



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 10, 2026 – 06:48 AM UTC

PDB ID : 1NWY / pdb_00001nwy
Title : COMPLEX OF THE LARGE RIBOSOMAL SUBUNIT FROM DEINOCOC-
CUS RADIODURANS WITH AZITHROMYCIN
Authors : Schlutzen, F.; Harms, J.; Franceschi, F.; Hansen, H.A.S.; Bartels, H.; Zari-
vach, R.; Yonath, A.
Deposited on : 2003-02-07
Resolution : 3.30 Å(reported)

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

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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)
Xtrriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

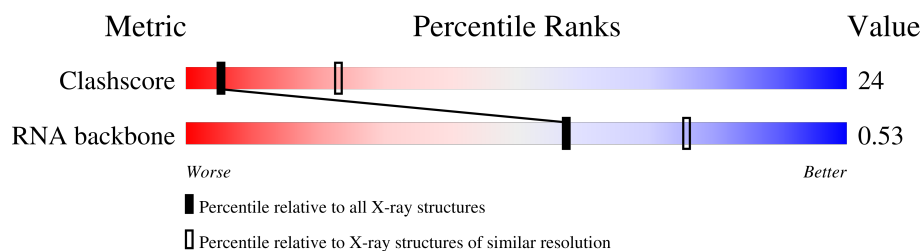
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 Å.

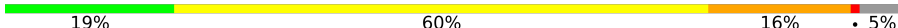
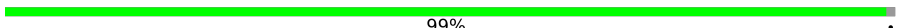
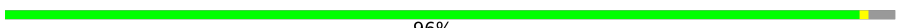
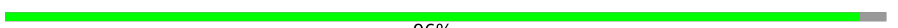
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	1209 (3.32-3.28)
RNA backbone	3983	1048 (3.60-3.00)

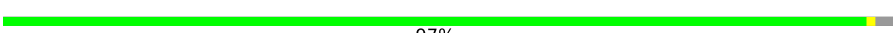
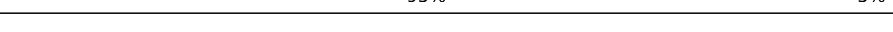
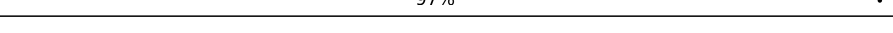
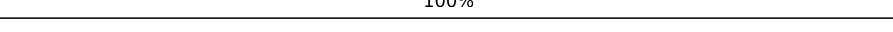
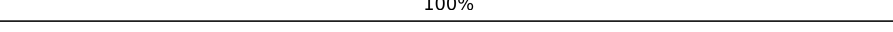
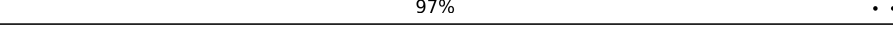
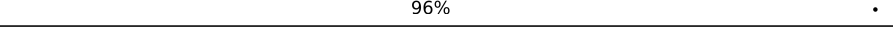
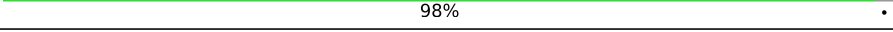
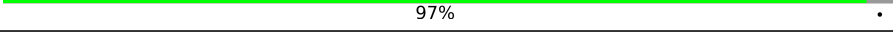
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	0	2880	 26% 57% 13% .
2	9	124	 19% 60% 16% . 5%
3	A	274	 99% .
4	B	211	 96% ..
5	C	204	 96% .
6	D	180	 98% ..
7	E	185	 95% . .
8	F	146	 34% . 64%
9	G	144	 99% .

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Mol	Chain	Length	Quality of chain
10	H	174	 82% 18%
11	I	134	 99% .
12	J	156	 90% 10%
13	K	141	 87% . 12%
14	L	116	 97% ..
15	M	113	 97% ..
16	N	166	 75% . 25%
17	O	118	 99% .
18	P	100	 100%
19	Q	134	 97% .
20	R	94	 99% .
21	S	115	 98% .
22	T	237	 94% 6%
23	U	91	 95% 5%
24	W	67	 97% .
25	X	55	 100%
26	Y	73	 100%
27	Z	59	 97% ..
28	1	55	 96% .
29	2	47	 98% .
30	3	65	 97% .
31	4	37	 95% 5%

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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
32	ZIT	0	2881	-	-	X	-
32	ZIT	0	2882	-	-	X	-

2 Entry composition

There are 32 unique types of molecules in this entry. The entry contains 65404 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	0	2766	Total	C	N	O	P	0	0	0
			59359	26479	10949	19166	2765			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	9	118	Total	C	N	O	P	0	0	0
			2519	1124	464	813	118			

