



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 03:45 AM UTC

PDB ID : 2UXB / pdb_00002uxb
Title : Crystal structure of an extended tRNA anticodon stem loop in complex with its cognate mRNA GGGU 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 : 3.10 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](#) ①) were used in the production of this report:

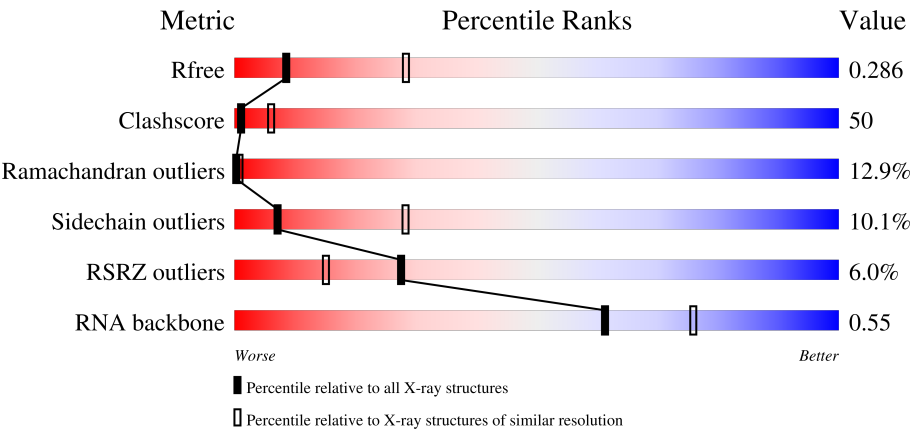
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtrriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

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 3.10 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}	180053	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)
RNA backbone	3983	1022 (3.32-2.88)

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	4% 19% 66% 12% • •
2	B	256	8% 16% 57% 17% • 8%
3	C	239	8% 18% 47% 19% • 13%
4	D	209	13% 15% 62% 21% •

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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	
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	3004	-	-	-	X
25	MG	G	3005	-	-	-	X
25	MG	G	3006	-	-	-	X
25	MG	G	3009	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	MG	G	3010	-	-	-	X
25	MG	G	3011	-	-	-	X
25	MG	G	3012	-	-	-	X
25	MG	G	3013	-	-	-	X
25	MG	G	3015	-	-	-	X
25	MG	G	3017	-	-	-	X
25	MG	G	3018	-	-	-	X
25	MG	G	3019	-	-	-	X
25	MG	G	3020	-	-	-	X
25	MG	G	3021	-	-	-	X
25	MG	G	3022	-	-	-	X
25	MG	G	3023	-	-	-	X
25	MG	G	3024	-	-	-	X
25	MG	G	3025	-	-	-	X
25	MG	G	3026	-	-	-	X
25	MG	G	3027	-	-	-	X
25	MG	G	3028	-	-	-	X
25	MG	G	3029	-	-	-	X
25	MG	G	3030	-	-	-	X
25	MG	G	3031	-	-	-	X
25	MG	G	3033	-	-	-	X
25	MG	G	3034	-	-	-	X
25	MG	G	3035	-	-	-	X
25	MG	G	3036	-	-	-	X
25	MG	G	3037	-	-	-	X
25	MG	G	3038	-	-	-	X
25	MG	G	3040	-	-	-	X
25	MG	G	3041	-	-	-	X
25	MG	G	3042	-	-	-	X
25	MG	G	3043	-	-	-	X
25	MG	G	3044	-	-	-	X
25	MG	G	3047	-	-	-	X
25	MG	G	3048	-	-	-	X
25	MG	G	3050	-	-	-	X
25	MG	G	3051	-	-	-	X
25	MG	G	3052	-	-	-	X
25	MG	G	3053	-	-	-	X
25	MG	G	3054	-	-	-	X
25	MG	G	3056	-	-	-	X
25	MG	G	3057	-	-	-	X
25	MG	G	3058	-	-	-	X
25	MG	G	3059	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	MG	G	3061	-	-	-	X
25	MG	G	3062	-	-	-	X
25	MG	G	3063	-	-	-	X
25	MG	G	3066	-	-	-	X
25	MG	G	3067	-	-	-	X
25	MG	G	3068	-	-	-	X
25	MG	G	3069	-	-	-	X
25	MG	G	3070	-	-	-	X
25	MG	G	3071	-	-	-	X
25	MG	G	3074	-	-	-	X
25	MG	G	3075	-	-	-	X
25	MG	G	3076	-	-	-	X
25	MG	G	3078	-	-	-	X
25	MG	G	3079	-	-	-	X
25	MG	G	3080	-	-	-	X
25	MG	G	3081	-	-	-	X
25	MG	G	3082	-	-	-	X
25	MG	G	3083	-	-	-	X
25	MG	G	3084	-	-	-	X
25	MG	G	3085	-	-	-	X
25	MG	G	3086	-	-	-	X
25	MG	G	3087	-	-	-	X
25	MG	G	3089	-	-	-	X
25	MG	G	3090	-	-	-	X
25	MG	G	3092	-	-	-	X
25	MG	G	3095	-	-	-	X
25	MG	G	3097	-	-	-	X
25	MG	G	3098	-	-	-	X
25	MG	G	3099	-	-	-	X
26	K	G	3134	-	-	-	X
26	K	G	3135	-	-	-	X
26	K	G	3138	-	-	-	X
26	K	G	3141	-	-	-	X

2 Entry composition

There are 27 unique types of molecules in this entry. The entry contains 52165 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	1513	Total	C	N	O	P	0	0	0
			32514	14472	6016	10513	1513			

- 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	S	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	U	25	Total	C	N	O	0	0	1
			209	128	51	30			

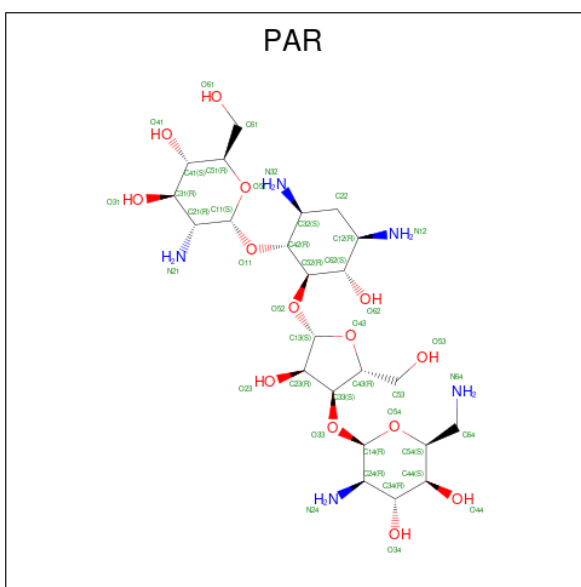
- Molecule 22 is a RNA chain called A-SITE MESSENGER RNA FRAGMENT GGGU.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	X	4	Total	C	N	O	P	0	0	0
			86	39	17	27	3			

- Molecule 23 is a RNA chain called ANTICODON STEM-LOOP OF TRANSFER RNA WITH ANTICODON ACCC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	Y	7	Total	C	N	O	P	0	0	0
			143	66	26	45	6			

- Molecule 24 is PAROMOMYCIN (CCD ID: PAR) (formula: C₂₃H₄₅N₅O₁₄).



