



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 11:35 PM GMT

PDB ID : 1XMO
Title : Crystal Structure of mnm5U34t6A37-tRNA^{Lys}UUU Complexed with AAG-mRNA in the Decoding Center
Authors : Murphy, F.V.; Ramakrishnan, V.; Malkiewicz, A.; Agris, P.F.
Deposited on : 2004-10-04
Resolution : 3.25 Å(reported)

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

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

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

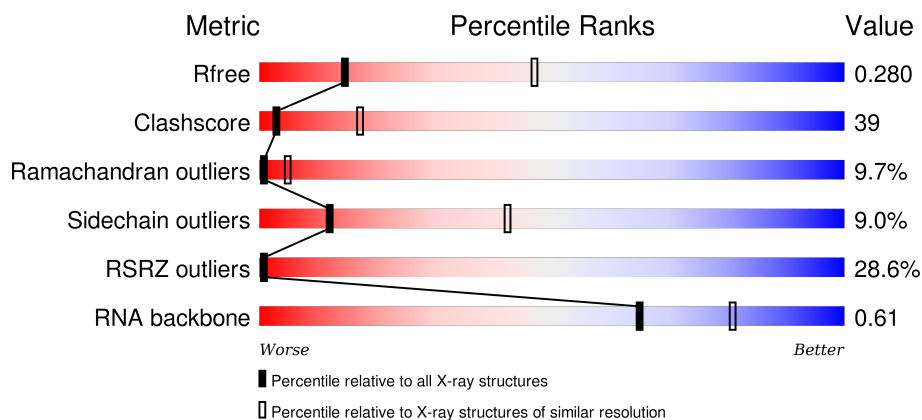
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.25 Å.

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



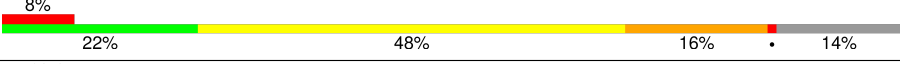
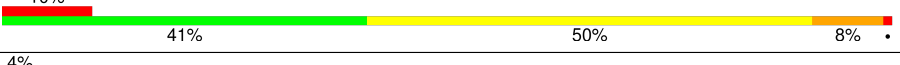
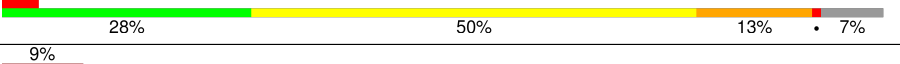
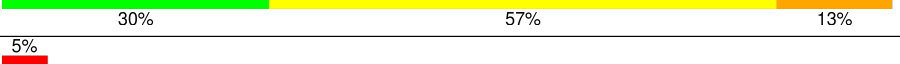
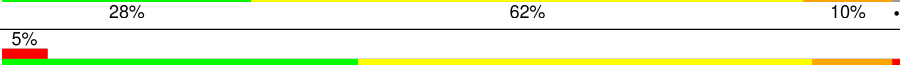
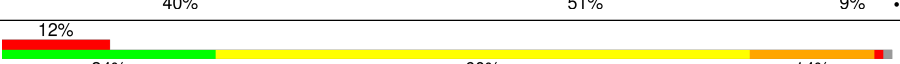
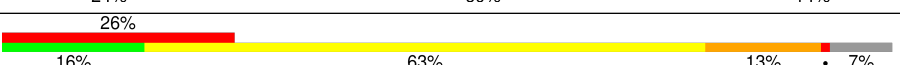
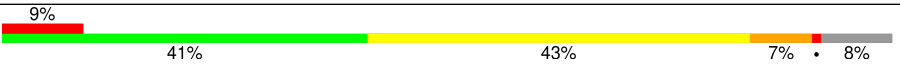
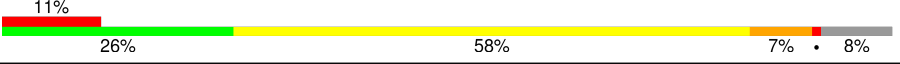
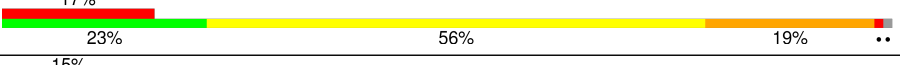
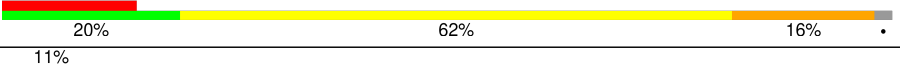
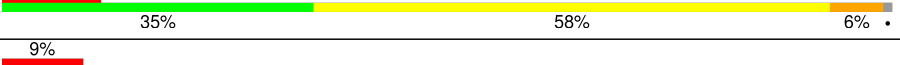

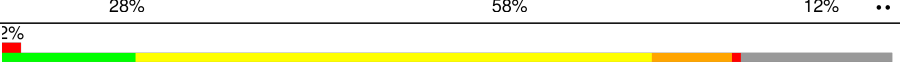
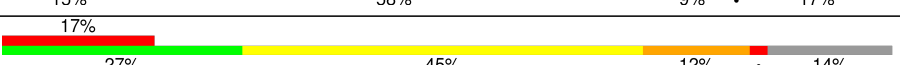
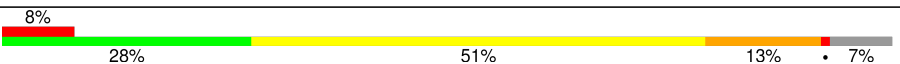
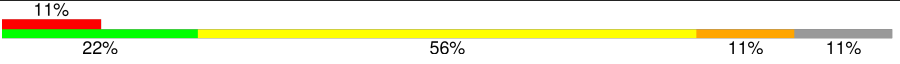
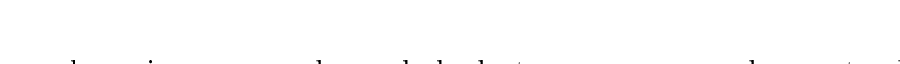
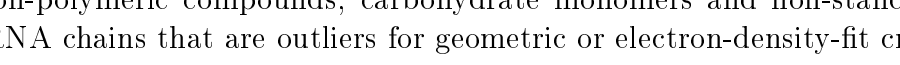
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1624 (3.32-3.20)
Clashscore	102246	1806 (3.32-3.20)
Ramachandran outliers	100387	1773 (3.32-3.20)
Sidechain outliers	100360	1771 (3.32-3.20)
RSRZ outliers	91569	1632 (3.32-3.20)
RNA backbone	2183	1001 (3.76-2.76)

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

Mol	Chain	Length	Quality of chain
1	A	1522	<div> <div>57%</div> <div>28% 55% 14% ..</div> </div>
2	W	3	<div> <div>100%</div> <div>33% 67%</div> </div>
3	X	11	<div> <div>45%</div> <div>36% 64%</div> </div>
4	B	256	<div> <div>7%</div> <div>15% 65% 9% • 9%</div> </div>

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Mol	Chain	Length	Quality of chain
5	C	239	
6	D	209	
7	E	162	
8	F	101	
9	G	156	
10	H	138	
11	I	128	
12	J	105	
13	K	129	
14	L	135	
15	M	126	
16	N	61	
17	O	89	
18	P	88	
19	Q	105	
20	R	88	
21	S	93	
22	T	106	
23	V	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
25	MG	A	1595	-	-	-	X
25	MG	A	1601	-	-	-	X
25	MG	A	1606	-	-	-	X
25	MG	A	210	-	-	-	X
3	T6A	X	37	X	-	-	-

2 Entry composition [i](#)

There are 26 unique types of molecules in this entry. The entry contains 52063 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 ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1507	Total	C	N	O	P	0	0	0
			32380	14414	5990	10470	1506			

- Molecule 2 is a RNA chain called A-Site Messenger RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	W	3	Total	C	N	O	P	0	0	0
			64	30	15	17	2			

- Molecule 3 is a RNA chain called Anticodon Transfer RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	X	11	Total	C	N	O	P	0	0	0
			239	110	38	81	10			

- Molecule 4 is a protein called 30S ribosomal protein S2.