- Molecule 3 is a protein called ribosomal protein L2.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
3	A	270	Total	C	0	0	270
			270	270			

- Molecule 4 is a protein called ribosomal protein L3.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
4	B	205	Total	C	0	0	205
			205	205			

- Molecule 5 is a protein called ribosomal protein L4.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
5	C	197	Total	C	0	0	197
			197	197			

- Molecule 6 is a protein called ribosomal protein L5.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
6	D	178	Total	C	0	0	178
			178	178			

- Molecule 7 is a protein called ribosomal protein L6.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
7	E	177	Total	C	0	0	177
			177	177			

- Molecule 8 is a protein called ribosomal protein L9.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
8	F	52	Total	C	0	0	52
			52	52			

- Molecule 9 is a protein called ribosomal protein L11.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
9	G	143	Total	C	0	0	143
			143	143			

- Molecule 10 is a protein called ribosomal protein L13.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
10	H	143	Total	C	0	0	143
			143	143			

- Molecule 11 is a protein called ribosomal protein L14.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
11	I	132	Total	C	0	0	132
			132	132			

- Molecule 12 is a protein called ribosomal protein L15.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
12	J	141	Total	C	0	0	141
			141	141			

- Molecule 13 is a protein called ribosomal protein L16.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
13	K	124	Total	C	0	0	124
			124	124			

- Molecule 14 is a protein called ribosomal protein L17.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
14	L	114	Total 114	C 114	0	0	114

- Molecule 15 is a protein called ribosomal protein L18.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
15	M	111	Total 111	C 111	8	0	111

- Molecule 16 is a protein called ribosomal protein L19.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
16	N	125	Total 125	C 125	0	0	125

- Molecule 17 is a protein called ribosomal protein L20.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
17	O	117	Total 117	C 117	16	0	117

- Molecule 18 is a protein called ribosomal protein L21.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
18	P	100	Total 100	C 100	0	0	100

- Molecule 19 is a protein called ribosomal protein L22.

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

- Molecule 20 is a protein called ribosomal protein L23.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
20	R	93	Total 93	C 93	0	0	93

- Molecule 21 is a protein called ribosomal protein L24.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
21	S	113	Total C 113 113	0	0	113

- Molecule 22 is a protein called general stress protein Ctc.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
22	T	223	Total C 223 223	43	0	223

- Molecule 23 is a protein called ribosomal protein L27.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
23	U	86	Total C 86 86	0	0	86

- Molecule 24 is a protein called ribosomal protein L29.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
24	W	65	Total C 65 65	0	0	65

- Molecule 25 is a protein called ribosomal protein L30.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
25	X	55	Total C 55 55	4	0	55

- Molecule 26 is a protein called ribosomal protein L31.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
26	Y	73	Total C 73 73	0	0	73

- Molecule 27 is a protein called ribosomal protein L32.

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

- Molecule 28 is a protein called ribosomal protein L33.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
28	1	53	Total	C		0	0	53
			53	53				

- Molecule 29 is a protein called ribosomal protein L34.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
29	2	46	Total	C		0	0	46
			46	46				

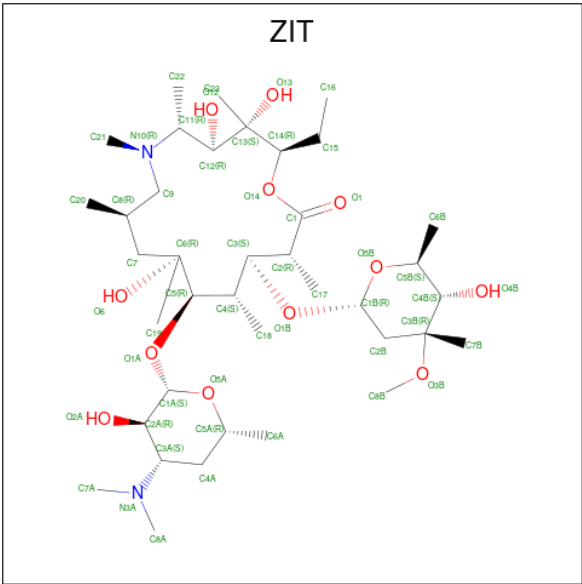
- Molecule 30 is a protein called ribosomal protein L35.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
30	3	63	Total	C		0	0	63
			63	63				

- Molecule 31 is a protein called ribosomal protein L36.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
31	4	35	Total	C		0	0	35
			35	35				

