



## wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 5, 2024 – 01:55 pm BST

PDB ID : 2UXD  
Title : Crystal structure of an extended tRNA anticodon stem loop in complex with its cognate mRNA CGGG in the context of the *Thermus thermophilus* 30S subunit.  
Authors : Dunham, C.M.; Selmer, M.; Phelps, S.S.; Kelley, A.C.; Suzuki, T.; Joseph, S.; Ramakrishnan, V.  
Deposited on : 2007-03-28  
Resolution : 3.20 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<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>.

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The following versions of software and data (see [references](#) ①) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

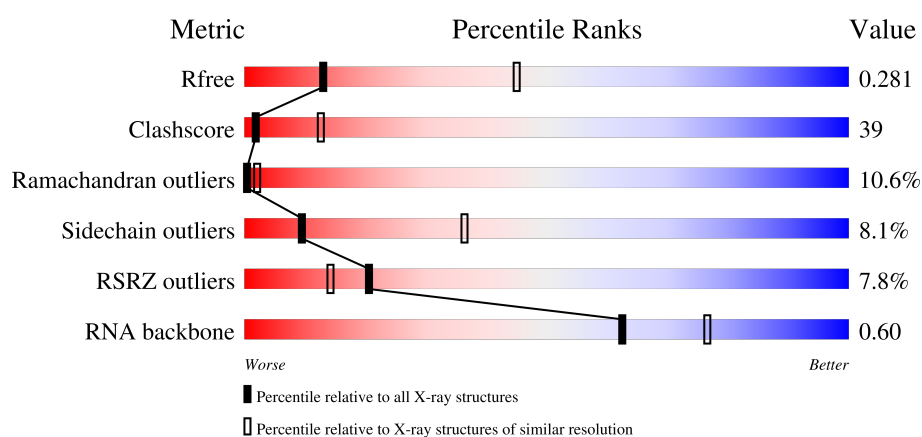
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 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	1370 (3.20-3.20)
Clashscore	180529	1497 (3.20-3.20)
Ramachandran outliers	177936	1479 (3.20-3.20)
Sidechain outliers	177891	1478 (3.20-3.20)
RSRZ outliers	164620	1371 (3.20-3.20)
RNA backbone	3690	1111 (3.50-2.90)

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  $\geq 3$ , 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	1523	<div> <div>9%</div> <div>28%</div> <div>54%</div> <div>13%</div> <div>• •</div> </div>
2	B	256	<div> <div>5%</div> <div>22%</div> <div>57%</div> <div>11%</div> <div>• 8%</div> </div>
3	C	239	<div> <div>10%</div> <div>18%</div> <div>52%</div> <div>15%</div> <div>• 13%</div> </div>
4	D	209	<div> <div>10%</div> <div>32%</div> <div>55%</div> <div>11%</div> <div>•</div> </div>

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Mol	Chain	Length	Quality of chain
5	E	162	
6	F	101	
7	G	156	
8	H	138	
9	I	128	
10	J	105	
11	K	129	
12	L	135	
13	M	126	
14	N	61	
15	O	89	
16	P	88	
17	Q	105	
18	R	88	
19	S	93	
20	T	106	
21	V	27	
22	X	4	
23	Y	18	

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	G	3003	-	-	-	X
25	MG	G	3015	-	-	-	X
25	MG	G	3016	-	-	-	X
25	MG	G	3019	-	-	-	X
25	MG	G	3024	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	MG	G	3025	-	-	-	X
25	MG	G	3027	-	-	-	X
25	MG	G	3028	-	-	-	X
25	MG	G	3029	-	-	-	X
25	MG	G	3033	-	-	-	X
25	MG	G	3034	-	-	-	X
25	MG	G	3037	-	-	-	X
25	MG	G	3039	-	-	-	X
25	MG	G	3046	-	-	-	X
25	MG	G	3050	-	-	-	X
25	MG	G	3055	-	-	-	X
25	MG	G	3058	-	-	-	X

## 2 Entry composition

There are 27 unique types of molecules in this entry. The entry contains 51468 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	1484	Total	C	N	O	P	0	0	0
			31852	14194	5901	10285	1472			

- Molecule 2 is a protein called RIBOSOMAL PROTEIN S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	235	Total	C	N	O	S	0	0	1
			1901	1213	342	341	5			

- Molecule 3 is a protein called RIBOSOMAL PROTEIN S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	207	Total	C	N	O	S	0	0	1
			1613	1016	315	281	1			

- Molecule 4 is a protein called 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	151	Total	C	N	O	S	0	0	1
			1147	724	218	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
			1011	639	198	174			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	58	ARG	HIS	conflict	UNP P80374

- Molecule 10 is a protein called RIBOSOMAL PROTEIN S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	99	Total	C	N	O	S	0	0	1
			793	498	157	137	1			

- Molecule 11 is a protein called RIBOSOMAL PROTEIN S11.

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

- Molecule 12 is a protein called RIBOSOMAL PROTEIN S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	125	Total	C	N	O	S	0	0	1
			971	611	196	163	1			

- Molecule 13 is a protein called RIBOSOMAL PROTEIN S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	125	Total	C	N	O	S	0	0	0
			997	617	207	171	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	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			

- Molecule 16 is a protein called RIBOSOMAL PROTEIN S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	P	84	Total	C	N	O	S	0	0	1
			701	443	140	117	1			

- Molecule 17 is a protein called RIBOSOMAL PROTEIN S17.

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	96	GLN	GLU	conflict	UNP Q5SHP7

- Molecule 18 is a protein called RIBOSOMAL PROTEIN S18.

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

- Molecule 19 is a protein called RIBOSOMAL PROTEIN S19.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	S	81	Total	C	N	O	S	0	0	1
			648	414	120	112	2			

- Molecule 20 is a protein called RIBOSOMAL PROTEIN S20.

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
T	41	VAL	ILE	conflict	UNP P80380

- Molecule 21 is a protein called RIBOSOMAL PROTEIN THX.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	V	25	Total	C	N	O	0	0	1
			209	128	51	30			

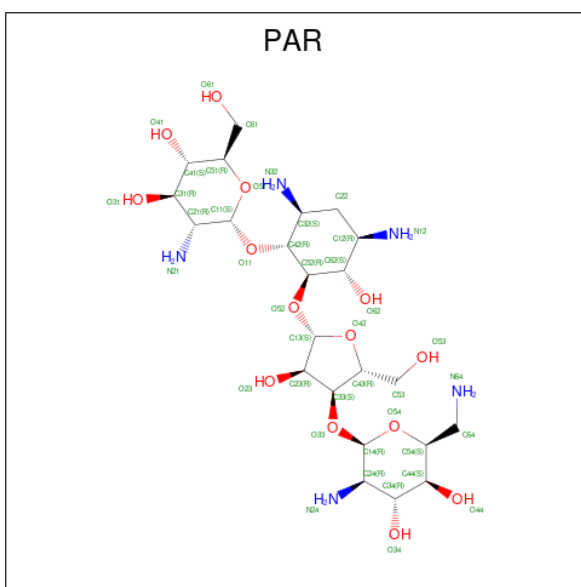
- Molecule 22 is a RNA chain called ANTICODON STEM-LOOP OF TRANSFER RNA WITH ANTICODON CCCG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	X	4	Total	C	N	O	P	0	0	0
			90	39	18	29	4			

- Molecule 23 is a RNA chain called A-SITE MESSENGER RNA FRAGMENT CGGG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	Y	8	Total	C	N	O	P	0	0	0
			167	75	28	56	8			

- Molecule 24 is PAROMOMYCIN (three-letter code: PAR) (formula: C<sub>23</sub>H<sub>45</sub>N<sub>5</sub>O<sub>14</sub>).