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

- Molecule 25 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
25	G	131	Total	Mg	0	0
			131	131		

- Molecule 26 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
26	G	10	Total	K	0	0
			10	10		

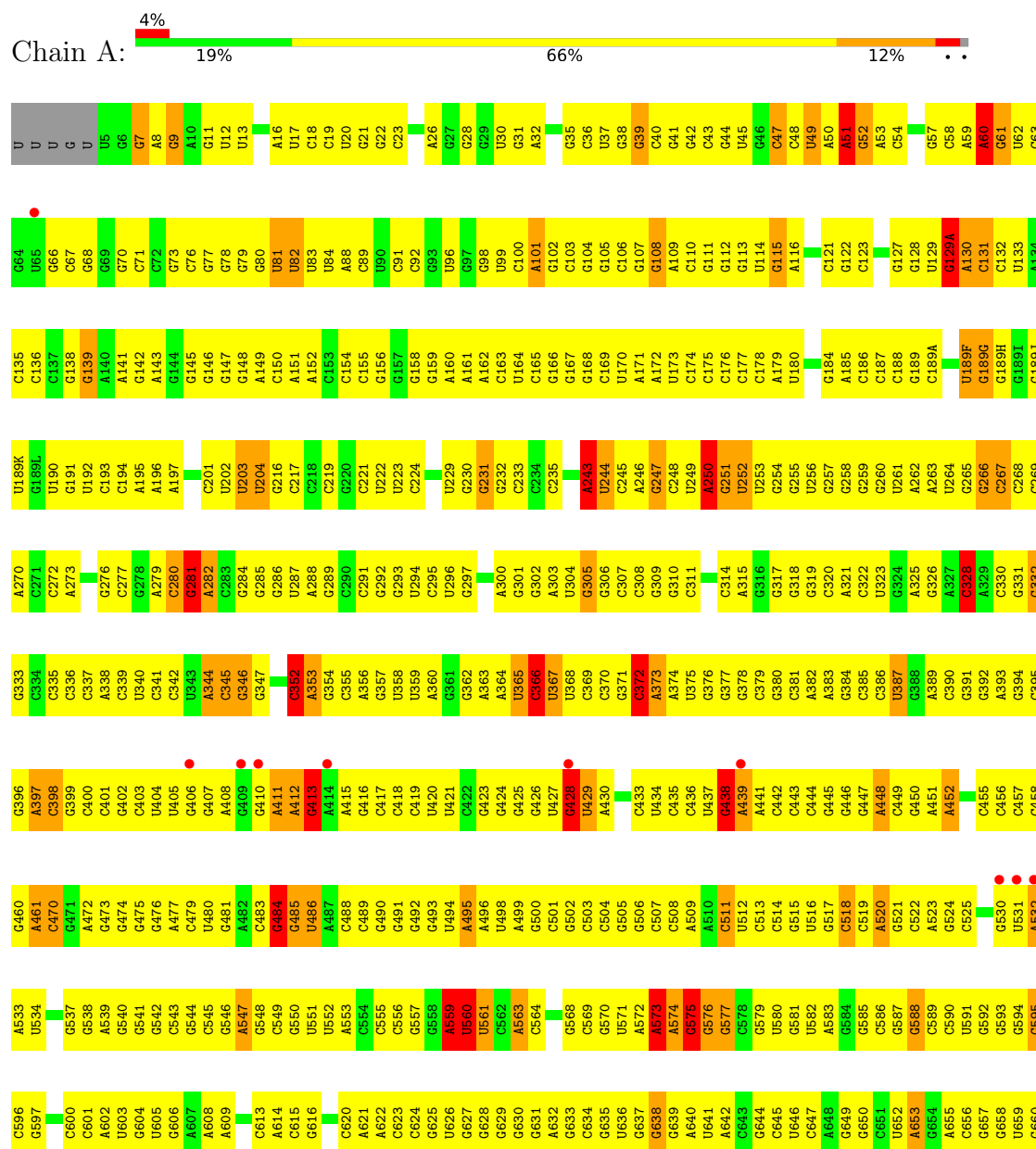
- Molecule 27 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

3 Residue-property plots

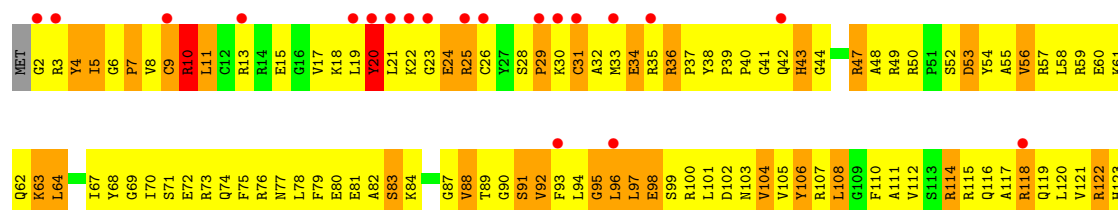
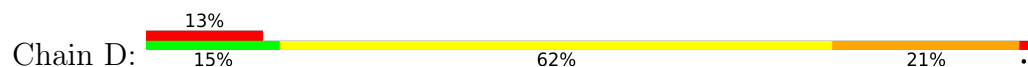
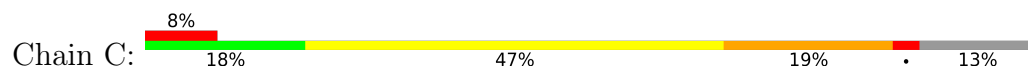
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

