



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 19, 2026 – 12:08 AM UTC

PDB ID : 5JVH / pdb_00005jvh
Title : The crystal structure large ribosomal subunit (50S) of *Deinococcus radiodurans* in complex with evernimicin
Authors : Yonath, A.
Deposited on : 2016-05-11
Resolution : 3.58 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) : 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

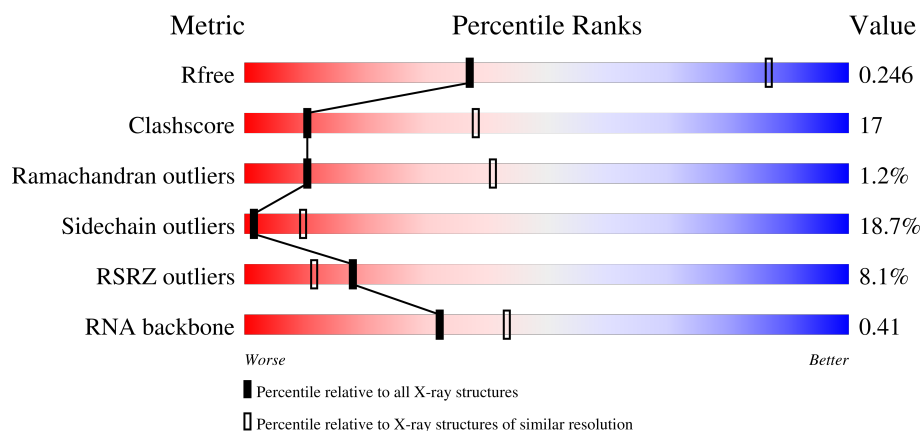
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.58 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	1521 (3.66-3.50)
Clashscore	190562	1595 (3.66-3.50)
Ramachandran outliers	187476	1551 (3.66-3.50)
Sidechain outliers	187428	1551 (3.66-3.50)
RSRZ outliers	180081	1520 (3.66-3.50)
RNA backbone	3983	1013 (4.10-3.06)

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	X	2880	5% 38% 43% 12% 8%
2	Y	123	9% 46% 41% 11%
3	A	275	15% 39% 44% 11% 6%
4	B	211	5% 46% 39% 9%

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Mol	Chain	Length	Quality of chain
5	C	205	
6	D	180	
7	E	185	
8	G	174	
9	H	134	
10	I	156	
11	J	141	
12	K	116	
13	L	114	
14	M	166	
15	N	118	
16	O	100	
17	P	134	
18	Q	95	
19	R	115	
20	S	237	
21	T	91	
22	U	81	
23	V	67	
24	W	55	
25	Z	60	
26	1	54	
27	2	47	
28	3	66	

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
30	MG	X	2906	-	-	-	X
30	MG	X	2909	-	-	-	X
30	MG	X	2916	-	-	-	X
30	MG	X	2921	-	-	-	X
30	MG	X	2927	-	-	-	X
30	MG	X	2931	-	-	-	X
30	MG	X	2939	-	-	-	X
30	MG	X	2944	-	-	-	X
30	MG	X	2952	-	-	-	X
30	MG	X	2964	-	-	-	X
30	MG	X	2967	-	-	-	X
30	MG	X	2970	-	-	-	X
30	MG	X	2976	-	-	-	X
30	MG	X	2977	-	-	-	X
30	MG	X	2988	-	-	-	X
30	MG	X	2999	-	-	-	X
30	MG	X	3001	-	-	-	X
30	MG	X	3015	-	-	-	X
30	MG	X	3016	-	-	-	X
30	MG	X	3019	-	-	-	X
30	MG	X	3020	-	-	-	X

2 Entry composition

There are 30 unique types of molecules in this entry. The entry contains 83681 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 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	X	2658	Total	C	N	O	P	0	0	0
			57052	25450	10532	18413	2657			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	1526	U	C	conflict	GB 1026245073

- Molecule 2 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	Y	120	Total	C	N	O	P	0	0	0
			2561	1143	471	827	120			

- Molecule 3 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	259	Total	C	N	O	S	0	0	0
			1973	1226	395	349	3			

- Molecule 4 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	205	Total	C	N	O	S	0	0	0
			1539	965	295	271	8			

- Molecule 5 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	C	194	Total	C	N	O	S	0	0	0
			1481	920	284	275	2			

- Molecule 6 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	D	177	Total	C	N	O	S	0	0	0
			1400	892	247	254	7			

- Molecule 7 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	E	171	Total	C	N	O	S	0	0	0
			1286	812	237	236	1			

- Molecule 8 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	G	142	Total	C	N	O	S	0	0	0
			1114	704	209	198	3			

- Molecule 9 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	H	134	Total	C	N	O	S	0	0	0
			997	614	198	180	5			

- Molecule 10 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	I	134	Total	C	N	O	S	0	0	0
			1011	619	206	186				

- Molecule 11 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	J	136	Total	C	N	O	S	0	0	0
			1078	690	196	185	7			

- Molecule 12 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	K	113	Total	C	N	O	S	0	0	0
			878	541	178	157	2			

- Molecule 13 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	L	104	Total	C	N	O	0	0	0
			779	476	161	142			

- Molecule 14 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	M	108	Total	C	N	O	0	0	0
			859	537	166	156			

- Molecule 15 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	N	117	Total	C	N	O	S	0	0	0
			978	608	210	159	1			

- Molecule 16 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
16	O	94	Total	C	N	O	0	0	0
			741	465	139	137			

- Molecule 17 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	P	127	Total	C	N	O	S	0	0	0
			1014	639	199	174	2			

- Molecule 18 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	Q	93	Total	C	N	O	S	0	0	0
			726	458	136	130	2			

- Molecule 19 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	R	110	Total	C	N	O	S	0	0	0
			825	513	160	151	1			

- Molecule 20 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	S	179	Total	C	N	O	S	0	0	0
			1374	867	240	261	6			

- Molecule 21 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	T	74	Total	C	N	O	S	0	0	0
			556	351	107	97	1			

- Molecule 22 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	U	72	Total	C	N	O		0	0	0
			552	341	116	95				

- Molecule 23 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	V	65	Total	C	N	O	S	0	0	0
			525	322	106	95	2			

- Molecule 24 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	W	55	Total	C	N	O	S	0	0	0
			424	264	82	76	2			

- Molecule 25 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	Z	57	Total	C	N	O	S	0	0	0
			452	278	93	76	5			

- Molecule 26 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	1	53	Total	C	N	O	S	0	0	0
			427	271	79	76	1			

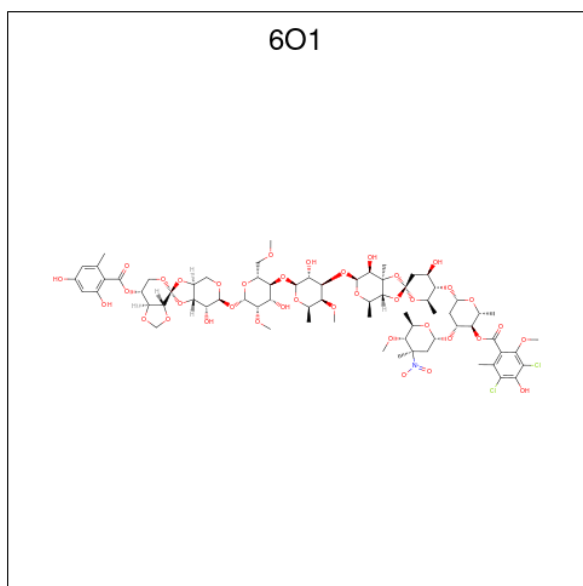
- Molecule 27 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	2	46	Total	C	N	O	S	0	0	0
			383	230	91	60	2			

- Molecule 28 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	3	59	Total	C	N	O	S	0	0	0
			462	290	95	73	4			

- Molecule 29 is Evernimicin (CCD ID: 6O1) (formula: $C_{70}H_{97}Cl_2NO_{38}$).

