



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 24, 2026 – 01:44 AM UTC

PDB ID : 2F4V / pdb_00002f4v
Title : 30S ribosome + designer antibiotic
Authors : Murray, J.B.; Meroueh, S.O.; Russell, R.J.; Lentzen, G.; Haddad, J.; Mobashery, S.
Deposited on : 2005-11-24
Resolution : 3.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

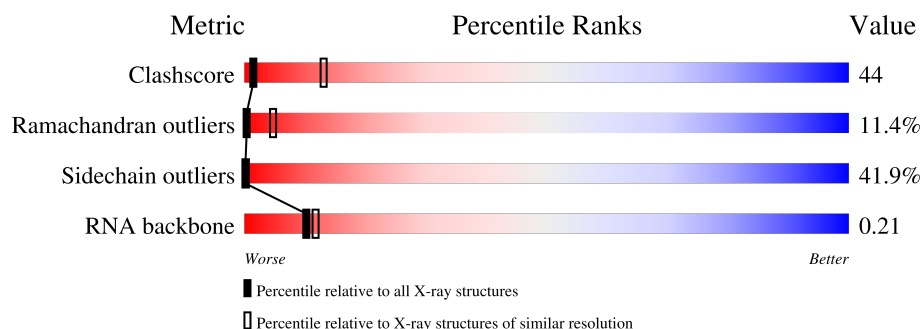
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.80 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))
Clashscore	190562	1012 (3.94-3.66)
Ramachandran outliers	187476	1048 (3.96-3.64)
Sidechain outliers	187428	1043 (3.96-3.64)
RNA backbone	3983	1007 (4.50-3.10)

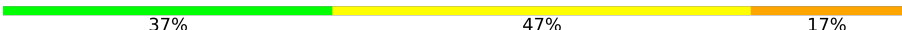
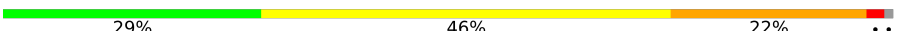
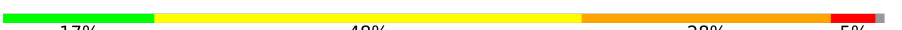
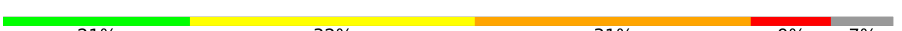
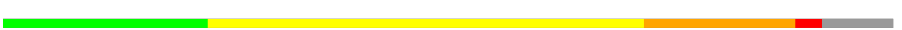
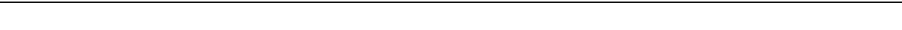
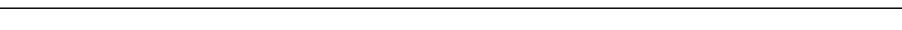
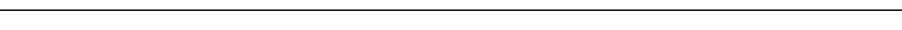
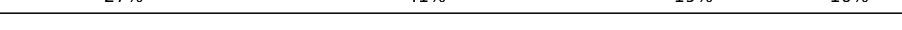
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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 $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	1511	14% 41% 34% 11%
2	Z	4	75% 25%
3	B	256	15% 48% 26% • 7%
4	C	239	18% 38% 24% 6% 14%
5	D	209	21% 47% 27% 5%
6	E	162	16% 39% 30% 7% 7%

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Mol	Chain	Length	Quality of chain
7	F	101	
8	G	156	
9	H	138	
10	I	128	
11	J	105	
12	K	129	
13	L	132	
14	M	126	
15	N	61	
16	O	89	
17	P	88	
18	Q	105	
19	R	88	
20	S	93	
21	T	106	

2 Entry composition [i](#)

There are 26 unique types of molecules in this entry. The entry contains 51728 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	22	0	0
			32391	14418	6002	10465	1506			

- Molecule 2 is a RNA chain called 5'-R(P*UP*UP*CP*U)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	Z	4	Total	C	N	O	P	0	0	0
			80	36	9	31	4			

- Molecule 3 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	B	237	Total	C	N	O	S	0	0	0
			1923	1226	344	348	5			

- Molecule 4 is a protein called 30S ribosomal protein S3.

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

- Molecule 5 is a protein called 30S ribosomal protein S4.

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	199	GLN	ASN	conflict	UNP P80373
D	201	ASN	GLN	conflict	UNP P80373

- Molecule 6 is a protein called 30S ribosomal protein S5.

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

- Molecule 7 is a protein called 30S ribosomal protein S6.

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

- Molecule 8 is a protein called 30S ribosomal protein S7.

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

- Molecule 9 is a protein called 30S ribosomal protein S8.

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

- Molecule 10 is a protein called 30S ribosomal protein S9.

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

- Molecule 11 is a protein called 30S ribosomal protein S10.

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

- Molecule 12 is a protein called 30S ribosomal protein S11.

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

- Molecule 13 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	L	125	Total	C	N	O	S	0	0	0
			975	614	196	164	1			

- Molecule 14 is a protein called 30S ribosomal protein S13.

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

- Molecule 15 is a protein called 30S ribosomal protein S14.

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

- Molecule 16 is a protein called 30S ribosomal protein S15.

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

- Molecule 17 is a protein called 30S ribosomal protein S16.

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

- Molecule 18 is a protein called 30S ribosomal protein S17.

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

- Molecule 19 is a protein called 30S ribosomal protein S18.

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

- Molecule 20 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	S	84	Total	C	N	O	S	0	0	0
			674	430	126	116	2			

- Molecule 21 is a protein called 30S ribosomal protein S20.

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

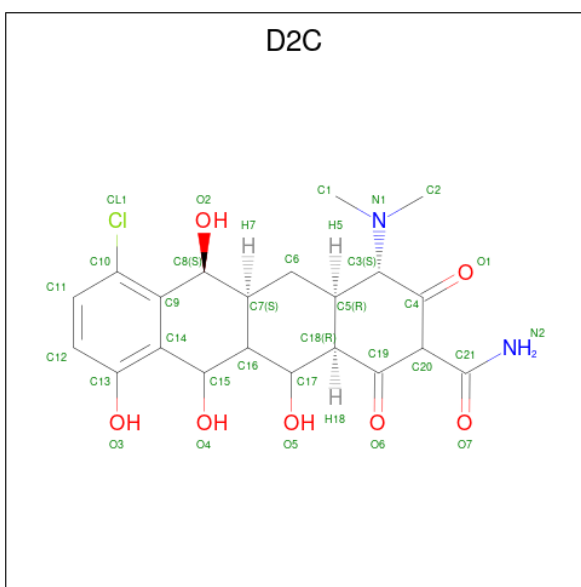
- Molecule 22 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	A	98	Total	Mg	0	0
			98	98		
22	Z	1	Total	Mg	0	0
			1	1		
22	D	1	Total	Mg	0	0
			1	1		
22	M	1	Total	Mg	0	0
			1	1		

- Molecule 23 is POTASSIUM ION (CCD ID: K) (formula: K).

