



wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 11:16 AM GMT

PDB ID : 1OND
Title : THE CRYSTAL STRUCTURE OF THE 50S LARGE RIBOSOMAL SUB-UNIT FROM DEINOCOCCUS RADIODURANS COMPLEXED WITH TROLEANDOMYCIN MACROLIDE ANTIBIOTIC
Authors : Berisio, R.; Schlutzen, F.; Harms, J.; Bashan, A.; Auerbach, T.; Baram, D.; Yonath, A.
Deposited on : 2003-02-27
Resolution : 3.40 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

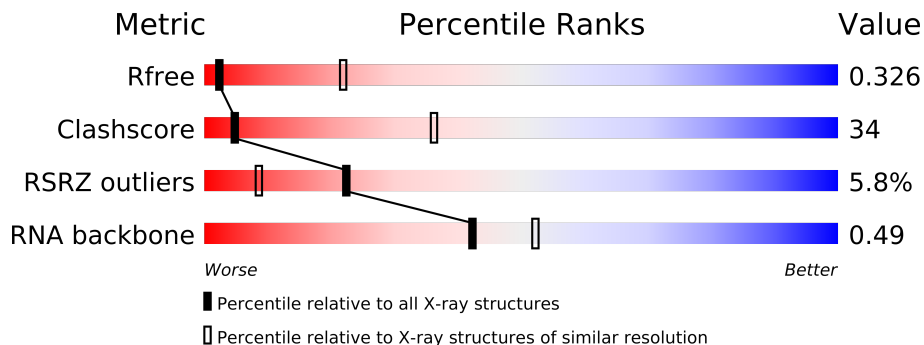
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 3.40 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}	66092	1017 (3.52-3.28)
Clashscore	79885	1214 (3.50-3.30)
RSRZ outliers	66119	1017 (3.52-3.28)
RNA backbone	1838	1002 (4.02-2.76)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	0	2880	
2	Q	134	
3	Z	60	

2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 59581 atoms, of which 0 are hydrogen and 0 are deuterium.

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	0	2765	Total	C	N	O	P	0	0	0
			59336	26469	10944	19159	2764			

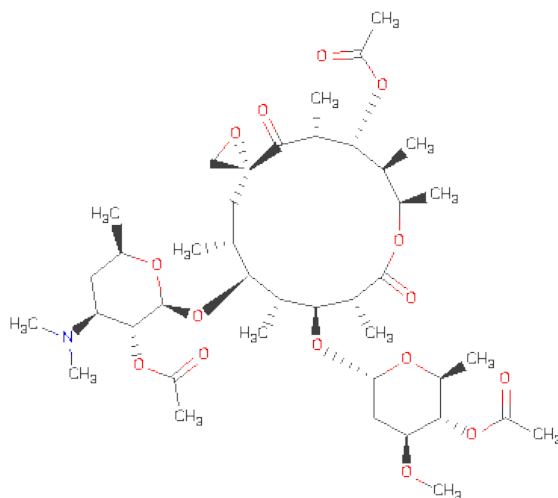
- Molecule 2 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
2	Q	130	Total	C	0	0	130
			130	130			

- Molecule 3 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
3	Z	58	Total	C	0	0	58
			58	58			