- Molecule 32 is AZITHROMYCIN (CCD ID: ZIT) (formula: C₃₈H₇₂N₂O₁₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
32	0	1	Total	C	N	O	0	0
			52	38	2	12		

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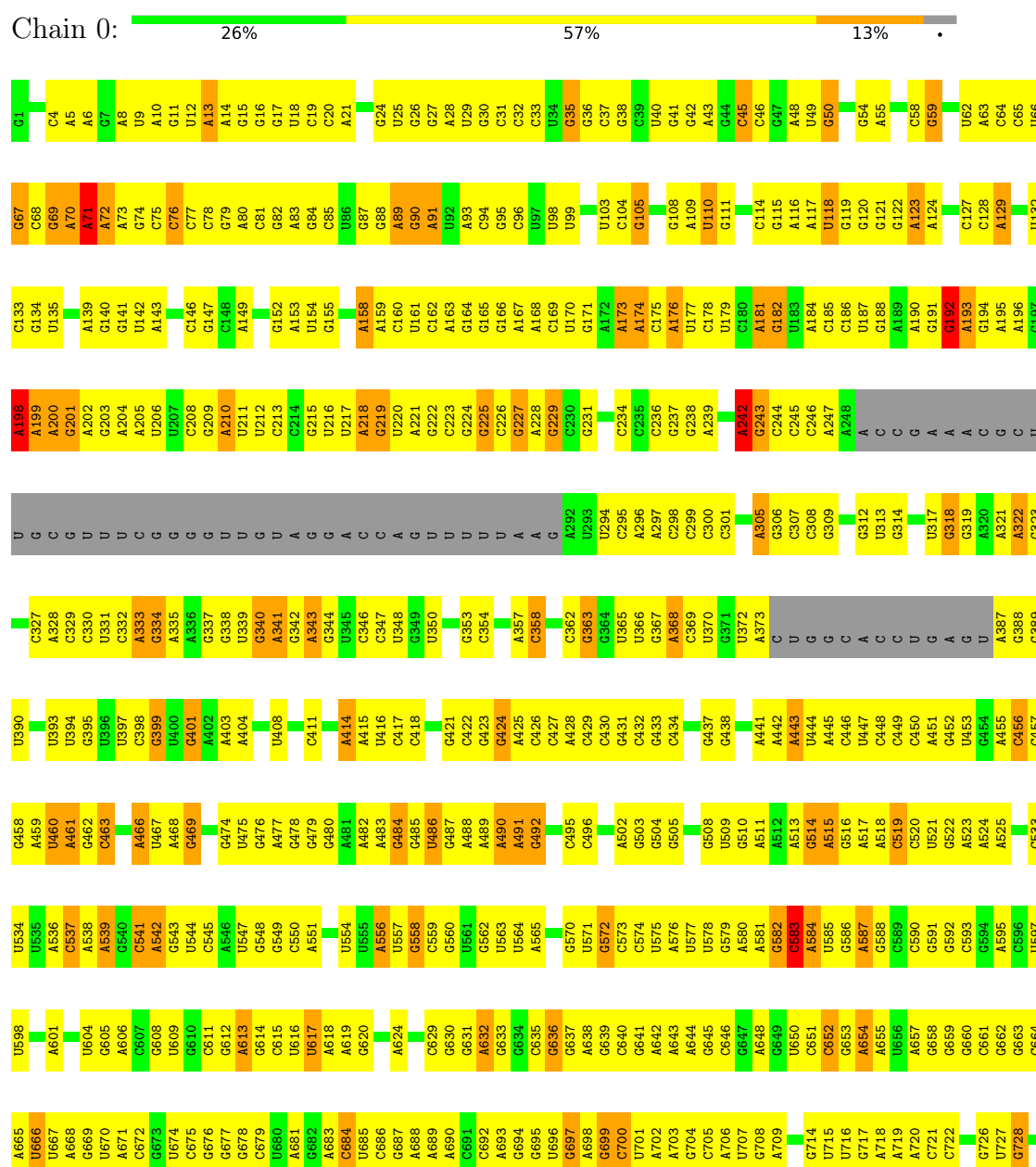
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
32	0	1	52	38	2	12	0	0

3 Residue-property plots

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

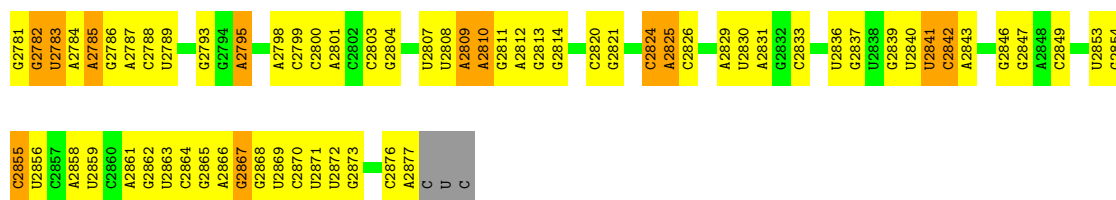
Note EDS was not executed.