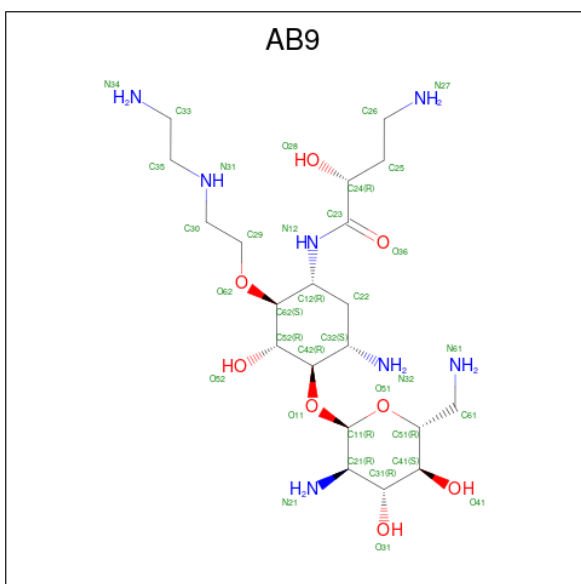
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
23	A	12	Total	K	0	0
			12	12		

- Molecule 24 is (2S,4S,4AR,5AS,6S,11R,11AS,12R,12AR)-7-CHLORO-4-(DIMETHYLAMINO)-6,10,11,12-TETRAHYDROXY-1,3-DIOXO-1,2,3,4,4A,5,5A,6,11,11A,12,12A-DODECAHYDROTETRACENE-2-CARBOXAMIDE (CCD ID: D2C) (formula: C₂₁H₂₅ClN₂O₇).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
24	A	1	Total	C	Cl	N	O	
			31	21	1	2	7	

- Molecule 25 is (2R)-4-AMINO-N-{(1R,2S,3R,4R,5S)-5-AMINO-2-{2-[(2-AMINOETHYL)AMINO]ETHOXY}-4-[(2,6-DIAMINO-2,6-DIDEOXY-ALPHA-D-GLUCOPYRANOSYL)OXY]-3-HYDROXYCYCLOHEXYL}-2-HYDROXYBUTANAMIDE (CCD ID: AB9) (formula: C₂₀H₄₃N₇O₈).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
25	A	1	Total	C	N	O		
			35	20	7	8		

- Molecule 26 is ZINC ION (CCD ID: ZN) (formula: Zn).

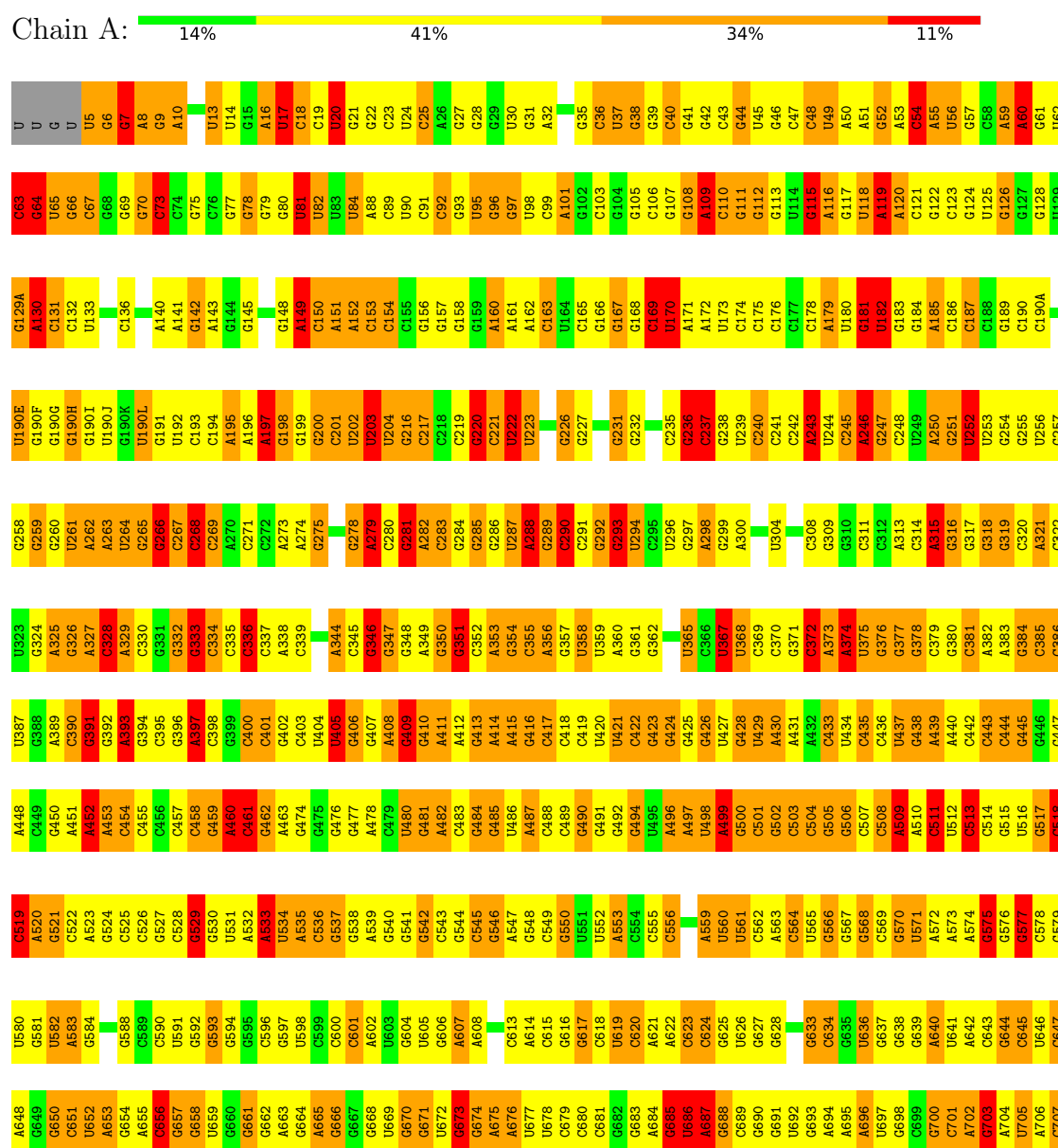
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
26	D	1	Total 1	Zn 1	0	0
26	N	1	Total 1	Zn 1	0	0

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. 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. 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.

Note EDS was not executed.

