



# wwPDB X-ray Structure Validation Summary Report

Feb 27, 2014 – 11:13 PM GMT

PDB ID : 1J5A  
Title : STRUCTURAL BASIS FOR THE INTERACTION OF ANTIBIOTICS  
WITH THE PEPTIDYL TRANSFERASE CENTER IN EUBACTERIA  
Authors : Schlutzen, F.; Zarivach, R.; Harms, J.; Bashan, A.; Tocilj, A.; Albrecht, R.;  
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Deposited on : 2002-03-06  
Resolution : 3.50 Å(reported)

This is a wwPDB 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 <http://wwpdb.org/ValidationPDFNotes.html>

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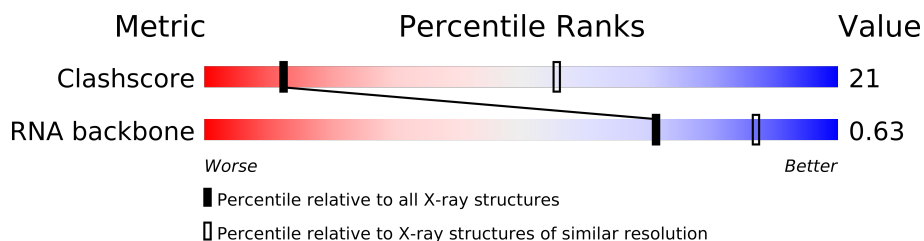
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 21963  
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 3.50 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	79885	1039 (3.66-3.34)
RNA backbone	1838	1007 (4.22-2.76)

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  $\geq 3$ , 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	2880	
2	K	205	
3	L	134	
4	M	60	

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 59971 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 RRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	2774	Total	C	N	O	P	0	0	0
			59532	26556	10982	19221	2773			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1526	U	Y	SEE REMARK 999	GB 15805042

- Molecule 2 is a protein called RIBOSOMAL PROTEIN L4.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
2	K	197	Total	C	0	0	197
			197	197			

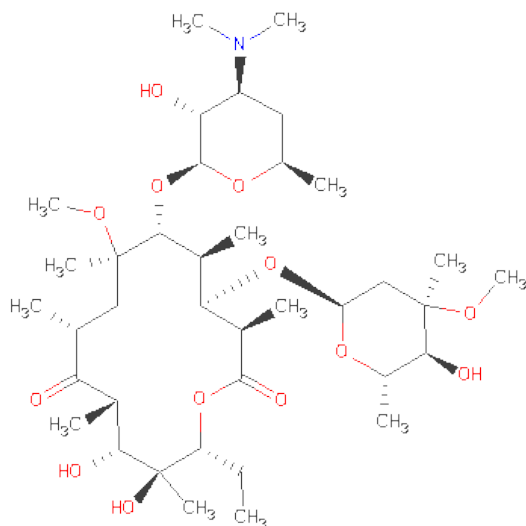
- Molecule 3 is a protein called RIBOSOMAL PROTEIN L22.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
3	L	130	Total	C	0	0	130
			130	130			

- Molecule 4 is a protein called RIBOSOMAL PROTEIN L32.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
4	M	58	Total	C	0	0	58
			58	58			

- Molecule 5 is CLARITHROMYCIN (three-letter code: CTY) (formula: C<sub>38</sub>H<sub>69</sub>NO<sub>13</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			52	38	1	13		