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

- Molecule 5 is a protein called 30S ribosomal protein S3.

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

- Molecule 6 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	D	208	Total	C	N	O	S	0	0	0
			1703	1066	339	291	7			

- Molecule 7 is a protein called 30S ribosomal protein S5.

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

- Molecule 8 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	F	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			

- Molecule 9 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	G	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			

- Molecule 10 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	H	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			

- Molecule 11 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	I	127	Total	C	N	O	0	0	0
			1011	639	198	174			

- Molecule 12 is a protein called 30S ribosomal protein S10.

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

- Molecule 13 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	K	119	Total	C	N	O	S	0	0	0
			885	549	168	165	3			

- Molecule 14 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	L	124	Total	C	N	O	S	0	0	0
			970	611	195	163	1			

- Molecule 15 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	M	125	Total	C	N	O	S	0	0	0
			997	617	207	171	2			

- Molecule 16 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	N	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			

- Molecule 17 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	O	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			

- Molecule 18 is a protein called 30S ribosomal protein S16.

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

- Molecule 19 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	Q	104	Total	C	N	O	S	0	0	0
			857	547	161	147	2			

- Molecule 20 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
20	R	73	Total	C	N	O	0	0	0
			597	380	118	99			

- Molecule 21 is a protein called 30S ribosomal protein S19.

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

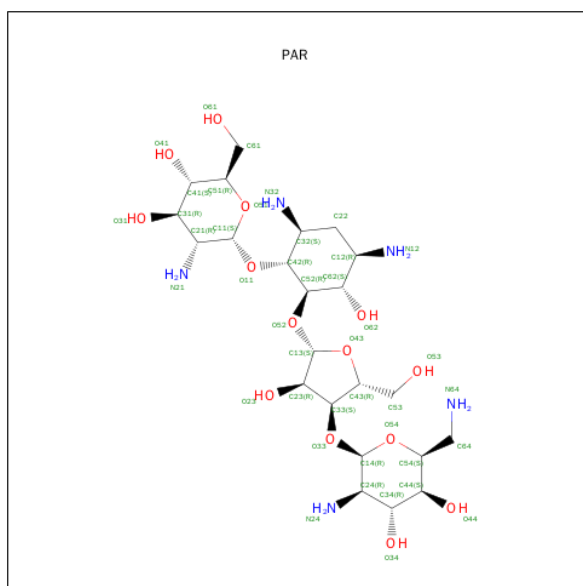
- Molecule 22 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	T	99	Total	C	N	O	S	0	0	0
			762	469	162	129	2			

- Molecule 23 is a protein called 30S ribosomal protein Thx.

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

- Molecule 24 is PAROMOMYCIN (three-letter code: PAR) (formula: $C_{23}H_{45}N_5O_{14}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
24	A	1	Total	C	N	O	0	0
			42	23	5	14		

- Molecule 25 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
25	X	2	Total	Mg	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
25	J	1	Total 1	Mg 1	0	0
25	A	104	Total 104	Mg 104	0	0

- Molecule 26 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

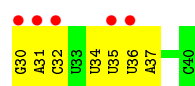
A1446	G1447	U1381	C1322	G1260	U1135	C1075	C1019	A958	G894	A828	G760	G638
G1447	U1450	C1382	G1323	A1261	U1136	C1076	U1020	A959	G895	G829	G761	G639
U1450	C1383	C1383	A1324	C1262	G1137	U1077	G1021	U960	G896	G830	U701	G640
A1451	C1384	C1263	C1325	C1263	G1138	U1078	G1022	U961	G897	U831	A702	U641
A1452	G1385	C1264	C1326	C1264	G1139	U1079	G1023	C962	G898	C932	G703	G644
G1453	G1386	C1265	G1327	C1265	C1140	A1080	G1024	G963	C899	U833	A704	C945
G1454	C1387	C1266	C1328	C1266	C1141	G1081	U1025	A964	A900	C934	U705	C946
G1455	C1388	C1267	C1329	C1267	C1142	U1082	G1026	U965	A901	U835	A706	U647
C1455	C1389	C1268	U1330	C1268	G1143	U1083	C1027	G966	G902	G836	C707	C708
C1459	U1390	A1269	G1331	A1269	G1144	U1084	C1028	C967	G903	G837	C709	G648
A1460	U1391	C1270	A1332	C1270	G1145	U1085	C1029	A968	G904	G838	G710	G650
G1461	G1392	G1271	G1333	G1271	A1146	U1086	C1030	A969	U905	U839	G711	G651
G1462	U1393	C1272	G1334	C1272	C1147	G1087	G	C970	G906	C940	G712	U652
C1463	A1394	G1273	C1335	G1273	U1148	U1088	C	G971	A907	U841	A713	U653
G1464	C1395	G1274	G1336	G1274	U1149	U1089	G	C972	A908	C948	G714	A854
C1465	G1337	A1275	U1150	U1090	U1150	U1090	A	G973	A909	U849	G715	A855
C1466	G1338	G1276	A1213	U1091	A1151	U1091	G1031	A974	C910	U850	A716	A856
G1467	A1397	C1277	G1214	A1092	A1152	A1092	G1032	A975	U911	G851	A717	C856
A1468	C1399	C1277	G1215	A1093	C1153	A1093	G1033	G976	C912	G852	C717	G657
C1400	C1400	U1278	G1216	U1094	G1154	U1094	G1034	A977	A913	G853	G718	G658
G1401	C1401	A1279	G1217	U1095	G1155	U1095	A1035	A978	A914	G854	C719	U659
G1470	G1402	A1280	C1218	U1096	G1156	C1096	G1036	A979	A915	G855	C720	G660
C1402	C1403	U1281	U1219	C1097	A1157	C1097	C1037	C980	G916	G856	G721	G661
G1471	C1343	C1282	G1220	C1098	U1158	C1098	G1038	U981	G917	G857	A722	G662
A1473	G1404	G1283	G1221	G1098	U1159	G1098	C1039	U982	A918	G858	U723	A663
G1474	C1405	C1284	G1222	C1100	G1160	C1100	U1040	A983	A919	A859	U724	G664
G1475	U1406	A1285	C1223	A1101	C1161	A1101	A1041	C984	U920	A860	A725	A665
G1476	C1407	A1286	G1224	A1102	C1162	A1102	G1042	C985	U921	G861	C726	G666
C1477	A1349	A1287	A1225	A1103	G1163	C1103	C1043	A986	G922	C862	G727	G667
A1413	C1413	A1288	C1226	G1104	C1164	G1104	A1044	G987	U923	U863	A728	G668
C1478	U1414	A1289	A1227	G1105	C1165	A1105	C1045	G988	C924	A864	A729	U669
G1480	G1415	G1290	C1228	G1106	C1166	G1106	A1046	C989	G925	A865	C730	G670
U1481	G1416	G1291	A1229	C1107	U1167	C1107	G1047	C990	G926	C866	G731	G671
G1482	G1417	U1292	C1230	G1108	A1168	G1108	G1048	U991	G927	G867	C732	U672
A1483	C1355	G1293	U1231	C1109	A1169	C1109	U1049	U992	G928	G868	G733	G673
C1484	G1356	G1294	U1232	A1110	G1171	A1110	G1050	G993	G929	G869	G734	G674
U1485	A1357	G1295	G1233	A1111	C1172	A1111	C1051	A994	C934	U870	C735	A675
G1486	U1358	C1296	C1234	C1112	G1173	C1112	U1052	C995	A935	U871	A737	A676
G1487	C1359	G1297	U1235	C1113	A1175	C1113	C1053	A996	C936	A872	C738	U677
G1488	A1360	C1298	A1236	C1114	G1176	C1114	C1054	U1000	A937	A873	C739	U678
G1489	C1423	A1299	C1237	C1115	G1177	C1115	A1055	A938	U804	C874	U740	C679
C1490	U1424	G1300	A1238	C1116	G1178	C1116	U1056	A939	C805	C875	G741	C680
G1491	C1425	U1301	A1239	C1117	A1179	G1117	G1057	G	C806	G876	G742	C681
A1492	U1426	U1302	U1240	C1118	A1180	C1118	U1058	G1002	A807	C877	U743	G682
U1493	C1427	C1303	G1241	C1119	G1181	C1119	C1059	G1003	C811	G878	C744	G683
G1494	A1428	G1304	C1242	C1120	A1182	G1120	G1060	A1004	C812	C879	C745	A684
U1495	C1429	G1305	C1243	U1121	G1183	U1121	G1061	A1005	U813	C880	A746	A685
C1496	C1367	A1306	C1254	U1122	G1184	U1122	U1062	C1006	U814	C881	C747	U686
G1497	G1368	U1307	C1244	A1123	G1185	A1123	C1063	G1007	A815	C882	G748	A687
U1498	C1432	G1369	A1248	G1124	G1186	G1124	G1064	C1008	A816	C883	C749	G688
A1499	A1433	C1370	C1249	U1125	C1188	U1125	U1065	G1009	A817	U884	G750	C689
A1500	A1434	G1371	A1250	U1126	C1189	U1126	C1066	G1010	C817	G885	U751	G690
C1501	G1435	U1372	A1251	U1127	G1190	U1127	A1067	G1011	G818	G886	G752	G691
A1503	U1436	C1373	A1252	C1128	A1191	C1128	G1068	U1012	A819	G887	A753	U692
G1504	C1437	A1374	G1253	U1129	C1192	G1129	G1069	G1013	U820	G888	C754	G693
G1505	G1438	A1375	G1316	C1130	G1193	A1130	U1070	A1014	G821	A889	G755	A694
G1506	C1439	U1376	G1255	A1131	U1194	A1131	C1071	A1015	G825	G890	G756	A695
U1507	C1440	A1377	A1256	G1132	U1195	A1256	C1072	A1016	G826	U891	U757	A696
G1508	G1441	C1378	U1257	C1133	U1196	C1132	U1073	G1017	G827	A892	G758	U697
G1509	C1443	U1380	C1259	G1134	G1197	G1134	G1074	C1018	U827	C893	U759	G698