• Molecule 1: 16S ribosomal RNA



A1519	G1453	U1390	G1331	G1267	G1207	G1144	G1084	U1025	A964	C899	U833	C770	C708
G1520	G1454	U1391	A1532	A1268	C1208	C1145	U1085	G1026	A965	A900	C834	G771	G709
G1521	G1455	U1392	A1333	A1269	C1209	A1146	U1086	G1027	G966	A901	U835	U772	G710
U1522	G1459	U1393	G1334	C1270	C1210	C1147	G1087	C1028	G967	G902	G836	G773	
G1523	A1460	A1394	C1335	G1271	U1211	U1148	G1088	C1029	A968	G903	G837	G774	G713
G1524	G1461	A1395	G1336	G1272	U1212	C1149	G1089		A969		G838	G775	G714
G1525		A1396	G1337	G1273	A1213	U1150	U1090	C1030B	C970	A908	U839	A776	A715
G1526	G1464	C1397	G1338		C1214	A1151	U1091	A1030C	G971	A909	C840	A777	A716
G1527	G1465	A1398	A1339	G1276	G1215	A1152	U1092	A1030D	C972	A910	U841	G778	G717
U1528	G1466	C1399	A1340	C1277	G1216	A1153	A1093	G1031	G973	U911	C848	G779	G718
G1529	G1467	C1400	U1341	U1278	C1217	G1154	G1094	G1032	A974	G912	C849	G780	G719
U1530	A1468	G1401	C1342	A1279	G1218	U1155	U1095	G1033	A975	A913	U850	A781	G720
A1531		C1402	G1343	A1280	U1219	G1156	C1096	G1034	G976	A914	G851	A782	G721
U1532	G1471	C1403	C1344	U1281	G1220	A1157	C1097	A1035	A977	A915	G852	G783	A722
A1534	U1472	C1404	U1345	C1282	G1221	C1158	G1098	G1036	A978	G916	G853	G784	U723
	A1473	G1405	A1346	G1283	G1222	U1159	G1099	C1037	C979	G917	G854	G785	G724
	G1474	U1406	G1347	C1284	G1223	U1160	C1100	G1038	A980	A918	G855	G786	G725
		C1407	U1348	A1285	G1224	C1161	A1101	C1039	U981	A919	C856	G787	G726
		A1408	A1349	A1286	A1225	C1162	A1102	U1040	U982	U920	C857	U788	G727
	C1478	C1409	A1350	A1287	C1226	C1163	C1103	A1041	A983	U921	C858	A789	A728
	C1479	G1410	U1351	A1288	C1227		G1104	G1042	C984	G922	A859	U790	A729
	G1480	C1411	C1352	A1289	C1228	G1166	A1105	C1043	C985	A923	G860	G791	G730
	U1481	C1412	G1353	G1290	A1229	A1167	G1106	A1044	A986	G924	G861	A792	G731
	G1482	A1413	C1354	G1291	C1230	A1168	G1107	C1045	G987	G925	C862	U793	G732
	A1483	U1414	G1355	G1291	G1231	A1169	G1108	A1046	G988	G926	U863	A794	A733
	C1484	G1415	G1356		U1232	G1171	C1109	G1047	C989	G927	A864	C795	G734
	U1485	G1416	A1357	C1296	G1233	C1172	A1110	G1048	C990		A865	C796	C735
	G1486	C1417	U1358	C1297	C1234	G1173	U1111	U1049	C991	C930	C866	C797	C736
	G1487	A1418	G1359	C1298	U1235	C1174	C1112	G1050	U992	C931	G867	A737	C737
	U1488	C1419	A1360	A1299	A1236	A1176	C1113		G983	C932	C868	G798	C738
	G1489	G1361	C1361	G1300	C1237	G1177	C1114	G1053	G983	G933	G869	G800	C739
	A1490	U1301	C1361A	U1301	A1238	G1178	C1115	C1054	C984	C934	U870	A801	C740
	G1491	C1362	C1362	U1302	A1239	A1179	C1116	A1055	U997	A935	U871	A802	G741
	A1492	G1363	C1363	C1303	U1240	G1180	C1117	U1056	G998	C936	A872	G803	U742
	A1493	U1364	G1364	G1304	G1241	A1181	C1118	G1057	C999	A937	A873	U804	G743
	G1494	G1365	C1365	G1305	C1242	G1182	C1119	G1058	U1000	A938	G874	C805	C744
	U1495	C1426	C1366	A1306	C1243	A1183	G1120	G1059	A1001	G939	C875	G806	C745
	A1496	U1427	C1367	U1307	G1244	G1184	U1121	C1060	G1002	C940	G876	A807	
	G1497	A1428	G1368	U1308	A1245	G1185	U1122	G1061	G1003	G941	C877	C748	
	U1498	C1429	C1369	G1309	C1246	G1186	A1123	U1062	G1003A	G942	G878	G809	C749
	A1499	G1430	G1370	C1310	U1247	G1187	G1124	C1063	A1004	U943	C879	C810	G750
	A1500	G1431	G1371	G1311	A1248	A1188	U1125	G1064	A1005	G944	C880	C811	U751
	C1501	A1433	U1372	G1312	C1249	G1189	U1126	U1065	C1006	A945	G881	C812	G752
	A1502	U1434	G1373	U1313	A1250	G1190	G1127	C1066	G1007	A946	C882	U813	A753
	A1503	G1435	A1374	C1314	A1251	A1191	C1128	A1067	C1008	G947	C883	A814	C754
	G1504	U1436	U1375	G1315	A1252	C1192	C1129	G1068	U1009	C948	U884	A815	G755
	U1505	G1437	U1376	G1316	G1253	G1193	A1130	C1069	G1010	A949	G885	A816	G756
	U1506	G1438	A1377	C1317	G1254	U1194	G1131	U1070	G1011	U950	G886	C817	U757
	A1507	C1439	C1378	A1318	G1255	G1195	C1132			G951	G887	G818	G758
	G1508	C1440	G1379	A1319	A1256	U1196	G1133	U1073	A1014	U952	G888	A819	A759
	C1509	G1441	U1380	C1320	U1257	G1197	G1134	G1074	A1015	G953	A889	U820	G760
	U1510	G1442	C1381	C1321	G1258	G1198	U1135	C1075	A1016	G954	G890	G761	
	G1511	A1443	C1382	C1322	U1259	U1199	U1136	G1076	U891	U955	G892	C824	G762
	U1512	A1446	C1383	G1323	C1260	C1200	C1137	C1077	C1018	U956	A892	G763	G763
	A1513	G1447	C1384	A1324	A1261	A1201	G1139	U1078	G1019	U957	G893	G825	G764
	U1514	G1448	G1385	C1262	G1262	G1202	G1139	G1079	U1020	A958	G894	G826	G765
	C1515	C1449	G1386	C1263	C1263	C1203	C1140	A1080	G1021	A959	C895	U827	A766
	G1516	U1450	G1387	G1264	C1265	A1204	C1141	G1081	G1022	U960	C896	A828	A767
	U1517	A1451	C1388	G1265	G1265	U1205	G1142	G1082	U961		C897	A768	
	A1518	C1452	C1389	G1266		G1206	G1143	U1083	G1024		G898	C832	G769

• Molecule 2: 5'-R(P*UP*UP*CP*U)-3'

Chain Z:

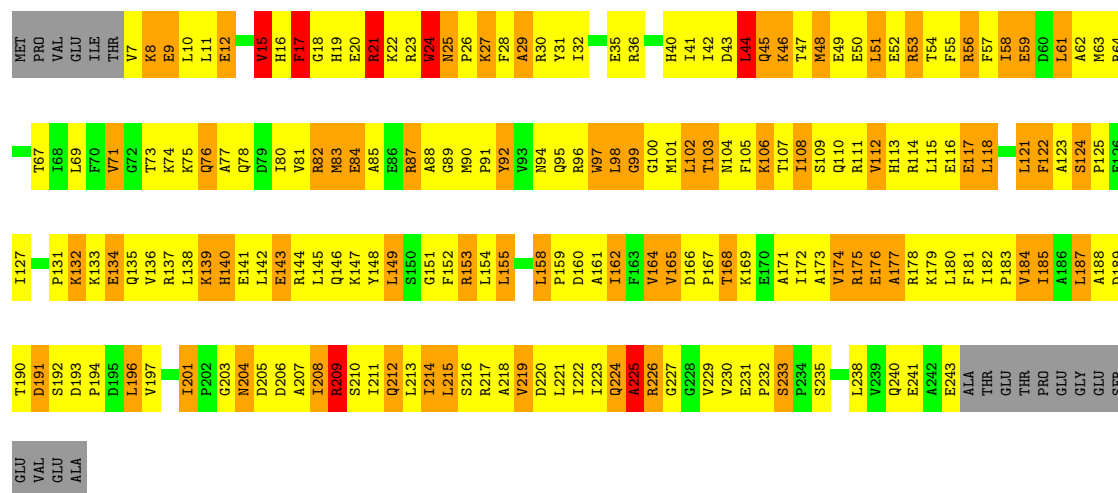


75%

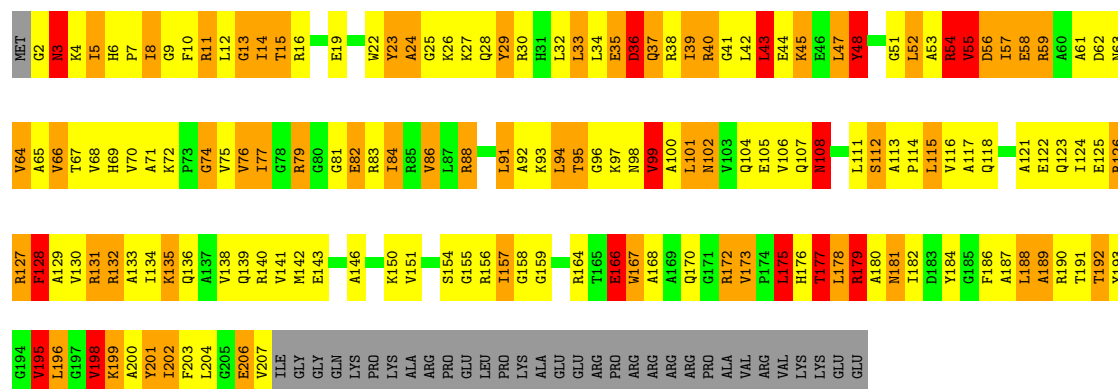
25%

U3
U4
U5
U6

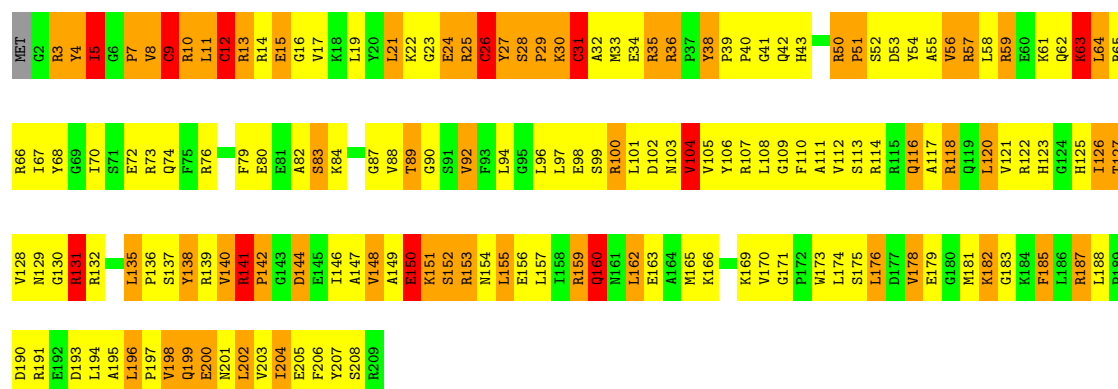
Chain B: 15% 48% 26% 7%



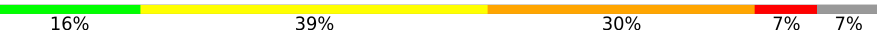
Chain C:

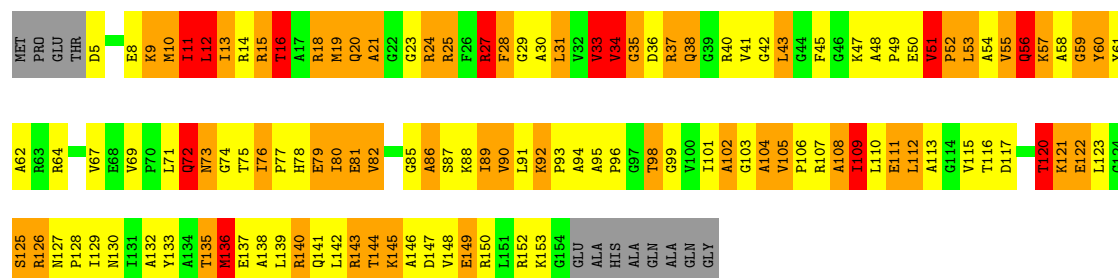


Chain D:

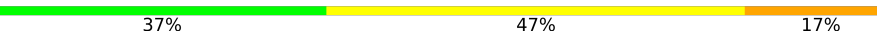


- Molecule 6: 30S ribosomal protein S5

Chain E: 

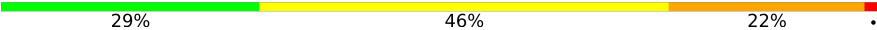


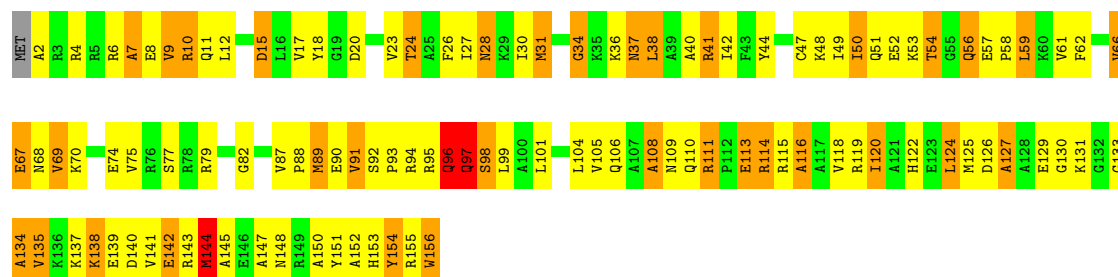
- Molecule 7: 30S ribosomal protein S6

Chain F: 