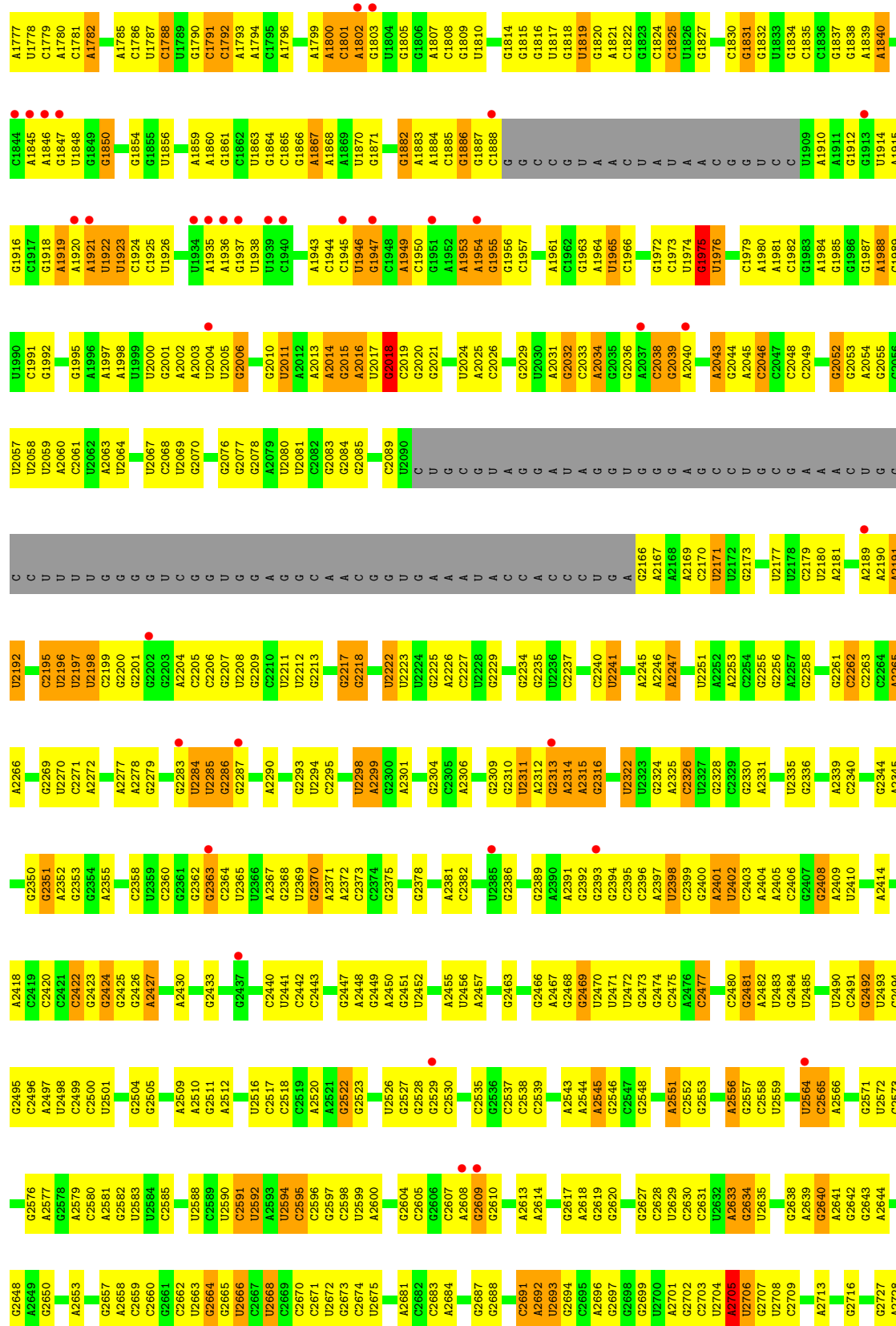


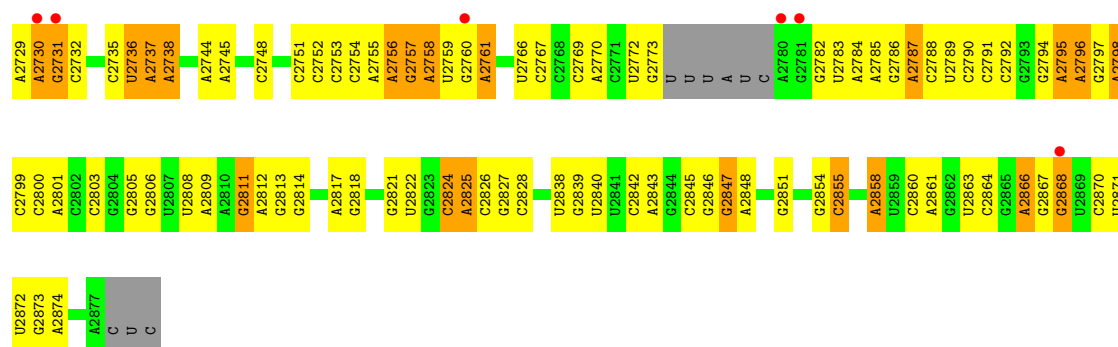
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
29	X	1	Total	C	Cl	N	O	0	0
			111	70	2	1	38		

- Molecule 30 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

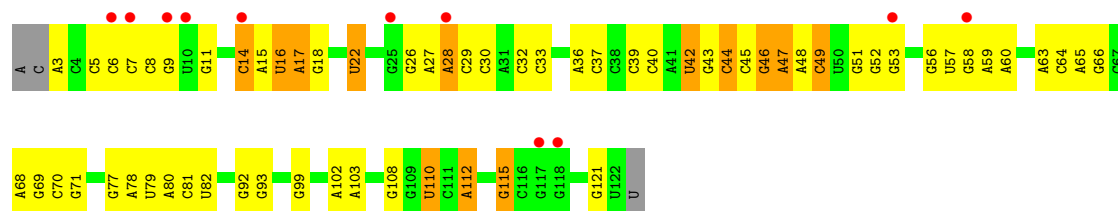
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
30	X	119	Total	Mg	0	0
			119	119		
30	Y	1	Total	Mg	0	0
			1	1		
30	K	2	Total	Mg	0	0
			2	2		
30	M	1	Total	Mg	0	0
			1	1		

U1697	A1810	G1532	C1462	C1385	A1314	A1231	G1165	C	C1029	G951	A879	U810	G742
C1698	C1614	G1533	A1463	A1386	A1315	C1235	A1166	U	U1030	A952	C880	C811	A743
A1699	C1615	A1534	G1465	G1390	G1316	C1236	C1236	C	C1031	G953	U881	C812	A746
C1700	C1616	G1542	G1466	A1391	G1317	G1237	G1173	A	A1032	G955	U890	C813	A747
U1705	G1617	G1543	U1467	U1392	C1321	G1240	A1174	A	G1033	A956	G	C818	C750
C1623	C1623	A1544	A1468	G1393	C1322	G1241	A1175	A	U1034	G957	G	C819	G751
A1624	A1624	U1547	U1469	A1397	G1323	G1242	U1176	G	G1035	G958	A	U820	G752
A1625	A1625	G1548	G1470	G1398	U1325	A1242	U1177	A	U1036	G959	G	C820	G753
A1630	A1630	C1550	U1475	C1399	U1326	G1245	C1178	G	U1037	A964	G	C821	G754
G1713	G1713	U1551	G1476	U1403	C1327	G1246	A1179	U1101	A1039	G965	G	C822	G755
A1714	A1714	C1552	C1477	C1404	G1328	U1247	G1181	C1103	A1040	A966	C	U823	C756
A1715	A1715	C1553	U1478	C1404	U1329	G1248	U1182	G1104	G1041	G967	C	C824	C757
G1716	G1716	G1554	G1479	G1407	G1330	A1250	C1183	U1105	U1044	C968	U	C825	U757
A1717	A1634	A1555	U1481	A1408	G1331	A1251	A1106	A1106	A1045	U969	A	C829	G758
A1718	G1635	A1556	U1482	U1409	G1332	C1252	C1185	U1107	U1046	C970	C	C830	U760
		G1557	G1483	U1411	A1334	A1255	C1187	A1109	G1047	C972	A	A832	A762
A1643	A1643	C1558	C1412	C1412	G1336	C1256	A1188	G1110	U1048	G977	C	A833	A763
G1721	G1721	G1559	A1416	A1416	G1337	A1260	G1189	U1112	U1050	U978	U	A834	A764
G1722	G1646	A1560	C1487	C1412	G1340	C1261	C1191	G1117	C1052	A979	A	U837	A766
U1723	U1647	U1561	G1488	C1412	G1341	U1262	G1193	C1120	G1053	A984	C	U840	G767
C1724	C1648	A1562	C1489	C1412	G1342	U1263	U1194	G1121	C1054	G985	C	U841	C769
A1728	A1649	U1563	C1490	C1419	U1343	C1264	U1195	A1122	A1055	A986	C	A842	G773
G1735	G1652	U1564	C1491	A1420	C1344	G1265	C1197	G1123	U1056	G987	C	U845	A774
G1742	A1654	G1565	A1492	U1421	G1345	A1267	U1197	U1124	A1057	G988	C	U846	A777
C1743	C1655	C1570	A1493	C1422	G1346	U1268	U1198	G1125	G1058	G989	C	A847	C778
G1744	U1656	G1573	G1496	U1424	C1348	U1269	G1201	C1126	C1063	A992	U	C847	U779
A1657	A1657	C1574	C1497	U1425	A1349	G1270	U1202	A1127	C	G993	U	A848	
A1658	A1658	U1575	G1498	U1426	G1350	C1271	A1203	G1128	A	A994	U	C849	U784
C1746	G1659	G1576	G1499	G1427	G1351	C1272	G1204	A1129	A995	A922	C	C850	U785
G1747	G1660	G1577	U1500	G1428	G1352	G1273	G1205	G1130	G	C996	C	U852	U786
A1750	A1661	U1578	C1501	A1429	A1353	C1274	G1206	U1136	A	G997	U	C853	A787
A1751	C1665	G1579	G1430	U1431	A1354	A1275	G1207	G1136	G	C998	U	C854	G788
U1752		U1582	U1432	G1432	A1355	U1276	A1208	A1139	U	A999	C	U857	G789
A1753	A1669	C1506	A1433	A1433	G1356	U1277	G1209	A1140	C	C1003	U	U858	A790
G1754	G1670	G1507	U1434	G1435	U1357	A1278	U1212	U1141	A1004	A928	U	U859	G791
C1755	A1671	G1508	U1436	U1436	C1358	G1279	G1213	G1142	U1005	A930	U	C860	U792
C1756	A1672	A1509	G1437	G1437	G1359	C1283	G1214	G1073	C1006	G931	U	U861	G793
C1757	C1673	A1510	A1438	G1438	G1361	G1284	A1215	U1072	A1007	G932	U	C862	A794
C1758	C1674	A1511	G1439	G1439	A1362	U1285	G1216	C1075	G1008	G933	U	C863	A795
C1675	C1675	U1583	G1440	G1440	C1363	U1287	U1217	U1076	C1009	G934	U	C864	U796
U1676	U1676	A1516	A1441	C1442	U1365	A1288	G1218	A1079	G1013	G938	U	A865	A797
C1677	C1677	C1517	U1454	C1443	U1370	A1289	G1220	C1150	U1014	C939	U	U866	G798
G1678	G1678	U1515	U1455	G1444	G1371	A1290	G1221	A1081	G1015	G940	U	U867	U800
A1682	A1682	G1520	C1455	C1444	A1372	G1296	C1152	C1016	C1016	G941	U	C870	A801
G1683	G1683	U1521	U1456	A1448	G1374	G1297	G1222	C1017	C1017	U942	U	U871	A802
G1684	A1684	C1522	C1457	C1448	G1374	G1298	G1223	C1018	C1018	U943	U	C872	C803
A1685	A1685	A1523	U1458	U1458	G1374	A1299	A1224	U1019	U1019	U944	U	A873	G804
A1686	A1686	C1524	C1459	C1455	A1378	C1310	G1225	C	G	A944	U	A874	G805
C1687	C1687	A1604	U1460	C1455	A1378	C1311	G1226	C	C	G945	U	C875	A806
A1691	A1691	U1526	U1461	C1455	A1378	C1312	A1227	A	A	U946	U	A876	A807
C1692	C1692	G1527	U1462	U1459	G1381	G1312	G1228	C	C	C947	U	C877	C808
A1693	A1693	C1528	G1460	G1460	G1384	U1313	G1230	C	C	C948	U	C878	C809
A1694	A1694	C1531	C1461	C1461	G1384	U1313	C1230			G1024	U		