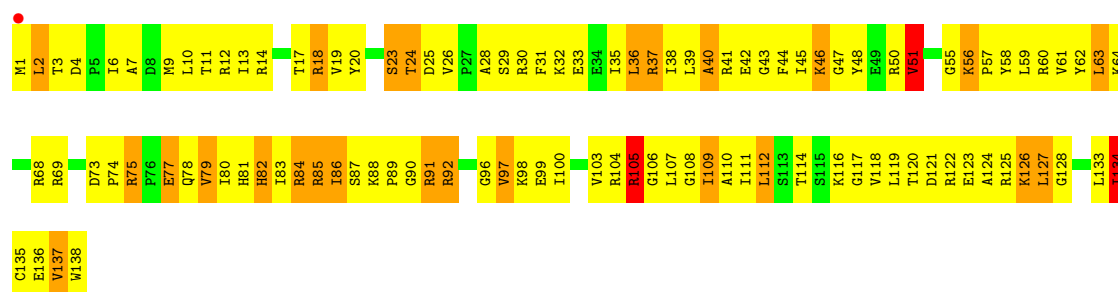
• Molecule 1: 16S RIBOSOMAL RNA



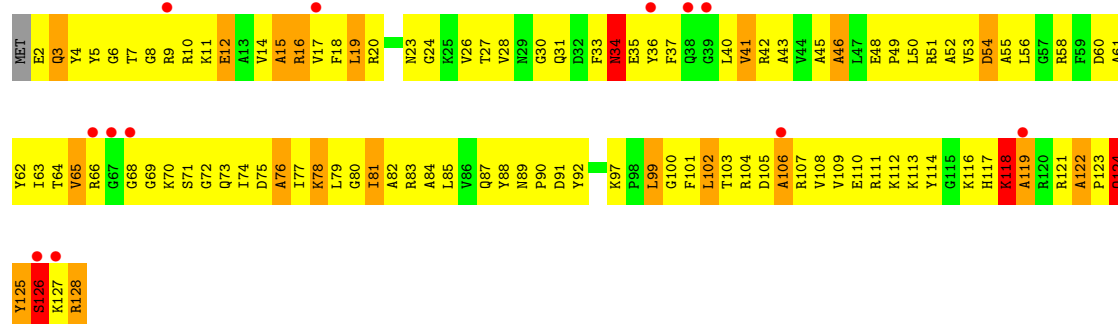
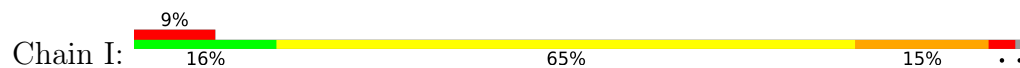
A1500	A1428	G1365	A1180	G1117	U1052	A996	C936	G867	A794	G727	G661
C1501	C1429	A1306	G1181	C1118	G1053	U997	A937	C868	C795	A728	G662
A1502	C1430	U1307	A1182	C1119	C1054	G998	A938	G869	C796		A663
A1503	C1431	G1368	A1183	G1120	A1055		A939		C797	G731	G664
G1504	G1432	C1369	A1245	U1121	U1056	A1001A	G941	A872	G798	C732	A665
G1505	A1433	G1370	G1185	U1122	U1057	G1001A	G942	A873	G799	A733	G666
U1506	A1434	G1371	G1186	A1123	G1058	G1002	G943	G874	G800	C734	G667
A1507	G1435	G1372	G1187	G1124	G1059	G1003	U943	C877	U801	C735	G668
G1508	U1436	U1373	A1188	G1125	C1060	A1004	G944	G878	A802	C736	U669
G1509	A1437	C1374	C1189	U1126	A1061	A1005	G945	C879	A807	A737	G670
U1510	A1438	U1375	G1190	G1127	U1062	C1006	A946	C890	C808	C738	
G1511	U1439	G1376	A1191	C1128	C1063	C1007	G947	C880			
U1512	C1440	C1377	C1192	C1129	G1064	C1008	C948	G881	G739	C739	G673
A1513	G1441	A1318	G1193	A1130	U1065	G1009	A949	C882	C812	U740	G674
C1514	G1442	A1319	U1194	G1131	C1066	G1010	U950	C883	U813	G741	A675
C1515	A1442A	C1320	C1196	C1132	A1067	G1011	G951		U814	G742	A676
G1516	A1442B	C1321	G1196	G1133	U1068	U1012	U952	G887	A815	U743	U677
G1517	C1443	C1322	G1197	G1134	C1069	U1013	G953	G888	A816	C744	
A1518	C1444		G1198	U1135		A1014	G954		C817	C745	G682
A1519	C1445		U1199	U1136		A1015	U955	A892	C818	A746	A684
G1520	A1446		C1200	C1137	U1072	A1016	U956	C893	A819	C747	
A1447	C1447	C1326	A1201	U1073	U1073	G1017	U957	G894	U820	G750	U686
C1452	A1452	C1327	G1202	G1074	C1075	C1018	U958	G895	G821	U751	A687
G1523	G1456	C1328	C1203	C1140	G1076	U1019	U959	C896	C822	G752	G688
C1524	A1457	U1329	C1204	C1141	U1077	U1020	U960	C899	G823	A753	G689
G1525	G1458	U1330	U1205	G1142	U1078	G1021	U961	A900	C824	G754	G690
G1526	A1459	G1331	G1206	G1143	G1079	U1022	C962	A901		G755	G691
C1527	A1460	A1332	G1207	G1144	U1080	G1023	G963	A902	A828	C756	U692
U1528	G1461	C1333	G1271	C1145	G1081	U1024	A964	G902	G829	U757	G693
G1529	C1462	G1334	G1272	U1146	C1208	G1025	A965	G903	G830	G758	A694
G1530		C1335	G1273	C1147	C1209	U1026	G966	C904	U831	A759	A695
A1531		C1336	C1210	U1085	U1085	C1027	C967	U905	C832	G760	A696
A1532	G1470	G1337	U1211	U1086	U1086	C1028	A968	G906	U833	G761	U697
C1533	G1471	U1338	U1212	G1089	G1089	C1029	A969	A907	C834	C762	G698
A1534	A1472	A1339	A1213	U1150	U1090	C1030	C970	A908	U835	G763	
C	A1473	C1340	C1214	A1151	U1091	G1030A	G971	A909	G836	C764	C701
C	G1474	U1341	G1215	A1152	A1092	G1030B	C972	C910	G837	G765	A702
C	G1475	C1342	G1216	C1153	A1093	G1030C	G973	U911	G838	A766	G703
U	G1476	G1343	C1217	G1154	U1094	A1030D	A974	C912	U839	A767	
C	U1477	C1344	C1218	G1155	U1095	G1031	A975	A914	U840	A768	A706
C1539	C1478	U1345	U1219	G1156	G1220	U1032	G976	A915	U841	C769	C707
U1540	G1479	A1346	G1221	U1157	C1096	G1033	A977	G916	C848	C708	C709
U1541	C1480	C1284	G1222	U1158		G1034	A978	G917	C849	G774	G710
U1542	U1481	A1285	G1223	U1159	G1099	A1035	C979	G918	U850	G775	G711
C1543	G1482	A1287	C1224	G1160	G1100	G1036	C980	A918	G851	G776	G712
U1544	A1483	A1288	A1225	C1161	A1101	C1037	U981	A919	G852	A777	A713
		A1289	C1226	C1162	A1102	C1038	U982	U920	G853	G778	G714
		G1290	A1227	G1163	C1103	U982	A983	U921	G854	C779	G715
	G1487	G1291	C1228	G1164	G1104	C1039	C984	G922	G855	A780	A716
	G1488	U1292	A1229	A1105	U1040	A1041	C985	A923	C856	A781	
	G1489	G1293	C1230	G1106	U1041	G1042	A986	C924	C857	A782	G717
	C1490	G1294	U1231	C1107	G1043	C1044	G987	G925	C858	C783	G718
	A1491	U1295	U1232	C1108	C1044	C1045	G988	G926	A859	A787	C719
	A1492	C1296	U1233	C1109	A1044	C1046	G989	G927	A860	C720	G721
	A1493	G1297	G1233	A1110	C1045	G1047	C990	G928	G861	U788	G722
	U1494	A1298	C1237	C1111	G1047	G1048	C991	G929	C862	U789	A723
	U1495	A1299	A1288	C1112	G1048	U1049	U992	G933	U863	A790	G724
	C1496	G1300	A1289	C1113	G1049	C1050	G993	G934	A864	G791	G725
	U1497	U1301	A1299	C1114	U1049	C1051	A994	A994	A865	A792	
	U1498	C1363	A1230	C1115	C1115		C995		C866	U793	C726
	C1426	A1363A	U1240	C1116	C1116						
	U1427	U1364	G1241	A1179							

Chain B: 8% 16% 57% 17% 8%

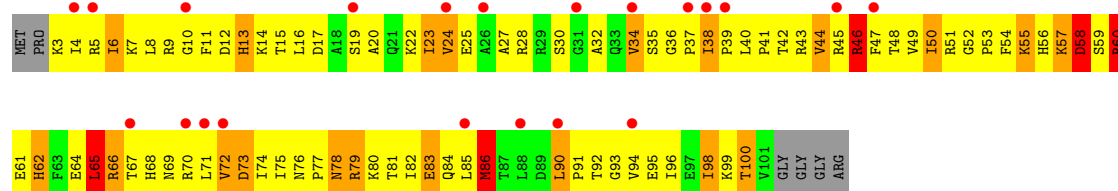
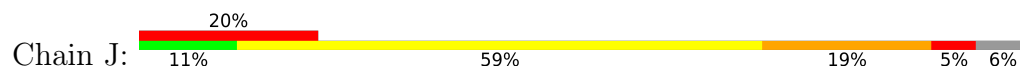