• Molecule 1: 23S RIBOSOMAL RRNA



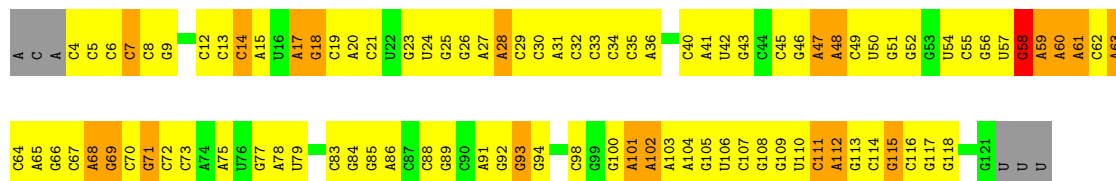
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C1622	C1623	A1624	A1625	A1626	C1627		C1630	C1631	C1632	C1633	A1634	C1635		G1638		C1641	C1642	A1643	C1644	U1645		C1648		U1651	C1652	C1653	C1654	C1655	C1656	C1657		C1661	C1662	C1663	C1664	C1665	C1666	C1667	C1668	C1669	C1670	C1671	C1672	C1673		C1677	C1678	C1679	C1680	C1681	C1682	C1683	C1684	C1685	C1686	C1687	C1688	C1689	C1690	C1691																																																	
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C1358	C1359		C1363	C1364	C1365		C1368	C1370	C1371	C1372	C1373	C1374	C1375	C1376	C1377	C1378	C1379	C1380	C1381	C1382	C1383	C1384	C1385	C1386	C1387		C1388	C1389	C1390	C1391	C1392	C1393		C1397	C1398	C1399	C1400	C1401	C1402	C1403	C1404	C1405	C1406	C1407	C1408	C1409	C1410	C1411	C1412		C1416	C1417	C1418	C1419	C1420	C1421	C1422	C1423	C1424	C1425	C1426																																																
A1297	G1298	A1299	A1300	C1301	C1302	C1303	C1304	C1305	C1306	C1307	C1308	C1309	C1310	C1311	C1312	C1313	C1314	C1315	C1316	C1317	C1318	C1319	C1320	C1321	C1322	C1323	C1324	C1325	C1326	C1327	C1328	C1329		C1332	C1333	C1334	C1335	C1336	C1337	C1338	C1339	C1340	C1341	C1342	C1343	C1344	C1345	C1346	C1347	C1348	C1349	C1350	C1351	C1352	C1353	C1354	C1355	C1356	C1357																																																		
A1283	C1284	C1285	C1286		A1288		G1241	A1242	C1243	C1244	C1245	C1246	C1247	C1248	C1249	C1250	C1251	C1252	C1253	C1254	C1255	C1256	C1257	C1258	C1259	C1260	C1261	C1262	C1263	C1264	C1265	C1266	C1267	C1268	C1269	C1270	C1271	C1272	C1273		C1277	C1278	C1279	C1280	C1281	C1282	C1283	C1284	C1285	C1286	C1287	C1288	C1289	C1290	C1291	C1292	C1293	C1294	C1295	C1296																																																	
U1156		A1162	C1163	C1164	C1165	C1166	A1167	C1168	C1169	C1170	A1171	C1172		A1179	A1180	C1181	C1182	C1183	C1184	C1185		C1190	C1191	C1192	C1193	C1194	C1195	C1196	C1197	C1198	C1199	C1200	C1201	C1202	C1203	C1204	C1205	C1206	C1207		C1212	C1213	C1214	C1215	C1216	C1217	C1218	C1219	C1220	C1221	C1222	C1223	C1224	C1225	C1226	C1227	C1228	C1229	C1230																																																		
G1082	C1083		C1086	C1087	C1088	C1089	C1090	C1091	C1092		A1095	A1096		A1099	C1100	C1101	C1102	C1103		C1110	C1111	C1112	C1113	C1114	C1115	C1116	C1117		C1121	C1122	C1123	C1124	C1125	C1126		C1130	C1131	C1132	C1133	C1134	C1135	C1136	C1137	C1138	C1139	C1140	C1141	C1142	C1143	C1144	C1145	C1146	C1147	C1148	C1149	C1150	C1151	C1152	C1153	C1154	C1155																																																
C1002	C1003	A1004	C1005	C1006	C1007	C1008	C1009	C1010	C1011	A1012		C1016	C1017	C1018	C1019	A1020	C1021	C1022	C1023	C1024	A1025	C1026	C1027	C1028	C1029	C1030	C1031	C1032	C1033	C1034	C1035	C1036	C1037	C1038	C1039	C1040	C1041		C1044		C1054	C1055	C1056	C1057	C1058	C1059	C1060	C1061	C1062	C1063	C1064	C1065	C1066	C1067	C1068	C1069	C1070	C1071	C1072	C1073	C1074	C1075	C1076	C1077	C1078	C1079	C1080	C1081																																									
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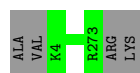
• Molecule 2: 5S RIBOSOMAL RRNA