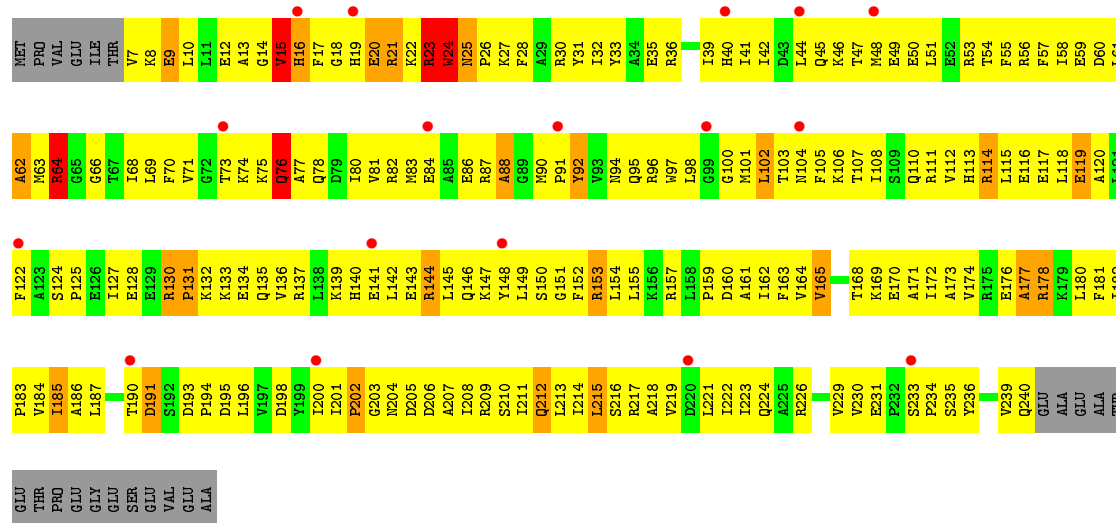
• Molecule 2: A-Site Messenger RNA



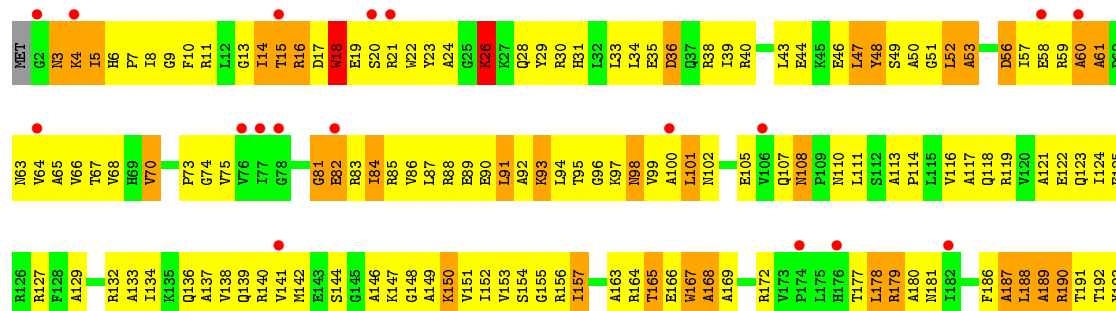
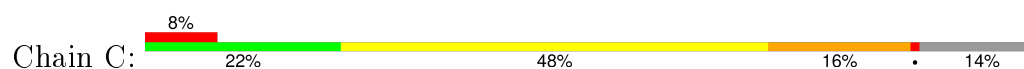
• Molecule 3: Anticodon Transfer RNA

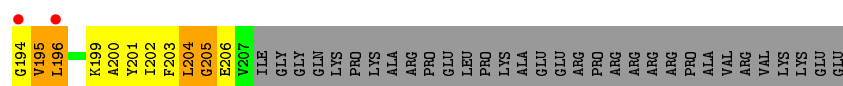


• Molecule 4: 30S ribosomal protein S2

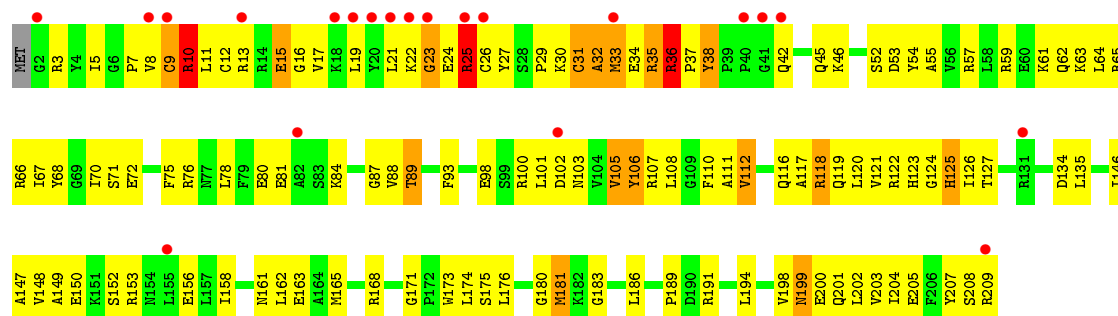
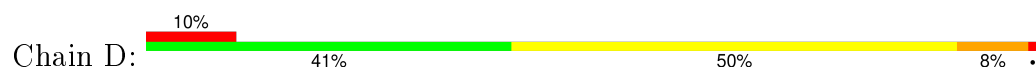