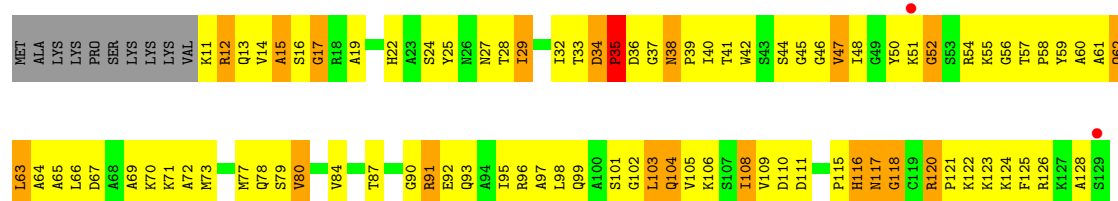
• Molecule 9: RIBOSOMAL PROTEIN S9



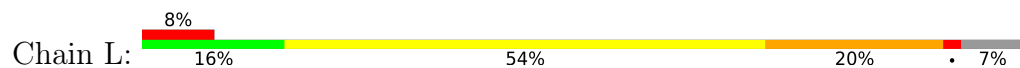
• Molecule 10: RIBOSOMAL PROTEIN S10

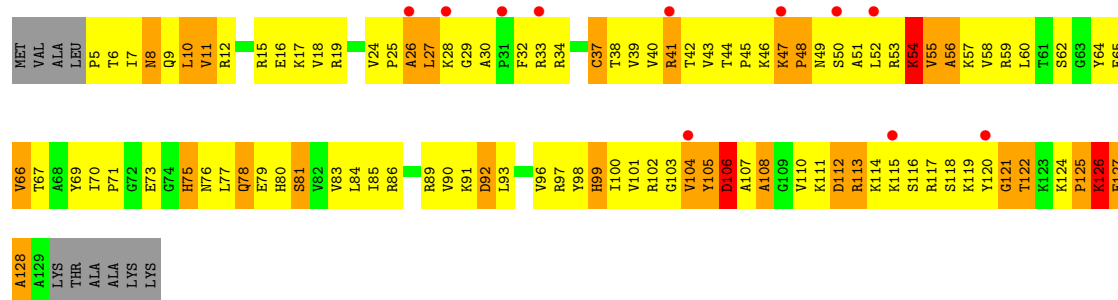


• Molecule 11: RIBOSOMAL PROTEIN S11



• Molecule 12: RIBOSOMAL PROTEIN S12

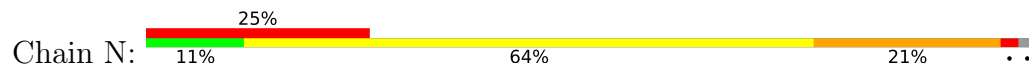




• Molecule 13: RIBOSOMAL PROTEIN S13



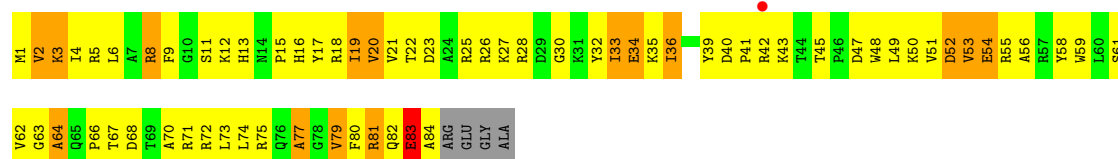
• Molecule 14: RIBOSOMAL PROTEIN S14



• Molecule 15: RIBOSOMAL PROTEIN S15



• Molecule 16: RIBOSOMAL PROTEIN S16



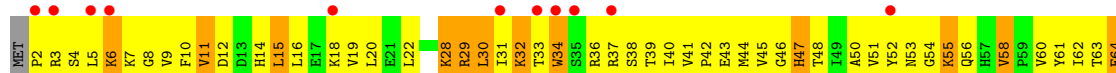
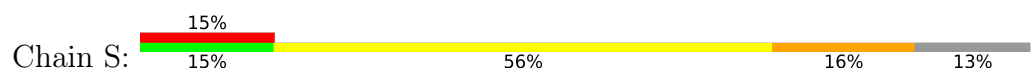
- Molecule 17: RIBOSOMAL PROTEIN S17



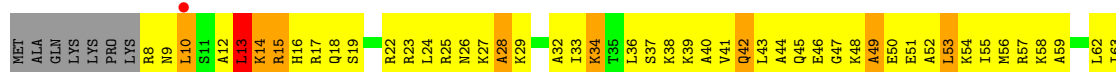
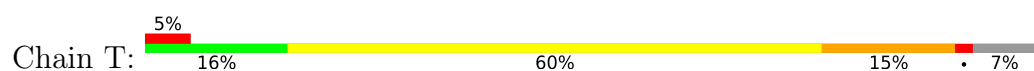
- Molecule 18: RIBOSOMAL PROTEIN S18



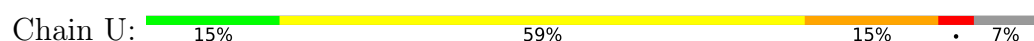
- Molecule 19: RIBOSOMAL PROTEIN S19



- Molecule 20: RIBOSOMAL PROTEIN S20



- Molecule 21: RIBOSOMAL PROTEIN THX



- Molecule 22: A-SITE MESSENGER RNA FRAGMENT GGGU



● Molecule 23: ANTICODON STEM-LOOP OF TRANSFER RNA WITH ANTICODON ACCC



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	401.95Å 401.95Å 174.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.88 – 3.10 29.88 – 3.10	Depositor EDS
% Data completeness (in resolution range)	98.1 (29.88-3.10) 98.0 (29.88-3.10)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.74 (at 3.01Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.295 , 0.328 0.239 , 0.286	Depositor DCC
R_{free} test set	13830 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	67.7	Xtriage
Anisotropy	0.071	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.23 , 70.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	52165	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.55% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, K, PAR, 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	0.49	1/36393 (0.0%)	0.74	52/56797 (0.1%)
2	B	0.47	1/1936 (0.1%)	1.02	10/2611 (0.4%)
3	C	0.43	1/1637 (0.1%)	0.97	11/2207 (0.5%)
4	D	0.42	0/1733	1.00	9/2318 (0.4%)
5	E	0.67	1/1163 (0.1%)	1.08	9/1566 (0.6%)
6	F	0.41	0/856	0.92	1/1154 (0.1%)
7	G	0.38	0/1276	0.94	11/1709 (0.6%)
8	H	0.75	0/1136	1.35	16/1527 (1.0%)
9	I	0.43	0/1029	1.08	11/1378 (0.8%)
10	J	0.45	1/806 (0.1%)	1.03	5/1084 (0.5%)
11	K	0.56	0/900	1.10	8/1213 (0.7%)
12	L	0.54	1/987 (0.1%)	1.13	6/1322 (0.5%)
13	M	0.43	0/1008	0.95	5/1347 (0.4%)
14	N	0.40	0/501	0.95	1/664 (0.2%)
15	O	0.54	0/745	0.92	2/992 (0.2%)
16	P	0.65	1/717 (0.1%)	1.13	7/965 (0.7%)
17	Q	0.62	0/870	1.12	4/1159 (0.3%)
18	R	0.49	0/603	1.02	4/799 (0.5%)
19	S	0.43	1/662 (0.2%)	0.97	2/892 (0.2%)
20	T	0.50	0/764	1.09	6/1006 (0.6%)
21	U	0.66	1/213 (0.5%)	1.03	1/279 (0.4%)
22	X	0.41	0/96	0.78	0/149
23	Y	0.52	0/159	0.83	0/245
All	All	0.50	9/56190 (0.0%)	0.85	181/83383 (0.2%)

