



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 15, 2024 – 11:33 PM EDT

PDB ID : 2F4V  
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](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 ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.37.1

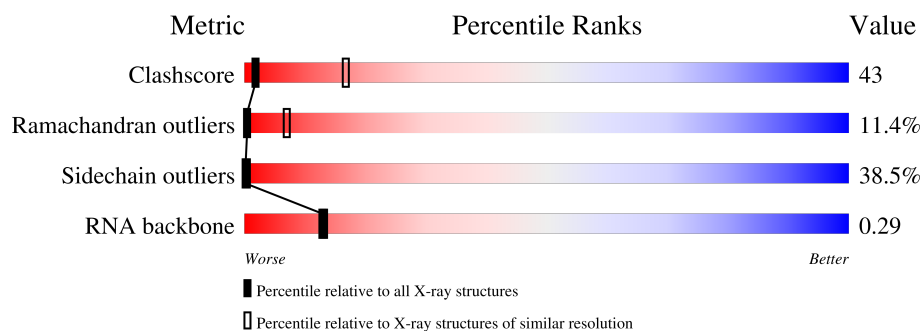
# 1 Overall quality at a glance ⓘ

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	141614	1288 (4.00-3.60)
Ramachandran outliers	138981	1243 (4.00-3.60)
Sidechain outliers	138945	1237 (4.00-3.60)
RNA backbone	3102	1036 (4.60-3.00)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	1511	11% 37% 36% 17%
2	Z	4	100%
3	B	256	20% 45% 24% • 7%
4	C	239	20% 37% 24% 5% 14%
5	D	209	21% 45% 28% 5%
6	E	162	20% 40% 31% • 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

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			

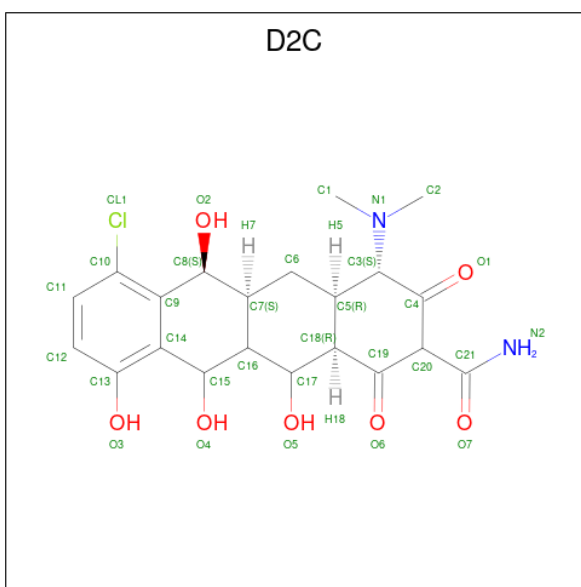
- Molecule 22 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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 (three-letter code: K) (formula: K).

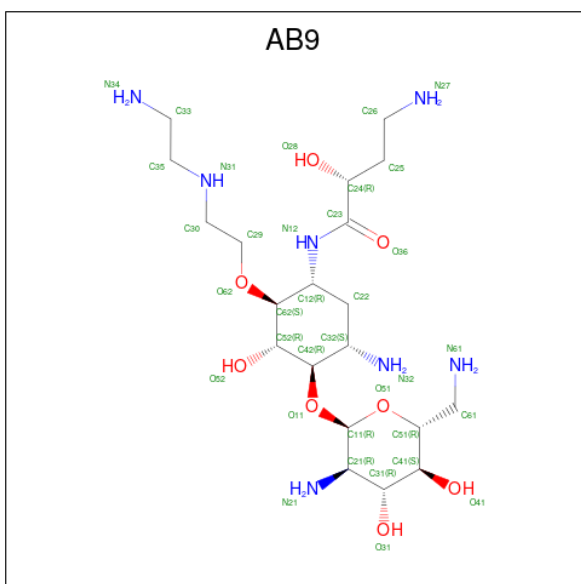
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
23	A	12	Total	K	0	0
			12	12		

- 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 (three-letter code: D2C) (formula: C<sub>21</sub>H<sub>25</sub>ClN<sub>2</sub>O<sub>7</sub>).



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 (three-letter code: AB9) (formula:  $C_{20}H_{43}N_7O_8$ ).