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	G	70	Total Mg 70 70	0	0

- Molecule 26 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	G	8	Total K 8 8	0	0

- Molecule 27 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	G	2	Total Zn 2 2	0	0

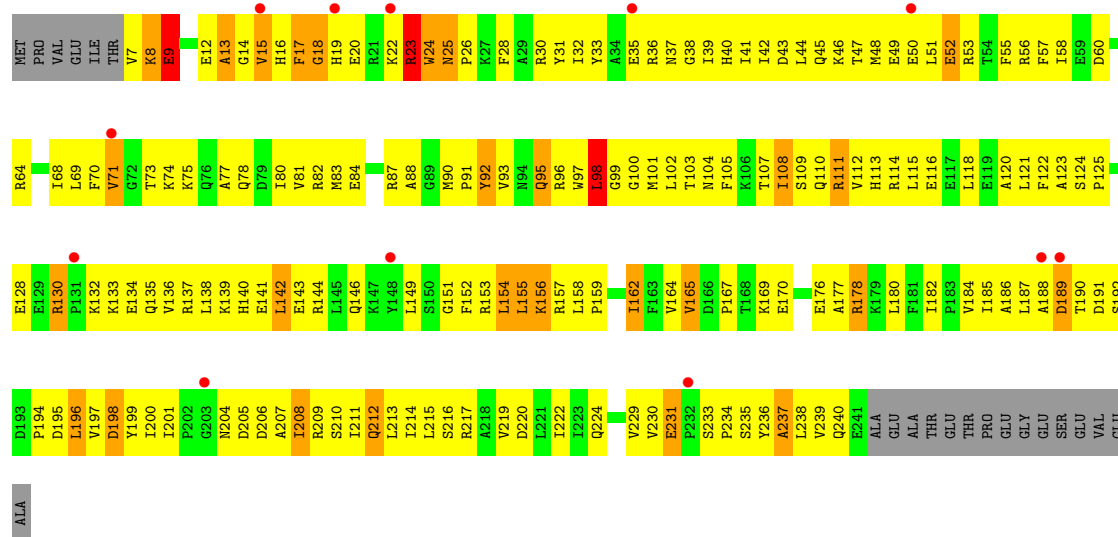


● Molecule 1: 16S RIBOSOMAL RNA

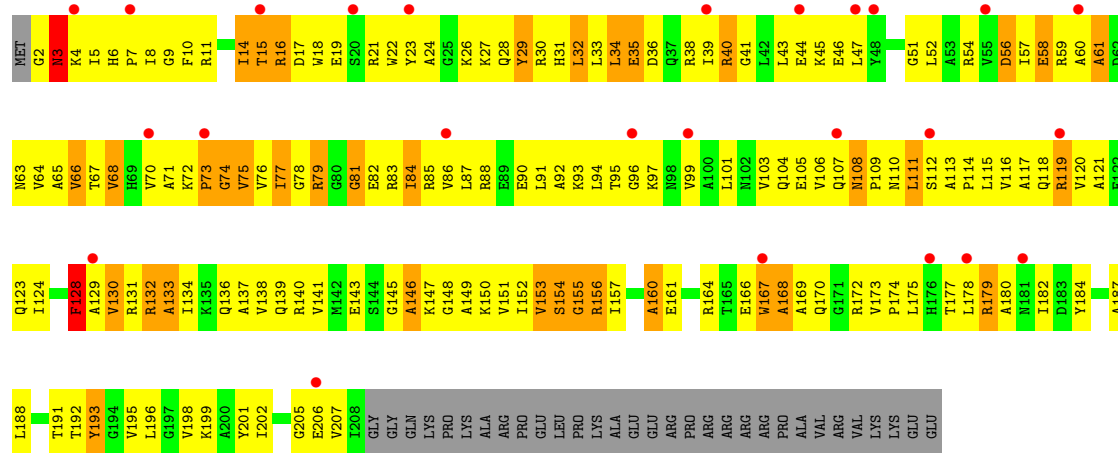
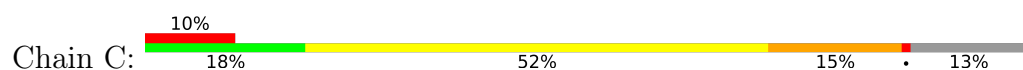