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	2	Total	Mg	0	0
			2	2		

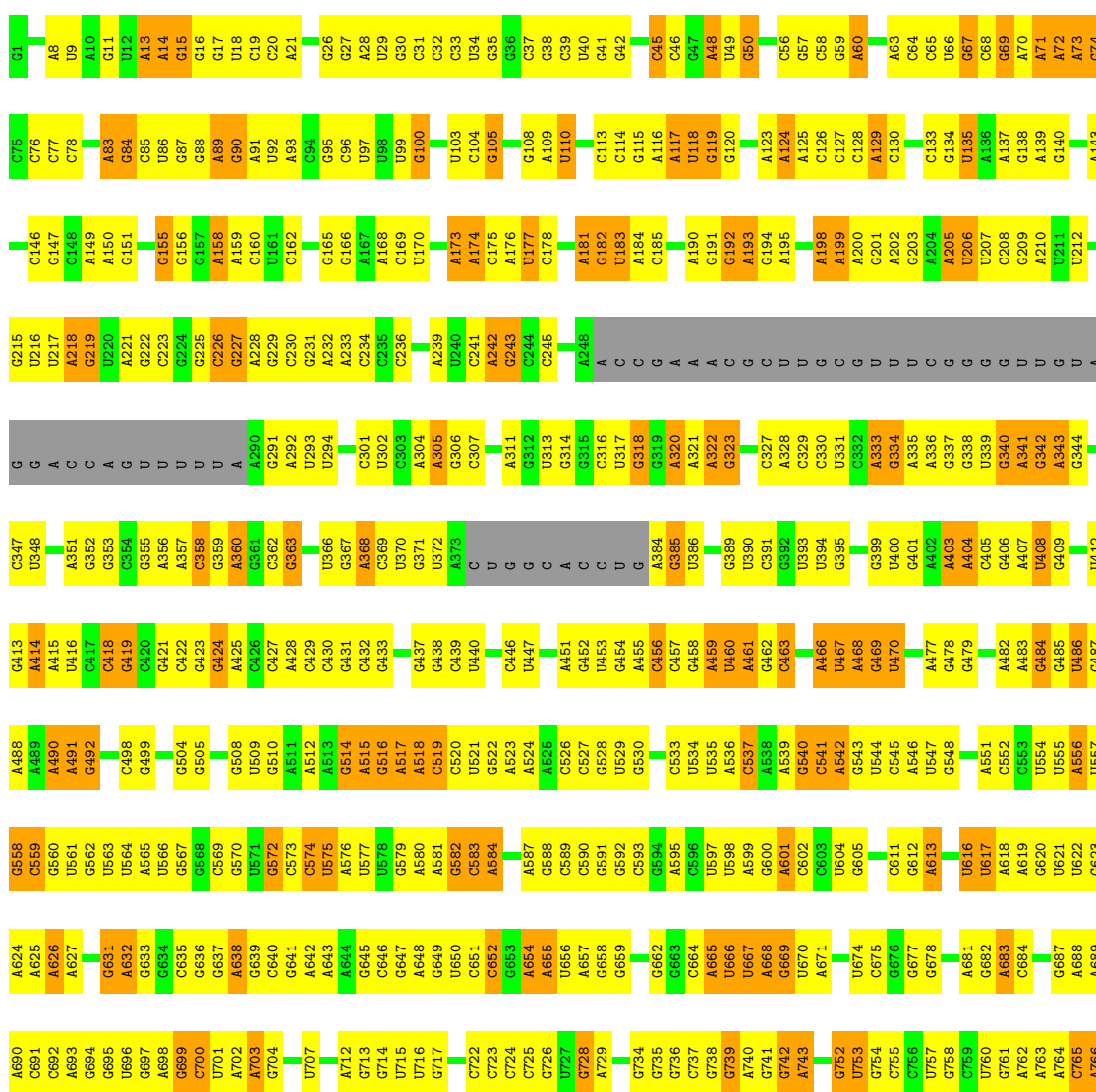
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

#### • Molecule 1: 23S rRNA

Chain A:

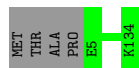


C1824	U1752	G1683	U1612	G1542	G1338	G1269	G1193	G1124	A1055	G977	C908	U840	G773
C1825	A1753	G1684	G1613	G1543	U1339	C1270	U1194	G1125	U1056	U978	C910	G841	A774
U1826	G1754	A1685	C1614	A1544	C1340	C1271	U1195	A1126	A1057	A979	A911	A842	U775
G1827	G1755	A1686	C1615	C1411	G1341	G1272	G1196	C1127	G1058	G980	A912	G843	G776
C1828	G1756	U1687	G1616	U1548	C1342	C1273	U1197	G1128	A1059	C981	A913	G844	A777
C1829	C1757	U1688	G1617	C1549	C1343	C1274	U1198	A1129	C1060	C982	C914	U845	G778
C1830	C1758	U1689	U1618	C1550	C1344	A1275	U1199	U1130	A1061	G983	C915	A846	
G1831		U1690	A1619	U1551	G1345	U1276	G1200	C1134	A1065	A984	A918	C850	U784
	C1762	C1691	C1623	C1552	C1346	G1277	G1201	C1135	G1066	G985	U919	C851	U785
G1834	G1763	G1553	A1624	G1554	C1347	A1278	U1202	G1136	G1067			U852	U786
C1835	A1764	C1554	C1625	C1488	C1348	G1279	A1203	G1137	A1068	A994	A922		A787
C1836	C1765	A1555	U1490	U1490	A1349	U1280	G1204	A1138	G1069	A995	A923	U857	G788
	U1626	A1556			G1350	A1281	G1205	A1139	G1070	C996	C924	G858	G789
A1840	C1627	G1557	U1424	U1424	G1351	A1282				C997		U859	U790
		C1558	G1425	G1425	G1352	C1283	G1209	U1140	U1071	C998	U925	U860	G791
A1851	C1628	G1559	U1426	U1426	A1353	G1284		U1141	U1072	A999	U926	G861	
	A1632	G1496	G1427	G1427	A1354	A1285	U1211	G1142	G1073	G1000	C927		
G1854	C1633	C1497	G1428	G1428	A1355	U1286	U1212	A1143	G1074	A1001	G928	C863	A794
G1855	A1561	C1497	G1428	G1428	A1356	U1287	U1213	U1144	C1075	C1002	A929	C864	A795
C1856	U1562	G1498	A1429	A1429	G1357	A1288	G1214	G1145		C1003	A930	C865	A796
U1857	U1564	U1500	G1430	G1430	C1358	A1289	C1215	G1146	G1079	G1004	A931	C866	A797
		C1501	G1432	G1432	G1359	A1290	G1216			U1005	G932	U866	G798
A1867	G1571	G1502	A1433	A1433		G1291	U1217	G1149	A1080	A1007	G933	U867	C799
	C1572	G1503	U1434	U1434	C1364	A1292	C1218	U1150	G1082	A1008	G934	U868	U800
	G1573	U1504	G1435	G1435	U1365	A1293	C1219	U1151	C1083	C1007		C869	A801
	A1574	U1505	G1436	G1436	A1366		G1220	C1152	A1084		C937	C870	A802
		C1506	A1437	A1437	U1367	G1298	C1221	A1153	G1085	A1012	G938	U871	C803
	C1575	A1507	G1438	G1438	G1368	U1299	G1222	U1154	C1086	G1013	C939	G872	C804
	G1576	G1508	G1439	G1439	G1369	A1300	G1223	G1155	C1087	G1014	G940	U873	G805
		A1509	G1440	G1440	U1370	U1301	A1224		C1088	U1015	U941	A874	A806
	G1579	C1510	A1441	A1441	G1371	C1302	G1225	C1160	C1089	C1016	U942	G875	A807
	C1580	A1511	G1442	G1442	A1372		A1226	U1161	C1090		U943	A876	C808
	C1581	A1512	G1443	G1443	U1373	U1306	A1227	A1162	C1091	U1019	A944	G877	C809
	A1582	U1513	C1444	C1444	G1374	U1307		C1163	C1092	A1020	G945	C878	U810
	G1583	C1514	U1445	U1445		G1308	A1233	C1164	U1093	A1021	G946	A879	G811
	G1584	U1515	U1446	U1446	G1377	G1309	C1234	G1165	U1093		C948	C880	
	A1585		U1447	U1447		C1310		A1166	A1096	U1023	G949	A886	A813
		G1519	G1450	G1450	C1380	C1311	G1240	A1167	A1097	G1024	G950	G887	G812
	A1588	U1520	C1451	C1451	G1381	U1312	G1241	G1168	C1098		G951	G888	G814
	G1589	U1521	U1452	U1452	G1382	U1313		C1169	A1099	U1030	A952	C889	A815
	C1590	C1522	A1453	A1453	C1383	A1314	U1244	U1170	G1100	C1031	G953	U890	U816
	U1591	A1523	A1453	A1453	G1384	A1315	G1245	U1171	U1101	A1032	U954	C891	A817
	U1592	C1524	C1456	C1456	C1385	G1316		U1172	G1102	G1033	G955	A891	G818
	C1593	A1525	C1457	C1457	U1387		G1249	G1173	C1103	U1034	A956	C892	C819
	U1594	U1526	A1457	A1457	G1387	A1321	A1250	G1174	G1104	G1035	G957	U820	A821
	A1595	G1528	U1458	U1458	A1391	G1322	G1251	A1175	U1105	C1036	G958	G	G822
	U1596	C1529	G1459	G1459	U1392	G1323	C1252	U1176	A1106	U1037	C959	G	U823
	A1597	U1530	U1460	U1460	G1393	G1324	C1253	U1177	A1107	U1038	U960	G	U824
	C1598	C1531	G1465	G1465	G1394	U1325		C1178	U1108	A1039		C	C825
	U1599	U1532	C1466	C1466	U1394	U1326	G1258	A1109	A1109	A1040	A964	U	U826
	U1600	G1533	U1467	U1467	G1397	C1327	A1259	C1183	G1110	G1041		C	C827
	U1601	U1534	C1467	C1467	A1397	C1328	A1260	G1184	C1111		C968	A	G828
	C1602	A1535	U1468	U1468	G1398	C1329	G1261	C1185	U1112	U1044	C969	C	U829
	A1603	C1536	U1469	U1469	C1399	G1330	U1262	G1186	C1113	G1045	A970	C	C830
	U1604	G1537	G1470	G1470	A1401	G1333	G1263	A1187	G1118	U1046	A971	A	G831
	A1605	U1537	G1471	G1471	G1402	G1334	C1264	A1188	U1119	G1047	C972	G	A832
	C1606	A1538	U1473	U1473	G1402	A1334	G1265	G1189	G1119	U1048	U973	C	A833
	U1607	U1539	U1474	U1474	G1403	A1335	G1266	C1190	U1122	C1049	U974	U	
	A1608	C1540	U1475	U1475	U1404	A1336	A1267	G1191	A1122		C975	A	A838
	U1609	G1541	G1476	G1476	A1405	G1337	U1268	A1192	G1123	C1054	C976		U839