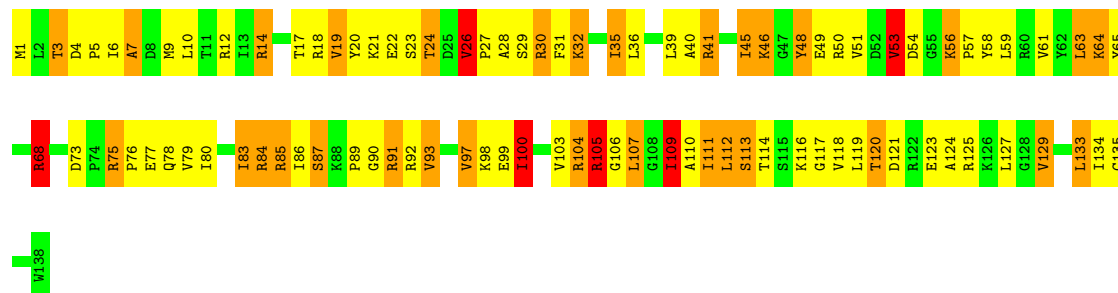
- Molecule 8: 30S ribosomal protein S7

Chain G: 



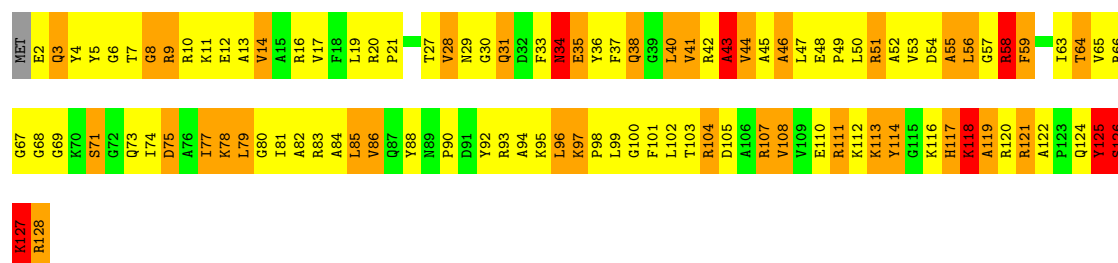
- Molecule 9: 30S ribosomal protein S8

Chain H: 



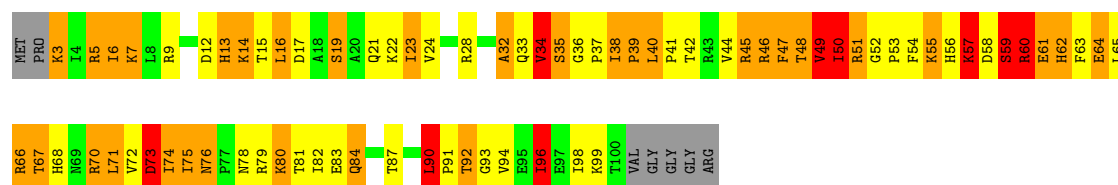
- Molecule 10: 30S ribosomal protein S9

Chain I: 17% 48% 28% 5% •



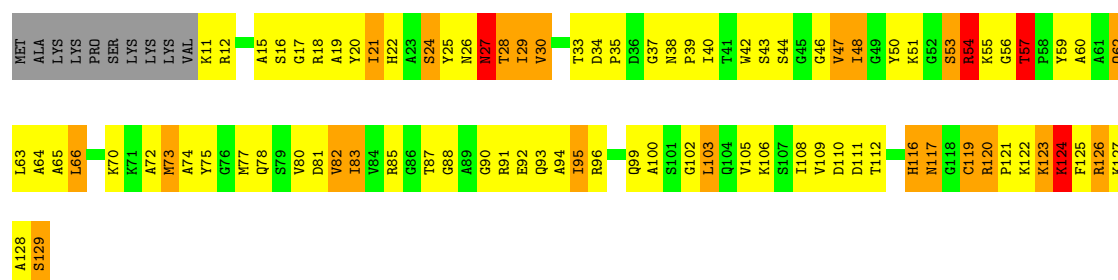
- Molecule 11: 30S ribosomal protein S10

Chain J: 21% 32% 31% 9% 7%



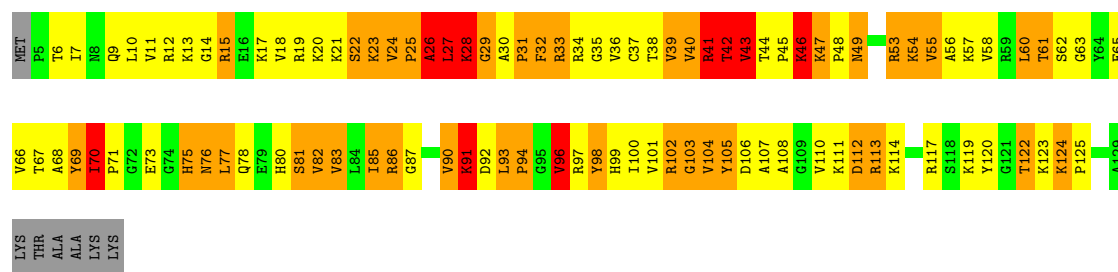
- Molecule 12: 30S ribosomal protein S11

Chain K: 23% 49% 17% • 8%



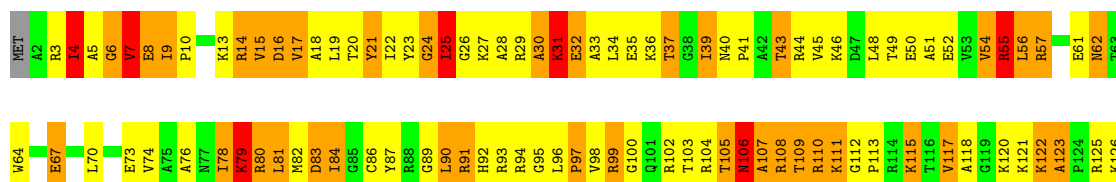
- Molecule 13: 30S ribosomal protein S12

Chain L: 18% 39% 30% 8% 5%

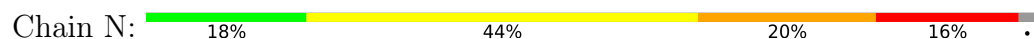


- Molecule 14: 30S ribosomal protein S13

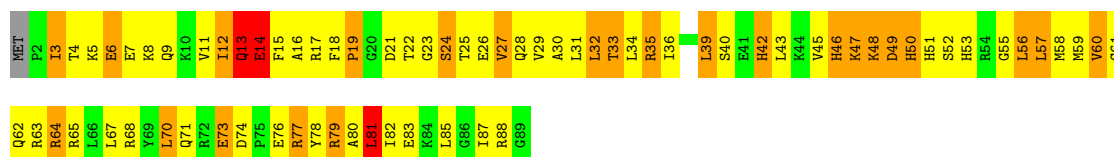
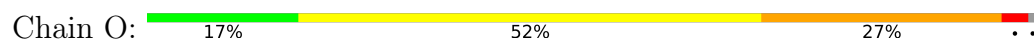
Chain M: 21% 43% 30% 6% •



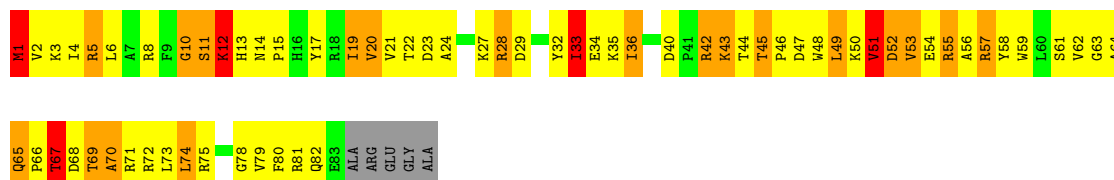
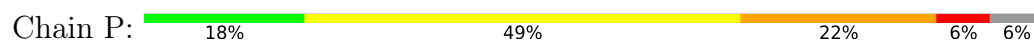
• Molecule 15: 30S ribosomal protein S14