U1542	C1479	C1402	A1339	G1272	A1146	G1074	G1017	G953	G869	C783	A706
C1543	G1490	C1403	U1340	G1273	C1147	C1075	G1018	G954	C877	C784	C707
U1544	G1481	G1404	U1341	G1274	C1148	C1076	C1019		G878		C708
	G1482	G1405	U1342	U1211	C1149	G1077	U1020	U957	C879	A787	G709
		U1406	G1343	U1212	U1150	U1078	G1021	A958	C882	U788	G710
		U1407	G1344	G1213	A1151	G1079	G1022	A959	C883	U789	G711
		A1408	C1344	G1214	A1152		G1023	U960	C897	A790	A712
	G1488	G1409	U1345	G1215	C1153	U1086	G1024	U961	C898	G791	G713
G1489	C1490	G1410	U1346	G1216	G1154		U1025	G962	G899	A792	G714
G1491	G1411	G1412	G1347	U1218	G1155	U1090	G1026	G963	U891	U793	A715
A1492	G1413	A1414	U1348	U1219	G1156	U1091	C1027	A964	A892	A794	A716
A1493	A1413	U1414		G1220	A1157		C1028	A965	G895	C795	G717
U1494	U1351	G1415		G1221	C1158	G1094	C1029	G966	C896	G796	G718
U1495	C1352			G1222	U1159	U1095	C1030	C967	C897	C797	
C1496	G1353			G1223	G1160	U1096	G1030A	A968	C897	G798	
C1497	C1354			G1224	C1161	C1097	C1030B	A969	C898	G799	
U1498	G1355			A1225	C1162	C1098	C1030C	A970	C899	C808	
A1499	G1356			C1226	C1163	G1099	A1030D	G971	A900	A816	
A1500	U1357			A1227	G1164	C1100	G1031	C972	A901	C817	
C1501	U1358			C1228	C1165	A1101	G1032	C973	G902	G818	
A1502	C1359			U1292	G1166	A1102	G1033	A974	G906	G819	
A1503	A1360			G1293	A1168	G1103	G1034	A975	A909	G820	
C1504	G1361			G1294	A	G1104	A1035	G976	U911	C824	
G1505	C1362			G1295	A1169	A1105	G1036	A977	C912	G825	
U1506	C1363			G1296	G1171	G1106	C1037	A978	A914	A828	
A1507	A1363A			C1234	C1172	C1107	G1038	C979	A918	G829	
G1508	U1364			U1235		G1108	C1039	C980	A919	G830	
C1509	G1365			A1236	A1176	C1109	U1040	U981	A920	U831	
U1510	C1366			C1237	G1177	A1110	U1041	U982	U921	C832	
G1511	C1367			U1302	G1178	G1115	G1042	A983	G922	U833	
U1512	G1368			A1238	C1179	C1116	C1043	C984	A923	U834	
A1513	C1369			U1239	A1180	G1117	A1044	C985	A924	G835	
C1514	G1370			G1240	G1181	C1118	C1045	A986	C925	G836	
G1515	G1371			C1242	A1182		G1046	C989	G926	G837	
U1517	G1372			C1243	A1183	U1121	G1048	C990	G927	G838	
A1518	A1374			C1244	G1184	U1122	U1049	U991	G933	U839	
A1519	A1375			A1245	G1185	A1123	G1050	U992	C934	U840	
G1520	U1376				G1186	G1124	G1051	C993	A935	U841	
U1521	A1377			C1249	G1187	U1125	U1052	C994	A938	G851	
U1522	C1378			A1250	A1188	U1126	G1053	A994	G939	G852	
G1523	G1379			A1251	C1189	U1127	C1054	A996	C940	G853	
C1524	U1380			A1252	G1190	G1128	C1055	U997	G941	G854	
A	U1381			G1253	A1191	C1129	U1056	G998	U943	G858	
C	U1382			G1254	C1192	A1130	G1057		U944	A859	
G	C1382			G1255	G1193	G1131	G1058	A1001	G945	A860	
G	G1385			A1256	U1194	C1132	C1059	G1001A	G946	G861	
G	C1386			U1257	C1195	G1133	C1060	G1002	U947	C862	
C				G1258	U1196	G1134	G1061	G1003	U948	A865	
U1529				C1259	G1197	U1135	U1062	G1004	A949	C866	
G1530	U1391			C1260	U1198	U1136	C1063	A1005	U950	G867	
A1531	G1392			A1261	C1200	C1137	G1064	A1006	G951	A781	
U1532	U1393			C1262	A1201	G1138	U1065	C1006A	A1015	A782	
A1534	A1394			C1263	G1202	G1139	C1066	C1007	A1016		
C	C1395			C1264	A1203	G1140	A1067	C1008			
U	A1396				C1203	C1141	G1068				
C	C1397			C1267	U1204	G1142	C1069	G1013			
U	U1398			A1268	U1205	G1143		A1014			
C	A1398			C1269	G1206	G1144	G1072	A1015			
C1539	C1399			A1332	G1207	G1207	U1073	A1016			
U1540	C1400			C1270	G1208						
U1541	G1401			G1271							

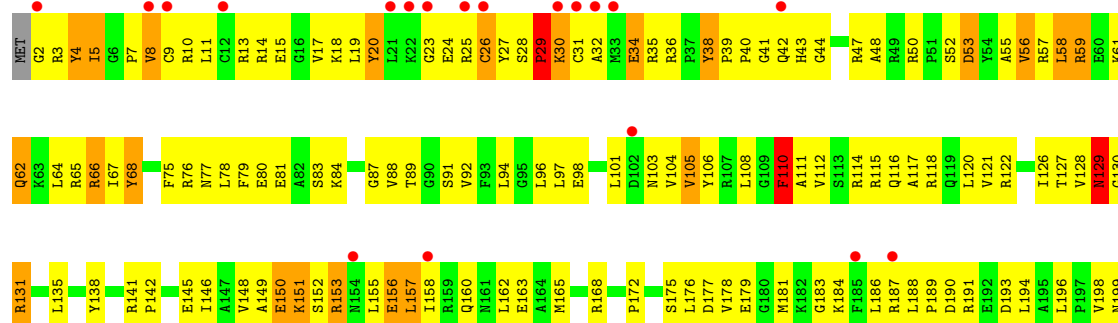
• Molecule 2: RIBOSOMAL PROTEIN S2



• Molecule 3: RIBOSOMAL PROTEIN S3

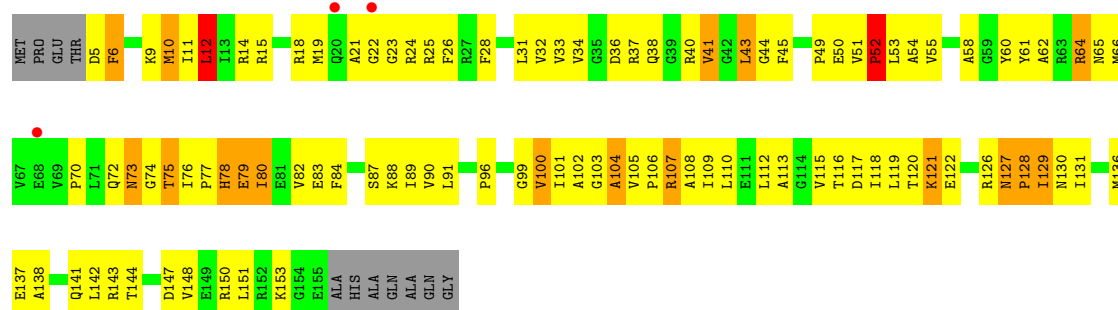


• Molecule 4: RIBOSOMAL PROTEIN S4

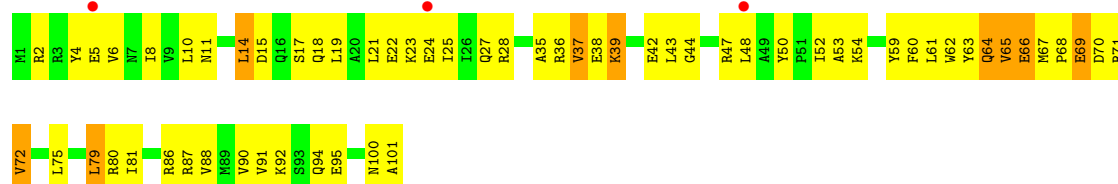
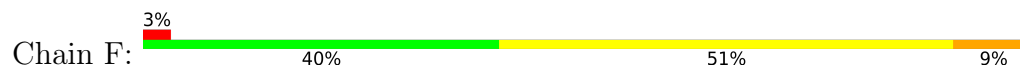