Chain 9: 19% 60% 16% 5%



• Molecule 3: ribosomal protein L2

Chain A: 99%



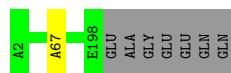
• Molecule 4: ribosomal protein L3

Chain B: 96%



• Molecule 5: ribosomal protein L4

Chain C: 96%



• Molecule 6: ribosomal protein L5

Chain D: 98%

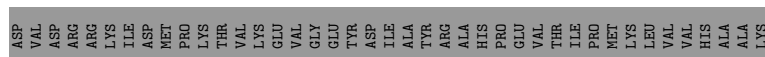
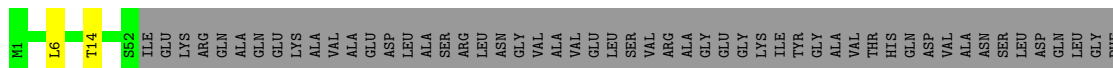


• Molecule 7: ribosomal protein L6

Chain E: 95%



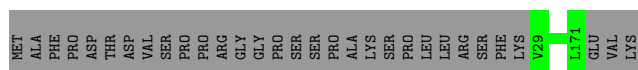
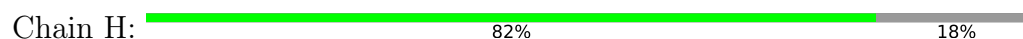
- Molecule 8: ribosomal protein L9



- Molecule 9: ribosomal protein L11



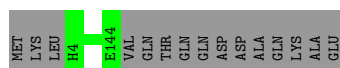
- Molecule 10: ribosomal protein L13



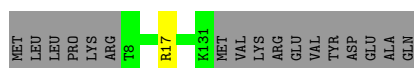
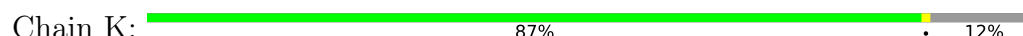
- Molecule 11: ribosomal protein L14



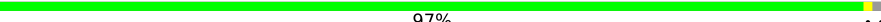
- Molecule 12: ribosomal protein L15



- Molecule 13: ribosomal protein L16

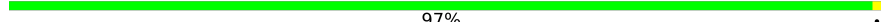


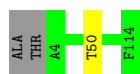
- Molecule 14: ribosomal protein L17

Chain L:  97% ..



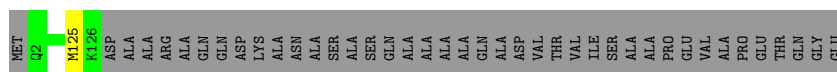
- Molecule 15: ribosomal protein L18

Chain M:  97% ..

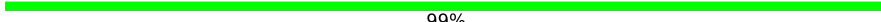


- Molecule 16: ribosomal protein L19

Chain N:  75% . 25%

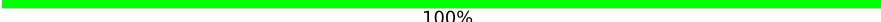


- Molecule 17: ribosomal protein L20

Chain O:  99% .

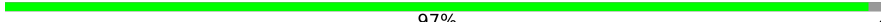


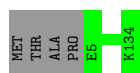
- Molecule 18: ribosomal protein L21

Chain P:  100%

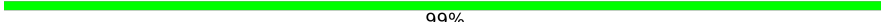
There are no outlier residues recorded for this chain.

- Molecule 19: ribosomal protein L22

Chain Q:  97% .

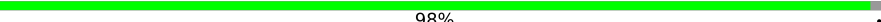


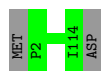
- Molecule 20: ribosomal protein L23

Chain R:  99% .



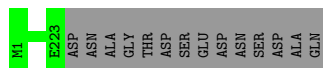
- Molecule 21: ribosomal protein L24

Chain S:  98% .