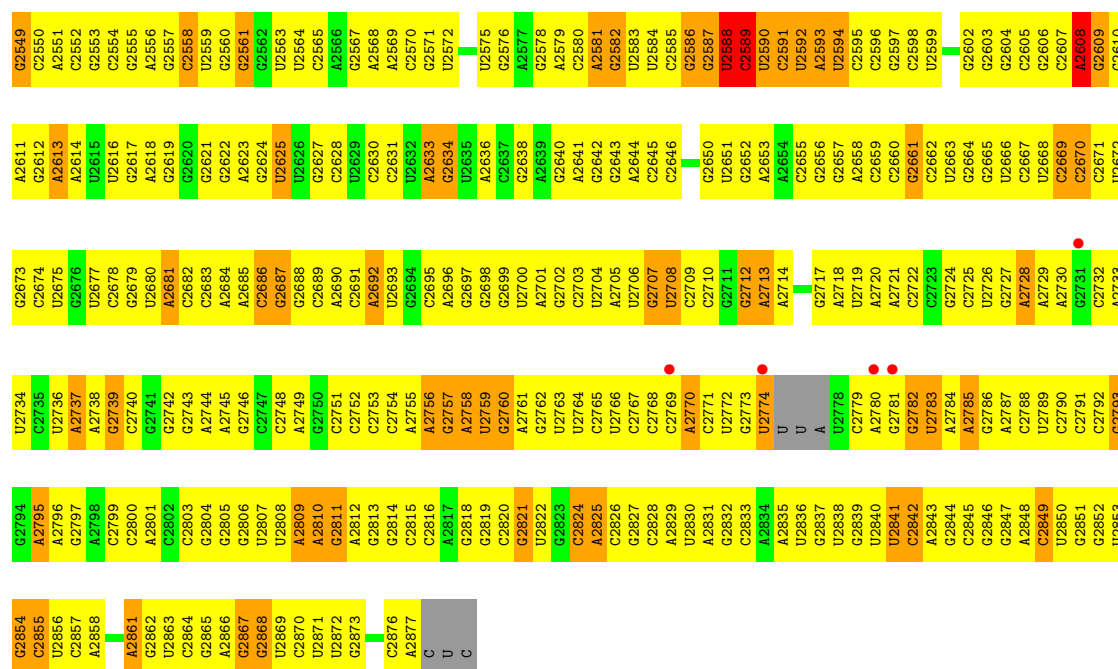
- Molecule 4 is TROLEANDOMYCIN (three-letter code: TAO) (formula: $C_{41}H_{67}NO_{15}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	0	1	Total	C	N	O	0	0
			57	41	1	15		