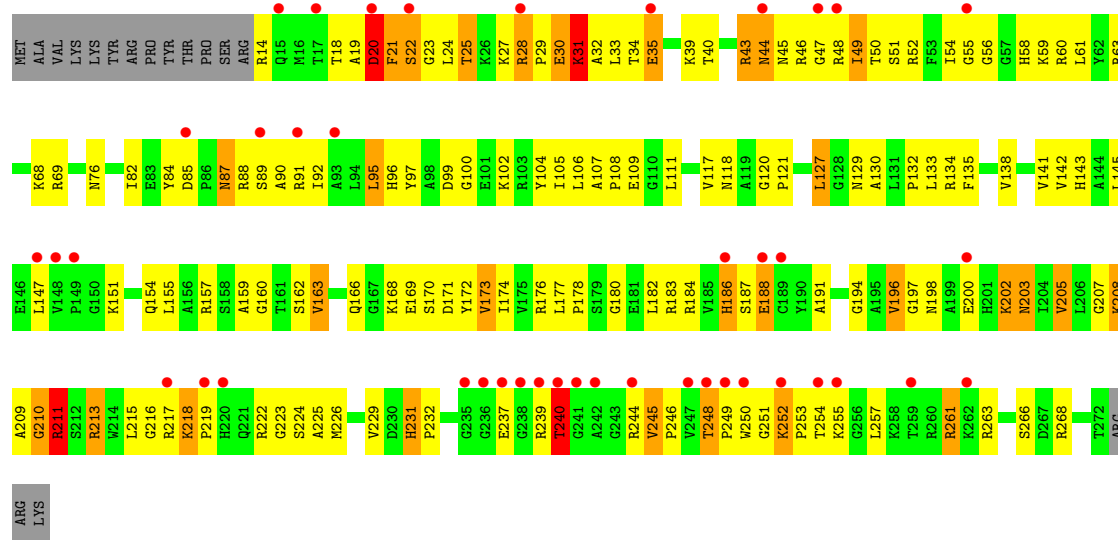




• Molecule 2: 5S ribosomal RNA

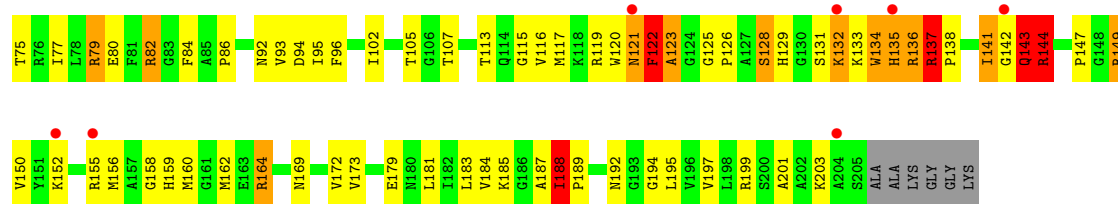


• Molecule 3: 50S ribosomal protein L2

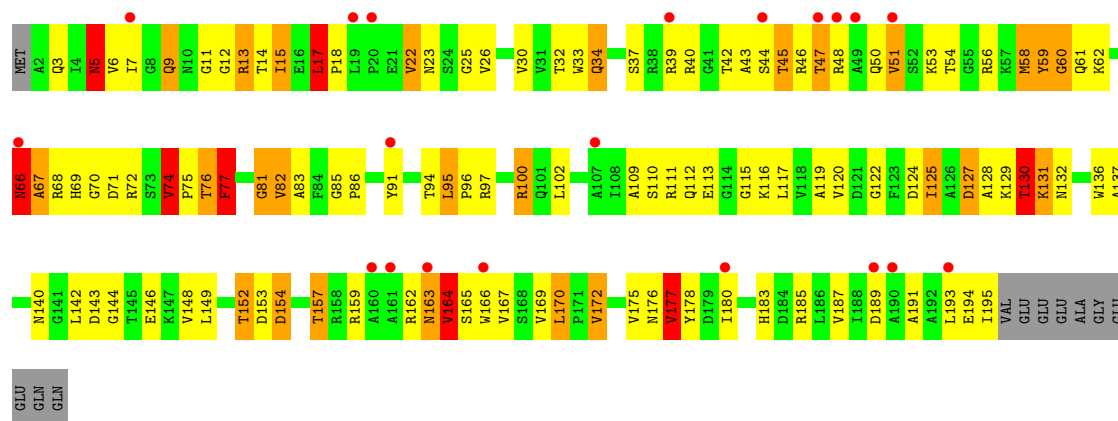


• Molecule 4: 50S ribosomal protein L3

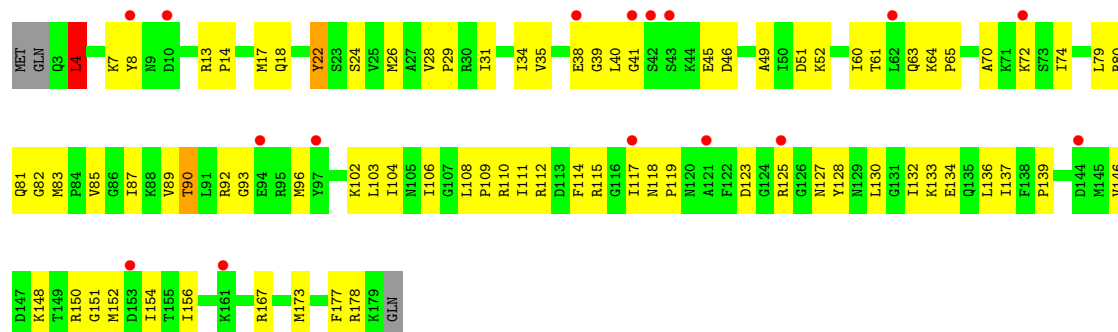




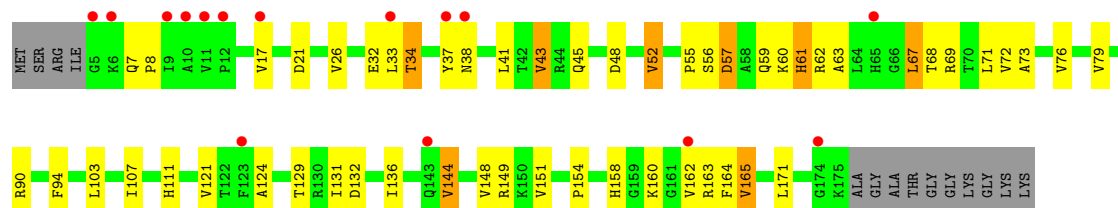
• Molecule 5: 50S ribosomal protein L4



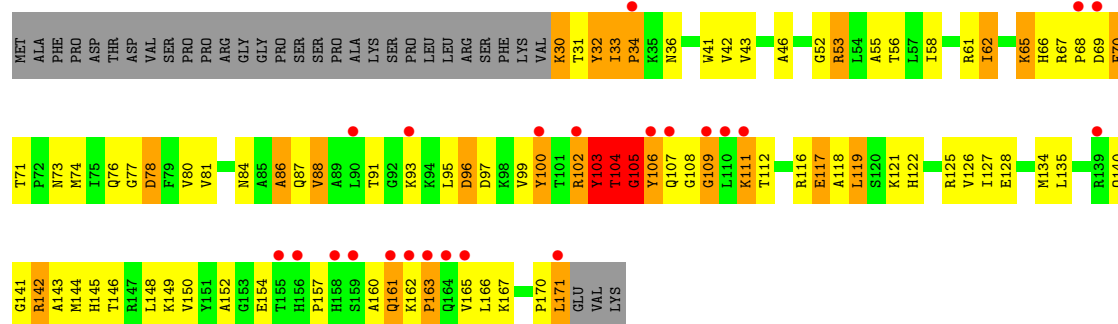
• Molecule 6: 50S ribosomal protein L5



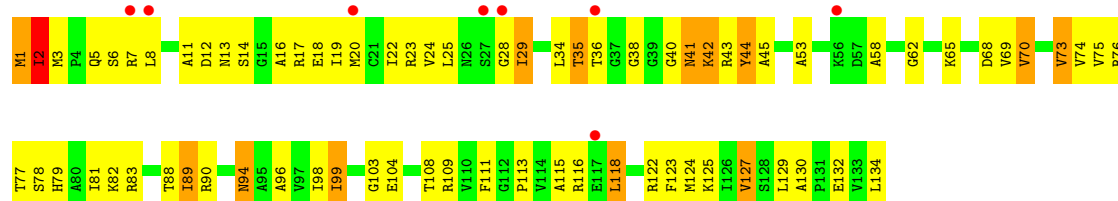
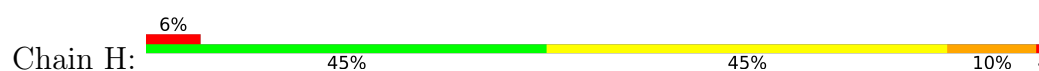
• Molecule 7: 50S ribosomal protein L6



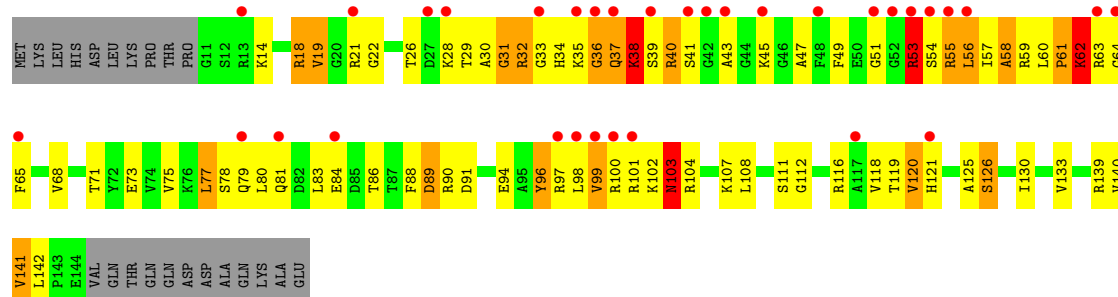