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	1	41

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	154	GLY	C-N	-5.72	1.25	1.33
3	C	207	VAL	C-N	-5.70	1.25	1.33
12	L	128	ALA	C-N	-5.68	1.25	1.33
16	P	83	GLU	C-N	-5.68	1.25	1.33
2	B	240	GLN	C-N	-5.68	1.25	1.33

The worst 5 of 181 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1532	U	P-O3'-C3'	21.15	151.92	120.20
1	A	1498	U	C2'-C3'-O3'	14.41	131.11	109.50
1	A	115	G	C2'-C3'-O3'	13.15	129.22	109.50
1	A	1532	U	C4'-C3'-O3'	12.96	132.44	113.00
19	S	58	VAL	N-CA-C	11.90	118.86	108.63

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	1498	U	C3'

5 of 41 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	108	G	Sidechain
1	A	189(G)	G	Sidechain
1	A	250	A	Sidechain
1	A	280	C	Sidechain
1	A	297	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	32514	0	16412	1693	0
2	B	1901	0	1951	338	0
3	C	1613	0	1677	302	0
4	D	1703	0	1764	263	0
5	E	1147	0	1207	175	0
6	F	843	0	857	85	0
7	G	1257	0	1296	182	0
8	H	1116	0	1177	154	0
9	I	1011	0	1043	195	0
10	J	793	0	835	183	0
11	K	885	0	904	137	0
12	L	971	0	1057	181	0
13	M	997	0	1072	129	0
14	N	492	0	531	107	0
15	O	734	0	771	96	0
16	P	701	0	720	103	0
17	Q	857	0	930	117	0
18	R	597	0	666	89	0
19	S	648	0	673	86	0
20	T	762	0	859	111	0
21	U	209	0	221	36	0
22	X	86	0	45	6	0
23	Y	143	0	78	15	0
24	A	42	0	45	2	0
25	G	131	0	0	0	0
26	G	10	0	0	0	0
27	G	2	0	0	0	0
All	All	52165	0	36791	4398	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 50.

The worst 5 of 4398 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:1539:C:C5	7:G:81:GLY:O	1.88	1.24
1:A:1347:G:N2	1:A:1373:G:H2'	1.58	1.19
1:A:1442(A):G:H5''	1:A:1442(B):A:H5'	1.28	1.15
11:K:48:ILE:HD13	11:K:63:LEU:HB2	1.27	1.15
1:A:1347:G:H22	1:A:1373:G:H2'	1.09	1.15

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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%)	134 (58%)	72 (31%)	27 (12%)	0	1
3	C	205/239 (86%)	116 (57%)	42 (20%)	47 (23%)	0	0
4	D	206/209 (99%)	125 (61%)	47 (23%)	34 (16%)	0	0
5	E	149/162 (92%)	109 (73%)	25 (17%)	15 (10%)	0	3
6	F	99/101 (98%)	72 (73%)	24 (24%)	3 (3%)	3	19
7	G	153/156 (98%)	78 (51%)	44 (29%)	31 (20%)	0	0
8	H	136/138 (99%)	105 (77%)	23 (17%)	8 (6%)	1	8
9	I	125/128 (98%)	80 (64%)	34 (27%)	11 (9%)	0	3
10	J	97/105 (92%)	56 (58%)	24 (25%)	17 (18%)	0	0
11	K	117/129 (91%)	83 (71%)	25 (21%)	9 (8%)	1	4
12	L	123/135 (91%)	70 (57%)	33 (27%)	20 (16%)	0	0
13	M	123/126 (98%)	74 (60%)	29 (24%)	20 (16%)	0	0
14	N	58/61 (95%)	31 (53%)	18 (31%)	9 (16%)	0	0
15	O	86/89 (97%)	43 (50%)	38 (44%)	5 (6%)	1	8
16	P	82/88 (93%)	52 (63%)	22 (27%)	8 (10%)	0	3
17	Q	102/105 (97%)	70 (69%)	26 (26%)	6 (6%)	1	8
18	R	71/88 (81%)	47 (66%)	15 (21%)	9 (13%)	0	1
19	S	79/93 (85%)	47 (60%)	17 (22%)	15 (19%)	0	0
20	T	97/106 (92%)	52 (54%)	37 (38%)	8 (8%)	0	4
21	U	23/27 (85%)	17 (74%)	3 (13%)	3 (13%)	0	1
All	All	2364/2541 (93%)	1461 (62%)	598 (25%)	305 (13%)	0	1

5 of 305 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	9	GLU

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Mol	Chain	Res	Type
2	B	15	VAL
2	B	16	HIS
2	B	17	PHE
2	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	
2	B	202/220 (92%)	178 (88%)	24 (12%)	5	21
3	C	160/188 (85%)	147 (92%)	13 (8%)	11	36
4	D	180/181 (99%)	165 (92%)	15 (8%)	10	35
5	E	115/123 (94%)	96 (84%)	19 (16%)	2	11
6	F	90/90 (100%)	78 (87%)	12 (13%)	4	17
7	G	126/127 (99%)	117 (93%)	9 (7%)	13	41
8	H	119/119 (100%)	101 (85%)	18 (15%)	3	13
9	I	98/99 (99%)	86 (88%)	12 (12%)	5	20
10	J	87/92 (95%)	77 (88%)	10 (12%)	5	23
11	K	90/99 (91%)	81 (90%)	9 (10%)	7	29
12	L	104/111 (94%)	96 (92%)	8 (8%)	12	38
13	M	100/101 (99%)	93 (93%)	7 (7%)	14	41
14	N	49/50 (98%)	42 (86%)	7 (14%)	3	14
15	O	79/80 (99%)	70 (89%)	9 (11%)	5	23
16	P	72/74 (97%)	67 (93%)	5 (7%)	14	41
17	Q	96/97 (99%)	89 (93%)	7 (7%)	13	40
18	R	64/77 (83%)	64 (100%)	0	100	100
19	S	71/80 (89%)	67 (94%)	4 (6%)	19	49
20	T	76/82 (93%)	65 (86%)	11 (14%)	3	14
21	U	19/22 (86%)	16 (84%)	3 (16%)	2	12

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1997/2112 (95%)	1795 (90%)	202 (10%)	7 28

5 of 202 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
9	I	41	VAL
12	L	54	LYS
21	U	8	THR
9	I	118	LYS
10	J	95	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 68 such sidechains are listed below:

Mol	Chain	Res	Type
16	P	13	HIS
16	P	65	GLN
20	T	18	GLN
6	F	13	ASN
5	E	127	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1512/1522 (99%)	221 (14%)	50 (3%)
22	X	3/4 (75%)	1 (33%)	0
23	Y	6/18 (33%)	1 (16%)	0
All	All	1521/1544 (98%)	223 (14%)	50 (3%)

