	0
22	MG	A	1777	1/1	0.97	0.15	111,111,111,111	0
22	MG	A	1757	1/1	0.97	0.13	103,103,103,103	0
22	MG	A	1779	1/1	0.97	0.11	112,112,112,112	0
22	MG	A	1669	1/1	0.97	0.04	149,149,149,149	0
22	MG	A	1620	1/1	0.97	0.13	162,162,162,162	0
22	MG	A	1671	1/1	0.97	0.11	170,170,170,170	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
22	MG	A	1635	1/1	0.97	0.06	99,99,99,99	0
22	MG	A	1728	1/1	0.97	0.43	138,138,138,138	0
22	MG	A	1629	1/1	0.97	0.34	131,131,131,131	0
22	MG	A	1786	1/1	0.97	0.16	131,131,131,131	0
22	MG	A	1787	1/1	0.97	0.04	147,147,147,147	0
22	MG	A	1788	1/1	0.97	0.07	151,151,151,151	0
22	MG	A	1651	1/1	0.97	0.09	113,113,113,113	0
22	MG	A	1676	1/1	0.97	0.04	136,136,136,136	0
22	MG	A	1767	1/1	0.97	0.14	130,130,130,130	0
22	MG	E	201	1/1	0.97	0.07	177,177,177,177	0
22	MG	A	1602	1/1	0.97	0.11	168,168,168,168	0
22	MG	A	1631	1/1	0.97	0.09	154,154,154,154	0
22	MG	A	1691	1/1	0.97	0.06	155,155,155,155	0
22	MG	A	1720	1/1	0.97	0.27	196,196,196,196	0
22	MG	A	1737	1/1	0.97	0.12	119,119,119,119	0
23	ZN	D	301	1/1	0.97	0.19	154,154,154,154	0
22	MG	A	1701	1/1	0.98	0.06	161,161,161,161	0
22	MG	A	1606	1/1	0.98	0.05	107,107,107,107	0
22	MG	A	1609	1/1	0.98	0.05	120,120,120,120	0
22	MG	A	1607	1/1	0.98	0.08	105,105,105,105	0
22	MG	A	1647	1/1	0.98	0.07	175,175,175,175	0
22	MG	A	1801	1/1	0.98	0.12	129,129,129,129	0
22	MG	A	1706	1/1	0.98	0.09	105,105,105,105	0
22	MG	A	1707	1/1	0.98	0.07	208,208,208,208	0
22	MG	A	1709	1/1	0.98	0.18	169,169,169,169	0
22	MG	A	1649	1/1	0.98	0.05	150,150,150,150	0
22	MG	A	1650	1/1	0.98	0.07	104,104,104,104	0
22	MG	A	1736	1/1	0.98	0.07	99,99,99,99	0
22	MG	A	1713	1/1	0.98	0.05	229,229,229,229	0
22	MG	A	1616	1/1	0.98	0.11	85,85,85,85	0
22	MG	A	1621	1/1	0.98	0.05	149,149,149,149	0
22	MG	A	1692	1/1	0.98	0.05	165,165,165,165	0
22	MG	A	1837	1/1	0.98	0.08	87,87,87,87	0
22	MG	A	1633	1/1	0.98	0.06	198,198,198,198	0
22	MG	A	1839	1/1	0.98	0.24	144,144,144,144	0
22	MG	A	1695	1/1	0.98	0.06	113,113,113,113	0
22	MG	A	1642	1/1	0.98	0.13	98,98,98,98	0
22	MG	A	1697	1/1	0.98	0.05	133,133,133,133	0
22	MG	A	1768	1/1	0.98	0.05	166,166,166,166	0
22	MG	A	1698	1/1	0.98	0.04	186,186,186,186	0
22	MG	A	1658	1/1	0.98	0.05	156,156,156,156	0
22	MG	A	1794	1/1	0.98	0.13	278,278,278,278	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
22	MG	A	1700	1/1	0.98	0.03	204,204,204,204	0
23	ZN	N	101	1/1	0.98	0.07	223,223,223,223	0
22	MG	A	1716	1/1	0.99	0.06	118,118,118,118	0
22	MG	A	1717	1/1	0.99	0.08	157,157,157,157	0
22	MG	A	1652	1/1	0.99	0.03	132,132,132,132	0
22	MG	A	1674	1/1	0.99	0.05	136,136,136,136	0
22	MG	A	1663	1/1	0.99	0.04	162,162,162,162	0
22	MG	A	1653	1/1	0.99	0.07	76,76,76,76	0
22	MG	A	1639	1/1	0.99	0.05	82,82,82,82	0
22	MG	A	1655	1/1	0.99	0.14	156,156,156,156	0
22	MG	A	1640	1/1	0.99	0.13	186,186,186,186	0
22	MG	A	1693	1/1	0.99	0.05	160,160,160,160	0
22	MG	A	1614	1/1	0.99	0.04	141,141,141,141	0
22	MG	F	201	1/1	0.99	0.03	127,127,127,127	0
22	MG	A	1681	1/1	0.99	0.10	167,167,167,167	0
22	MG	A	1648	1/1	0.99	0.15	149,149,149,149	0
22	MG	A	1712	1/1	0.99	0.18	324,324,324,324	0
22	MG	A	1622	1/1	0.99	0.04	106,106,106,106	0
22	MG	A	1603	1/1	0.99	0.02	137,137,137,137	0
22	MG	A	1766	1/1	0.99	0.05	126,126,126,126	0
22	MG	A	1644	1/1	0.99	0.03	111,111,111,111	0
22	MG	A	1615	1/1	1.00	0.06	81,81,81,81	0
22	MG	A	1708	1/1	1.00	0.04	155,155,155,155	0

6.5 Other polymers [i](#)

There are no such residues in this entry.