• Molecule 5: 30S ribosomal protein S3

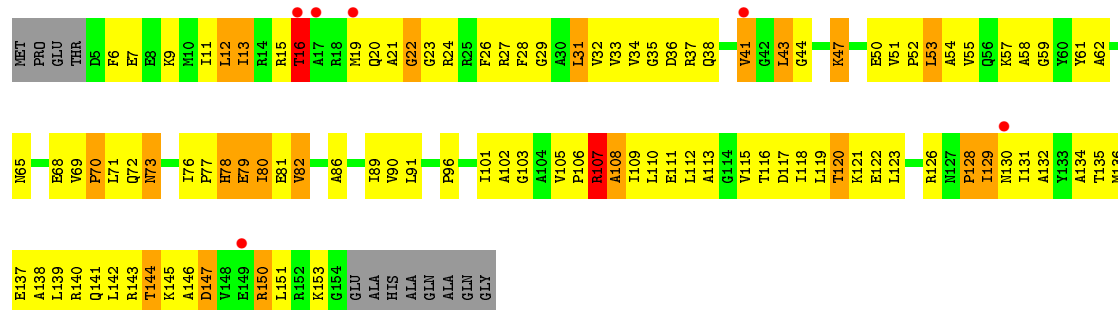




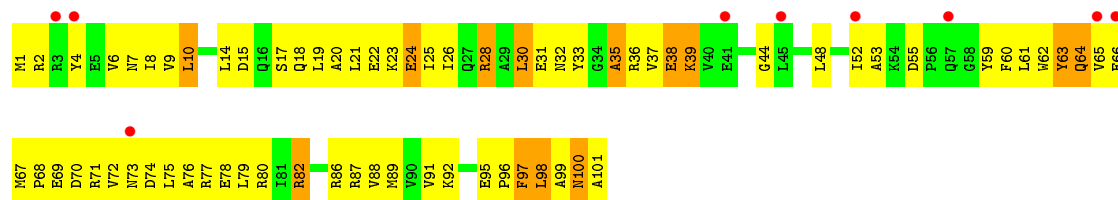
• Molecule 6: 30S ribosomal protein S4



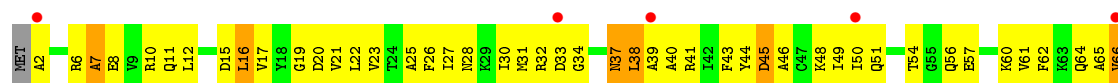
• Molecule 7: 30S ribosomal protein S5

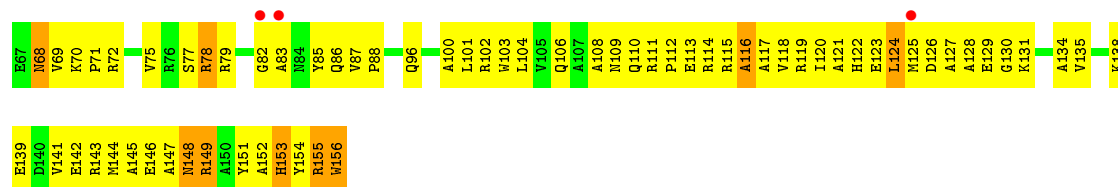


• Molecule 8: 30S ribosomal protein S6

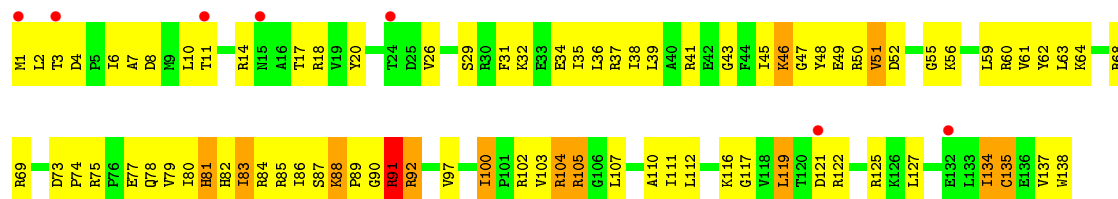


• Molecule 9: 30S ribosomal protein S7

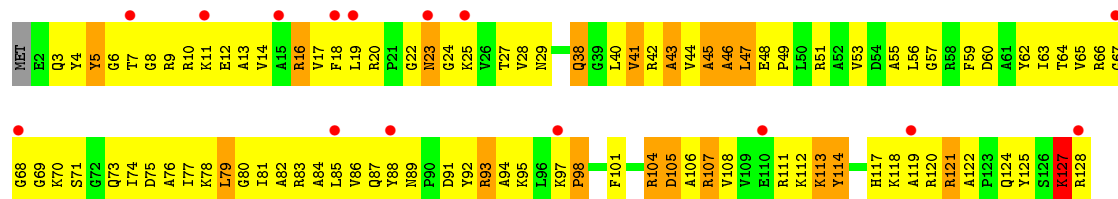




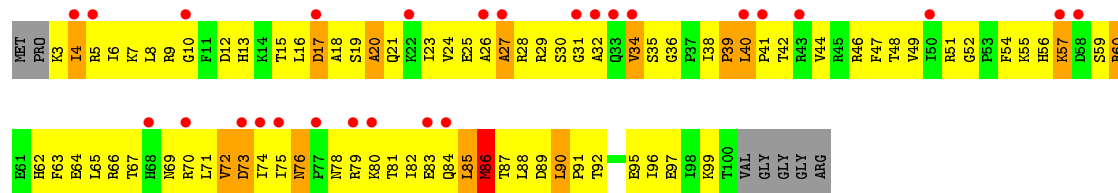
• Molecule 10: 30S ribosomal protein S8



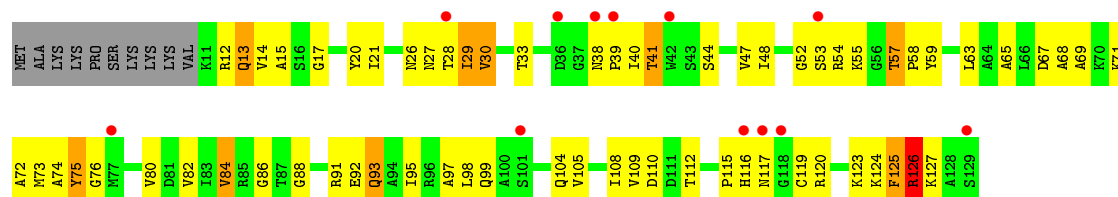
• Molecule 11: 30S ribosomal protein S9



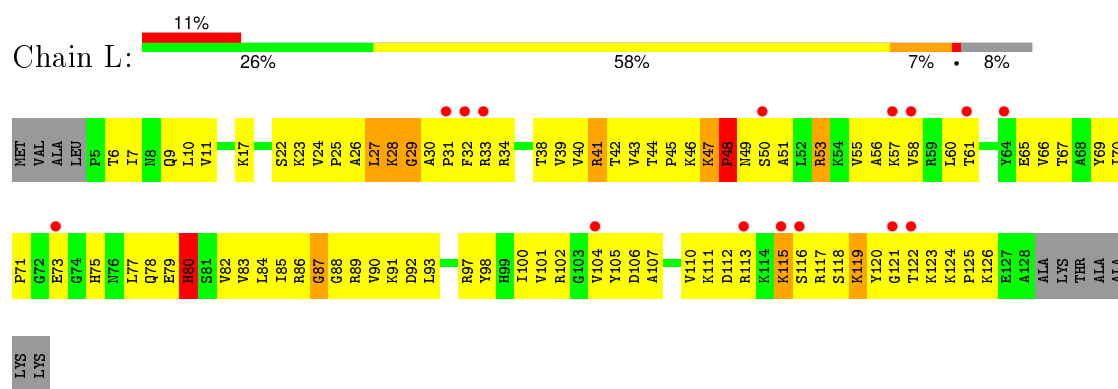
• Molecule 12: 30S ribosomal protein S10



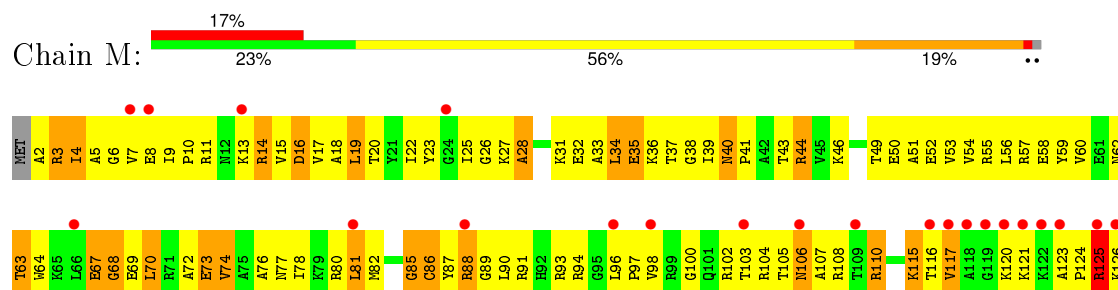
• Molecule 13: 30S ribosomal protein S11