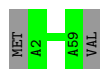
- Molecule 3: RIBOSOMAL PROTEIN L22

Chain L: 



- Molecule 4: RIBOSOMAL PROTEIN L32

Chain M: 





## 4 Data and refinement statistics

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

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	169.90Å 412.70Å 697.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.50	Depositor
% Data completeness (in resolution range)	(Not available) (50.00-3.50)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS, REFMAC	Depositor
R, $R_{free}$	0.273 , 0.323	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	59971	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	51.0	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, CTY

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.23	0/66661	0.66	2/103976 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	1746	A	C2'-C3'-O3'	5.89	123.12	113.70
1	A	777	A	C2'-C3'-O3'	5.52	122.53	113.70

There are no chirality outliers.

There are no planarity outliers.

### 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	A	59532	0	30004	1877	0
2	K	197	0	0	0	0
3	L	130	0	0	0	0
4	M	58	0	0	0	0
5	A	52	0	69	32	0
6	A	2	0	0	0	0
All	All	59971	0	30073	1896	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 21.

The worst 5 of 1896 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:2042:A:C2	5:A:2881:CTY:H383	1.63	1.30
1:A:2042:A:N3	5:A:2881:CTY:H383	1.62	1.14
1:A:1747:G:H4'	1:A:1749:G:H1'	1.29	1.12
1:A:940:G:H3'	1:A:941:U:H5''	1.34	1.09
1:A:1199:U:H3'	1:A:1200:G:H5''	1.35	1.08

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	A	2765/2880 (96%)	555 (20%)	142 (5%)

5 of 555 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	13	A
1	A	14	A
1	A	15	G
1	A	45	C
1	A	48	A

5 of 142 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	1278	A

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Mol	Chain	Res	Type
1	A	1563	U
1	A	2633	A
1	A	1285	A
1	A	1354	A

## 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 ⓘ

Of 3 ligands modelled in this entry, 2 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$
5	CTY	A	2881	-	54,54,54	1.52	8 (14%)	83,83,83	2.99	41 (49%)

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
5	CTY	A	2881	-	-	1/75/110/110	1/3/3/3

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	2881	CTY	C7-C6	4.70	1.60	1.52
5	A	2881	CTY	C7-C8	4.17	1.60	1.54
5	A	2881	CTY	O2-C13	-2.94	1.40	1.46
5	A	2881	CTY	C15-C14	2.78	1.58	1.51
5	A	2881	CTY	C35-C12	2.69	1.58	1.52

The worst 5 of 41 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	2881	CTY	O3-C3-C4	7.54	116.97	108.14
5	A	2881	CTY	O5-C16-C19	-7.20	98.20	110.85
5	A	2881	CTY	C33-C8-C7	6.98	122.79	109.97
5	A	2881	CTY	O5-C16-C17	6.31	113.53	103.73
5	A	2881	CTY	C6-C5-C4	6.12	123.20	113.60

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	2881	CTY	C20-O5-C16-C17

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	2881	CTY	C14-C15-C16-C17-C18-O4

## 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 ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.