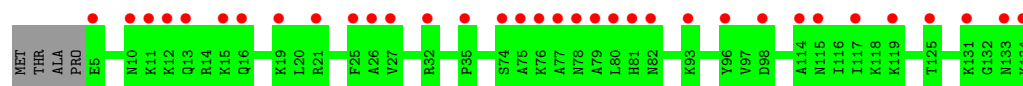
U1594	G1461	G1465	C1531	G1485	G1401	G1338	U1276	C1214	G1147	G1082	U1015	A952	A891	G822	U760	C700
A1595	G1402	C1466	A1532	C1467	G1403	U1339	G1277	A1215	G1148	C1083	C1016	G953	G	U823	G761	U701
A1596	G1403	C1467	G1340	U1403	C1404	C1341	G1278	U1216	G1149	C1086	C1017	U954	G	U954	A762	A703
A1597	C1404	A1468	U1467	C1405	U1405	C1342	G1279	U1217	G1150	C1087	C1018	G955	G	C925	A763	A704
C1598	A1406	U1469	U1343	U1406	C1406	U1343	U1280	C1218	U1151	C1088	C1019	U956	G	U956	A764	C705
G1599	A1406	C1470	U1343	A1406	C1406	U1343	U1281	C1219	G1152	C1089	A1020	G957	C	C827	A766	A706
U1600	G1407	G1471	C1344	G1471	G1407	C1344	G1284	G1220	A1153	C1090	A1021	C958	C	C928	A767	U707
U1601	A1408	C1472	G1345	C1472	A1408	G1345	A1285	C1221	A1154	C1091	A1022	C959	C	C929	G767	U708
G1602	U1409	U1473	G1346	U1473	U1409	C1346	U1286	G1222	A1155	C1092	U1023	U960	U	C930	U768	G709
A1603	C1410	C1474	C1347	C1474	C1410	C1347	U1287	G1223	G1156	U1093	A1024	G961	A	G831	C769	A709
A1604	C1411	U1475	C1348	U1475	C1411	C1348	U1287	A1224	G1160	U1094	A1025	G962	C	A832	U770	C710
A1605	C1412	C1476	C1412	C1476	C1412	C1412	A1288	G1225	U1161	C1095	U1026	G963	C	A833	C771	C711
U1608	C1418	C1477	G1350	C1477	C1418	G1350	A1289	A1226	A1162	A1096	G1027	G964	A	A834	C772	A712
G1609	G1419	U1478	G1351	U1478	G1419	G1351	A1290	A1227	C1163	A1097	G1028	G965	C	U835	C773	G713
A1610	G1420	G1479	G1352	G1479	G1420	G1352	G1291	G1228	G1164	U1098	U1030	C968	C	G836	A774	G714
U1611	A1421	C1480	A1353	C1480	A1421	A1353	A1292	G1229	G1165	C1031	C1031	U969	U	U837	U775	U715
U1612	U1422	U1481	U1354	U1481	U1422	A1354	A1293	C1230	A1166	A1099	A1032	U970	U	A838	C776	U716
G1613	A1423	C1482	C1355	C1482	A1423	A1355	G1294	C1231	A1167	G1100	G1033	A971	A	U839	A777	A717
C1614	U1424	G1483	G1356	G1483	U1424	G1356	U1295	U1232	G1168	U1101	U1034	C972	C	U840	C778	A718
C1615	U1425	G1484	U1357	G1484	U1425	U1357	U1296	A1233	G1169	C1102	U1034	C972	C	G841	A719	A719
G1616	G1426	U1485	C1358	U1485	G1426	C1358	A1297	C1234	U1170	G1103	G1035	U973	A911	A842	G726	G726
G1617	G1427	C1487	G1359	C1487	G1427	G1359	U1298	C1235	U1171	G1104	G1036	U974	A912	G843	U727	U727
U1618	G1428	G1488	A1362	G1488	G1428	A1362	A1300	A1238	G1172	U1105	U1037	U975	A913	G844	C722	C722
A1619	A1429	C1489	C1363	C1489	A1429	C1363	U1301	A1238	G1173	A1106	U1038	C976	C914	U845	U784	C723
C1620	G1430	U1490	C1364	U1490	G1430	C1364	C1302	G1241	C1178	G1110	U1044	U980	A921	U846	U785	C724
G1621	U1431	C1491	U1365	C1491	U1431	U1365	U1303	A1242	C1179	U1112	G1045	U981	A922	C947	U786	C725
A1622	G1432	A1492	C1366	A1492	G1432	C1366	U1304	G1243	A1179	U1113	G1046	U982	A922	A848	G726	G726
C1623	A1433	G1493	C1367	G1493	A1433	C1367	U1305	U1244	A1180	U1114	U1046	U983	A922	U852	U727	U727
A1624	U1434	C1494	G1368	C1494	U1434	G1368	U1306	G1245	A1181	C1115	G1053	U984	A922	U857	G732	G732