• Molecule 8: 50S ribosomal protein L13



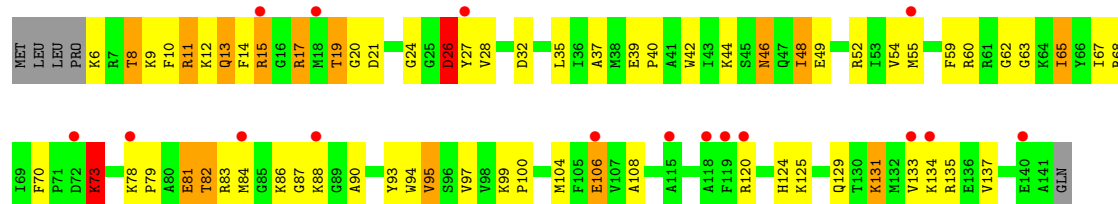
• Molecule 9: 50S ribosomal protein L14



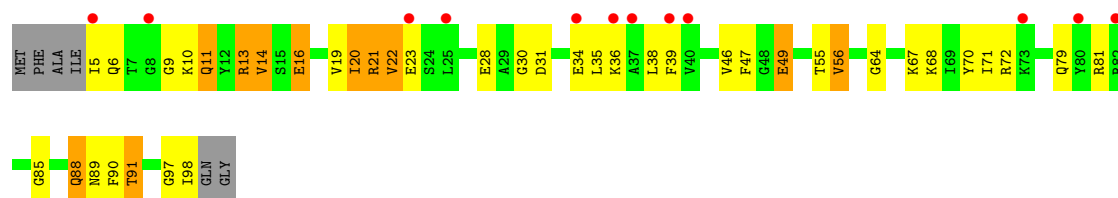
• Molecule 10: 50S ribosomal protein L15



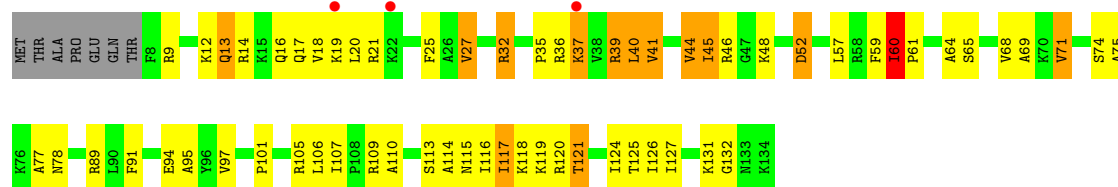
• Molecule 11: 50S ribosomal protein L16



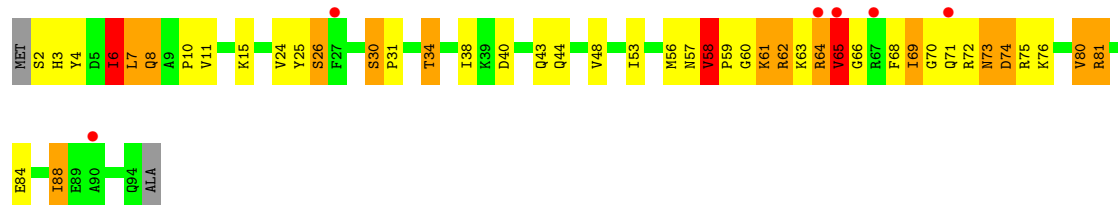
• Molecule 12: 50S ribosomal protein L17



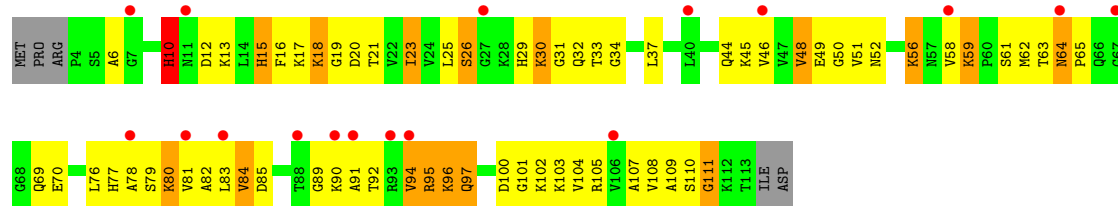
• Molecule 17: 50S ribosomal protein L22



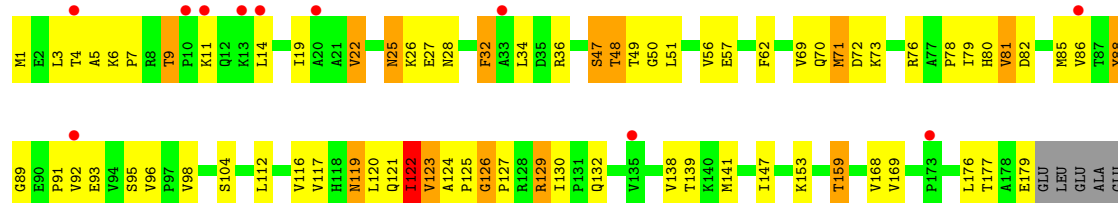
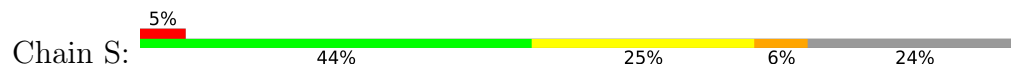
• Molecule 18: 50S ribosomal protein L23