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



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

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



C1496	U1427	C1366	A1428	G1184	U1122	U1062	C1006	G945	U884	C817	U757	A695
G1497	A1428	C1367	U1307	G1185	A1123	C1063	C1007	A946	G885	G818	G758	A696
A1498	C1429	G1368	U1308	G1186	G1124	G1064	G1008	G947	G886	A819	A759	U697
A1499	C1430	C1369	U1309	G1187	U1125	G1065	G1009	C948	G887	U820	G760	G698
A1500	C1431	G1370	G1310	A1188	C1249	C1066	G1010	A949	G888	G821	G761	C699
A1501	G1432	G1371	G1311	C1189	G1127	A1067	G1011	U950	A889	G822	G762	G700
A1502	A1433	U1372	G1312	G1190	C1128	G1068	U1012	G951	G890	G823	G763	C701
A1503	G1434	G1373	U1313	A1191	C1129	C1069	G1013	U952	U891	G824	C764	A702
G1504	A1435	U1374	C1314	C1192	A1130	U1070	A1014	G953	A892	G825	G765	G703
G1505	U1436	G1375	U1315	G1254	C1131	C1071	A1015	G954	C893	G826	A766	A704
A1506	C1437	U1376	G1316	U1194	G1132	G1072	A1016	U955	G894	U827	A767	U705
A1507	A1438	C1377	U1317	C1195	C1133	U1073	G1017	U956	G895	A828	A768	A706
A1508	C1439	C1378	U1318	U1196	G1134	G1074	C1018	U957	C896	G829	G769	C707
C1509	C1440	G1379	A1319	G1197	U1135	C1075	U1019	A958	C897	C770	C770	C708
U1510	G1441	U1380	C1320	U1198	U1136	C1076	U1020	A959	C898	C832	G771	G709
G1511	G1442	U1381	C1321	U1199	C1137	G1077	G1021	U960	C899	U833	U772	G710
A1512	G1443	C1382	C1322	U1200	G1138	U1078	G1022	U961	C900	C834	G773	G711
A1513	A1446	C1383	G1323	C1201	G1139	G1079	G1023	A901	A901	U835	G774	A712
C1514	G1447	C1384	A1324	G1202	C1140	A1080	G1024	G902	G902	U836	G775	G713
G1515	C1448	G1385	C1264	C1203	C1141	G1081	U1025	A965	C904	G837	G776	G714
C1449	C1449	G1386	G1265	G1204	G1142	U1082	G1026	G966	C907	G838	A777	A715
G1450	U1450	G1387	U1266	U1205	G1143	U1083	C1027	G967	C908	U839	G778	A716
A1518	A1451	C1388	C1267	G1206	G1144	U1084	C1028	A968	C909	C840	C779	G717
A1519	C1452	C1389	G1268	C1207	G1145	U1085	C1029	A969	A908	U841	G780	G718
G1520	G1453	U1390	A1269	C1208	A1146	U1086	U1030	C970	A909	C848	A781	C719
G1521	C1454	U1391	C1270	C1209	C1147	G1087	G1030A	C971	C910	C849	A782	C720
U1522	G1455	G1392	G1271	C1210	U1148	U1088	C1030B	C972	U911	U850	G783	G721
G1523	C1459	U1393	U1272	U1211	C1149	G1089	G1030C	C973	C912	G851	A722	G784
C1524	A1460	A1394	G1273	U1212	U1150	U1090	A1030D	A974	G785	U852	G723	U723
G1525	G1461	C1395	G1274	A1213	A1151	U1091	G1031	A975	A914	G853	G724	G724
G1526	C1462	A1396	A1275	C1214	A1152	A1092	G1032	G976	A915	G854	A787	G725
C1527	G1464	C1397	G1276	G1215	C1153	A1093	G1033	A977	C916	G855	U788	C726
U1528	C1465	A1398	C1277	G1216	G1094	U1095	G1034	A978	C917	C856	G727	G727
G1529	G1466	C1399	U1278	C1217	G1154	C1096	A1035	C979	A918	U857	U789	A728
G1530	A1467	C1400	A1279	G1218	G1155	C1097	G1036	C980	A919	C858	G791	A729
A1531	A1468	G1401	A1280	U1219	A1157	U1097	C1037	U981	U920	A859	A792	G730
U1532	C1469	G1402	U1281	G1220	G1158	C1098	C1038	U982	U921	A860	A793	G731
C1533	G1471	C1403	C1282	G1221	U1159	G1099	C1039	A983	C922	G861	A794	C732
A1534	U1472	G1404	G1283	C1222	C1160	C1100	U1040	C984	A923	C862	C795	A733
G1473	A1473	C1405	C1284	G1223	C1161	A1101	A1041	C985	C924	U863	G796	G734
G1474	G1474	U1406	A1285	G1224	C1162	A1102	G1042	A986	G925	U864	C797	C735
G1475	C1475	C1407	A1286	A1225	C1163	C1103	C1043	G987	G926	A865	G798	C736
C1408	C1478	A1408	A1287	C1226	G1165	G1104	A1044	G988	G927	C866	G799	A737
C1409	C1479	G1410	A1288	U1227	A1166	A1105	C1045	C989	G928	G867	G800	C738
G1410	C1410	U1351	A1289	C1228	A1167	G1106	A1046	C990	G929	C868	U801	C739
C1411	C1411	C1352	G1290	U1229	A1168	C1107	G1047	U991	C930	G869	A802	U740
C1412	C1412	G1353	G1291	C1230	A1169	G1108	U1048	U992	C931	U870	G803	G741
A1413	A1413	C1354	C1292	G1231	G1171	C1109	U1049	G993	C932	U871	U804	G742
U1414	C1484	G1355	G1294	U1232	G1172	A1110	G1050	A994	G933	A872	C805	U743
G1415	U1485	G1356	G1295	G1233	G1173	A1111	C1051	U997	C934	A873	C806	C744
G1416	G1486	A1357	C1296	U1234	G1174	C1112	U1052	A998	A935	G874	A807	C745
G1417	G1487	U1358	C1297	U1235	G1175	C1113	G1053	C999	C936	C875	G808	C746
A1418	G1488	C1359	A1236	A1236	A1176	C1114	C1054	C999	C937	G876	G809	C749
G1419	G1489	A1360	C1297	C1237	G1177	C1115	A1055	U1000	A938	C877	C810	G750
C1490	A1490	G1361	U1300	A1238	G1178	C1116	U1056	A1001	G939	G878	C811	U751
G1491	C1491	U1301	A1239	A1239	A1179	G1117	G1057	G1002	C940	G879	G812	G752
A1492	G1423	C1362	U1302	U1240	A1180	C1118	G1058	G1003	C941	C880	U813	A753
G1493	C1424	A1363	G1303	G1241	G1181	C1119	C1059	G1003A	G942	G881	A814	C754
G1494	U1364	G1304	C1304	C1242	G1182	C1120	G1060	A1004	U943	C882	A815	G755
U1495	C1426	G1305	G1305	A1183	A1183	U1121	G1061	A1005	G944	C883	A816	C756