A1625	G1435	G1495	G1369	G1495	G1435	G1369	U1307	G1246	U1182	U1116	G1054	U985	A922	G858	G733	G733
A1626	G1436	G1496	U1370	G1496	G1436	U1370	C1308	U1247	C1183	G1117	A1055	U986	A922	U859	G734	G734
C1627	A1437	C1497	G1371	C1497	A1437	G1371	C1309	G1248	C1185	U1118	U1056	U987	A922	U860	G735	G735
G1628	G1438	U1500	G1372	U1500	G1438	G1372	C1310	A1250	G1186	U1119	U1057	A990	A922	U861	G736	G736
A1630	A1439	G1501	G1373	G1501	A1439	G1373	C1311	C1251	G1187	C1120	G1058	A991	A922	U862	G737	G737
A1631	G1440	G1502	C1374	G1502	G1440	C1374	C1312	C1252	A1188	A1122	A1061	C993	A929	C864	G738	G738
A1632	A1441	G1503	C1375	G1503	A1441	C1375	U1313	C1253	C1189	G1123	C1062	A992	A929	A865	U800	G739
G1633	C1442	U1504	C1376	U1504	C1442	C1376	A1314	G1254	G1190	U1124	C1063	A994	A929	U866	A801	A740
A1634	G1443	C1444	G1377	C1444	G1443	G1377	A1315	A1255	G1191	G1125	C1064	A995	A929	G867	A802	G741
G1635	C1445	U1509	C1378	U1509	C1445	C1378	G1316	U1256	G1192	U1126	C1065	C996	A929	U868	C803	G742
G1636	U1446	C1446	C1380	C1446	U1446	C1380	A1317	G1263	G1193	G1126	A1065	C996	A929	U869	C804	A743
G1637	U1447	C1447	G1381	C1447	U1447	G1381	C1319	G1264	U1199	C1135	C1003	C996	A929	C870	G744	C744
U1638	A1448	U1512	G1382	U1512	A1448	G1382	A1320	G1265	U1194	U1130	G1066	A999	A929	C871	G745	G745
U1639	C1449	C1513	C1383	C1449	C1449	C1383	A1321	A1266	U1195	G1131	G1067	G1000	A929	U871	G746	G746
C1640	G1450	U1515	G1384	G1450	G1450	G1384	G1322	G1267	U1196	U1132	C1068	A1001	A929	C872	A747	A747
C1641	A1516	C1580	C1385	A1516	C1580	C1385	G1323	U1262	U1197	G1133	G1069	C937	A929	U872	C748	C748
G1642	C1581	C1517	C1386	C1581	C1517	C1386	G1324	G1263	U1198	C1134	C1070	C937	A929	A874	C749	C749
A1643	U1452	C1518	G1387	U1452	C1518	G1387	U1325	C1264	U1199	C1135	C1071	C937	A929	G875	C750	C750
G1644	U1454	G1519	C1388	U1454	G1519	C1388	U1326	G1265	G1200	U1136	U1072	U1005	A929	A876	C751	C751
U1645	C1455	G1520	C1389	C1455	G1520	C1389	C1327	G1266	G1201	G1137	C1073	U942	A929	G877	C752	C752
G1646	C1456	C1523	G1390	C1456	C1523	G1390	C1328	A1267	U1202	A1138	G1074	U943	A929	C878	C753	C753
U1647	A1457	C1524	U1391	A1457	C1524	U1391	U1329	U1268	U1203	G1139	C1075	U944	A929	A879	G754	G754
C1648	A1458	C1525	U1392	A1458	C1525	U1392	G1269	G1269	G1204	A1140	U1076	U945	A929	U880	C755	C755
A1649	U1459	U1526	G1393	U1459	U1526	G1393	G1332	C1270	G1205	U1141	U1077	U946	A929	A886	C756	C756
U1651	G1460	C1461	C1394	G1460	C1461	C1394	G1333	G1271	G1206	G1142	A1078	A1011	A929	C887	C757	C757
G1652	C1462	C1527	A1395	C1462	C1527	A1395	A1334	G1272	G1207	C1145	G1079	A1012	A929	G888	C758	C758
C1653	A1463	C1528	G1396	A1463	C1528	G1396	A1335	G1273	U1212	C1146	A1080	G1013	A929	C889	U820	U757
A1654	A1464	U1530	G1397	A1464	U1530	G1397	G1337	A1275	U1213	G1146	A1081	G1014	A929	U890	A821	C759