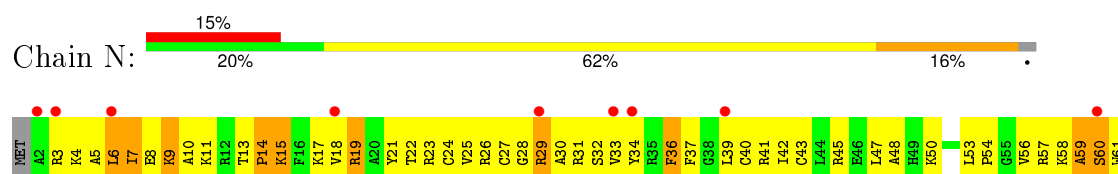
• Molecule 14: 30S ribosomal protein S12



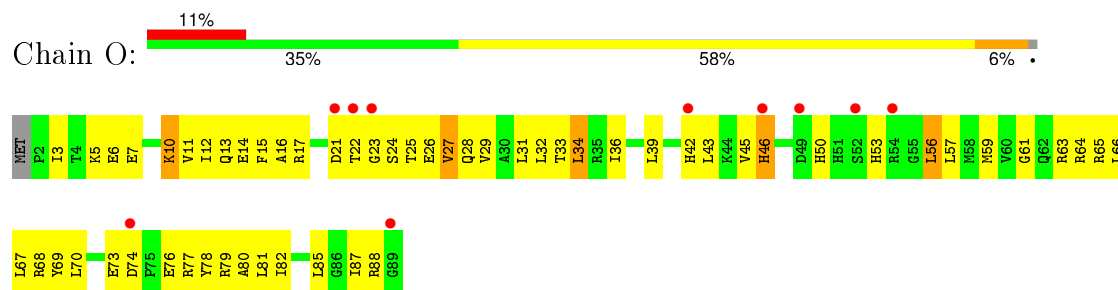
- Molecule 15: 30S ribosomal protein S13



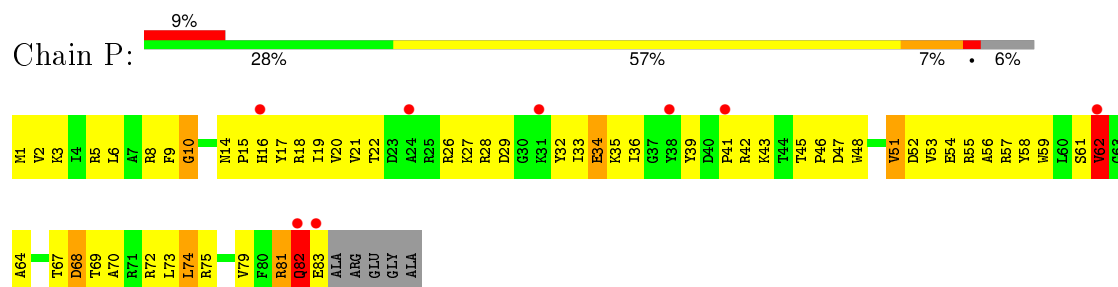
- Molecule 16: 30S ribosomal protein S14



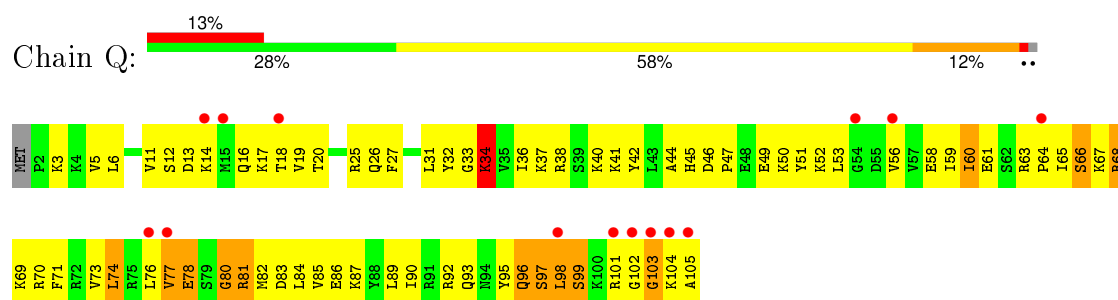
- Molecule 17: 30S ribosomal protein S15



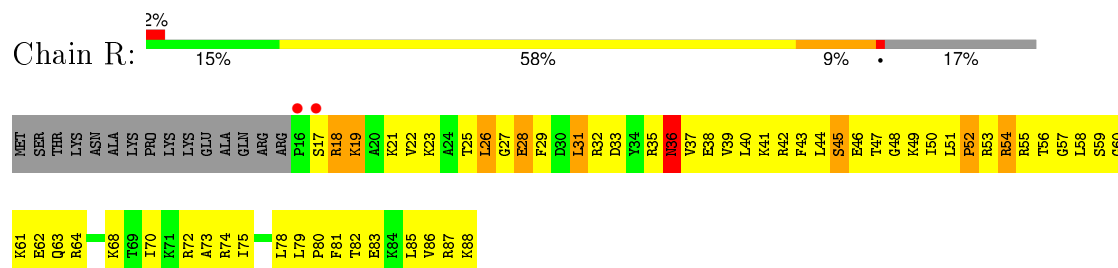
- Molecule 18: 30S ribosomal protein S16



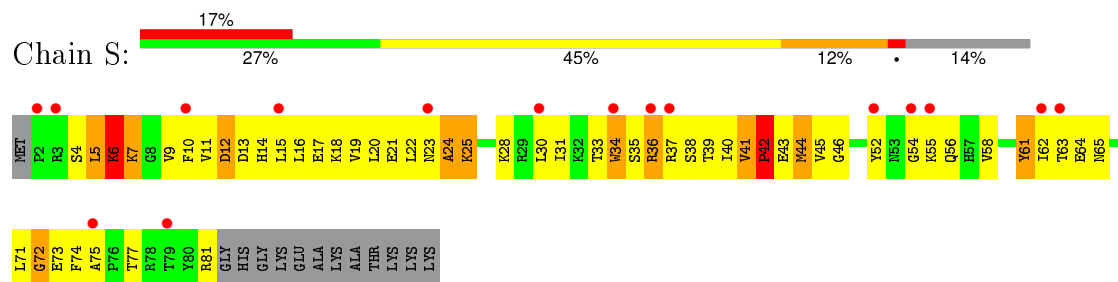
- Molecule 19: 30S ribosomal protein S17



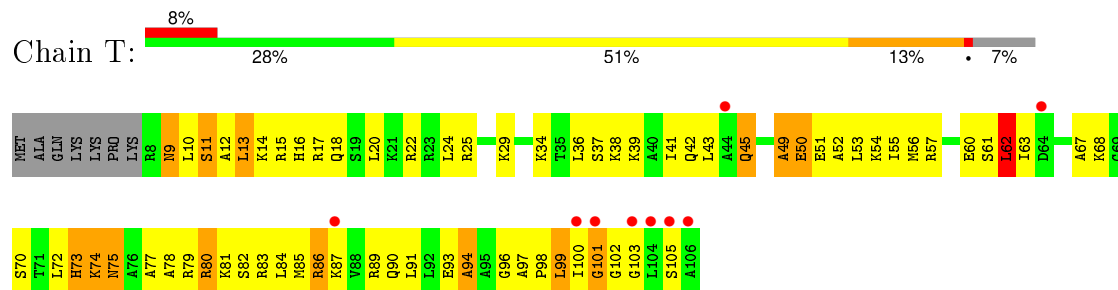
• Molecule 20: 30S ribosomal protein S18