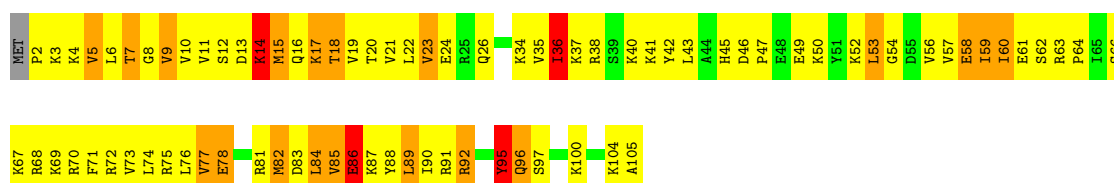
• Molecule 16: 30S ribosomal protein S15



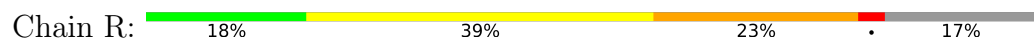
• Molecule 17: 30S ribosomal protein S16



• Molecule 18: 30S ribosomal protein S17

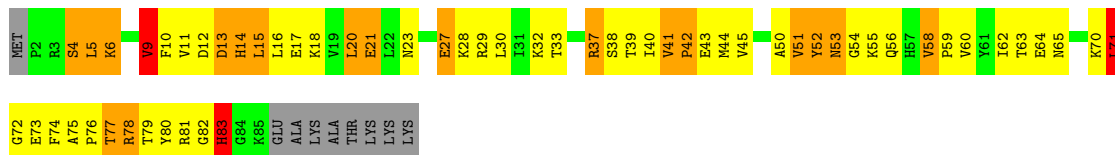


• Molecule 19: 30S ribosomal protein S18

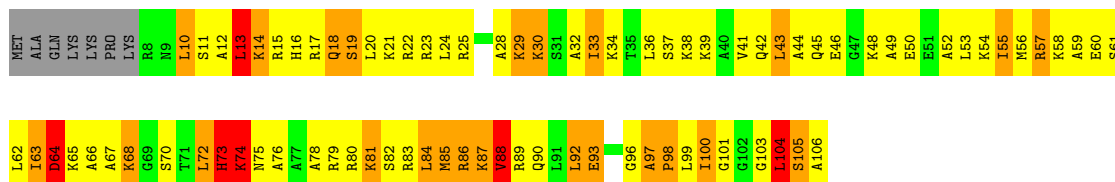
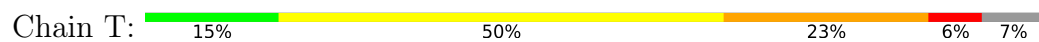




- Molecule 20: 30S ribosomal protein S19



- Molecule 21: 30S ribosomal protein S20



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	403.32Å 403.32Å 176.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.80	Depositor
% Data completeness (in resolution range)	97.2 (30.00-3.80)	Depositor
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.259 , 0.315	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	51728	wwPDB-VP
Average B, all atoms (Å ²)	84.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: K, AB9, MG, ZN, D2C

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.20	184/36247 (0.5%)	1.31	309/56545 (0.5%)
2	Z	1.68	1/87 (1.1%)	1.41	1/132 (0.8%)
3	B	1.04	3/1958 (0.2%)	0.85	0/2640
4	C	1.14	5/1636 (0.3%)	0.86	1/2205 (0.0%)
5	D	0.99	1/1733 (0.1%)	0.85	0/2318
6	E	1.46	10/1162 (0.9%)	1.02	4/1564 (0.3%)
7	F	0.89	1/856 (0.1%)	0.83	0/1154
8	G	1.08	2/1276 (0.2%)	0.80	0/1709
9	H	1.41	5/1136 (0.4%)	0.98	1/1527 (0.1%)
10	I	0.94	0/1029	0.82	1/1378 (0.1%)
11	J	1.08	1/805 (0.1%)	0.95	1/1082 (0.1%)
12	K	1.22	2/900 (0.2%)	0.89	1/1213 (0.1%)
13	L	1.05	0/991	0.92	1/1327 (0.1%)
14	M	1.05	1/1008 (0.1%)	0.83	0/1347
15	N	1.07	0/501	0.87	0/664
16	O	1.08	0/745	0.78	0/992
17	P	1.39	2/716 (0.3%)	0.93	0/963
18	Q	1.29	4/870 (0.5%)	0.91	0/1159
19	R	1.13	1/603 (0.2%)	0.89	0/799
20	S	0.87	0/689	0.85	0/926
21	T	1.33	1/764 (0.1%)	0.91	2/1006 (0.2%)
All	All	1.18	224/55712 (0.4%)	1.19	322/82650 (0.4%)

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
3	B	0	2
4	C	0	6

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Mol	Chain	#Chirality outliers	#Planarity outliers
5	D	0	6
6	E	0	5
7	F	0	1
9	H	0	5
10	I	0	4
11	J	0	6
12	K	0	5
13	L	0	8
14	M	0	4
15	N	0	8
17	P	0	4
18	Q	0	1
20	S	0	5
21	T	0	4
All	All	0	74

The worst 5 of 224 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1169	A	O3'-P	28.37	2.03	1.61
1	A	1129	C	C1'-N1	11.33	1.64	1.47
1	A	1346	A	C3'-O3'	9.73	1.57	1.43
1	A	1125	U	C3'-O3'	9.53	1.56	1.42
14	M	7	VAL	CA-CB	9.51	1.67	1.54

The worst 5 of 322 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1169	A	P-O3'-C3'	23.55	155.53	120.20
1	A	1525	G	C4'-C3'-C2'	-12.91	89.69	102.60
1	A	1169	A	O3'-P-O5'	-12.22	85.67	104.00
1	A	1380	U	C2'-C3'-O3'	10.47	125.20	109.50
1	A	115	G	C2'-C3'-O3'	10.40	125.10	109.50

There are no chirality outliers.

5 of 74 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	B	133	LYS	Peptide
3	B	225	ALA	Peptide
4	C	13	GLY	Peptide

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Mol	Chain	Res	Type	Group
4	C	166	GLU	Peptide
4	C	48	TYR	Peptide

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	32391	0	16359	1896	0
2	Z	80	0	42	4	0
3	B	1923	0	1968	226	0
4	C	1612	0	1677	183	0
5	D	1703	0	1763	209	0
6	E	1146	0	1207	171	0
7	F	843	0	857	61	0
8	G	1257	0	1296	110	0
9	H	1116	0	1177	96	0
10	I	1011	0	1043	127	0
11	J	792	0	835	125	0
12	K	885	0	904	83	0
13	L	975	0	1062	128	0
14	M	997	0	1072	120	0
15	N	492	0	530	88	0
16	O	734	0	771	80	0
17	P	700	0	720	80	0
18	Q	857	0	930	72	0
19	R	597	0	668	68	0
20	S	674	0	699	59	0
21	T	762	0	859	100	0
22	A	98	0	0	0	0
22	D	1	0	0	0	0
22	M	1	0	0	0	0
22	Z	1	0	0	0	0
23	A	12	0	0	0	0
24	A	31	0	19	4	0
25	A	35	0	43	1	0
26	D	1	0	0	0	0
26	N	1	0	0	0	0
All	All	51728	0	36501	3813	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 44.