• Molecule 2: 5'-R(P\*UP\*UP\*CP\*U)-3'

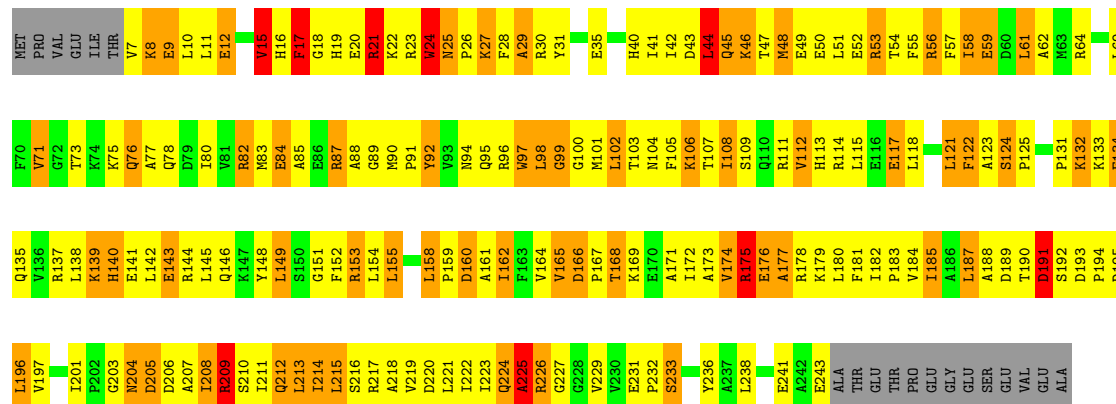
Chain Z:

100%

U3  
U4  
C5  
U6

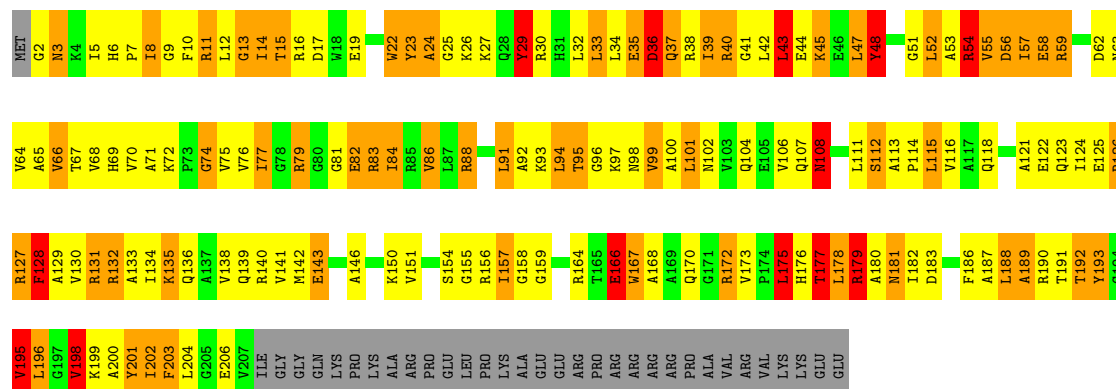
• Molecule 3: 30S ribosomal protein S2

Chain B: 20% 45% 24% 7%



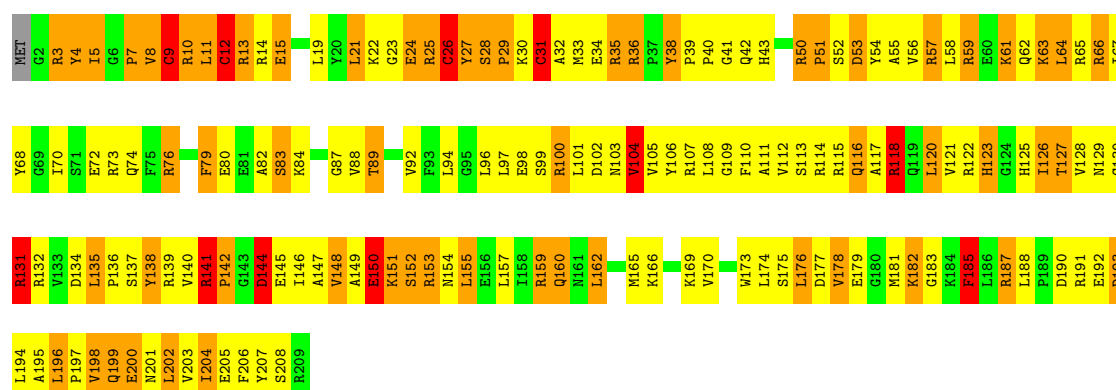
• Molecule 4: 30S ribosomal protein S3

Chain C: 20% 37% 24% 5% 14%

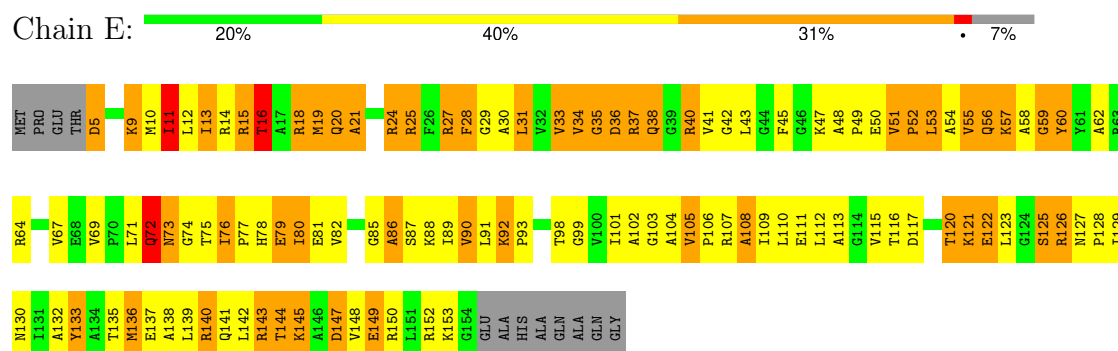


• Molecule 5: 30S ribosomal protein S4

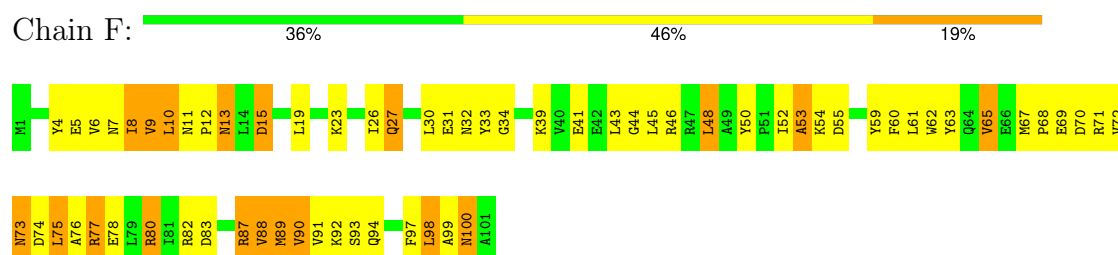
Chain D: 21% 45% 28% 5%



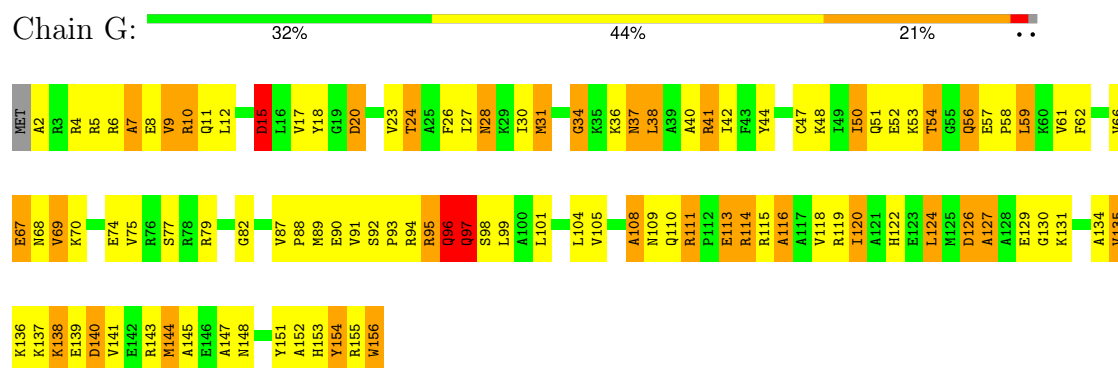
- Molecule 6: 30S ribosomal protein S5



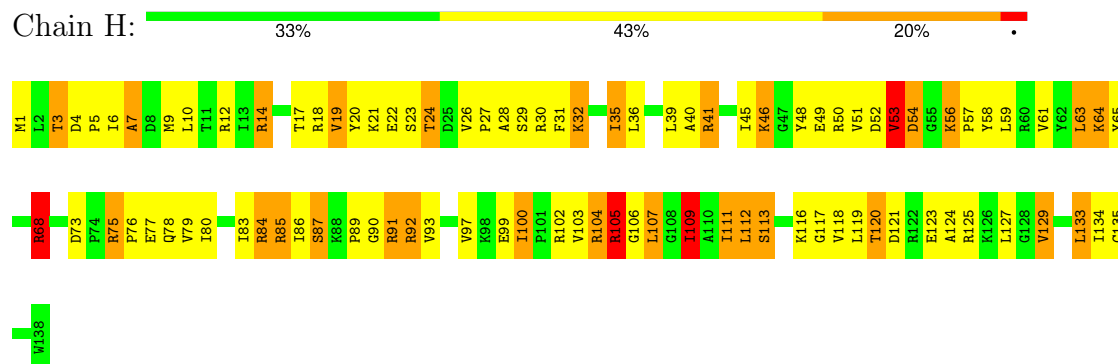
- Molecule 7: 30S ribosomal protein S6



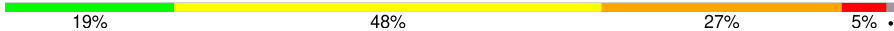
- Molecule 8: 30S ribosomal protein S7

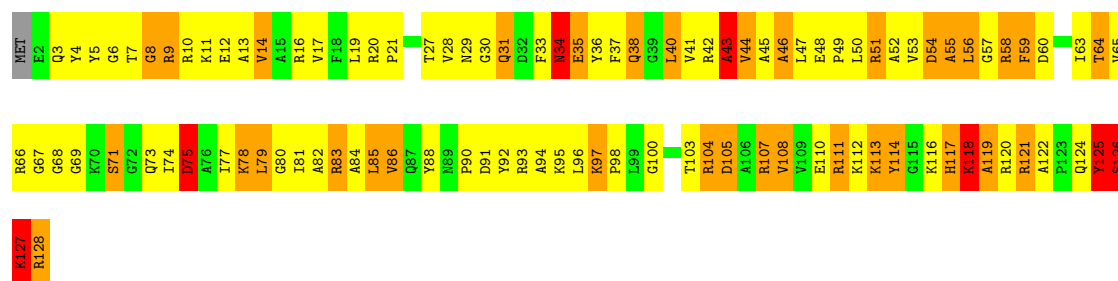


- Molecule 9: 30S ribosomal protein S8




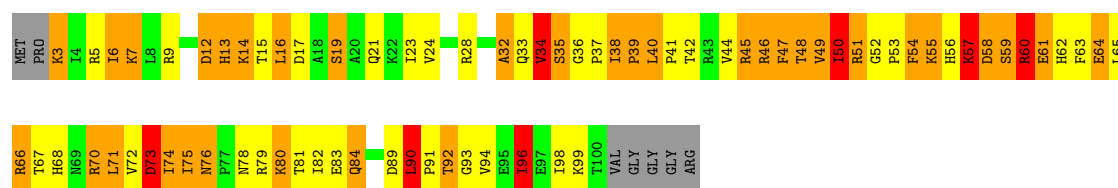
- Molecule 10: 30S ribosomal protein S9

Chain I: 



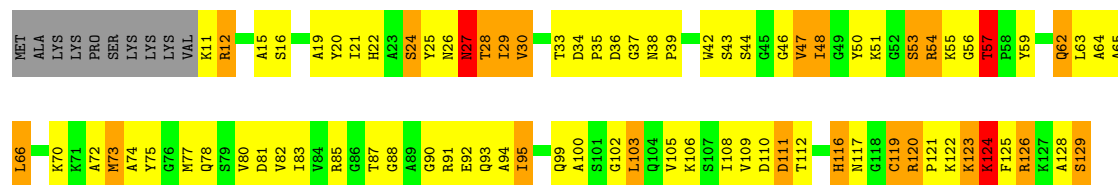