5 of 223 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	8	A
1	A	9	G
1	A	31	G
1	A	32	A
1	A	39	G

5 of 50 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	975	A
1	A	1183	A
1	A	1532	U
1	A	992	U
1	A	1067	A

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 144 ligands modelled in this entry, 143 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	-	44,45,45	1.40	6 (13%)	63,67,67	1.10	6 (9%)

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	-	-	3/18/94/94	0/4/4/4

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	3001	PAR	O54-C14	3.22	1.50	1.41
24	A	3001	PAR	C34-C24	3.09	1.57	1.53
24	A	3001	PAR	C52-C42	3.04	1.58	1.52
24	A	3001	PAR	C31-C21	2.44	1.56	1.53
24	A	3001	PAR	C11-C21	2.41	1.57	1.52

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	3001	PAR	O54-C54-C64	3.52	112.83	106.07
24	A	3001	PAR	C14-O54-C54	2.99	119.56	113.72
24	A	3001	PAR	O52-C13-O43	-2.54	108.77	111.37
24	A	3001	PAR	O11-C11-C21	2.28	111.81	108.08
24	A	3001	PAR	C11-O51-C51	2.15	117.91	113.72

There are no chirality outliers.

All (3) torsion outliers are listed below:

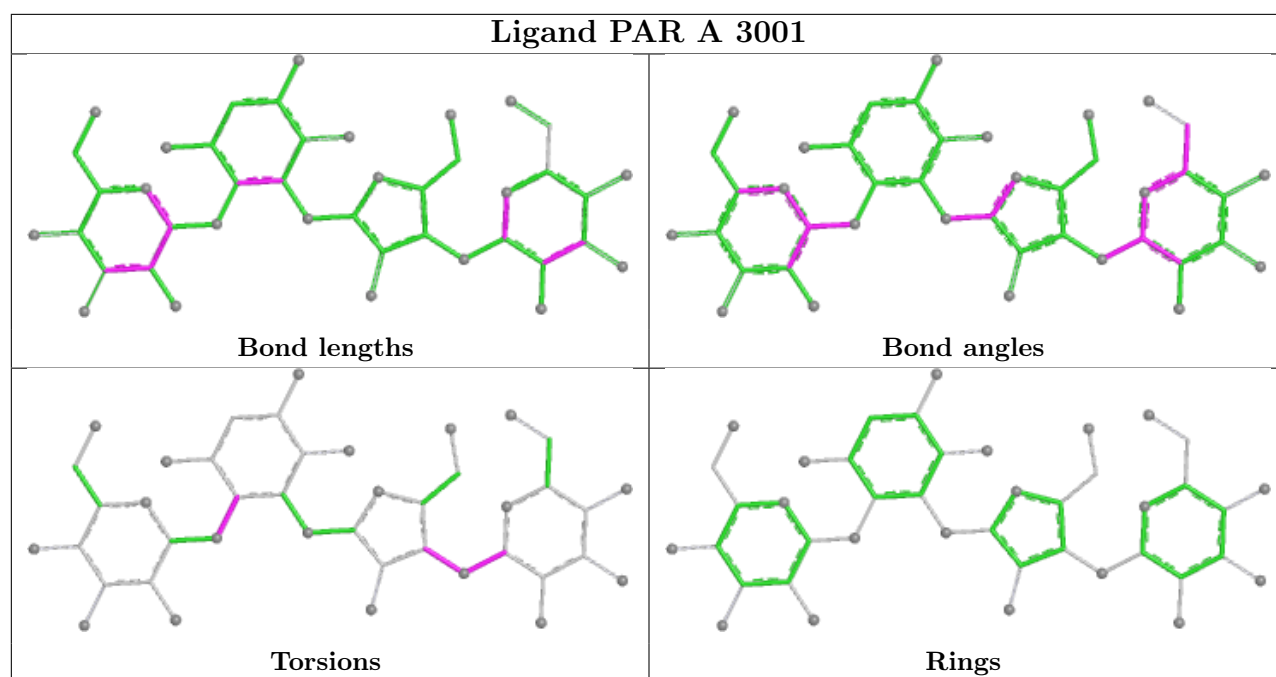
Mol	Chain	Res	Type	Atoms
24	A	3001	PAR	C52-C42-O11-C11
24	A	3001	PAR	C24-C14-O33-C33
24	A	3001	PAR	C43-C33-O33-C14

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	A	3001	PAR	2	0

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, 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	1513/1522 (99%)	0.11	60 (3%) 42 23	18, 65, 147, 201	0
2	B	235/256 (91%)	0.44	21 (8%) 15 8	27, 82, 159, 197	0
3	C	207/239 (86%)	0.57	18 (8%) 16 9	41, 101, 167, 197	0
4	D	208/209 (99%)	0.53	27 (12%) 7 4	28, 78, 139, 160	0
5	E	151/162 (93%)	-0.24	1 (0%) 84 68	14, 46, 91, 164	0
6	F	101/101 (100%)	0.10	1 (0%) 79 61	42, 83, 133, 151	0
7	G	155/156 (99%)	0.34	8 (5%) 33 17	36, 97, 162, 197	0
8	H	138/138 (100%)	-0.51	1 (0%) 84 68	9, 35, 83, 108	0
9	I	127/128 (99%)	0.65	12 (9%) 14 8	23, 98, 159, 190	0
10	J	99/105 (94%)	1.18	21 (21%) 2 1	41, 139, 192, 197	0
11	K	119/129 (92%)	-0.05	2 (1%) 69 48	19, 64, 129, 178	0
12	L	125/135 (92%)	0.38	11 (8%) 15 9	5, 75, 133, 187	0
13	M	125/126 (99%)	0.59	15 (12%) 9 5	36, 86, 165, 197	0
14	N	60/61 (98%)	1.29	15 (25%) 2 1	42, 92, 187, 193	0
15	O	88/89 (98%)	-0.34	0 100 100	21, 55, 102, 154	0
16	P	84/88 (95%)	-0.16	1 (1%) 76 58	24, 48, 91, 140	0
17	Q	104/105 (99%)	-0.07	3 (2%) 53 32	17, 49, 117, 197	0
18	R	73/88 (82%)	-0.21	0 100 100	29, 64, 142, 187	0
19	S	81/93 (87%)	1.25	14 (17%) 4 2	84, 133, 174, 197	0
20	T	99/106 (93%)	0.20	5 (5%) 33 18	33, 63, 121, 151	0
21	U	25/27 (92%)	0.37	0 100 100	47, 69, 115, 123	0
22	X	4/4 (100%)	0.88	1 (25%) 2 1	87, 92, 100, 115	0
23	Y	7/18 (38%)	0.58	0 100 100	88, 120, 170, 196	0
All	All	3928/4085 (96%)	0.23	237 (6%) 27 15	5, 72, 157, 201	0

The worst 5 of 237 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
19	S	82	GLY	13.2
13	M	124	PRO	8.6
14	N	30	ALA	8.6
4	D	2	GLY	7.9
14	N	2	ALA	6.9