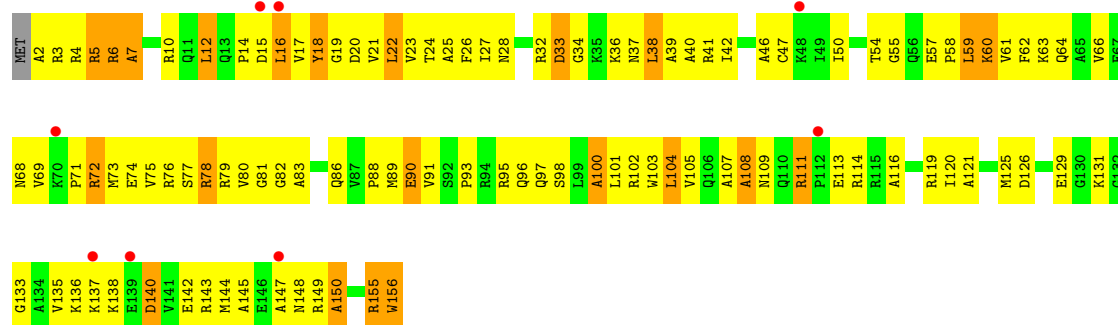
• Molecule 5: RIBOSOMAL PROTEIN S5



• Molecule 6: RIBOSOMAL PROTEIN S6



• Molecule 7: RIBOSOMAL PROTEIN S7



• Molecule 8: RIBOSOMAL PROTEIN S8





• Molecule 9: RIBOSOMAL PROTEIN S9



• Molecule 10: RIBOSOMAL PROTEIN S10



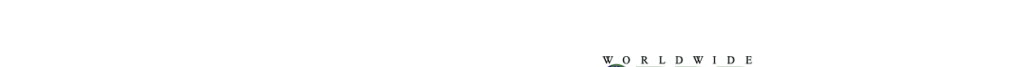
• Molecule 11: RIBOSOMAL PROTEIN S11



• Molecule 12: RIBOSOMAL PROTEIN S12

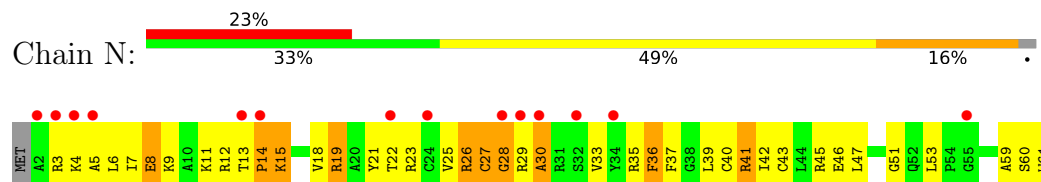


• Molecule 13: RIBOSOMAL PROTEIN S13

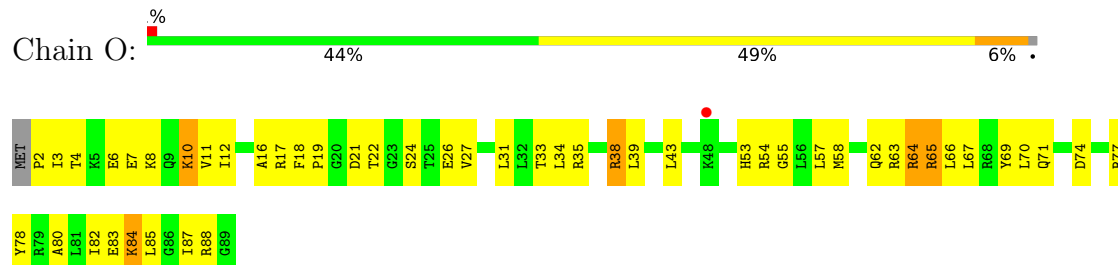


T63	W64	K65	L66	E67	G68	E69	L70	E73	V74	N77	I78	K79	R80	L81	M82	D83	I84	G85	G86	Y87	R88	G89	L90	R91	L96	P97	R98	R99	G100	Q101	R102	T103	R104	T105	N106	A107	R108	T109	R110	K111	R114	K115	T116	V117	A118	G119	K120	K121	K122	A123	P124	R125	K126
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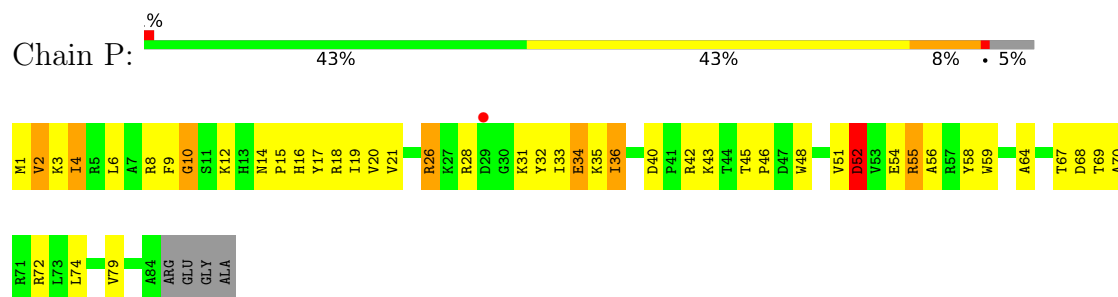
- Molecule 14: RIBOSOMAL PROTEIN S14