• Molecule 11: 30S ribosomal protein S10

Chain J: 



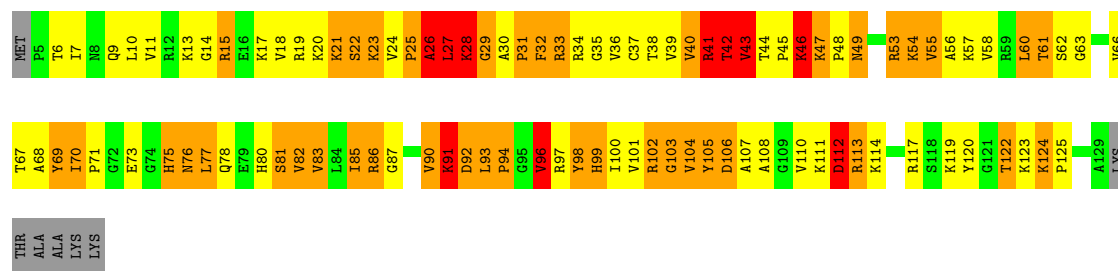
• Molecule 12: 30S ribosomal protein S11

Chain K: 

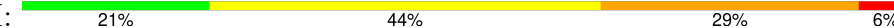


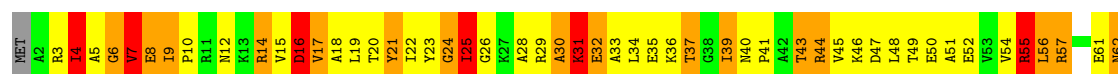
• Molecule 13: 30S ribosomal protein S12

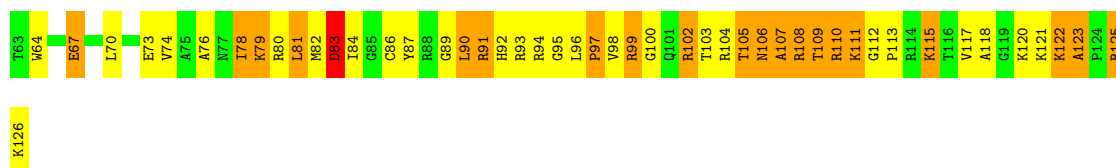
Chain L: 



• Molecule 14: 30S ribosomal protein S13

Chain M: 





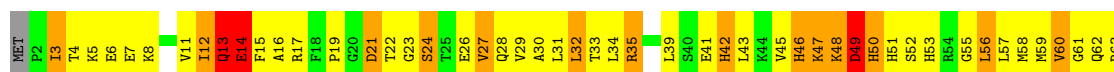
- Molecule 15: 30S ribosomal protein S14

Chain N: 20% 43% 23% 13%



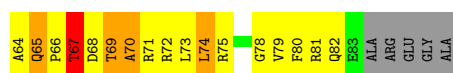
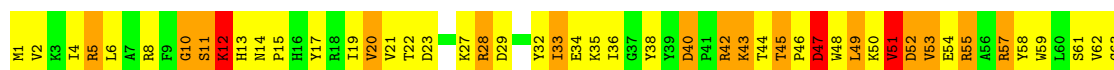
- Molecule 16: 30S ribosomal protein S15

Chain O: 22% 49% 22%



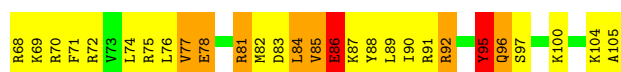
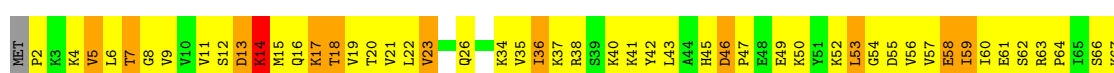
- Molecule 17: 30S ribosomal protein S16

Chain P: 20% 48% 22% 5% 6%



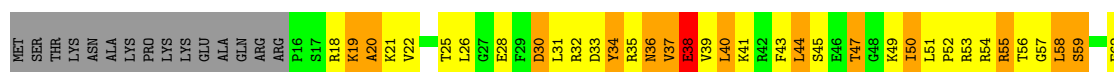
- Molecule 18: 30S ribosomal protein S17