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 oligosaccharides 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($\text{\AA}^2$)	Q<0.9
25	MG	G	3083	1/1	0.01	1.23	162,162,162,162	0
25	MG	G	3027	1/1	0.05	0.72	89,89,89,89	0
25	MG	G	3025	1/1	0.11	1.85	113,113,113,113	0
25	MG	G	3044	1/1	0.12	1.02	109,109,109,109	0
25	MG	G	3082	1/1	0.18	0.43	121,121,121,121	0
25	MG	G	3079	1/1	0.19	0.89	128,128,128,128	0
25	MG	G	3076	1/1	0.21	0.94	143,143,143,143	0
25	MG	G	3056	1/1	0.21	2.17	113,113,113,113	0
25	MG	G	3038	1/1	0.27	1.20	99,99,99,99	0
25	MG	G	3034	1/1	0.28	0.53	103,103,103,103	0
25	MG	G	3018	1/1	0.32	0.71	96,96,96,96	0
25	MG	G	3066	1/1	0.34	0.54	102,102,102,102	0
25	MG	G	3052	1/1	0.36	1.19	99,99,99,99	0
25	MG	G	3068	1/1	0.36	1.22	102,102,102,102	0
25	MG	G	3061	1/1	0.37	2.20	124,124,124,124	0
25	MG	G	3022	1/1	0.41	1.53	126,126,126,126	0
25	MG	G	3040	1/1	0.41	1.48	121,121,121,121	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
25	MG	G	3098	1/1	0.42	0.45	81,81,81,81	0
25	MG	G	3005	1/1	0.44	1.01	95,95,95,95	0
25	MG	G	3058	1/1	0.47	0.85	89,89,89,89	0
25	MG	G	3009	1/1	0.49	1.16	90,90,90,90	0
25	MG	G	3078	1/1	0.50	0.67	118,118,118,118	0
25	MG	G	3003	1/1	0.51	1.38	102,102,102,102	0
25	MG	G	3043	1/1	0.52	0.66	105,105,105,105	0
25	MG	G	3090	1/1	0.52	1.14	123,123,123,123	0
25	MG	G	3031	1/1	0.52	1.29	82,82,82,82	0
26	K	G	3142	1/1	0.52	0.27	156,156,156,156	0
25	MG	G	3089	1/1	0.53	0.69	106,106,106,106	0
25	MG	G	3099	1/1	0.54	0.62	102,102,102,102	0
25	MG	G	3092	1/1	0.55	0.68	97,97,97,97	0
25	MG	G	3020	1/1	0.55	1.27	115,115,115,115	0
25	MG	G	3075	1/1	0.56	1.24	134,134,134,134	0
25	MG	G	3122	1/1	0.57	0.34	77,77,77,77	0
25	MG	G	3010	1/1	0.58	1.38	103,103,103,103	0
25	MG	G	3012	1/1	0.58	1.50	101,101,101,101	0
25	MG	G	3057	1/1	0.59	0.87	86,86,86,86	0
25	MG	G	3048	1/1	0.59	1.37	100,100,100,100	0
25	MG	G	3019	1/1	0.60	0.57	92,92,92,92	0
25	MG	G	3035	1/1	0.60	1.14	103,103,103,103	0
25	MG	G	3017	1/1	0.60	0.77	110,110,110,110	0
25	MG	G	3042	1/1	0.61	1.03	103,103,103,103	0
25	MG	G	3030	1/1	0.61	0.59	83,83,83,83	0
25	MG	G	3059	1/1	0.63	0.77	93,93,93,93	0
25	MG	G	3037	1/1	0.64	0.64	90,90,90,90	0
25	MG	G	3053	1/1	0.64	1.46	96,96,96,96	0
26	K	G	3138	1/1	0.65	0.47	146,146,146,146	0
25	MG	G	3084	1/1	0.65	0.75	97,97,97,97	0
25	MG	G	3036	1/1	0.66	1.52	96,96,96,96	0
25	MG	G	3028	1/1	0.66	0.69	90,90,90,90	0
25	MG	G	3118	1/1	0.67	0.22	46,46,46,46	0
25	MG	G	3081	1/1	0.67	1.15	110,110,110,110	0
25	MG	G	3004	1/1	0.67	0.48	89,89,89,89	0
26	K	G	3141	1/1	0.67	0.57	145,145,145,145	0
25	MG	G	3080	1/1	0.67	0.58	108,108,108,108	0
25	MG	G	3033	1/1	0.68	0.67	84,84,84,84	0
25	MG	G	3013	1/1	0.68	0.59	103,103,103,103	0
25	MG	G	3015	1/1	0.68	0.90	87,87,87,87	0
26	K	G	3140	1/1	0.69	0.34	161,161,161,161	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
25	MG	G	3041	1/1	0.71	1.45	116,116,116,116	0
25	MG	G	3067	1/1	0.71	1.67	102,102,102,102	0
25	MG	G	3024	1/1	0.71	0.80	102,102,102,102	0
25	MG	G	3070	1/1	0.71	1.17	106,106,106,106	0
25	MG	G	3054	1/1	0.72	0.65	95,95,95,95	0
25	MG	G	3047	1/1	0.72	1.08	87,87,87,87	0
25	MG	G	3096	1/1	0.72	0.19	43,43,43,43	0
25	MG	G	3097	1/1	0.72	0.58	100,100,100,100	0
26	K	G	3137	1/1	0.73	0.26	123,123,123,123	0
25	MG	G	3021	1/1	0.73	0.68	108,108,108,108	0
25	MG	G	3071	1/1	0.73	0.74	89,89,89,89	0
25	MG	G	3006	1/1	0.73	0.80	92,92,92,92	0
25	MG	G	3069	1/1	0.73	0.76	97,97,97,97	0
26	K	G	3135	1/1	0.74	0.58	135,135,135,135	0
26	K	G	3133	1/1	0.74	0.30	107,107,107,107	0
25	MG	G	3029	1/1	0.75	0.81	112,112,112,112	0
25	MG	G	3011	1/1	0.75	0.63	106,106,106,106	0
25	MG	G	3023	1/1	0.75	0.80	91,91,91,91	0
25	MG	G	3087	1/1	0.75	0.69	102,102,102,102	0
25	MG	G	3062	1/1	0.75	1.07	114,114,114,114	0
25	MG	G	3110	1/1	0.76	0.19	44,44,44,44	0
25	MG	G	3074	1/1	0.76	0.92	112,112,112,112	0
26	K	G	3134	1/1	0.76	0.64	131,131,131,131	0
25	MG	G	3086	1/1	0.77	0.59	102,102,102,102	0
25	MG	G	3063	1/1	0.78	0.97	96,96,96,96	0
25	MG	G	3026	1/1	0.79	0.73	108,108,108,108	0
25	MG	G	3051	1/1	0.79	0.46	80,80,80,80	0
25	MG	G	3095	1/1	0.79	0.49	74,74,74,74	0
25	MG	G	3085	1/1	0.79	1.18	116,116,116,116	0
25	MG	G	3113	1/1	0.79	0.16	31,31,31,31	0
25	MG	G	3050	1/1	0.80	0.96	97,97,97,97	0
25	MG	G	3102	1/1	0.80	0.10	53,53,53,53	0
25	MG	G	3039	1/1	0.81	0.97	96,96,96,96	0
25	MG	G	3117	1/1	0.81	0.26	53,53,53,53	0
25	MG	G	3032	1/1	0.82	0.82	107,107,107,107	0
25	MG	G	3073	1/1	0.83	0.30	93,93,93,93	0
25	MG	G	3055	1/1	0.83	1.07	91,91,91,91	0
25	MG	G	3108	1/1	0.84	0.45	58,58,58,58	0
25	MG	G	3045	1/1	0.84	1.08	87,87,87,87	0
25	MG	G	3007	1/1	0.84	1.20	89,89,89,89	0
25	MG	G	3100	1/1	0.84	0.59	45,45,45,45	0