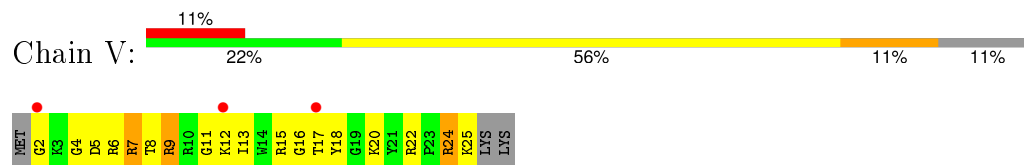
• Molecule 21: 30S ribosomal protein S19



• Molecule 22: 30S ribosomal protein S20



• Molecule 23: 30S 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	400.81Å 400.81Å 176.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	99.00 – 3.25 200.41 – 3.23	Depositor EDS
% Data completeness (in resolution range)	5.0 (99.00-3.25) 88.5 (200.41-3.23)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.14	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.05 (at 3.26Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.231 , 0.284 0.228 , 0.280	Depositor DCC
R_{free} test set	10001 reflections (5.02%)	DCC
Wilson B-factor (Å ²)	85.2	Xtriage
Anisotropy	0.267	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 146.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 209982 reflections	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	52063	wwPDB-VP
Average B, all atoms (Å ²)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.22% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG, T6A, PAR, MNU

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	0.57	2/36244 (0.0%)	0.74	36/56567 (0.1%)
2	W	0.55	0/72	0.95	1/111 (0.9%)
3	X	0.41	0/203	0.78	0/311
4	B	0.34	0/1935	0.65	0/2609
5	C	0.36	0/1636	0.63	0/2205
6	D	0.39	0/1733	0.65	0/2318
7	E	0.44	0/1162	0.74	0/1564
8	F	0.32	0/856	0.59	0/1154
9	G	0.35	0/1276	0.61	0/1709
10	H	0.44	0/1136	0.75	0/1527
11	I	0.35	0/1029	0.63	0/1378
12	J	0.35	0/805	0.69	0/1082
13	K	0.41	0/900	0.68	0/1213
14	L	0.45	0/986	0.77	0/1320
15	M	0.35	0/1008	0.67	0/1347
16	N	0.43	0/501	0.74	0/664
17	O	0.36	0/745	0.63	0/992
18	P	0.47	0/716	0.74	0/963
19	Q	0.47	0/870	0.77	0/1159
20	R	0.35	0/603	0.65	0/799
21	S	0.32	0/661	0.63	0/890
22	T	0.41	0/764	0.77	0/1006
23	V	0.42	0/212	0.72	0/277
All	All	0.52	2/56053 (0.0%)	0.73	37/83165 (0.0%)

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
1	A	4	60
3	X	1	0
All	All	5	60

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1361	G	C3'-O3'	5.22	1.49	1.42
1	A	1361	G	O3'-P	5.14	1.67	1.61

The worst 5 of 37 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	575	G	C2'-C3'-O3'	9.66	130.74	109.50
1	A	115	G	C2'-C3'-O3'	9.52	130.44	109.50
1	A	559	A	C2'-C3'-O3'	9.37	130.12	109.50
1	A	243	A	C2'-C3'-O3'	9.32	130.01	109.50
1	A	1528	U	C2'-C3'-O3'	8.97	129.23	109.50

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	181	G	C3'
1	A	243	A	C3'
1	A	559	A	C3'
1	A	1528	U	C3'
3	X	37	T6A	C14

5 of 60 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	107	G	Sidechain
1	A	108	G	Sidechain
1	A	39	G	Sidechain
1	A	77	G	Sidechain
1	A	84	U	Sidechain

5.2 Too-close contacts ⓘ

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

the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	32380	0	16346	1337	0
2	W	64	0	35	4	0
3	X	239	0	127	7	0
4	B	1900	0	1951	305	0
5	C	1612	0	1677	245	0
6	D	1703	0	1764	150	0
7	E	1146	0	1207	140	0
8	F	843	0	857	102	0
9	G	1257	0	1296	131	0
10	H	1116	0	1177	112	0
11	I	1011	0	1043	153	0
12	J	792	0	835	127	0
13	K	885	0	904	71	0
14	L	970	0	1057	130	0
15	M	997	0	1072	155	0
16	N	492	0	530	67	0
17	O	734	0	771	78	0
18	P	700	0	720	81	0
19	Q	857	0	930	125	0
20	R	597	0	668	100	0
21	S	647	0	673	83	0
22	T	762	0	856	87	0
23	V	208	0	221	19	0
24	A	42	0	45	2	0
25	A	104	0	0	0	0
25	J	1	0	0	0	0
25	X	2	0	0	0	0
26	D	1	0	0	0	0
26	N	1	0	0	1	0
All	All	52063	0	36762	3496	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 39.

The worst 5 of 3496 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1489:G:H2'	1:A:1490:C:H5''	1.26	1.10
6:D:36:ARG:H	6:D:37:PRO:HD3	1.13	1.08
5:C:179:ARG:HG2	5:C:180:ALA:H	0.98	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:26:LYS:HD3	5:C:26:LYS:H	1.14	1.06
4:B:132:LYS:HA	4:B:135:GLN:HB3	1.36	1.05

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	
4	B	232/256 (91%)	129 (56%)	80 (34%)	23 (10%)	1	4
5	C	204/239 (85%)	123 (60%)	48 (24%)	33 (16%)	0	1
6	D	206/209 (99%)	151 (73%)	38 (18%)	17 (8%)	1	7
7	E	148/162 (91%)	120 (81%)	18 (12%)	10 (7%)	1	11
8	F	99/101 (98%)	68 (69%)	24 (24%)	7 (7%)	1	10
9	G	153/156 (98%)	99 (65%)	41 (27%)	13 (8%)	1	6
10	H	136/138 (99%)	106 (78%)	25 (18%)	5 (4%)	4	28
11	I	125/128 (98%)	85 (68%)	27 (22%)	13 (10%)	1	4
12	J	96/105 (91%)	57 (59%)	23 (24%)	16 (17%)	0	1
13	K	117/129 (91%)	85 (73%)	26 (22%)	6 (5%)	2	20
14	L	122/135 (90%)	85 (70%)	24 (20%)	13 (11%)	0	3
15	M	123/126 (98%)	75 (61%)	30 (24%)	18 (15%)	0	1
16	N	58/61 (95%)	34 (59%)	16 (28%)	8 (14%)	0	1
17	O	86/89 (97%)	54 (63%)	28 (33%)	4 (5%)	3	22
18	P	81/88 (92%)	59 (73%)	16 (20%)	6 (7%)	1	10
19	Q	102/105 (97%)	75 (74%)	17 (17%)	10 (10%)	1	5
20	R	71/88 (81%)	50 (70%)	16 (22%)	5 (7%)	1	10
21	S	78/93 (84%)	56 (72%)	14 (18%)	8 (10%)	1	4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
22	T	97/106 (92%)	56 (58%)	30 (31%)	11 (11%)	0	3
23	V	22/27 (82%)	18 (82%)	2 (9%)	2 (9%)	1	5
All	All	2356/2541 (93%)	1585 (67%)	543 (23%)	228 (10%)	1	5

5 of 228 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	B	13	ALA
4	B	15	VAL
4	B	16	HIS
4	B	21	ARG
4	B	24	TRP

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	
4	B	202/220 (92%)	181 (90%)	21 (10%)	9	34
5	C	160/188 (85%)	145 (91%)	15 (9%)	11	40
6	D	180/181 (99%)	164 (91%)	16 (9%)	12	43
7	E	115/123 (94%)	96 (84%)	19 (16%)	3	14
8	F	90/90 (100%)	83 (92%)	7 (8%)	16	51
9	G	126/127 (99%)	115 (91%)	11 (9%)	13	45
10	H	119/119 (100%)	107 (90%)	12 (10%)	9	36
11	I	98/99 (99%)	87 (89%)	11 (11%)	7	31
12	J	87/92 (95%)	85 (98%)	2 (2%)	58	85
13	K	90/99 (91%)	79 (88%)	11 (12%)	6	27
14	L	104/111 (94%)	100 (96%)	4 (4%)	40	76
15	M	100/101 (99%)	88 (88%)	12 (12%)	6	28
16	N	49/50 (98%)	47 (96%)	2 (4%)	37	75
17	O	79/80 (99%)	76 (96%)	3 (4%)	40	76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	P	72/74 (97%)	66 (92%)	6 (8%)	14	48
19	Q	96/97 (99%)	90 (94%)	6 (6%)	22	62
20	R	64/77 (83%)	59 (92%)	5 (8%)	16	51
21	S	71/80 (89%)	63 (89%)	8 (11%)	7	31
22	T	75/82 (92%)	67 (89%)	8 (11%)	8	33
23	V	19/22 (86%)	18 (95%)	1 (5%)	28	68
All	All	1996/2112 (94%)	1816 (91%)	180 (9%)	12	42