Chain Q: 25% 54% 17%



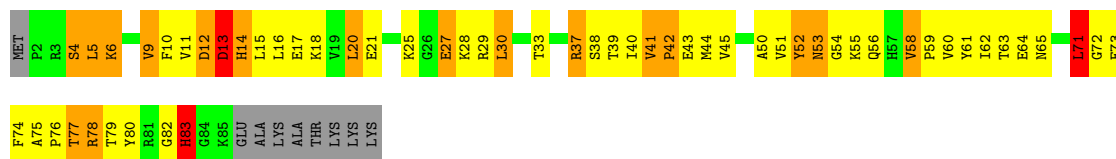
- Molecule 19: 30S ribosomal protein S18

Chain R: 19% 39% 23% 17%

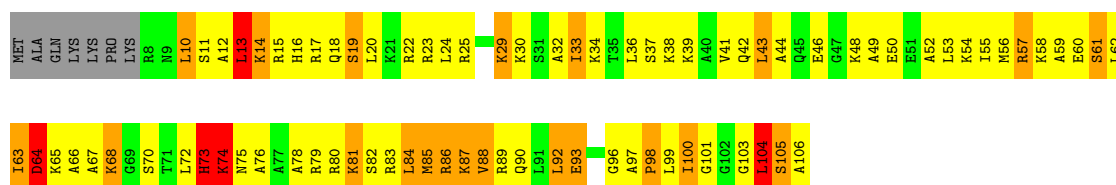
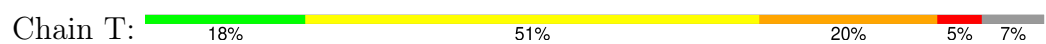




- Molecule 20: 30S ribosomal protein S19



- 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, $\alpha$ , $\beta$ , $\gamma$	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 <sup>2</sup> )	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: MG, AB9, K, 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	1.70	440/36247 (1.2%)	1.64	607/56545 (1.1%)
2	Z	2.01	1/87 (1.1%)	1.60	0/132
3	B	0.84	1/1958 (0.1%)	0.69	5/2640 (0.2%)
4	C	0.91	1/1636 (0.1%)	0.66	3/2205 (0.1%)
5	D	0.81	1/1733 (0.1%)	0.66	5/2318 (0.2%)
6	E	1.14	1/1162 (0.1%)	0.75	3/1564 (0.2%)
7	F	0.73	0/856	0.65	2/1154 (0.2%)
8	G	0.89	1/1276 (0.1%)	0.64	4/1709 (0.2%)
9	H	1.18	1/1136 (0.1%)	0.80	2/1527 (0.1%)
10	I	0.79	0/1029	0.67	5/1378 (0.4%)
11	J	0.81	1/805 (0.1%)	0.75	3/1082 (0.3%)
12	K	0.99	0/900	0.73	2/1213 (0.2%)
13	L	0.87	0/991	0.67	3/1327 (0.2%)
14	M	0.87	1/1008 (0.1%)	0.69	3/1347 (0.2%)
15	N	0.86	0/501	0.63	0/664
16	O	0.88	0/745	0.67	3/992 (0.3%)
17	P	1.16	1/716 (0.1%)	0.82	2/963 (0.2%)
18	Q	1.01	0/870	0.71	3/1159 (0.3%)
19	R	0.92	0/603	0.72	1/799 (0.1%)
20	S	0.70	0/689	0.66	2/926 (0.2%)
21	T	1.07	0/764	0.68	0/1006
All	All	1.47	450/55712 (0.8%)	1.41	658/82650 (0.8%)

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 450 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1169	A	O3'-P	35.46	2.03	1.61
1	A	1227	A	N9-C4	-13.10	1.29	1.37
1	A	1346	A	C3'-O3'	11.14	1.57	1.42
1	A	1224	G	C3'-O3'	10.61	1.57	1.42
1	A	1129	C	C1'-N1	10.46	1.64	1.48

The worst 5 of 658 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1169	A	P-O3'-C3'	29.86	155.53	119.70
1	A	1525	G	C4'-C3'-C2'	-12.91	89.69	102.60
1	A	1346	A	P-O3'-C3'	11.99	134.09	119.70
1	A	1345	U	C1'-O4'-C4'	-11.81	100.45	109.90
1	A	1025	U	C1'-O4'-C4'	-11.60	100.62	109.90

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	1894	0
2	Z	80	0	42	4	0
3	B	1923	0	1968	218	0
4	C	1612	0	1677	175	0
5	D	1703	0	1763	198	0
6	E	1146	0	1207	161	0
7	F	843	0	857	58	0
8	G	1257	0	1296	105	0
9	H	1116	0	1177	93	0
10	I	1011	0	1043	122	0
11	J	792	0	835	125	0
12	K	885	0	904	80	0
13	L	975	0	1062	129	0
14	M	997	0	1072	111	0
15	N	492	0	530	84	0
16	O	734	0	771	70	0
17	P	700	0	720	72	0
18	Q	857	0	930	70	0
19	R	597	0	668	68	0
20	S	674	0	699	56	0
21	T	762	0	859	97	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	3715	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 43.