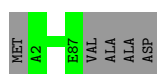
- Molecule 22: general stress protein Ctc

Chain T: 94% 6%



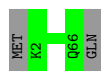
- Molecule 23: ribosomal protein L27

Chain U: 95% 5%



- Molecule 24: ribosomal protein L29

Chain W: 97% .



- Molecule 25: ribosomal protein L30

Chain X: 100%

There are no outlier residues recorded for this chain.

- Molecule 26: ribosomal protein L31

Chain Y: 100%

There are no outlier residues recorded for this chain.

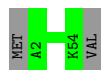
- Molecule 27: ribosomal protein L32

Chain Z: 97% ..

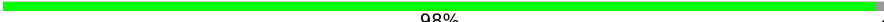


- Molecule 28: ribosomal protein L33

Chain 1: 96% .

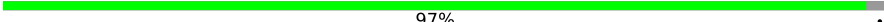


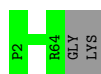
- Molecule 29: ribosomal protein L34

Chain 2:  98% .



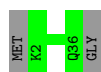
- Molecule 30: ribosomal protein L35

Chain 3:  97% .



- Molecule 31: ribosomal protein L36

Chain 4:  95% 5%



4 Data and refinement statistics

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

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	170.80 Å 409.50 Å 695.70 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 3.30	Depositor
% Data completeness (in resolution range)	(Not available) (15.00-3.30)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.279 , 0.304	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	65404	wwPDB-VP
Average B, all atoms (Å ²)	46.0	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: ZIT

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	0.26	0/66467	0.59	16/103673 (0.0%)
2	9	0.45	0/2816	0.80	1/4388 (0.0%)
All	All	0.27	0/69283	0.60	17/108061 (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	1

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	2588	U	C2'-C3'-O3'	7.20	120.29	109.50
1	0	2018	G	C2'-C3'-O3'	7.15	120.22	109.50
1	0	242	A	C2'-C3'-O3'	6.86	119.79	109.50
1	0	192	G	C2'-C3'-O3'	6.31	118.97	109.50
1	0	71	A	C2'-C3'-O3'	5.77	118.15	109.50

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	1342	U	Sidechain

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	0	59359	0	29917	2151	0
2	9	2519	0	1285	147	0
3	A	270	0	0	0	0
4	B	205	0	0	3	0
5	C	197	0	0	1	0
6	D	178	0	0	1	0
7	E	177	0	0	1	0
8	F	52	0	0	1	0
9	G	143	0	0	0	0
10	H	143	0	0	0	0
11	I	132	0	0	0	0
12	J	141	0	0	0	0
13	K	124	0	0	1	0
14	L	114	0	0	1	0
15	M	111	0	0	1	0
16	N	125	0	0	1	0
17	O	117	0	0	0	0
18	P	100	0	0	0	0
19	Q	130	0	0	0	0
20	R	93	0	0	0	0
21	S	113	0	0	0	0
22	T	223	0	0	0	0
23	U	86	0	0	0	0
24	W	65	0	0	0	0
25	X	55	0	0	0	0
26	Y	73	0	0	0	0
27	Z	58	0	0	1	0
28	1	53	0	0	0	0
29	2	46	0	0	0	0
30	3	63	0	0	0	0
31	4	35	0	0	0	0
32	0	104	0	144	47	0
All	All	65404	0	31346	2333	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 24.

The worst 5 of 2333 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)
32:0:2882:ZIT:H6A1	32:0:2882:ZIT:C6B	1.61	1.30
32:0:2881:ZIT:H6A1	32:0:2881:ZIT:C6B	1.61	1.29
1:0:1679:U:H2'	1:0:1680:U:H5''	1.27	1.16
1:0:2058:U:H1'	1:0:2576:G:H21	1.10	1.14
1:0:2548:G:H2'	1:0:2549:G:H5''	1.26	1.14

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

5.3.2 Protein sidechains [i](#)

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

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2757/2880 (95%)	485 (17%)	43 (1%)
2	9	117/124 (94%)	23 (19%)	1 (0%)
All	All	2874/3004 (95%)	508 (17%)	44 (1%)

5 of 508 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 44 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	2015	G

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Mol	Chain	Res	Type
1	0	2377	U
1	0	2018	G
1	0	2204	A
1	0	2560	G

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](#)

2 ligands are 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	$\# Z > 2$
32	ZIT	0	2881	-	54,54,54	0.86	1 (1%)	82,83,83	1.30	7 (8%)
32	ZIT	0	2882	-	54,54,54	0.86	1 (1%)	82,83,83	1.30	6 (7%)