5 of 180 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
9	G	45	ASP
10	H	134	ILE
21	S	34	TRP
9	G	124	LEU
10	H	51	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 59 such sidechains are listed below:

Mol	Chain	Res	Type
8	F	32	ASN
11	I	23	ASN
21	S	23	ASN
8	F	57	GLN
8	F	100	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1506/1522 (98%)	240 (15%)	62 (4%)
2	W	2/3 (66%)	1 (50%)	0
3	X	9/11 (81%)	0	0
All	All	1517/1536 (98%)	241 (15%)	62 (4%)

5 of 241 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	8	A

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Mol	Chain	Res	Type
1	A	9	G
1	A	31	G
1	A	32	A
1	A	39	G

5 of 62 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	701	C
1	A	965	A
1	A	1498	U
1	A	812	C
1	A	992	U

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

2 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$
3	MNU	X	34	3,2	14,24,25	1.11	2 (14%)	17,34,37	4.04	2 (11%)
3	T6A	X	37	3	22,34,35	1.42	3 (13%)	25,49,52	3.65	8 (32%)

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
3	MNU	X	34	3,2	-	0/5/28/29	0/2/2/2
3	T6A	X	37	3	1/1/9/11	0/15/41/42	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	X	37	T6A	O14-C14	-3.73	1.34	1.43
3	X	37	T6A	C15-C14	-3.27	1.43	1.51
3	X	37	T6A	C12-N11	-2.47	1.40	1.46
3	X	34	MNU	C6-N1	2.02	1.38	1.35
3	X	34	MNU	C4-N3	2.82	1.38	1.33

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	X	34	MNU	C5-C4-N3	-9.33	114.48	125.04
3	X	37	T6A	O14-C14-C12	-6.46	95.20	109.08
3	X	37	T6A	O10-C10-N6	-4.84	116.23	123.58
3	X	37	T6A	C2-N1-C6	3.14	118.74	116.48
3	X	37	T6A	C13-C12-N11	4.13	121.79	113.51

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	X	37	T6A	C14

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	X	34	MNU	3	0
3	X	37	T6A	2	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 110 ligands modelled in this entry, 109 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected

value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
24	PAR	A	1545	-	45,45,45	1.64	11 (24%)	59,67,67	1.16	4 (6%)

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
24	PAR	A	1545	-	-	0/18/94/94	0/4/4/4

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	1545	PAR	C11-C21	2.02	1.56	1.52
24	A	1545	PAR	O54-C54	2.26	1.50	1.44
24	A	1545	PAR	C34-C24	2.30	1.56	1.53
24	A	1545	PAR	O51-C51	2.38	1.50	1.44
24	A	1545	PAR	C64-C54	2.50	1.58	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	1545	PAR	O33-C14-C24	2.90	113.33	107.96
24	A	1545	PAR	C14-O54-C54	3.14	119.83	113.75
24	A	1545	PAR	O54-C54-C64	3.27	112.49	106.10
24	A	1545	PAR	O52-C13-C23	4.29	116.68	107.75

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	A	1545	PAR	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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	1507/1522 (99%)	2.29	863 (57%) 0 0	30, 65, 160, 200	0
2	W	3/3 (100%)	2.59	3 (100%) 0 0	56, 56, 63, 72	0
3	X	9/11 (81%)	2.02	5 (55%) 0 0	64, 101, 157, 157	0
4	B	234/256 (91%)	0.68	17 (7%) 18 13	37, 100, 173, 200	0
5	C	206/239 (86%)	0.74	20 (9%) 10 7	44, 93, 169, 200	0
6	D	208/209 (99%)	0.75	21 (10%) 9 6	33, 71, 149, 200	0
7	E	150/162 (92%)	0.75	6 (4%) 42 32	27, 63, 122, 200	0
8	F	101/101 (100%)	0.73	9 (8%) 12 8	48, 103, 154, 174	0
9	G	155/156 (99%)	0.67	8 (5%) 31 22	41, 81, 152, 200	0
10	H	138/138 (100%)	0.77	7 (5%) 32 23	20, 54, 113, 174	0
11	I	127/128 (99%)	0.86	15 (11%) 6 4	35, 90, 149, 178	0
12	J	98/105 (93%)	1.28	27 (27%) 1 1	44, 117, 186, 200	0
13	K	119/129 (92%)	0.86	12 (10%) 9 6	30, 67, 138, 187	0
14	L	124/135 (91%)	1.00	15 (12%) 6 4	31, 64, 139, 175	0
15	M	125/126 (99%)	1.29	22 (17%) 2 1	44, 85, 169, 200	0
16	N	60/61 (98%)	1.08	9 (15%) 3 2	42, 82, 139, 179	0
17	O	88/89 (98%)	0.89	10 (11%) 7 5	23, 76, 142, 192	0
18	P	83/88 (94%)	1.00	8 (9%) 10 7	27, 52, 96, 173	0
19	Q	104/105 (99%)	1.35	14 (13%) 4 3	22, 61, 146, 200	0
20	R	73/88 (82%)	0.78	2 (2%) 58 48	40, 79, 175, 188	0
21	S	80/93 (86%)	1.04	16 (20%) 1 1	62, 111, 162, 193	0
22	T	99/106 (93%)	0.89	9 (9%) 11 8	32, 58, 136, 168	0
23	V	24/27 (88%)	1.09	3 (12%) 5 3	41, 69, 118, 136	0
All	All	3915/4077 (96%)	1.43	1121 (28%) 1 1	20, 73, 159, 200	0

The worst 5 of 1121 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
19	Q	103	GLY	13.6
19	Q	104	LYS	13.2
15	M	120	LYS	11.6
1	A	202	U	11.5
19	Q	105	ALA	10.8