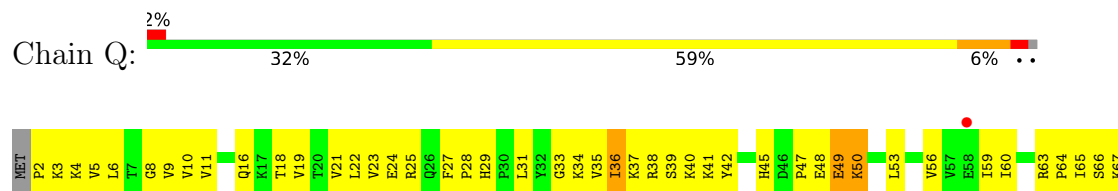
- Molecule 15: RIBOSOMAL PROTEIN S15



- Molecule 16: RIBOSOMAL PROTEIN S16



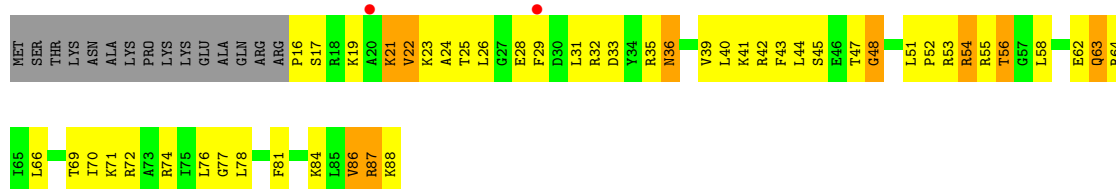
• Molecule 17: RIBOSOMAL PROTEIN S17



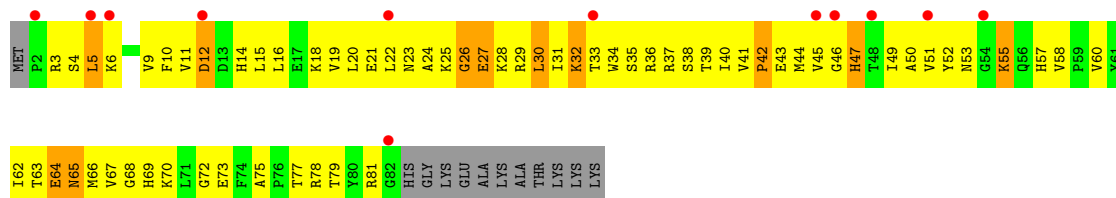
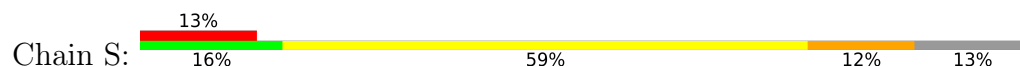
- Molecule 18: RIBOSOMAL PROTEIN S18



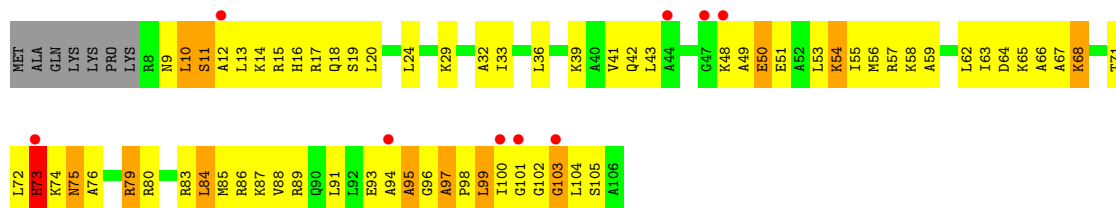




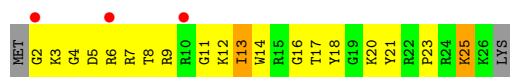
• Molecule 19: RIBOSOMAL PROTEIN S19



• Molecule 20: RIBOSOMAL PROTEIN S20



• Molecule 21: RIBOSOMAL PROTEIN THX



• Molecule 22: ANTICODON STEM-LOOP OF TRANSFER RNA WITH ANTICODON CCCG



• Molecule 23: A-SITE MESSENGER RNA FRAGMENT CGGG



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	401.90Å 401.90Å 174.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.38 – 3.20 49.38 – 3.20	Depositor EDS
% Data completeness (in resolution range)	98.4 (49.38-3.20) 98.3 (49.38-3.20)	Depositor EDS
$R_{merge}$	0.24	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.24 (at 2.81Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.238 , 0.282 0.240 , 0.281	Depositor DCC
$R_{free}$ test set	11541 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	89.1	Xtriage
Anisotropy	0.189	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 123.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	51468	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	99.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.62% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 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: PAR, ZN, MG, K

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	0.62	16/35645 (0.0%)	0.77	53/55610 (0.1%)
2	B	0.37	0/1936	0.62	0/2611
3	C	0.34	0/1637	0.58	0/2207
4	D	0.36	0/1733	0.60	0/2318
5	E	0.49	0/1163	0.75	1/1566 (0.1%)
6	F	0.32	0/856	0.58	0/1154
7	G	0.31	0/1276	0.58	0/1709
8	H	0.49	0/1136	0.76	1/1527 (0.1%)
9	I	0.33	0/1029	0.56	0/1378
10	J	0.35	0/806	0.60	0/1084
11	K	0.40	0/900	0.69	0/1213
12	L	0.42	0/987	0.71	0/1322
13	M	0.32	0/1008	0.62	0/1347
14	N	0.33	0/501	0.60	0/664
15	O	0.37	0/745	0.59	0/992
16	P	0.47	0/717	0.79	1/965 (0.1%)
17	Q	0.46	0/870	0.76	0/1159
18	R	0.35	0/603	0.63	0/799
19	S	0.32	0/662	0.58	0/892
20	T	0.41	0/764	0.70	0/1006
21	V	0.52	0/213	0.71	0/279
22	X	0.98	1/100 (1.0%)	0.93	0/153
23	Y	0.59	0/185	0.84	0/285
All	All	0.55	17/55472 (0.0%)	0.73	56/82240 (0.1%)

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	8	57

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	496	A	C3'-O3'	7.89	1.53	1.42
1	A	190	C	C3'-O3'	7.73	1.52	1.42
22	X	1	C	OP3-P	-7.35	1.52	1.61
1	A	129	U	C3'-O3'	7.24	1.52	1.42
1	A	73	C	C3'-O3'	7.07	1.52	1.42

The worst 5 of 56 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	575	G	C2'-C3'-O3'	10.78	133.22	109.50
1	A	190	C	N1-C1'-C2'	10.38	127.49	114.00
1	A	1498	U	C2'-C3'-O3'	9.97	131.43	109.50
1	A	748	C	C2'-C3'-O3'	9.67	130.78	109.50
1	A	129	U	C2'-C3'-O3'	9.59	130.60	109.50

5 of 8 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	115	G	C3'
1	A	129	U	C3'
1	A	281	G	C3'
1	A	748	C	C3'
1	A	1006	A	C1'

5 of 57 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	106	C	Sidechain
1	A	128	G	Sidechain
1	A	17	U	Sidechain
1	A	70	G	Sidechain
1	A	93	G	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	31852	0	16122	1389	0
2	B	1901	0	1951	247	0
3	C	1613	0	1677	261	0
4	D	1703	0	1764	178	0
5	E	1147	0	1207	112	0
6	F	843	0	857	75	0
7	G	1257	0	1296	141	0
8	H	1116	0	1177	114	0
9	I	1011	0	1043	134	0
10	J	793	0	835	145	0
11	K	885	0	904	87	0
12	L	971	0	1057	154	0
13	M	997	0	1072	115	0
14	N	492	0	531	66	0
15	O	734	0	771	65	0
16	P	701	0	720	58	0
17	Q	857	0	930	83	0
18	R	597	0	666	60	0
19	S	648	0	673	93	0
20	T	762	0	859	84	0
21	V	209	0	221	19	0
22	X	90	0	45	11	0
23	Y	167	0	87	14	0
24	A	42	0	45	0	0
25	G	70	0	0	0	0
26	G	8	0	0	0	0
27	G	2	0	0	0	0
All	All	51468	0	36510	3377	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 3377 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:189:G:H2'	1:A:190:C:C6	1.68	1.27
3:C:27:LYS:HA	3:C:30:ARG:HH12	1.09	1.13
10:J:38:ILE:HD11	10:J:71:LEU:HB2	1.20	1.11
1:A:1305:G:H22	1:A:1331:G:H2'	1.02	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1356:G:H2'	1:A:1357:A:C8	1.88	1.08