The worst 5 of 3813 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)
8:G:89:MET:CE	8:G:89:MET:SD	2.02	1.45
1:A:492:G:H3'	1:A:494:G:OP2	1.29	1.32
6:E:80:ILE:CD1	6:E:91:LEU:HB2	1.62	1.29
1:A:70:G:H3'	1:A:73:C:P	1.72	1.27
15:N:40:CYS:O	15:N:43:CYS:HB2	1.23	1.27

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	
3	B	235/256 (92%)	153 (65%)	48 (20%)	34 (14%)	0	2
4	C	204/239 (85%)	120 (59%)	51 (25%)	33 (16%)	0	2
5	D	206/209 (99%)	145 (70%)	37 (18%)	24 (12%)	0	4
6	E	148/162 (91%)	110 (74%)	24 (16%)	14 (10%)	0	8
7	F	99/101 (98%)	76 (77%)	17 (17%)	6 (6%)	1	14
8	G	153/156 (98%)	103 (67%)	36 (24%)	14 (9%)	0	8
9	H	136/138 (99%)	103 (76%)	26 (19%)	7 (5%)	1	17
10	I	125/128 (98%)	79 (63%)	33 (26%)	13 (10%)	0	6
11	J	96/105 (91%)	63 (66%)	20 (21%)	13 (14%)	0	3
12	K	117/129 (91%)	79 (68%)	25 (21%)	13 (11%)	0	5
13	L	123/132 (93%)	76 (62%)	29 (24%)	18 (15%)	0	2
14	M	123/126 (98%)	75 (61%)	31 (25%)	17 (14%)	0	3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	N	58/61 (95%)	43 (74%)	8 (14%)	7 (12%)	0	4
16	O	86/89 (97%)	56 (65%)	22 (26%)	8 (9%)	0	8
17	P	81/88 (92%)	55 (68%)	17 (21%)	9 (11%)	0	5
18	Q	102/105 (97%)	73 (72%)	21 (21%)	8 (8%)	1	11
19	R	71/88 (81%)	50 (70%)	14 (20%)	7 (10%)	0	7
20	S	82/93 (88%)	58 (71%)	17 (21%)	7 (8%)	0	9
21	T	97/106 (92%)	60 (62%)	21 (22%)	16 (16%)	0	2
All	All	2342/2511 (93%)	1577 (67%)	497 (21%)	268 (11%)	0	5

5 of 268 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	B	17	PHE
3	B	29	ALA
3	B	99	GLY
3	B	106	LYS
3	B	131	PRO

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	
3	B	204/220 (93%)	112 (55%)	92 (45%)	0	0
4	C	160/188 (85%)	86 (54%)	74 (46%)	0	0
5	D	180/181 (99%)	106 (59%)	74 (41%)	0	0
6	E	115/123 (94%)	62 (54%)	53 (46%)	0	0
7	F	90/90 (100%)	66 (73%)	24 (27%)	0	3
8	G	126/127 (99%)	78 (62%)	48 (38%)	0	0
9	H	119/119 (100%)	73 (61%)	46 (39%)	0	0
10	I	98/99 (99%)	54 (55%)	44 (45%)	0	0
11	J	87/92 (95%)	46 (53%)	41 (47%)	0	0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	K	90/99 (91%)	57 (63%)	33 (37%)	0	0
13	L	104/109 (95%)	51 (49%)	53 (51%)	0	0
14	M	100/101 (99%)	58 (58%)	42 (42%)	0	0
15	N	49/50 (98%)	24 (49%)	25 (51%)	0	0
16	O	79/80 (99%)	44 (56%)	35 (44%)	0	0
17	P	72/74 (97%)	44 (61%)	28 (39%)	0	0
18	Q	96/97 (99%)	65 (68%)	31 (32%)	0	1
19	R	64/77 (83%)	34 (53%)	30 (47%)	0	0
20	S	73/80 (91%)	44 (60%)	29 (40%)	0	0
21	T	76/82 (93%)	47 (62%)	29 (38%)	0	0
All	All	1982/2088 (95%)	1151 (58%)	831 (42%)	0	0

5 of 831 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	J	22	LYS
13	L	96	VAL
20	S	79	THR
11	J	59	SER
11	J	19	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 48 such sidechains are listed below:

Mol	Chain	Res	Type
11	J	78	ASN
13	L	99	HIS
11	J	84	GLN
13	L	49	ASN
14	M	62	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1504/1511 (99%)	671 (44%)	162 (10%)
2	Z	3/4 (75%)	0	0
All	All	1507/1515 (99%)	671 (44%)	162 (10%)

5 of 671 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	6	G
1	A	8	A
1	A	9	G
1	A	13	U
1	A	16	A

5 of 162 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	1192	C
1	A	1337	G
1	A	1212	U
1	A	1263	C
1	A	1396	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 117 ligands modelled in this entry, 115 are monoatomic - leaving 2 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
25	AB9	A	1637	-	35,36,36	2.20	3 (8%)	43,49,49	1.65	3 (6%)
24	D2C	A	1636	22	31,34,34	4.34	11 (35%)	37,54,54	2.47	16 (43%)

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
25	AB9	A	1637	-	-	11/24/64/64	0/2/2/2
24	D2C	A	1636	22	-	6/6/64/64	0/4/4/4

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	1636	D2C	C16-C15	-15.94	1.40	1.53
24	A	1636	D2C	C16-C17	-12.35	1.37	1.53
25	A	1637	AB9	O36-C23	10.63	1.43	1.23
24	A	1636	D2C	C18-C5	-7.06	1.44	1.54
24	A	1636	D2C	C14-C15	-6.64	1.43	1.52

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	1637	AB9	O36-C23-N12	-7.27	109.94	122.96
25	A	1637	AB9	O36-C23-C24	-6.29	111.32	120.61
24	A	1636	D2C	O5-C17-C18	5.18	121.55	109.80
24	A	1636	D2C	O4-C15-C14	5.09	122.53	110.56
24	A	1636	D2C	C18-C17-C16	4.88	118.55	110.45

There are no chirality outliers.