WORLDWIDE
PDB
PROTEIN DATA BANK



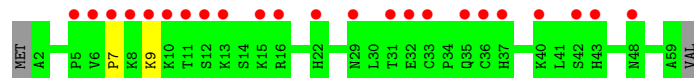
- Molecule 2: 50S ribosomal protein L22

Chain Q:



- Molecule 3: 50S ribosomal protein L32

Chain Z:



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	170.25Å 411.09Å 695.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 3.40 20.02 – 3.40	Depositor EDS
% Data completeness (in resolution range)	(Not available) (8.00-3.40) 88.0 (20.02-3.40)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.62 (at 3.36Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.261 , 0.310 0.325 , 0.326	Depositor DCC
R_{free} test set	8414 reflections (2.89%)	DCC
Wilson B-factor (Å ²)	69.2	Xtriage
Anisotropy	0.502	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.13 , -10.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	1 of 291031 reflections (0.000%)	Xtriage
F_o, F_c correlation	0.75	EDS
Total number of atoms	59581	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.19% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: TAO

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	0	0.83	17/66440 (0.0%)	0.75	34/103628 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	0	0	47

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	0	1549	C	N1-C2	11.30	1.51	1.40
1	0	1549	C	N3-C4	9.79	1.40	1.33
1	0	929	A	N1-C2	8.60	1.42	1.34
1	0	1149	G	C6-O6	-8.38	1.16	1.24
1	0	1549	C	C2-O2	7.25	1.30	1.24

The worst 5 of 34 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	2590	U	P-O3'-C3'	-9.16	108.70	119.70
1	0	633	G	N3-C2-N2	7.30	125.01	119.90
1	0	2591	C	OP1-P-OP2	-6.77	109.45	119.60
1	0	2428	U	N1-C1'-C2'	6.61	122.60	114.00
1	0	459	A	N9-C1'-C2'	6.53	122.49	114.00

There are no chirality outliers.

5 of 47 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	211	U	Sidechain
1	0	343	A	Sidechain
1	0	470	U	Sidechain
1	0	491	A	Sidechain
1	0	82	G	Sidechain

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	59336	0	29907	3024	0
2	Q	130	0	0	0	0
3	Z	58	0	0	4	0
4	0	57	0	67	22	0
All	All	59581	0	29974	3039	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 34.

The worst 5 of 3039 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:0:2881:TAO:C31	4:0:2881:TAO:C26	1.82	1.56
4:0:2881:TAO:C24	4:0:2881:TAO:O18	1.65	1.41
1:0:2058:U:H1'	1:0:2576:G:H21	1.09	1.17
1:0:1458:A:H3'	1:0:1459:U:C5'	1.74	1.17
1:0:2548:G:H2'	1:0:2549:G:H5''	1.17	1.15

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains ⓘ

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2755/2880 (95%)	523 (18%)	52 (1%)

5 of 523 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	0	13	A
1	0	35	G
1	0	45	C
1	0	48	A
1	0	49	U

5 of 52 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	1338	G
1	0	1651	U
1	0	2592	U
1	0	1354	A
1	0	1410	U

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

1 ligand is modelled in this entry.

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	$\# Z > 2$
4	TAO	0	2881	-	60,60,60	4.13	34 (56%)	89,89,89	4.25	50 (56%)

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
4	TAO	0	2881	-	-	2/41/113/113	0/0/4/4

The worst 5 of 34 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	0	2881	TAO	C31-C26	11.19	1.82	1.55
4	0	2881	TAO	O11-C9	9.89	1.60	1.44
4	0	2881	TAO	O11-C15	8.87	1.55	1.35
4	0	2881	TAO	O18-C24	8.83	1.65	1.41
4	0	2881	TAO	C31-C27	7.92	1.71	1.51

The worst 5 of 50 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	0	2881	TAO	C16-C12-C17	-11.77	97.66	112.10
4	0	2881	TAO	C26-C31-C27	11.12	132.86	110.06
4	0	2881	TAO	O23-C27-C31	11.07	137.34	111.64
4	0	2881	TAO	C22-C17-C12	-10.79	103.21	114.42
4	0	2881	TAO	O18-C14-C19	10.12	119.99	108.14

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	0	2881	TAO	C17-O23-C27-C31
4	0	2881	TAO	C17-O23-C27-O32

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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	0	2765/2880 (96%)	0.29	113 (4%)	35 14	10, 30, 100, 100	0
2	Q	130/134 (97%)	1.49	34 (26%)	1 2	10, 28, 83, 167	0
3	Z	58/60 (96%)	1.86	23 (39%)	1 1	10, 18, 60, 89	0
All	All	2953/3074 (96%)	0.37	170 (5%)	22 8	10, 30, 100, 167	0

The worst 5 of 170 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	Z	8	LYS	8.1
2	Q	76	LYS	7.7
3	Z	11	THR	6.7
2	Q	134	LYS	6.0
1	0	1083	C	5.5

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	TAO	0	2881	57/57	0.29	1.99	27,27,27,27	0

6.5 Other polymers ⓘ

There are no such residues in this entry.