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	233/256 (91%)	149 (64%)	60 (26%)	24 (10%)	0	2
3	C	205/239 (86%)	119 (58%)	53 (26%)	33 (16%)	0	0
4	D	206/209 (99%)	131 (64%)	54 (26%)	21 (10%)	0	2
5	E	149/162 (92%)	124 (83%)	15 (10%)	10 (7%)	1	7
6	F	99/101 (98%)	73 (74%)	19 (19%)	7 (7%)	1	6
7	G	153/156 (98%)	100 (65%)	35 (23%)	18 (12%)	0	1
8	H	136/138 (99%)	107 (79%)	19 (14%)	10 (7%)	1	6
9	I	125/128 (98%)	78 (62%)	34 (27%)	13 (10%)	0	2
10	J	97/105 (92%)	53 (55%)	29 (30%)	15 (16%)	0	0
11	K	117/129 (91%)	85 (73%)	18 (15%)	14 (12%)	0	1
12	L	123/135 (91%)	92 (75%)	16 (13%)	15 (12%)	0	1
13	M	123/126 (98%)	89 (72%)	21 (17%)	13 (11%)	0	2
14	N	58/61 (95%)	33 (57%)	19 (33%)	6 (10%)	0	2
15	O	86/89 (97%)	60 (70%)	23 (27%)	3 (4%)	3	20
16	P	82/88 (93%)	62 (76%)	16 (20%)	4 (5%)	2	14
17	Q	102/105 (97%)	82 (80%)	10 (10%)	10 (10%)	0	3
18	R	71/88 (81%)	49 (69%)	15 (21%)	7 (10%)	0	2
19	S	79/93 (85%)	50 (63%)	15 (19%)	14 (18%)	0	0
20	T	97/106 (92%)	67 (69%)	19 (20%)	11 (11%)	0	2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
21	V	23/27 (85%)	18 (78%)	2 (9%)	3 (13%)	0	1
All	All	2364/2541 (93%)	1621 (69%)	492 (21%)	251 (11%)	0	2

5 of 251 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	8	LYS
2	B	17	PHE
2	B	23	ARG
2	B	95	GLN
2	B	98	LEU

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	202/220 (92%)	182 (90%)	20 (10%)	6	26
3	C	160/188 (85%)	151 (94%)	9 (6%)	17	50
4	D	180/181 (99%)	165 (92%)	15 (8%)	9	35
5	E	115/123 (94%)	98 (85%)	17 (15%)	2	12
6	F	90/90 (100%)	84 (93%)	6 (7%)	13	44
7	G	126/127 (99%)	115 (91%)	11 (9%)	8	32
8	H	119/119 (100%)	104 (87%)	15 (13%)	3	18
9	I	98/99 (99%)	94 (96%)	4 (4%)	26	59
10	J	87/92 (95%)	80 (92%)	7 (8%)	10	37
11	K	90/99 (91%)	85 (94%)	5 (6%)	17	50
12	L	104/111 (94%)	96 (92%)	8 (8%)	10	39
13	M	100/101 (99%)	90 (90%)	10 (10%)	6	26
14	N	49/50 (98%)	44 (90%)	5 (10%)	6	26
15	O	79/80 (99%)	74 (94%)	5 (6%)	15	46
16	P	72/74 (97%)	68 (94%)	4 (6%)	17	50

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	Q	96/97 (99%)	90 (94%)	6 (6%)	15	46
18	R	64/77 (83%)	60 (94%)	4 (6%)	15	46
19	S	71/80 (89%)	69 (97%)	2 (3%)	38	68
20	T	76/82 (93%)	68 (90%)	8 (10%)	5	24
21	V	19/22 (86%)	19 (100%)	0	100	100
All	All	1997/2112 (95%)	1836 (92%)	161 (8%)	9	36

5 of 161 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	L	99	HIS
17	Q	38	ARG
13	M	44	ARG
14	N	27	CYS
18	R	87	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 54 such sidechains are listed below:

Mol	Chain	Res	Type
7	G	106	GLN
12	L	49	ASN
19	S	23	ASN
8	H	78	GLN
10	J	84	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1472/1523 (96%)	218 (14%)	66 (4%)
22	X	3/4 (75%)	1 (33%)	0
23	Y	7/18 (38%)	4 (57%)	0
All	All	1482/1545 (95%)	223 (15%)	66 (4%)

5 of 223 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	8	A
1	A	9	G

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Mol	Chain	Res	Type
1	A	32	A
1	A	39	G
1	A	47	C

5 of 66 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	1347	G
1	A	1452	C
1	A	1528	U
1	A	484	G
1	A	442	C

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 81 ligands modelled in this entry, 80 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	3001	-	45,45,45	1.49	8 (17%)	64,67,67	1.23	8 (12%)

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	3001	-	-	2/18/94/94	0/4/4/4

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	3001	PAR	C64-C54	3.79	1.57	1.52
24	A	3001	PAR	C52-C42	3.53	1.59	1.52
24	A	3001	PAR	O54-C14	2.82	1.49	1.41
24	A	3001	PAR	C11-C21	2.76	1.57	1.52
24	A	3001	PAR	C31-C21	2.59	1.56	1.53

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	3001	PAR	O54-C54-C64	3.55	112.62	106.01
24	A	3001	PAR	O33-C14-C24	3.26	113.84	108.22
24	A	3001	PAR	C14-O54-C54	3.10	119.78	113.69
24	A	3001	PAR	O52-C13-C23	2.99	114.16	107.96
24	A	3001	PAR	O11-C11-C21	2.76	112.97	108.22

There are no chirality outliers.