5 of 17 torsion outliers are listed below:

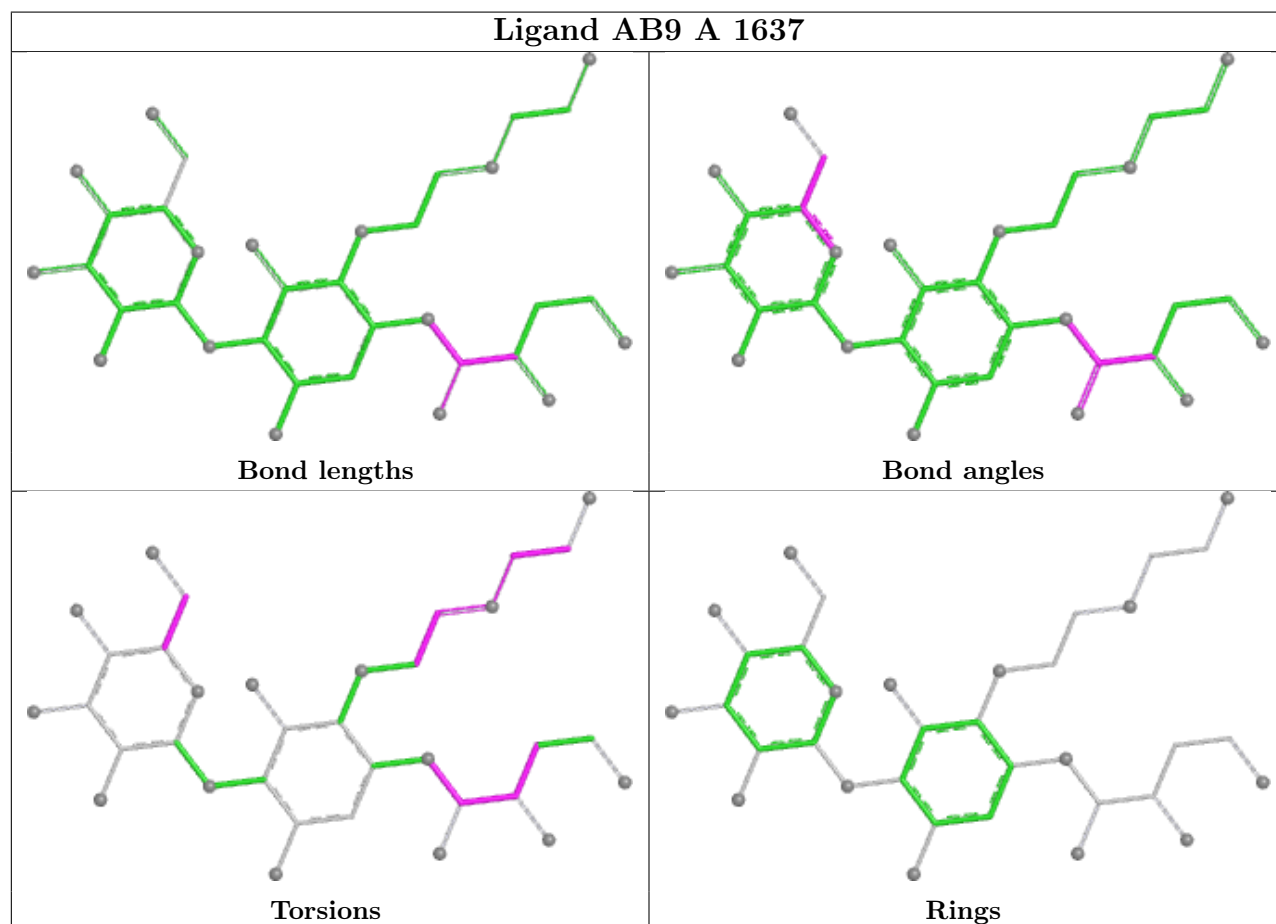
Mol	Chain	Res	Type	Atoms
24	A	1636	D2C	C4-C3-N1-C1
24	A	1636	D2C	C5-C3-N1-C1
24	A	1636	D2C	C4-C3-N1-C2
24	A	1636	D2C	C4-C20-C21-O7
24	A	1636	D2C	C19-C20-C21-O7

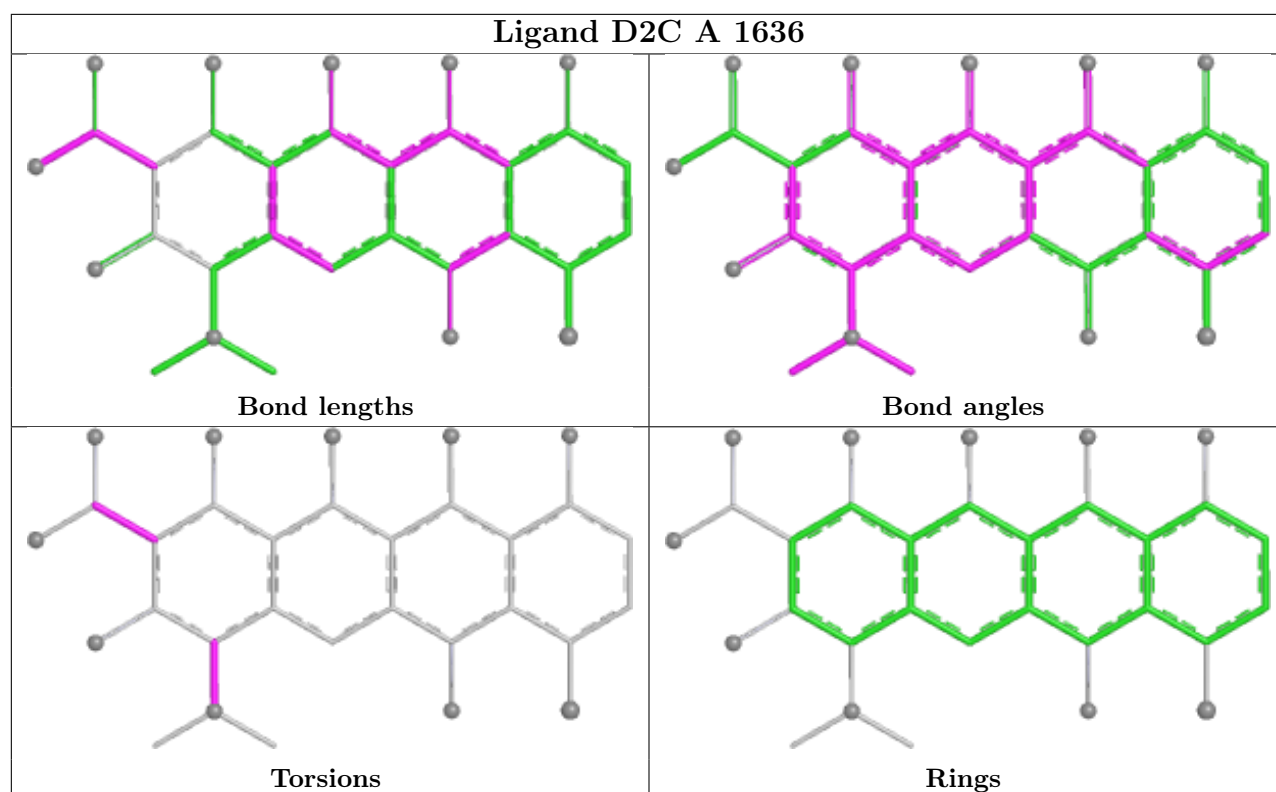
There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	A	1637	AB9	1	0
24	A	1636	D2C	4	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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	13

The worst 5 of 13 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	841:U	O3'	848:C	P	5.02
1	A	84:U	O3'	88:A	P	3.79
1	A	1533:C	O3'	1534:A	P	3.45
1	A	70:G	O3'	73:C	P	3.36
1	A	204:U	O3'	216:G	P	3.36

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.