• Molecule 19: 50S ribosomal protein L24



• Molecule 20: 50S ribosomal protein L25



VAL GLN ALA ALA ALA GLN VAL ALA GLY VAL SER VAL ALA ALA GLY GLU LEU SER SER GLU GLU ALA ALA GLU VAL ALA VAL VAL LEU GLU GLY ASP SER SER LEU GLU VAL VAL LYS ALA ALA GLU SER GLU ASP ASN ALA GLY THR ASP SER GLU ASP ASN SER ASP ALA GLN

• Molecule 21: 50S ribosomal protein L27

Chain T: 10% 51% 24% 7% 19%

MET ALA HIS LYS LYS VAL GLY SER SER LYS N12 N13 R14 D15 S16 N17 P18 K19 Y20 V23 K24 K25 F26 E29 V30 T36 L37 V38 K44 F45 K46 A47 V51 F60 D64 G65 K66 V67 V68 K72 G73 G74 G75 A76 R77 F78 I79 S80 Q85 THR

GLU VAL ALA ALA ASP

• Molecule 22: 50S ribosomal protein L28

Chain U: 14% 40% 32% 15% 11%

MET SER ARG GLU CYS TYR LEU T8 G9 L13 V14 V15 N16 V17 S18 I19 R20 R21 R22 K23 D27 G28 G29 V30 G31 R32 K33 T34 T35 G36 L37 T38 K39 R40 V41 Q42 R43 A44 N45 L46 H47 K48 K49 A50 I51 R52 R53 R54 K58 T59 V60 W61 L62 S63 A66 L67

L70 Y75 Y76 G77 I78 E79 LEU ILE

• Molecule 23: 50S ribosomal protein L29

Chain V: 3% 58% 39%

MET K2 P3 S4 E5 M6 T12 D13 F14 E17 I18 D19 A20 K22 K23 L28 R29 F30 Q31 A32 Q36 L37 R42 V43 R44 Q45 L46 R47 R48 Q52 L53 R62 Q66 GLN

• Molecule 24: 50S ribosomal protein L30

Chain W: 5% 51% 38% 11%

M1 K2 T3 K4 P5 L5 V6 R7 S8 V9 T10 G11 R12 P13 G14 T19 L23 L25 R26 K27 D30 D36 T37 P38 C33 V40 R41 Q42 M43 T46 V47 L50 L51 E52 V53 Q54 E55

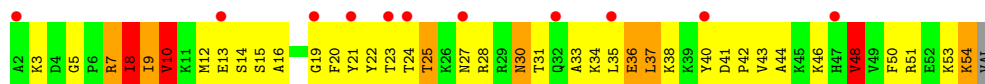
• Molecule 25: 50S ribosomal protein L32

Chain Z: 5% 37% 40% 15% 5%

MET ALA K3 H4 P5 V6 P7 K8 K9 K10 K13 S14 K15 R16 D17 M18 R19 R20 S21 L25 T26 A27 L30 T31 E32 C33 P34 Q35 K40 L41 S42 I45 C46 C49 G50 Y51 D52 D53 G54 R55 Q56 V57 L58 A59 VAL

• Molecule 26: 50S ribosomal protein L33

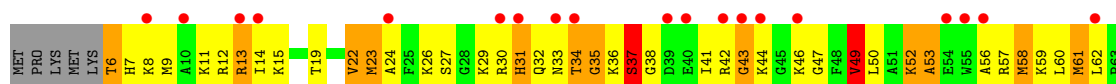
Chain 1: 20% 26% 54% 13% 6%



- Molecule 27: 50S ribosomal protein L34



- Molecule 28: 50S ribosomal protein L35



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	169.47Å 407.38Å 692.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.84 – 3.58 29.84 – 3.58	Depositor EDS
% Data completeness (in resolution range)	94.3 (29.84-3.58) 94.2 (29.84-3.58)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.91 (at 3.56Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.204 , 0.247 0.203 , 0.246	Depositor DCC
R_{free} test set	13397 reflections (4.76%)	wwPDB-VP
Wilson B-factor (Å ²)	112.0	Xtriage
Anisotropy	0.654	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.23 , 55.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	83681	wwPDB-VP
Average B, all atoms (Å ²)	96.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.34% 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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 6O1, 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	X	0.37	0/63887	0.56	5/99650 (0.0%)
2	Y	0.23	0/2863	0.42	0/4461
3	A	0.70	3/2011 (0.1%)	1.27	23/2708 (0.8%)
4	B	0.78	0/1567	1.29	16/2105 (0.8%)
5	C	0.67	1/1504 (0.1%)	1.26	19/2036 (0.9%)
6	D	0.40	0/1419	0.92	3/1903 (0.2%)
7	E	0.44	0/1308	0.94	2/1771 (0.1%)
8	G	0.63	0/1138	1.25	16/1539 (1.0%)
9	H	0.77	1/1007 (0.1%)	1.15	5/1352 (0.4%)
10	I	0.82	0/1022	1.45	15/1366 (1.1%)
11	J	0.66	1/1101 (0.1%)	1.22	14/1472 (1.0%)
12	K	0.88	1/886 (0.1%)	1.34	12/1188 (1.0%)
13	L	0.55	0/785	1.09	3/1048 (0.3%)
14	M	0.88	1/872 (0.1%)	1.34	11/1172 (0.9%)
15	N	0.67	0/994	1.15	9/1323 (0.7%)
16	O	0.55	0/750	1.19	6/1000 (0.6%)
17	P	0.74	0/1027	1.19	6/1373 (0.4%)
18	Q	0.66	0/737	1.41	6/988 (0.6%)
19	R	0.61	1/835 (0.1%)	1.25	15/1121 (1.3%)
20	S	0.46	0/1399	0.99	7/1902 (0.4%)
21	T	0.55	0/563	1.18	4/747 (0.5%)
22	U	0.59	0/556	1.08	2/741 (0.3%)
23	V	0.42	0/529	0.89	0/704
24	W	0.56	0/426	0.98	2/568 (0.4%)
25	Z	0.75	0/464	1.36	8/622 (1.3%)
26	1	0.67	0/434	1.39	10/579 (1.7%)
27	2	0.78	0/387	1.55	9/509 (1.8%)
28	3	0.74	0/468	1.46	9/614 (1.5%)
All	All	0.46	9/90939 (0.0%)	0.76	237/136562 (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
3	A	0	1
4	B	0	1
5	C	0	2
8	G	0	4
10	I	0	5
11	J	0	1
13	L	0	1
15	N	0	2
19	R	0	1
25	Z	0	1
27	2	0	3
28	3	0	2
All	All	0	24

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	M	29	PRO	CA-C	9.62	1.66	1.52
3	A	20	ASP	N-CA	7.46	1.55	1.46
5	C	51	VAL	CA-CB	6.51	1.64	1.54
12	K	12	ARG	CA-C	6.32	1.61	1.52
3	A	20	ASP	CA-C	5.92	1.60	1.52

The worst 5 of 237 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	Q	58	VAL	CA-C-N	16.57	136.47	119.24
18	Q	58	VAL	C-N-CA	16.57	136.47	119.24
3	A	35	GLU	N-CA-C	14.34	127.69	110.91
17	P	60	ILE	CA-C-N	13.30	132.86	119.82
17	P	60	ILE	C-N-CA	13.30	132.86	119.82

There are no chirality outliers.

5 of 24 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	58	HIS	Peptide
4	B	122	PHE	Peptide
5	C	176	ASN	Peptide

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Mol	Chain	Res	Type	Group
5	C	66	ASN	Peptide
8	G	34	PRO	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	X	57052	0	28750	1266	0
2	Y	2561	0	1306	57	0
3	A	1973	0	2034	136	0
4	B	1539	0	1600	85	0
5	C	1481	0	1504	99	0
6	D	1400	0	1481	61	0
7	E	1286	0	1336	31	0
8	G	1114	0	1144	83	0
9	H	997	0	1046	58	0
10	I	1011	0	1047	77	0
11	J	1078	0	1103	48	0
12	K	878	0	930	36	0
13	L	779	0	820	50	0
14	M	859	0	872	35	0
15	N	978	0	1020	73	0
16	O	741	0	756	34	0
17	P	1014	0	1096	51	0
18	Q	726	0	753	31	0
19	R	825	0	881	59	0
20	S	1374	0	1401	48	0
21	T	556	0	579	25	0
22	U	552	0	604	43	0
23	V	525	0	546	14	0
24	W	424	0	470	17	0
25	Z	452	0	457	36	0
26	1	427	0	445	36	0
27	2	383	0	414	38	0
28	3	462	0	506	37	0
29	X	111	0	0	2	0
30	K	2	0	0	0	0
30	M	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	X	119	0	0	0	0
30	Y	1	0	0	0	0
All	All	83681	0	54901	2321	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 17.