The worst 5 of 3715 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

### 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	
3	B	235/256 (92%)	153 (65%)	48 (20%)	34 (14%)	0	4
4	C	204/239 (85%)	120 (59%)	51 (25%)	33 (16%)	0	3
5	D	206/209 (99%)	145 (70%)	37 (18%)	24 (12%)	0	6
6	E	148/162 (91%)	110 (74%)	24 (16%)	14 (10%)	0	11
7	F	99/101 (98%)	76 (77%)	17 (17%)	6 (6%)	1	20
8	G	153/156 (98%)	103 (67%)	36 (24%)	14 (9%)	1	12
9	H	136/138 (99%)	103 (76%)	26 (19%)	7 (5%)	2	23
10	I	125/128 (98%)	79 (63%)	33 (26%)	13 (10%)	0	9
11	J	96/105 (91%)	63 (66%)	20 (21%)	13 (14%)	0	4
12	K	117/129 (91%)	79 (68%)	25 (21%)	13 (11%)	0	7
13	L	123/132 (93%)	76 (62%)	29 (24%)	18 (15%)	0	4
14	M	123/126 (98%)	75 (61%)	31 (25%)	17 (14%)	0	4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	N	58/61 (95%)	43 (74%)	8 (14%)	7 (12%)	0	6
16	O	86/89 (97%)	56 (65%)	22 (26%)	8 (9%)	0	11
17	P	81/88 (92%)	55 (68%)	17 (21%)	9 (11%)	0	7
18	Q	102/105 (97%)	73 (72%)	21 (21%)	8 (8%)	1	15
19	R	71/88 (81%)	50 (70%)	14 (20%)	7 (10%)	0	10
20	S	82/93 (88%)	58 (71%)	17 (21%)	7 (8%)	1	12
21	T	97/106 (92%)	60 (62%)	21 (22%)	16 (16%)	0	3
All	All	2342/2511 (93%)	1577 (67%)	497 (21%)	268 (11%)	0	7

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%)	125 (61%)	79 (39%)	0	0
4	C	160/188 (85%)	90 (56%)	70 (44%)	0	0
5	D	180/181 (99%)	105 (58%)	75 (42%)	0	0
6	E	115/123 (94%)	70 (61%)	45 (39%)	0	0
7	F	90/90 (100%)	63 (70%)	27 (30%)	0	2
8	G	126/127 (99%)	80 (64%)	46 (36%)	0	0
9	H	119/119 (100%)	78 (66%)	41 (34%)	0	1
10	I	98/99 (99%)	61 (62%)	37 (38%)	0	0
11	J	87/92 (95%)	51 (59%)	36 (41%)	0	0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	K	90/99 (91%)	62 (69%)	28 (31%)	0	2
13	L	104/109 (95%)	53 (51%)	51 (49%)	0	0
14	M	100/101 (99%)	59 (59%)	41 (41%)	0	0
15	N	49/50 (98%)	26 (53%)	23 (47%)	0	0
16	O	79/80 (99%)	48 (61%)	31 (39%)	0	0
17	P	72/74 (97%)	45 (62%)	27 (38%)	0	0
18	Q	96/97 (99%)	69 (72%)	27 (28%)	0	3
19	R	64/77 (83%)	37 (58%)	27 (42%)	0	0
20	S	73/80 (91%)	47 (64%)	26 (36%)	0	1
21	T	76/82 (93%)	50 (66%)	26 (34%)	0	1
All	All	1982/2088 (95%)	1219 (62%)	763 (38%)	0	0

5 of 763 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	K	30	VAL
14	M	121	LYS
12	K	93	GLN
12	K	29	ILE
13	L	85	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 38 such sidechains are listed below:

Mol	Chain	Res	Type
13	L	99	HIS
20	S	65	ASN
14	M	40	ASN
18	Q	16	GLN
21	T	73	HIS

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1494/1511 (98%)	656 (43%)	162 (10%)
2	Z	3/4 (75%)	0	0
All	All	1497/1515 (98%)	656 (43%)	162 (10%)

5 of 656 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 monosaccharides 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:

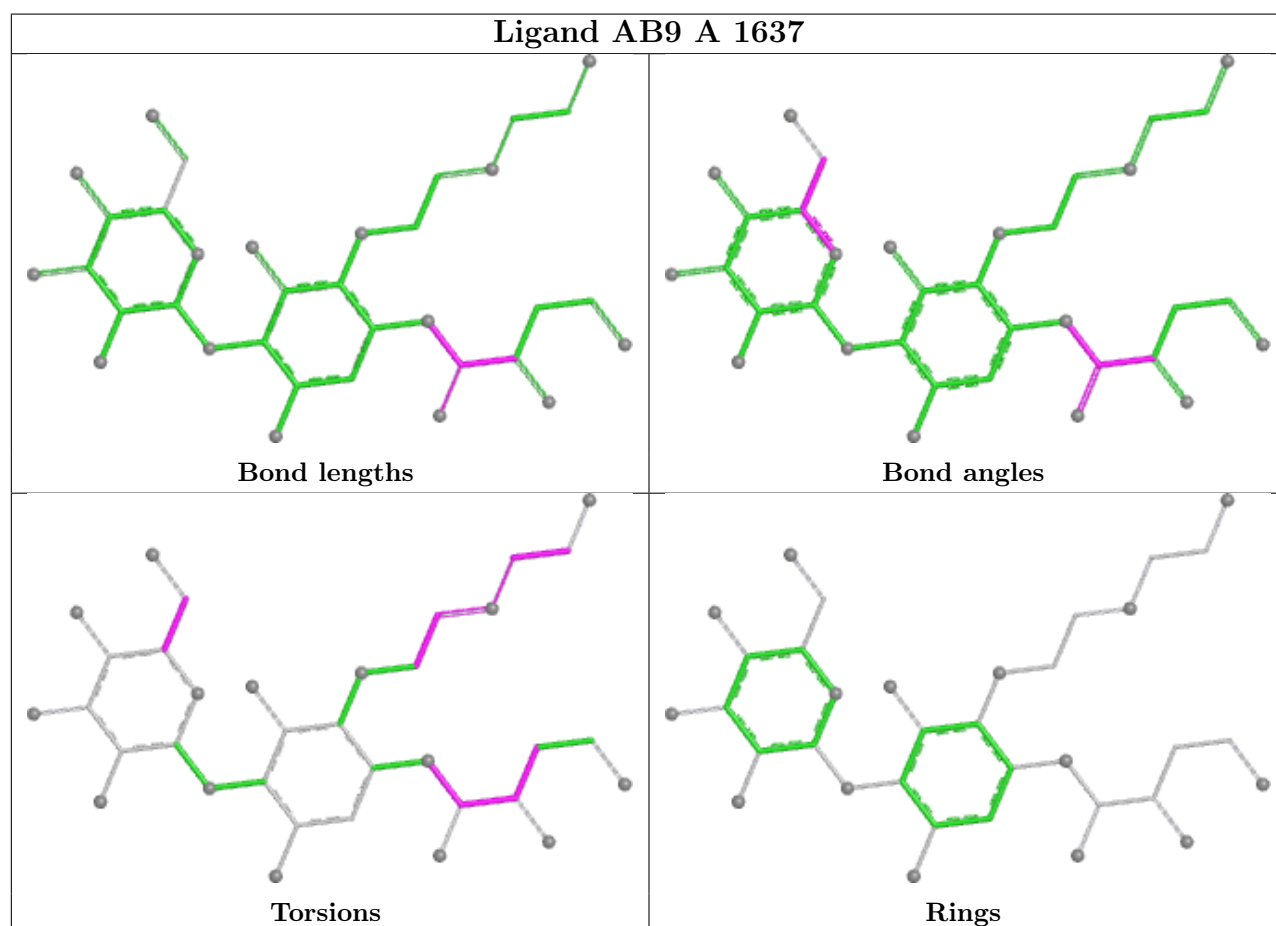
Mol	Chain	Res	Type	Atoms
24	A	1636	D2C	C4-C3-N1-C1
24	A	1636	D2C	C5-C3-N1-C1
24	A	1636	D2C	C4-C3-N1-C2
24	A	1636	D2C	C4-C20-C21-O7
24	A	1636	D2C	C19-C20-C21-O7

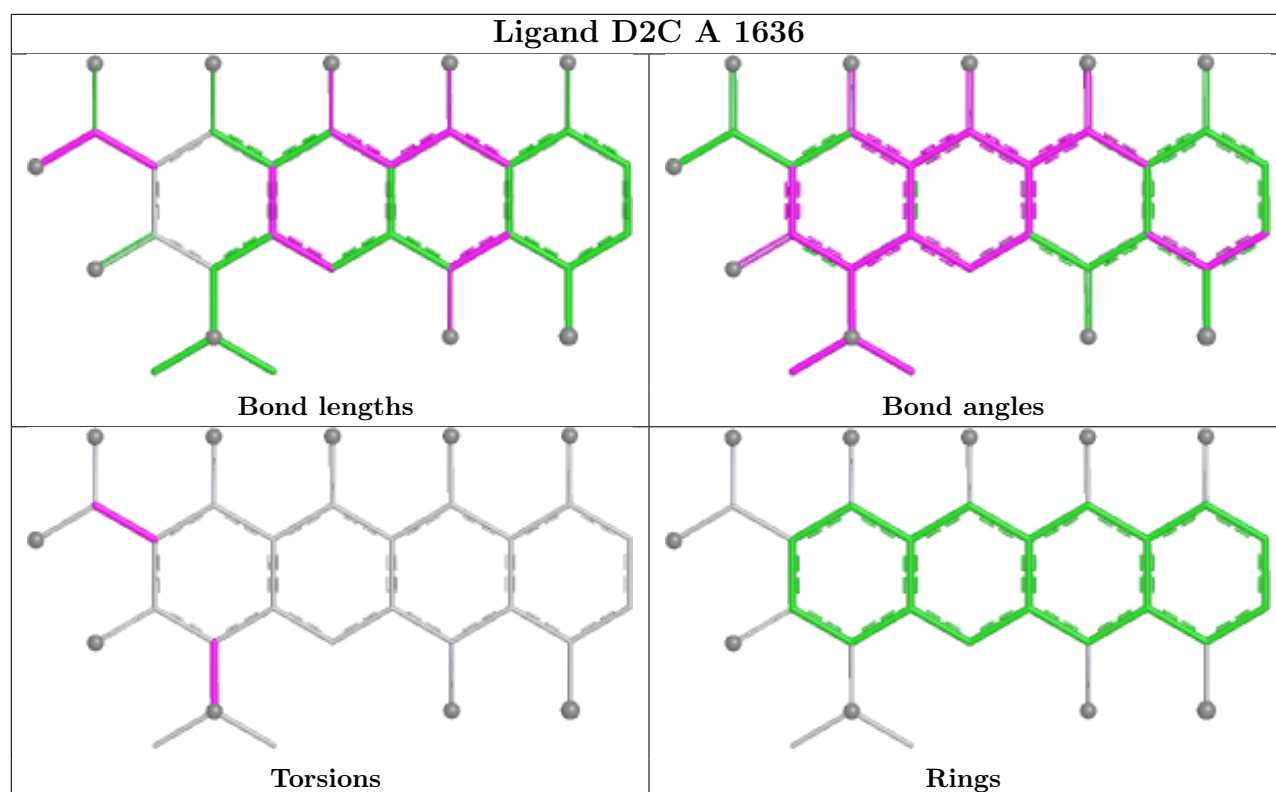
There are no ring outliers.

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.