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
32	ZIT	0	2881	-	-	3/72/107/107	0/3/3/3
32	ZIT	0	2882	-	-	5/72/107/107	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	0	2881	ZIT	C3A-N3A	-2.29	1.42	1.47
32	0	2882	ZIT	C3A-N3A	-2.20	1.42	1.47

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	0	2882	ZIT	C1A-O1A-C5	-7.31	103.82	116.26
32	0	2881	ZIT	C1A-O1A-C5	-7.24	103.94	116.26
32	0	2881	ZIT	C4A-C3A-C2A	-3.20	105.42	110.02
32	0	2882	ZIT	C4A-C3A-C2A	-3.16	105.47	110.02
32	0	2882	ZIT	O1B-C3-C4	2.73	111.45	108.23

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

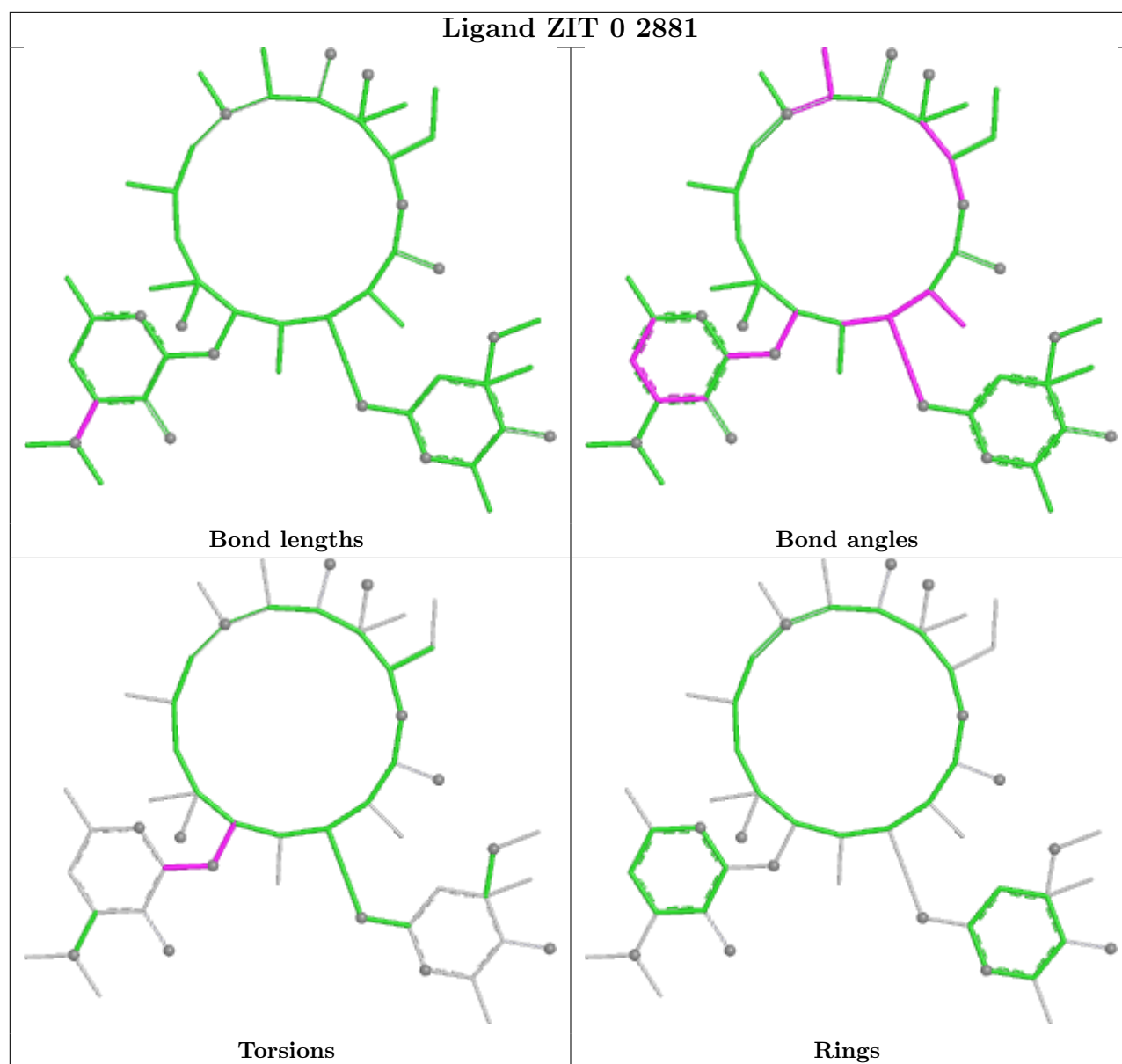
Mol	Chain	Res	Type	Atoms
32	0	2882	ZIT	C13-C14-C15-C16
32	0	2881	ZIT	O5A-C1A-O1A-C5
32	0	2882	ZIT	O5A-C1A-O1A-C5
32	0	2882	ZIT	O14-C14-C15-C16
32	0	2881	ZIT	C4-C5-O1A-C1A