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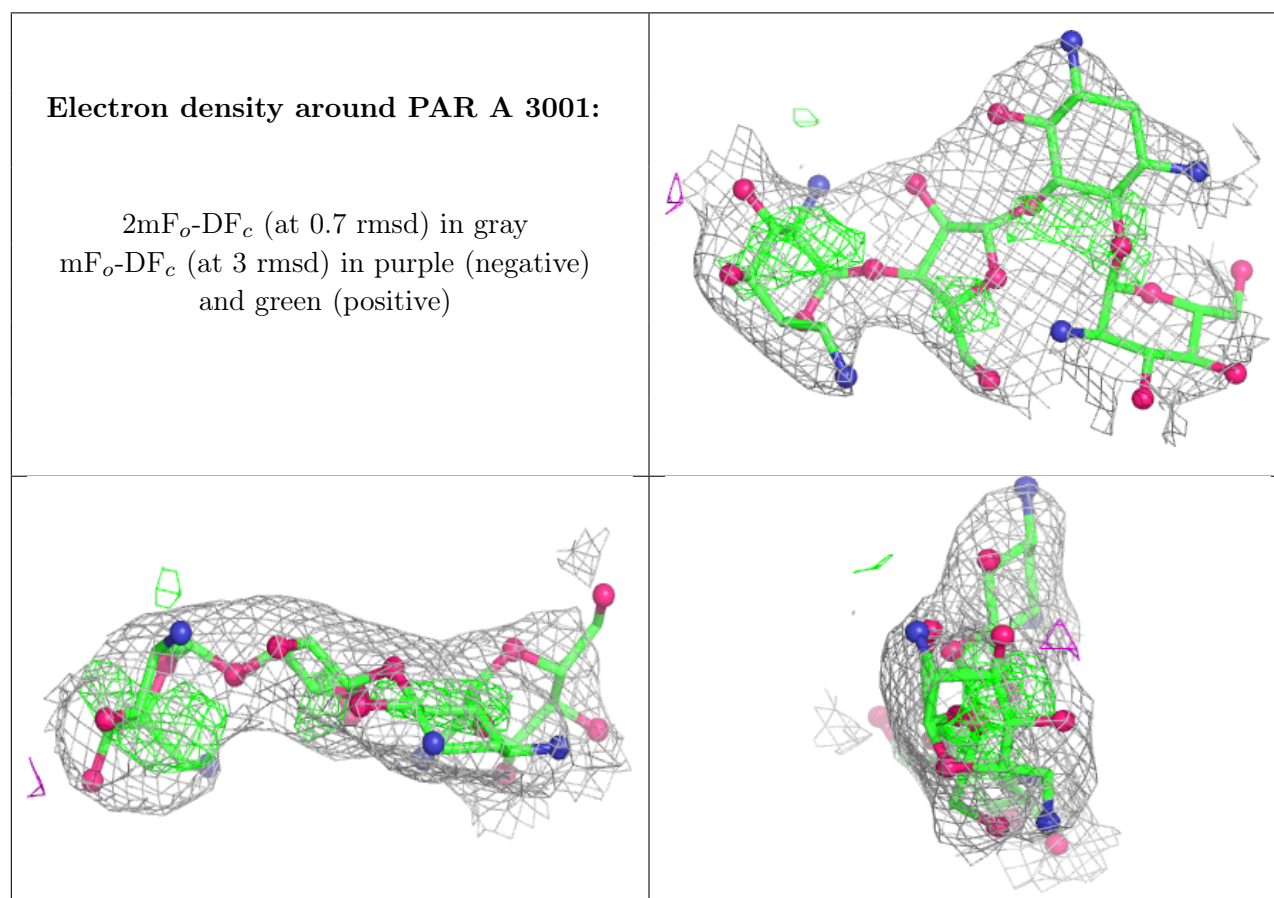
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
25	MG	G	3016	1/1	0.84	0.71	93,93,93,93	0
25	MG	G	3104	1/1	0.84	0.70	47,47,47,47	0
25	MG	G	3123	1/1	0.84	0.18	35,35,35,35	0
25	MG	G	3130	1/1	0.84	0.27	47,47,47,47	0
26	K	G	3139	1/1	0.85	0.49	150,150,150,150	0
25	MG	G	3088	1/1	0.85	1.07	113,113,113,113	0
25	MG	G	3116	1/1	0.85	0.14	43,43,43,43	0
25	MG	G	3072	1/1	0.85	0.32	61,61,61,61	0
25	MG	G	3014	1/1	0.86	0.87	101,101,101,101	0
25	MG	G	3077	1/1	0.86	0.86	103,103,103,103	0
25	MG	G	3121	1/1	0.86	0.22	56,56,56,56	0
25	MG	G	3094	1/1	0.87	0.27	49,49,49,49	0
25	MG	G	3064	1/1	0.88	0.89	83,83,83,83	0
25	MG	G	3049	1/1	0.88	0.48	78,78,78,78	0
25	MG	G	3132	1/1	0.88	0.54	51,51,51,51	0
25	MG	G	3091	1/1	0.88	1.07	110,110,110,110	0
25	MG	G	3008	1/1	0.89	1.42	100,100,100,100	0
25	MG	G	3120	1/1	0.89	0.17	59,59,59,59	0
25	MG	G	3119	1/1	0.90	0.20	47,47,47,47	0
26	K	G	3136	1/1	0.90	0.43	105,105,105,105	0
25	MG	G	3046	1/1	0.90	0.58	77,77,77,77	0
25	MG	G	3101	1/1	0.90	0.42	56,56,56,56	0
25	MG	G	3103	1/1	0.91	0.44	52,52,52,52	0
25	MG	G	3125	1/1	0.91	0.19	60,60,60,60	0
25	MG	G	3129	1/1	0.91	0.11	48,48,48,48	0
25	MG	G	3114	1/1	0.91	0.06	38,38,38,38	0
25	MG	G	3106	1/1	0.91	0.14	39,39,39,39	0
25	MG	G	3002	1/1	0.92	0.20	79,79,79,79	0
25	MG	G	3128	1/1	0.92	0.28	58,58,58,58	0
25	MG	G	3112	1/1	0.92	0.28	51,51,51,51	0
25	MG	G	3065	1/1	0.92	1.13	87,87,87,87	0
25	MG	G	3109	1/1	0.92	0.48	57,57,57,57	0
27	ZN	G	3143	1/1	0.92	0.37	118,118,118,118	0
25	MG	G	3093	1/1	0.93	0.61	71,71,71,71	0
24	PAR	A	3001	42/42	0.93	0.16	67,70,81,87	0
25	MG	G	3111	1/1	0.93	0.16	54,54,54,54	0
25	MG	G	3115	1/1	0.94	0.08	49,49,49,49	0
25	MG	G	3127	1/1	0.95	0.20	49,49,49,49	0
25	MG	G	3107	1/1	0.95	0.28	59,59,59,59	0
25	MG	G	3060	1/1	0.95	0.61	91,91,91,91	0
25	MG	G	3126	1/1	0.95	0.06	45,45,45,45	0
25	MG	G	3124	1/1	0.96	0.10	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
25	MG	G	3131	1/1	0.97	0.14	30,30,30,30	0
25	MG	G	3105	1/1	0.98	0.12	44,44,44,44	0
27	ZN	G	3144	1/1	0.99	0.12	97,97,97,97	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.



6.5 Other polymers [i](#)

There are no such residues in this entry.