The worst 5 of 2321 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:100:TYR:HB2	8:G:116:ARG:HE	1.25	0.96
10:I:56:LEU:H	10:I:59:ARG:HD3	1.30	0.94
1:X:1277:G:OP1	25:Z:19:ARG:NH2	2.01	0.93
1:X:1264:C:H5''	15:N:13:ARG:HH12	1.34	0.93
15:N:66:ASN:HB3	15:N:76:TYR:HB2	1.48	0.92

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	A	257/275 (94%)	219 (85%)	37 (14%)	1 (0%)	30	60
4	B	203/211 (96%)	183 (90%)	15 (7%)	5 (2%)	4	28
5	C	192/205 (94%)	161 (84%)	25 (13%)	6 (3%)	3	25
6	D	175/180 (97%)	151 (86%)	24 (14%)	0	100	100
7	E	169/185 (91%)	155 (92%)	13 (8%)	1 (1%)	21	54
8	G	140/174 (80%)	124 (89%)	15 (11%)	1 (1%)	18	51
9	H	132/134 (98%)	123 (93%)	8 (6%)	1 (1%)	16	49
10	I	132/156 (85%)	98 (74%)	30 (23%)	4 (3%)	3	25

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	J	134/141 (95%)	117 (87%)	16 (12%)	1 (1%)	18	51
12	K	111/116 (96%)	101 (91%)	9 (8%)	1 (1%)	14	46
13	L	102/114 (90%)	80 (78%)	22 (22%)	0	100	100
14	M	106/166 (64%)	100 (94%)	6 (6%)	0	100	100
15	N	115/118 (98%)	100 (87%)	13 (11%)	2 (2%)	7	35
16	O	92/100 (92%)	83 (90%)	9 (10%)	0	100	100
17	P	125/134 (93%)	121 (97%)	4 (3%)	0	100	100
18	Q	91/95 (96%)	69 (76%)	19 (21%)	3 (3%)	3	23
19	R	108/115 (94%)	80 (74%)	28 (26%)	0	100	100
20	S	177/237 (75%)	150 (85%)	25 (14%)	2 (1%)	11	43
21	T	72/91 (79%)	63 (88%)	9 (12%)	0	100	100
22	U	70/81 (86%)	51 (73%)	17 (24%)	2 (3%)	3	25
23	V	63/67 (94%)	58 (92%)	5 (8%)	0	100	100
24	W	53/55 (96%)	49 (92%)	4 (8%)	0	100	100
25	Z	55/60 (92%)	45 (82%)	10 (18%)	0	100	100
26	1	51/54 (94%)	36 (71%)	12 (24%)	3 (6%)	1	13
27	2	44/47 (94%)	37 (84%)	5 (11%)	2 (4%)	2	17
28	3	57/66 (86%)	44 (77%)	11 (19%)	2 (4%)	3	23
All	All	3026/3377 (90%)	2598 (86%)	391 (13%)	37 (1%)	10	41

5 of 37 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
15	N	94	VAL
18	Q	6	ILE
5	C	177	VAL
20	S	122	ILE
26	1	9	ILE

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	A	200/216 (93%)	161 (80%)	39 (20%)	1	9
4	B	155/157 (99%)	122 (79%)	33 (21%)	1	7
5	C	154/163 (94%)	119 (77%)	35 (23%)	1	6
6	D	153/156 (98%)	145 (95%)	8 (5%)	21	48
7	E	136/144 (94%)	121 (89%)	15 (11%)	6	27
8	G	118/146 (81%)	99 (84%)	19 (16%)	2	15
9	H	103/103 (100%)	83 (81%)	20 (19%)	1	9
10	I	101/121 (84%)	77 (76%)	24 (24%)	1	5
11	J	108/115 (94%)	90 (83%)	18 (17%)	2	14
12	K	90/93 (97%)	71 (79%)	19 (21%)	1	7
13	L	74/82 (90%)	51 (69%)	23 (31%)	0	2
14	M	92/134 (69%)	69 (75%)	23 (25%)	0	4
15	N	96/97 (99%)	87 (91%)	9 (9%)	8	32
16	O	75/79 (95%)	61 (81%)	14 (19%)	1	10
17	P	109/115 (95%)	88 (81%)	21 (19%)	1	9
18	Q	75/76 (99%)	55 (73%)	20 (27%)	0	3
19	R	91/96 (95%)	74 (81%)	17 (19%)	1	10
20	S	152/192 (79%)	127 (84%)	25 (16%)	2	14
21	T	55/67 (82%)	46 (84%)	9 (16%)	2	14
22	U	57/66 (86%)	42 (74%)	15 (26%)	0	4
23	V	53/55 (96%)	50 (94%)	3 (6%)	18	46
24	W	48/48 (100%)	38 (79%)	10 (21%)	1	7
25	Z	51/53 (96%)	39 (76%)	12 (24%)	1	5
26	1	45/47 (96%)	34 (76%)	11 (24%)	1	5
27	2	39/40 (98%)	30 (77%)	9 (23%)	1	6
28	3	46/52 (88%)	35 (76%)	11 (24%)	1	5
All	All	2476/2713 (91%)	2014 (81%)	462 (19%)	1	10

5 of 462 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
13	L	11	LEU

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Mol	Chain	Res	Type
27	2	6	GLN
16	O	16	GLU
26	1	36	GLU
22	U	49	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 60 such sidechains are listed below:

Mol	Chain	Res	Type
10	I	103	ASN
25	Z	23	HIS
12	K	35	GLN
24	W	54	GLN
27	2	41	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	X	2650/2880 (92%)	581 (21%)	49 (1%)
2	Y	119/123 (96%)	23 (19%)	1 (0%)
All	All	2769/3003 (92%)	604 (21%)	50 (1%)

5 of 604 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	X	2	G
1	X	4	C
1	X	7	G
1	X	10	A
1	X	14	A

5 of 50 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	X	1496	G
1	X	2015	G
2	Y	16	U
1	X	1607	A
1	X	1800	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 124 ligands modelled in this entry, 123 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$
29	6O1	X	2901	-	117,123,123	1.63	14 (11%)	155,191,191	1.84	30 (19%)

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
29	6O1	X	2901	-	-	10/50/234/234	0/13/13/13

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	X	2901	6O1	O71-N65	6.73	1.36	1.22
29	X	2901	6O1	C08-C05	-6.08	1.39	1.51
29	X	2901	6O1	C62-C61	-5.64	1.40	1.51
29	X	2901	6O1	O53-C49	5.39	1.45	1.40
29	X	2901	6O1	C04-C09	-4.43	1.40	1.50

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	X	2901	6O1	O50-C50-C51	-10.43	97.90	106.63
29	X	2901	6O1	O51-C51-C50	-6.40	98.11	106.41
29	X	2901	6O1	C44-O44-C36	-5.05	105.27	114.33
29	X	2901	6O1	C36-C37-C38	-5.03	102.16	110.37
29	X	2901	6O1	C06-C01-C02	4.13	122.20	117.78

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

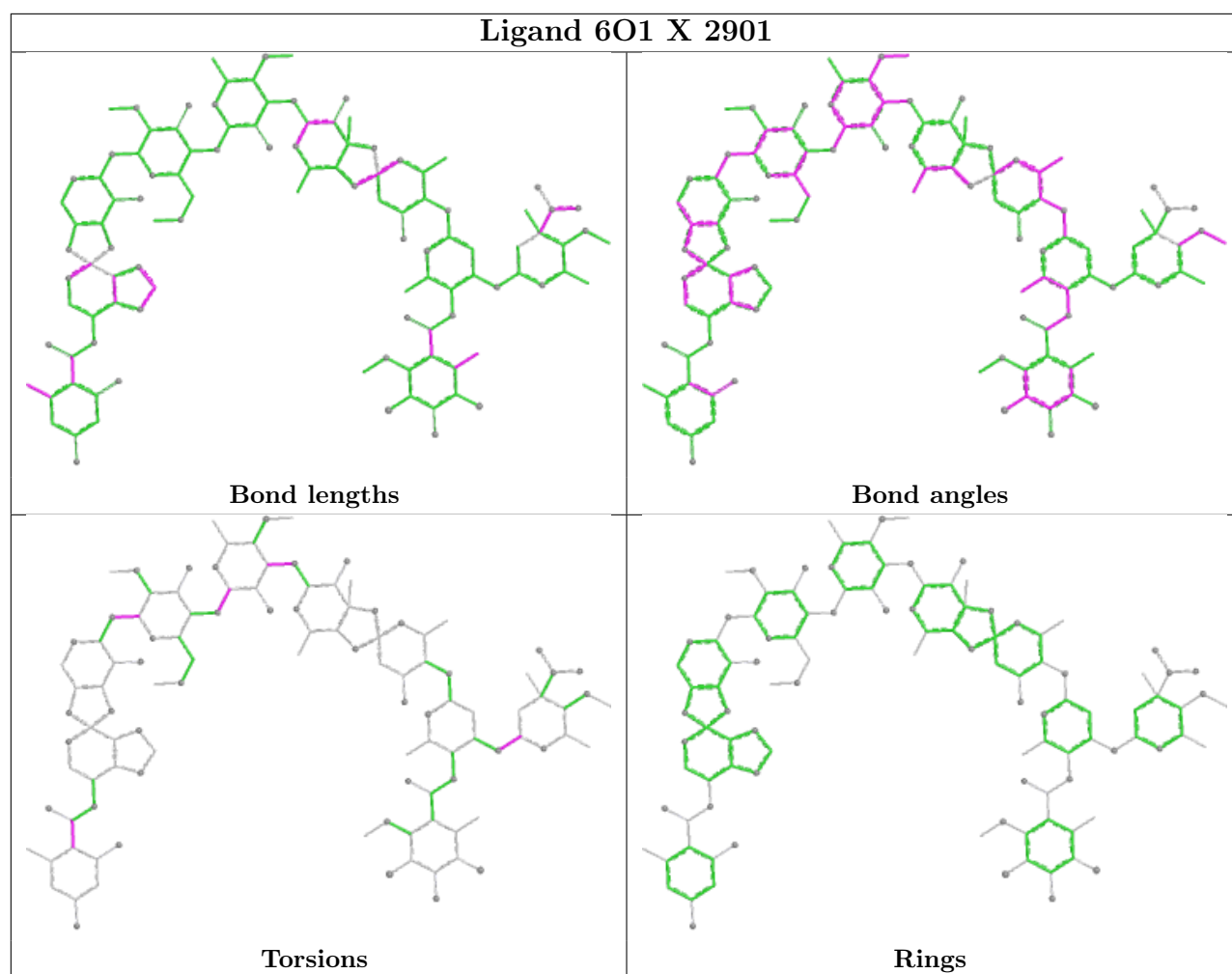
Mol	Chain	Res	Type	Atoms
29	X	2901	6O1	O67-C63-O12-C12
29	X	2901	6O1	O33-C29-O39-C39
29	X	2901	6O1	O40-C36-O44-C44
29	X	2901	6O1	C37-C36-O44-C44
29	X	2901	6O1	O55-C55-C56-C61