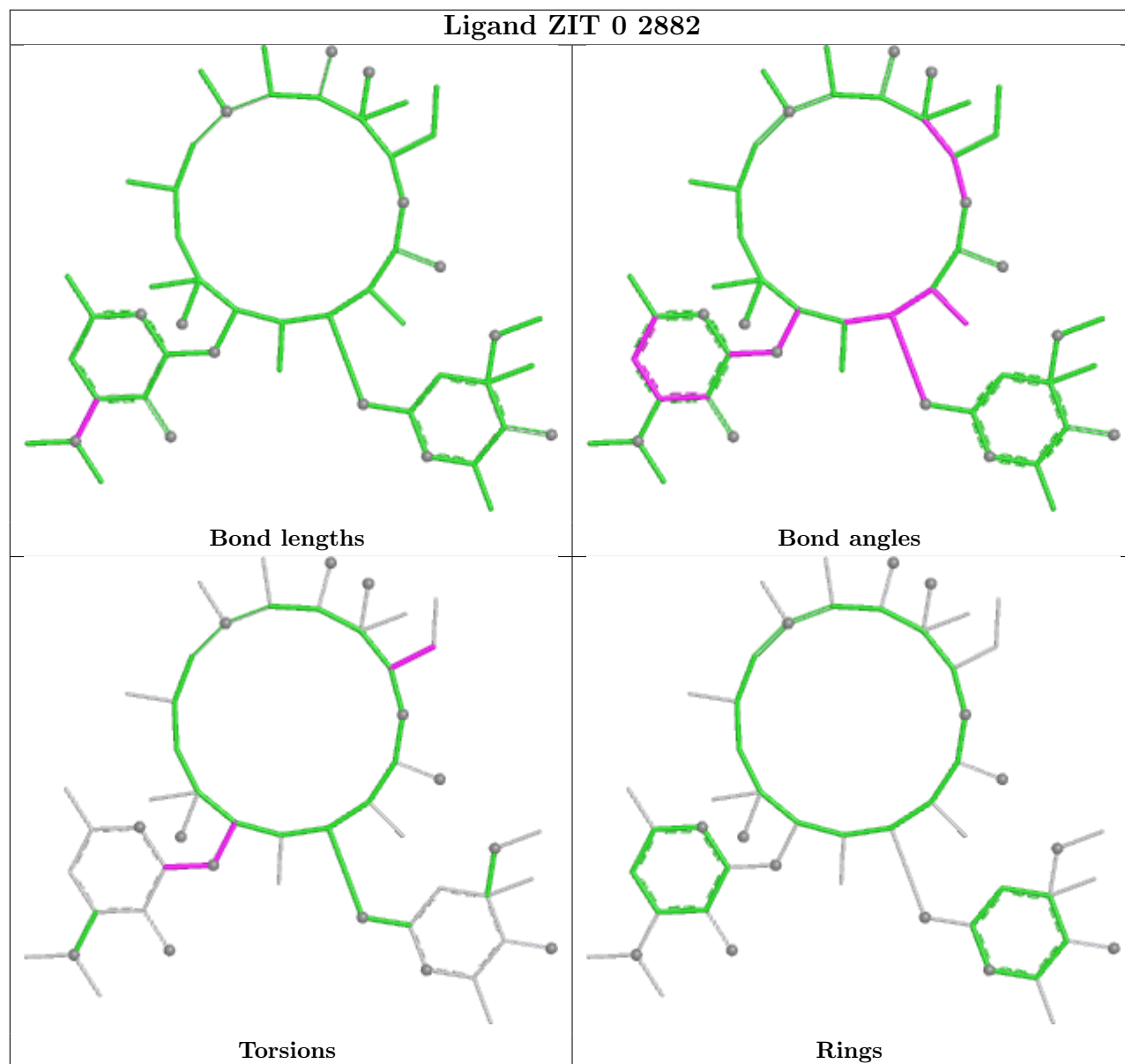
There are no ring outliers.

2 monomers are involved in 47 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	0	2881	ZIT	21	0
32	0	2882	ZIT	26	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 [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.