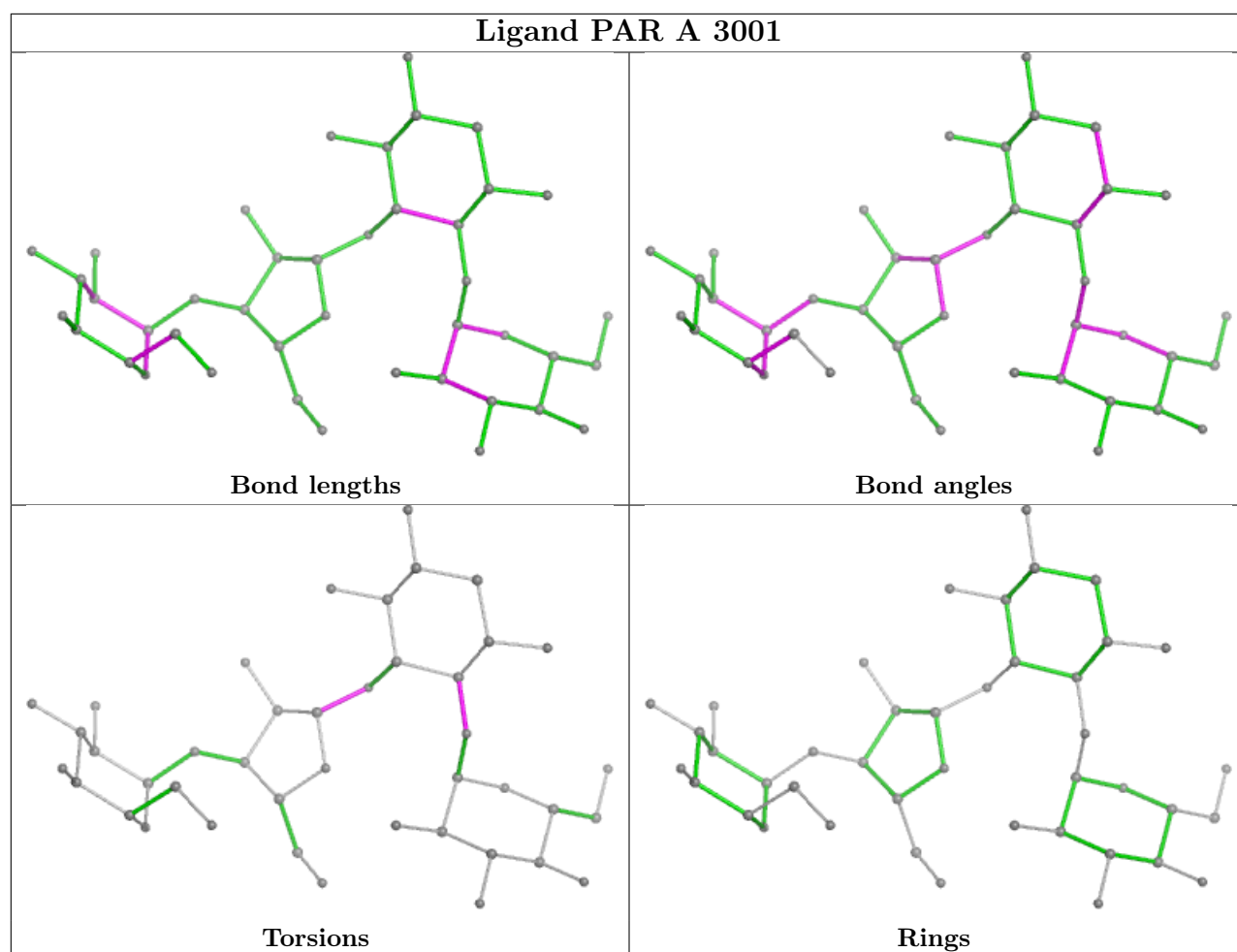
All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	A	3001	PAR	C52-C42-O11-C11
24	A	3001	PAR	C23-C13-O52-C52

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 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, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	1484/1523 (97%)	0.72	140 (9%) 15 11	40, 86, 171, 201	0
2	B	235/256 (91%)	0.61	12 (5%) 34 23	50, 117, 152, 155	0
3	C	207/239 (86%)	0.82	25 (12%) 10 7	61, 123, 153, 155	0
4	D	208/209 (99%)	0.58	20 (9%) 15 10	57, 101, 143, 155	0
5	E	151/162 (93%)	0.21	3 (1%) 64 49	43, 76, 119, 149	0
6	F	101/101 (100%)	0.51	3 (2%) 52 37	64, 116, 146, 151	0
7	G	155/156 (99%)	0.53	8 (5%) 34 23	63, 121, 153, 155	0
8	H	138/138 (100%)	-0.08	0 100 100	39, 67, 111, 132	0
9	I	127/128 (99%)	0.79	9 (7%) 23 16	54, 123, 155, 155	0
10	J	99/105 (94%)	1.17	14 (14%) 7 5	70, 139, 155, 155	0
11	K	119/129 (92%)	0.31	5 (4%) 41 28	44, 89, 134, 148	0
12	L	125/135 (92%)	0.57	9 (7%) 23 16	38, 96, 137, 155	0
13	M	125/126 (99%)	0.61	10 (8%) 20 14	68, 108, 144, 155	0
14	N	60/61 (98%)	1.21	14 (23%) 2 2	74, 116, 145, 155	0
15	O	88/89 (98%)	0.07	1 (1%) 77 63	49, 88, 136, 145	0
16	P	84/88 (95%)	0.23	1 (1%) 76 61	46, 75, 109, 154	0
17	Q	104/105 (99%)	0.27	2 (1%) 66 50	47, 76, 132, 155	0
18	R	73/88 (82%)	0.16	2 (2%) 56 40	52, 95, 141, 155	0
19	S	81/93 (87%)	1.01	12 (14%) 7 5	95, 136, 154, 155	0
20	T	99/106 (93%)	0.59	9 (9%) 16 11	51, 84, 139, 155	0
21	V	25/27 (92%)	0.56	3 (12%) 10 7	63, 89, 132, 152	0
22	X	4/4 (100%)	1.27	1 (25%) 2 2	102, 111, 115, 128	0
23	Y	8/18 (44%)	0.84	0 100 100	104, 144, 155, 155	0
All	All	3900/4086 (95%)	0.60	303 (7%) 20 14	38, 96, 154, 201	0

The worst 5 of 303 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1452	C	10.9
1	A	1447	G	10.1
1	A	474	G	8.5
1	A	73	C	8.4
1	A	190	C	7.8

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

There are no non-standard protein/DNA/RNA residues in this entry.