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	T6A	X	37	32/33	0.89	0.34	-	76,80,80,80	0
3	MNU	X	34	23/24	0.90	0.37	-	56,96,115,115	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
25	MG	A	1595	1/1	0.69	1.32	21.24	23,23,23,23	1
25	MG	A	1601	1/1	0.94	0.67	6.59	23,23,23,23	1
25	MG	A	210	1/1	0.41	0.53	5.03	23,23,23,23	1
25	MG	A	1606	1/1	0.93	0.49	2.34	23,23,23,23	1
24	PAR	A	1545	42/42	0.92	0.39	1.51	25,25,25,25	0
25	MG	A	1598	1/1	0.93	0.40	1.29	23,23,23,23	0
25	MG	A	1600	1/1	0.92	0.39	0.59	23,23,23,23	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
25	MG	A	1593	1/1	0.91	0.33	-0.31	23,23,23,23	1
26	ZN	N	307	1/1	1.00	0.24	-0.70	23,23,23,23	1
26	ZN	D	306	1/1	0.99	0.33	-0.73	23,23,23,23	1
25	MG	J	449	1/1	0.97	0.33	-0.78	23,23,23,23	1
25	MG	A	211	1/1	0.67	0.34	-1.03	23,23,23,23	0
25	MG	A	1597	1/1	0.86	0.30	-1.19	23,23,23,23	1
25	MG	A	1620	1/1	0.74	0.29	-1.48	23,23,23,23	1
25	MG	A	1611	1/1	0.64	0.31	-1.77	23,23,23,23	1
25	MG	A	1588	1/1	0.97	0.28	-1.98	23,23,23,23	0
25	MG	A	1569	1/1	0.90	0.23	-2.16	23,23,23,23	1
25	MG	A	1592	1/1	0.84	0.23	-2.18	23,23,23,23	0
25	MG	A	1546	1/1	0.96	0.28	-2.23	23,23,23,23	0
25	MG	A	1590	1/1	0.96	0.25	-2.41	23,23,23,23	0
25	MG	A	1626	1/1	0.97	0.19	-2.67	23,23,23,23	1
25	MG	A	1602	1/1	0.93	0.19	-2.69	23,23,23,23	0
25	MG	A	1561	1/1	0.80	0.28	-2.89	23,23,23,23	1
25	MG	A	1578	1/1	0.93	0.21	-3.01	23,23,23,23	0
25	MG	A	1570	1/1	0.95	0.20	-3.10	23,23,23,23	0
25	MG	A	1586	1/1	0.96	0.18	-3.16	23,23,23,23	1
25	MG	A	1555	1/1	0.97	0.27	-3.36	23,23,23,23	0
25	MG	A	1629	1/1	0.92	0.23	-3.62	23,23,23,23	0
25	MG	A	1551	1/1	0.96	0.25	-3.66	23,23,23,23	0
25	MG	A	1558	1/1	0.83	0.18	-5.73	23,23,23,23	0
25	MG	A	1572	1/1	0.98	0.16	-6.50	23,23,23,23	0
25	MG	A	1584	1/1	0.99	0.15	-6.72	23,23,23,23	0
25	MG	A	1582	1/1	0.91	0.12	-7.34	23,23,23,23	0
25	MG	A	1587	1/1	0.96	0.13	-8.73	23,23,23,23	0
25	MG	A	1621	1/1	0.48	0.33	-	23,23,23,23	1
25	MG	A	1574	1/1	0.97	0.22	-	23,23,23,23	0
25	MG	A	1562	1/1	0.79	0.76	-	23,23,23,23	1
25	MG	A	1609	1/1	0.92	0.27	-	23,23,23,23	0
25	MG	A	1589	1/1	0.94	0.33	-	23,23,23,23	0
25	MG	A	1563	1/1	0.94	0.47	-	23,23,23,23	1
25	MG	A	1625	1/1	0.95	0.27	-	23,23,23,23	1
25	MG	A	1550	1/1	0.86	0.30	-	23,23,23,23	1
25	MG	A	1579	1/1	0.96	0.29	-	23,23,23,23	1
25	MG	A	87	1/1	0.59	0.32	-	23,23,23,23	1
25	MG	A	471	1/1	0.86	0.29	-	23,23,23,23	1
25	MG	A	1564	1/1	0.85	0.28	-	23,23,23,23	0
25	MG	A	1585	1/1	0.82	0.38	-	23,23,23,23	1
25	MG	A	1603	1/1	0.94	0.30	-	23,23,23,23	1
25	MG	A	1630	1/1	0.91	0.26	-	23,23,23,23	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
25	MG	A	1614	1/1	0.98	0.22	-	23,23,23,23	1
25	MG	A	1565	1/1	0.93	0.27	-	23,23,23,23	0
25	MG	A	1552	1/1	0.94	0.21	-	23,23,23,23	0
25	MG	A	1624	1/1	0.93	0.20	-	23,23,23,23	1
25	MG	A	1618	1/1	0.97	0.23	-	23,23,23,23	0
25	MG	A	1616	1/1	0.74	0.30	-	23,23,23,23	1
25	MG	A	1615	1/1	0.79	0.27	-	23,23,23,23	1
25	MG	X	502	1/1	0.94	0.31	-	23,23,23,23	1
25	MG	A	1577	1/1	0.94	0.15	-	23,23,23,23	0
25	MG	A	1612	1/1	0.88	0.28	-	23,23,23,23	1
25	MG	A	1623	1/1	0.97	0.40	-	23,23,23,23	1
25	MG	A	1549	1/1	0.90	0.41	-	23,23,23,23	1
25	MG	A	1627	1/1	0.67	0.28	-	23,23,23,23	1
25	MG	A	1560	1/1	0.88	0.26	-	23,23,23,23	0
25	MG	A	1556	1/1	0.91	0.24	-	23,23,23,23	0
25	MG	A	1599	1/1	0.93	0.26	-	23,23,23,23	1
25	MG	A	1605	1/1	0.85	0.44	-	23,23,23,23	1
25	MG	A	1613	1/1	0.85	0.40	-	23,23,23,23	1
25	MG	A	1608	1/1	0.92	0.29	-	23,23,23,23	1
25	MG	A	1566	1/1	0.75	0.53	-	23,23,23,23	1
25	MG	A	1573	1/1	0.92	0.23	-	23,23,23,23	0
25	MG	A	1635	1/1	0.91	0.42	-	23,23,23,23	1
25	MG	X	500	1/1	0.96	0.23	-	23,23,23,23	1
25	MG	A	1548	1/1	0.88	0.32	-	23,23,23,23	1
25	MG	A	1576	1/1	0.98	0.26	-	23,23,23,23	0
25	MG	A	1567	1/1	0.96	0.32	-	23,23,23,23	0
25	MG	A	466	1/1	0.89	0.42	-	23,23,23,23	1
25	MG	A	1619	1/1	0.74	0.23	-	23,23,23,23	1
25	MG	A	441	1/1	0.78	0.22	-	23,23,23,23	1
25	MG	A	86	1/1	0.95	0.30	-	23,23,23,23	1
25	MG	A	1604	1/1	0.85	0.36	-	23,23,23,23	1
25	MG	A	473	1/1	0.92	0.36	-	23,23,23,23	1
25	MG	A	1631	1/1	0.91	0.14	-	23,23,23,23	1
25	MG	A	1575	1/1	0.43	1.13	-	23,23,23,23	1
25	MG	A	1581	1/1	0.89	0.46	-	23,23,23,23	1
25	MG	A	1554	1/1	0.90	0.31	-	23,23,23,23	1
25	MG	A	1596	1/1	0.58	1.50	-	23,23,23,23	1
25	MG	A	1594	1/1	0.97	0.23	-	23,23,23,23	1
25	MG	A	1553	1/1	0.95	0.35	-	23,23,23,23	0
25	MG	A	1617	1/1	0.96	0.18	-	23,23,23,23	1
25	MG	A	1571	1/1	0.92	0.15	-	23,23,23,23	0
25	MG	A	1547	1/1	0.95	0.34	-	23,23,23,23	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
25	MG	A	1557	1/1	0.97	0.22	-	23,23,23,23	0
25	MG	A	1559	1/1	0.84	0.33	-	23,23,23,23	0
25	MG	A	1607	1/1	0.45	0.69	-	23,23,23,23	1
25	MG	A	1622	1/1	0.62	0.51	-	23,23,23,23	1
25	MG	A	1628	1/1	0.85	0.30	-	23,23,23,23	1
25	MG	A	469	1/1	0.91	0.24	-	23,23,23,23	1
25	MG	A	71	1/1	0.78	0.34	-	23,23,23,23	1
25	MG	A	1610	1/1	0.90	0.54	-	23,23,23,23	1
25	MG	A	1568	1/1	0.94	0.16	-	23,23,23,23	0
25	MG	A	470	1/1	0.80	0.42	-	23,23,23,23	1
25	MG	A	1634	1/1	0.76	0.43	-	23,23,23,23	1
25	MG	A	1633	1/1	0.79	0.34	-	23,23,23,23	1
25	MG	A	1583	1/1	0.94	0.16	-	23,23,23,23	0
25	MG	A	1632	1/1	0.76	0.26	-	23,23,23,23	1
25	MG	A	467	1/1	0.89	0.91	-	23,23,23,23	1
25	MG	A	1580	1/1	0.80	0.31	-	23,23,23,23	1
25	MG	A	214	1/1	0.93	0.37	-	23,23,23,23	1
25	MG	A	493	1/1	0.56	1.21	-	23,23,23,23	1
25	MG	A	1591	1/1	0.96	0.29	-	23,23,23,23	1

6.5 Other polymers

There are no such residues in this entry.