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	X	2901	6O1	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	X	2658/2880 (92%)	0.16	131 (4%) 35 19	30, 77, 204, 337	0
2	Y	120/123 (97%)	0.54	11 (9%) 14 9	80, 150, 187, 207	0
3	A	259/275 (94%)	0.82	42 (16%) 4 4	50, 105, 160, 212	0
4	B	205/211 (97%)	0.13	10 (4%) 35 19	30, 51, 113, 199	0
5	C	194/205 (94%)	0.59	20 (10%) 12 8	35, 103, 180, 254	0
6	D	177/180 (98%)	0.49	16 (9%) 15 10	128, 183, 249, 280	0
7	E	171/185 (92%)	0.41	15 (8%) 15 10	70, 142, 203, 254	0
8	G	142/174 (81%)	0.88	23 (16%) 4 4	38, 78, 188, 245	0
9	H	134/134 (100%)	0.13	8 (5%) 27 16	40, 55, 108, 175	0
10	I	134/156 (85%)	1.23	33 (24%) 2 2	50, 120, 191, 236	0
11	J	136/141 (96%)	0.57	16 (11%) 9 7	65, 106, 170, 225	0
12	K	113/116 (97%)	0.33	7 (6%) 26 15	30, 37, 91, 200	0
13	L	104/114 (91%)	1.19	21 (20%) 3 3	120, 154, 189, 241	0
14	M	108/166 (65%)	-0.02	2 (1%) 66 38	37, 50, 117, 169	0
15	N	117/118 (99%)	0.51	8 (6%) 23 14	42, 82, 136, 279	0
16	O	94/100 (94%)	0.57	12 (12%) 7 6	48, 101, 170, 216	0
17	P	127/134 (94%)	-0.06	3 (2%) 59 34	34, 53, 105, 192	0
18	Q	93/95 (97%)	0.28	6 (6%) 25 15	49, 88, 174, 215	0
19	R	110/115 (95%)	0.68	17 (15%) 5 5	62, 117, 213, 259	0
20	S	179/237 (75%)	0.49	11 (6%) 27 15	97, 158, 213, 289	0
21	T	74/91 (81%)	0.61	9 (12%) 8 7	67, 104, 157, 206	0
22	U	72/81 (88%)	0.87	11 (15%) 5 5	70, 125, 187, 215	0
23	V	65/67 (97%)	0.20	2 (3%) 51 28	83, 125, 197, 216	0
24	W	55/55 (100%)	0.01	3 (5%) 30 17	68, 90, 135, 182	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	Z	57/60 (95%)	0.20	3 (5%) 32 18	32, 43, 104, 182	0
26	1	53/54 (98%)	1.37	11 (20%) 2 3	101, 129, 224, 259	0
27	2	46/47 (97%)	0.68	5 (10%) 10 8	44, 59, 103, 162	0
28	3	59/66 (89%)	1.71	20 (33%) 1 1	72, 100, 161, 239	0
All	All	5856/6380 (91%)	0.37	476 (8%) 18 11	30, 91, 201, 337	0

The worst 5 of 476 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
8	G	109	GLY	14.7
8	G	110	LEU	11.7
3	A	220	HIS	8.4
8	G	156	HIS	8.1
27	2	46	ASP	8.0

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(Å ²)	Q<0.9
30	MG	X	3020	1/1	0.40	0.66	64,64,64,64	0
30	MG	X	3015	1/1	0.47	0.55	98,98,98,98	0
30	MG	X	2994	1/1	0.53	0.40	77,77,77,77	0
30	MG	X	2977	1/1	0.56	0.60	78,78,78,78	0
30	MG	X	2914	1/1	0.57	0.39	43,43,43,43	0
30	MG	X	2906	1/1	0.58	0.52	42,42,42,42	0
30	MG	X	2967	1/1	0.63	0.50	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
30	MG	X	2944	1/1	0.67	0.51	37,37,37,37	0
30	MG	X	2976	1/1	0.67	0.49	53,53,53,53	0
30	MG	X	2952	1/1	0.67	0.51	54,54,54,54	0
30	MG	X	3011	1/1	0.69	0.28	58,58,58,58	0
30	MG	X	2960	1/1	0.69	0.36	34,34,34,34	0
30	MG	X	2964	1/1	0.69	0.43	60,60,60,60	0
30	MG	X	2970	1/1	0.72	0.72	63,63,63,63	0
30	MG	X	2909	1/1	0.72	0.43	36,36,36,36	0
30	MG	X	3005	1/1	0.72	0.39	66,66,66,66	0
30	MG	X	2981	1/1	0.73	0.33	99,99,99,99	0
30	MG	X	2921	1/1	0.73	1.07	37,37,37,37	0
30	MG	X	2922	1/1	0.73	0.34	35,35,35,35	0
30	MG	X	2927	1/1	0.74	0.48	57,57,57,57	0
30	MG	X	3016	1/1	0.75	0.60	74,74,74,74	0
30	MG	X	3019	1/1	0.75	0.52	46,46,46,46	0
30	MG	X	3001	1/1	0.75	0.56	86,86,86,86	0
30	MG	X	2931	1/1	0.76	0.47	32,32,32,32	0
30	MG	X	2999	1/1	0.77	0.49	74,74,74,74	0
30	MG	X	2958	1/1	0.77	0.36	38,38,38,38	0
30	MG	X	2916	1/1	0.78	0.72	51,51,51,51	0
30	MG	X	2939	1/1	0.78	0.41	30,30,30,30	0
30	MG	X	2986	1/1	0.78	0.37	46,46,46,46	0
30	MG	X	2988	1/1	0.79	0.59	55,55,55,55	0
30	MG	M	201	1/1	0.80	0.70	35,35,35,35	0
30	MG	X	2979	1/1	0.81	0.32	46,46,46,46	0
30	MG	X	2961	1/1	0.82	0.36	68,68,68,68	0
30	MG	X	2908	1/1	0.82	0.46	34,34,34,34	0
30	MG	X	2995	1/1	0.82	0.47	83,83,83,83	0
30	MG	X	2957	1/1	0.82	0.40	42,42,42,42	0
30	MG	X	2989	1/1	0.83	0.40	56,56,56,56	0
30	MG	X	2969	1/1	0.83	0.31	43,43,43,43	0
30	MG	X	2954	1/1	0.83	0.42	41,41,41,41	0
30	MG	X	2959	1/1	0.84	0.72	54,54,54,54	0
30	MG	X	2926	1/1	0.84	0.33	32,32,32,32	0
30	MG	X	3017	1/1	0.84	0.32	52,52,52,52	0
30	MG	X	3003	1/1	0.84	0.28	63,63,63,63	0
30	MG	X	2912	1/1	0.84	0.26	34,34,34,34	0
30	MG	Y	201	1/1	0.84	0.86	77,77,77,77	0
30	MG	X	2924	1/1	0.84	0.43	30,30,30,30	0
30	MG	X	2913	1/1	0.85	0.44	36,36,36,36	0
30	MG	X	2941	1/1	0.86	0.37	55,55,55,55	0
30	MG	X	2907	1/1	0.86	0.88	49,49,49,49	0