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
25	MG	G	3003	1/1	0.49	0.66	84,84,84,84	0
25	MG	G	3025	1/1	0.49	1.06	84,84,84,84	0
25	MG	G	3050	1/1	0.49	0.99	84,84,84,84	0
25	MG	G	3046	1/1	0.59	0.43	84,84,84,84	0
26	K	G	3077	1/1	0.61	0.37	84,84,84,84	1
25	MG	G	3013	1/1	0.63	0.31	84,84,84,84	0
25	MG	G	3034	1/1	0.65	0.47	84,84,84,84	0
25	MG	G	3064	1/1	0.66	0.29	84,84,84,84	0
25	MG	G	3055	1/1	0.68	0.71	84,84,84,84	0
25	MG	G	3028	1/1	0.68	0.44	84,84,84,84	0
25	MG	G	3015	1/1	0.68	0.84	84,84,84,84	0
25	MG	G	3039	1/1	0.70	0.69	84,84,84,84	0
25	MG	G	3027	1/1	0.70	0.60	84,84,84,84	0
25	MG	G	3033	1/1	0.71	0.50	84,84,84,84	0
25	MG	G	3010	1/1	0.72	0.34	84,84,84,84	0
25	MG	G	3038	1/1	0.72	0.23	84,84,84,84	0
25	MG	G	3058	1/1	0.75	0.66	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
25	MG	G	3008	1/1	0.75	0.18	84,84,84,84	0
25	MG	G	3016	1/1	0.75	0.55	84,84,84,84	0
26	K	G	3072	1/1	0.76	0.22	84,84,84,84	0
25	MG	G	3019	1/1	0.76	0.88	84,84,84,84	0
25	MG	G	3029	1/1	0.78	0.52	84,84,84,84	0
26	K	G	3075	1/1	0.78	0.19	84,84,84,84	1
25	MG	G	3024	1/1	0.78	0.58	84,84,84,84	0
25	MG	G	3069	1/1	0.80	0.30	84,84,84,84	0
25	MG	G	3041	1/1	0.80	0.58	84,84,84,84	0
25	MG	G	3037	1/1	0.80	0.40	84,84,84,84	0
25	MG	G	3067	1/1	0.80	0.34	84,84,84,84	0
26	K	G	3073	1/1	0.82	0.19	84,84,84,84	1
25	MG	G	3022	1/1	0.82	0.54	84,84,84,84	0
25	MG	G	3060	1/1	0.82	0.56	84,84,84,84	0
26	K	G	3076	1/1	0.83	0.15	84,84,84,84	0
26	K	G	3078	1/1	0.83	0.15	84,84,84,84	1
25	MG	G	3068	1/1	0.84	0.33	84,84,84,84	0
25	MG	G	3063	1/1	0.84	0.33	84,84,84,84	0
25	MG	G	3026	1/1	0.84	0.34	84,84,84,84	0
25	MG	G	3049	1/1	0.84	0.59	84,84,84,84	0
25	MG	G	3066	1/1	0.85	0.44	84,84,84,84	0
25	MG	G	3070	1/1	0.85	0.47	84,84,84,84	0
25	MG	G	3021	1/1	0.85	0.34	84,84,84,84	0
25	MG	G	3045	1/1	0.85	0.48	84,84,84,84	0
26	K	G	3074	1/1	0.86	0.11	84,84,84,84	1
25	MG	G	3018	1/1	0.86	0.90	84,84,84,84	0
25	MG	G	3004	1/1	0.86	0.31	84,84,84,84	0
25	MG	G	3020	1/1	0.86	0.68	84,84,84,84	0
25	MG	G	3053	1/1	0.86	0.45	84,84,84,84	0
24	PAR	A	3001	42/42	0.87	0.18	84,84,84,84	0
25	MG	G	3002	1/1	0.87	0.56	84,84,84,84	1
25	MG	G	3065	1/1	0.87	0.16	84,84,84,84	0
25	MG	G	3059	1/1	0.87	0.25	84,84,84,84	0
25	MG	G	3006	1/1	0.87	0.18	84,84,84,84	0
26	K	G	3079	1/1	0.87	0.28	84,84,84,84	1
25	MG	G	3035	1/1	0.88	0.84	84,84,84,84	0
25	MG	G	3032	1/1	0.88	0.54	84,84,84,84	0
25	MG	G	3061	1/1	0.89	0.33	84,84,84,84	0
25	MG	G	3071	1/1	0.89	0.12	84,84,84,84	0
25	MG	G	3014	1/1	0.89	0.46	84,84,84,84	0
25	MG	G	3017	1/1	0.89	0.59	84,84,84,84	0
25	MG	G	3012	1/1	0.89	0.25	84,84,84,84	0

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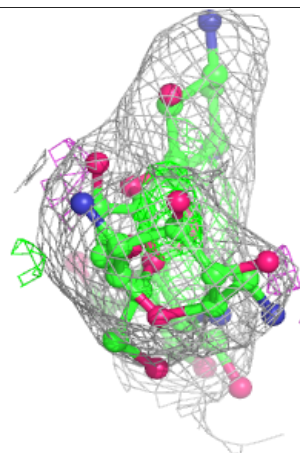
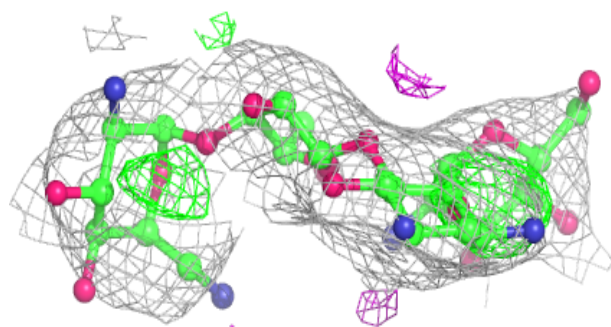
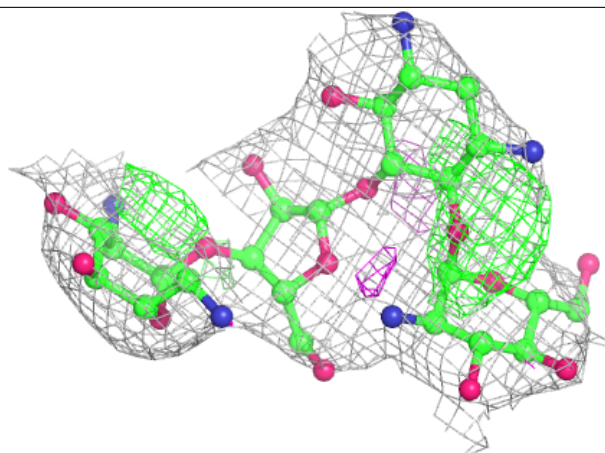
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
25	MG	G	3044	1/1	0.90	0.44	84,84,84,84	0
25	MG	G	3040	1/1	0.90	0.63	84,84,84,84	0
25	MG	G	3051	1/1	0.91	0.32	84,84,84,84	0
25	MG	G	3047	1/1	0.91	0.43	84,84,84,84	0
25	MG	G	3005	1/1	0.91	0.49	84,84,84,84	0
25	MG	G	3036	1/1	0.91	0.39	84,84,84,84	0
25	MG	G	3056	1/1	0.92	0.35	84,84,84,84	0
25	MG	G	3031	1/1	0.92	0.42	84,84,84,84	0
25	MG	G	3048	1/1	0.93	0.27	84,84,84,84	0
25	MG	G	3054	1/1	0.93	0.32	84,84,84,84	0
25	MG	G	3011	1/1	0.93	0.27	84,84,84,84	0
25	MG	G	3042	1/1	0.93	0.64	84,84,84,84	0
25	MG	G	3030	1/1	0.93	0.41	84,84,84,84	0
25	MG	G	3052	1/1	0.94	0.47	84,84,84,84	0
25	MG	G	3023	1/1	0.94	0.54	84,84,84,84	0
25	MG	G	3007	1/1	0.95	0.37	84,84,84,84	0
25	MG	G	3009	1/1	0.95	0.25	84,84,84,84	0
25	MG	G	3057	1/1	0.95	0.53	84,84,84,84	0
25	MG	G	3043	1/1	0.96	0.14	84,84,84,84	0
25	MG	G	3062	1/1	0.97	0.27	84,84,84,84	0
27	ZN	G	3080	1/1	0.97	0.17	84,84,84,84	1
27	ZN	G	3081	1/1	0.99	0.04	84,84,84,84	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around PAR A 3001:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.