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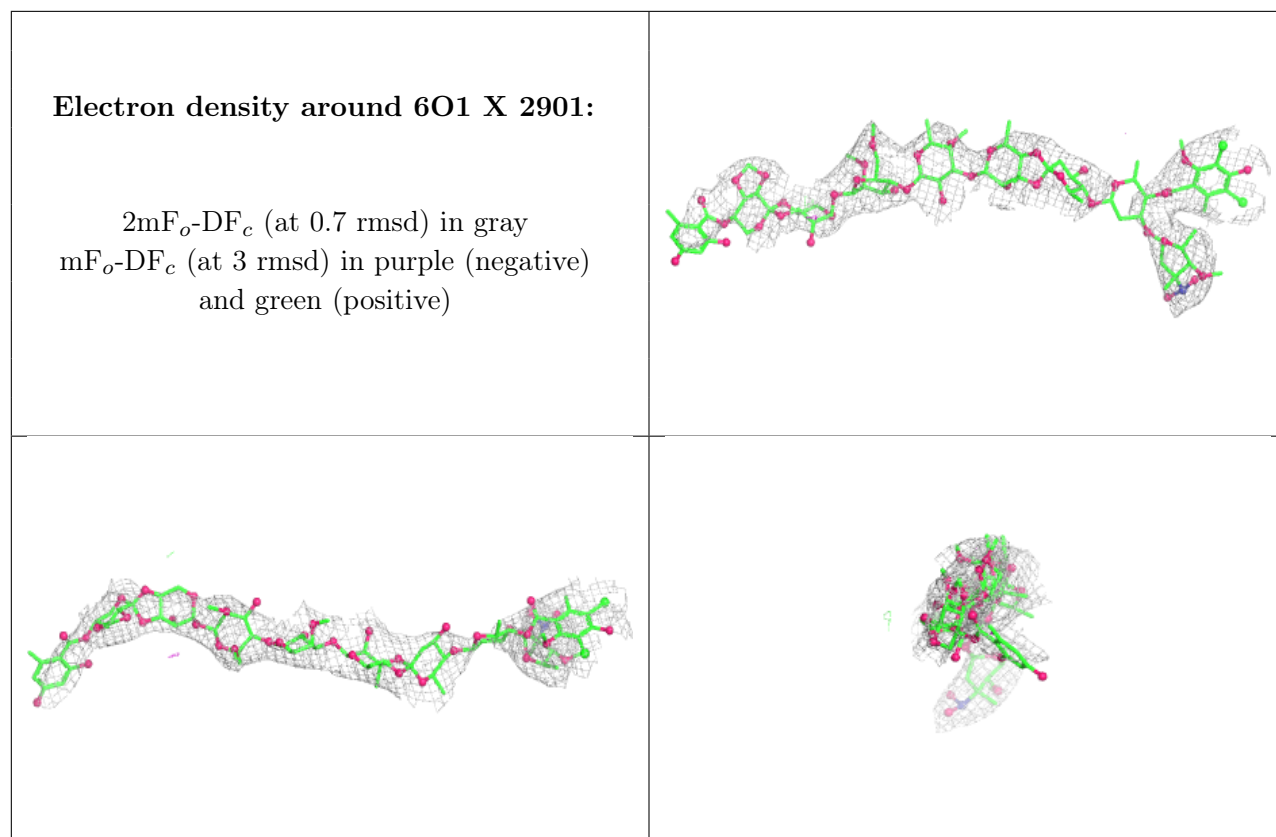
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
30	MG	X	2972	1/1	0.87	0.32	36,36,36,36	0
30	MG	X	2911	1/1	0.87	0.33	46,46,46,46	0
30	MG	X	2997	1/1	0.87	0.32	38,38,38,38	0
30	MG	X	2953	1/1	0.88	0.36	38,38,38,38	0
30	MG	X	2930	1/1	0.88	0.33	46,46,46,46	0
30	MG	X	3004	1/1	0.88	0.32	54,54,54,54	0
29	6O1	X	2901	111/111	0.88	0.11	106,116,136,139	0
30	MG	X	2915	1/1	0.88	0.26	36,36,36,36	0
30	MG	X	2965	1/1	0.88	0.34	40,40,40,40	0
30	MG	X	2923	1/1	0.89	0.27	30,30,30,30	0
30	MG	X	3013	1/1	0.89	0.39	47,47,47,47	0
30	MG	X	2984	1/1	0.89	0.39	49,49,49,49	0
30	MG	X	2998	1/1	0.89	0.48	35,35,35,35	0
30	MG	X	2910	1/1	0.89	0.56	34,34,34,34	0
30	MG	X	2917	1/1	0.89	0.20	33,33,33,33	0
30	MG	X	2978	1/1	0.89	0.24	49,49,49,49	0
30	MG	X	2991	1/1	0.89	0.38	72,72,72,72	0
30	MG	X	2936	1/1	0.89	0.24	53,53,53,53	0
30	MG	X	2962	1/1	0.90	0.31	41,41,41,41	0
30	MG	X	2946	1/1	0.90	0.26	34,34,34,34	0
30	MG	X	2987	1/1	0.90	0.28	43,43,43,43	0
30	MG	X	2932	1/1	0.90	0.17	53,53,53,53	0
30	MG	X	2935	1/1	0.90	0.54	41,41,41,41	0
30	MG	X	2983	1/1	0.90	0.20	63,63,63,63	0
30	MG	X	3007	1/1	0.91	0.28	40,40,40,40	0
30	MG	X	3009	1/1	0.91	0.18	41,41,41,41	0
30	MG	X	2903	1/1	0.91	0.41	37,37,37,37	0
30	MG	X	2955	1/1	0.91	0.41	31,31,31,31	0
30	MG	X	2947	1/1	0.91	0.44	52,52,52,52	0
30	MG	X	2948	1/1	0.91	0.28	30,30,30,30	0
30	MG	X	3002	1/1	0.91	0.25	44,44,44,44	0
30	MG	X	2950	1/1	0.91	0.44	36,36,36,36	0
30	MG	X	2940	1/1	0.91	0.33	34,34,34,34	0
30	MG	X	2945	1/1	0.91	0.53	55,55,55,55	0
30	MG	X	3006	1/1	0.91	0.34	34,34,34,34	0
30	MG	X	3014	1/1	0.92	0.17	43,43,43,43	0
30	MG	X	2928	1/1	0.92	0.21	41,41,41,41	0
30	MG	X	2904	1/1	0.92	0.68	32,32,32,32	0
30	MG	X	2951	1/1	0.92	0.19	35,35,35,35	0
30	MG	X	2971	1/1	0.92	0.28	33,33,33,33	0
30	MG	X	2938	1/1	0.92	0.21	36,36,36,36	0
30	MG	X	2993	1/1	0.92	0.16	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
30	MG	K	201	1/1	0.92	0.36	31,31,31,31	0
30	MG	X	2942	1/1	0.92	0.16	31,31,31,31	0
30	MG	X	2949	1/1	0.93	0.23	32,32,32,32	0
30	MG	X	2982	1/1	0.93	0.61	31,31,31,31	0
30	MG	X	2920	1/1	0.93	0.52	34,34,34,34	0
30	MG	X	2937	1/1	0.93	0.48	32,32,32,32	0
30	MG	X	2985	1/1	0.93	0.24	55,55,55,55	0
30	MG	X	2902	1/1	0.93	0.68	32,32,32,32	0
30	MG	K	202	1/1	0.93	0.37	31,31,31,31	0
30	MG	X	2980	1/1	0.93	0.26	49,49,49,49	0
30	MG	X	2996	1/1	0.94	0.17	43,43,43,43	0
30	MG	X	2918	1/1	0.94	0.34	45,45,45,45	0
30	MG	X	2990	1/1	0.94	0.39	39,39,39,39	0
30	MG	X	2925	1/1	0.94	0.45	43,43,43,43	0
30	MG	X	2919	1/1	0.95	0.14	33,33,33,33	0
30	MG	X	2943	1/1	0.95	0.17	33,33,33,33	0
30	MG	X	3000	1/1	0.95	0.10	39,39,39,39	0
30	MG	X	3018	1/1	0.95	0.23	32,32,32,32	0
30	MG	X	2974	1/1	0.95	0.48	30,30,30,30	0
30	MG	X	3010	1/1	0.95	0.21	41,41,41,41	0
30	MG	X	2934	1/1	0.95	0.56	39,39,39,39	0
30	MG	X	3012	1/1	0.95	0.31	52,52,52,52	0
30	MG	X	2905	1/1	0.95	0.47	30,30,30,30	0
30	MG	X	2963	1/1	0.95	0.35	71,71,71,71	0
30	MG	X	2956	1/1	0.96	0.36	32,32,32,32	0
30	MG	X	3008	1/1	0.96	0.75	39,39,39,39	0
30	MG	X	2929	1/1	0.96	0.56	39,39,39,39	0
30	MG	X	2933	1/1	0.97	0.49	38,38,38,38	0
30	MG	X	2975	1/1	0.97	0.81	49,49,49,49	0
30	MG	X	2992	1/1	0.97	0.59	34,34,34,34	0
30	MG	X	2968	1/1	0.97	0.15	35,35,35,35	0
30	MG	X	2966	1/1	0.97	0.24	37,37,37,37	0
30	MG	X	2973	1/1	0.98	0.17	52,52,52,52	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.