



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 05:46 PM UTC

PDB ID : 4WFN / pdb_00004wfn
Title : Crystal structure of the large ribosomal subunit (50S) of *Deinococcus radiodurans* containing a three residue insertion in L22 in complex with erythromycin
Authors : Wekselman, I.; Zimmerman, E.; Rozenberg, H.; Bashan, A.; Yonath, A.
Deposited on : 2014-09-16
Resolution : 3.54 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

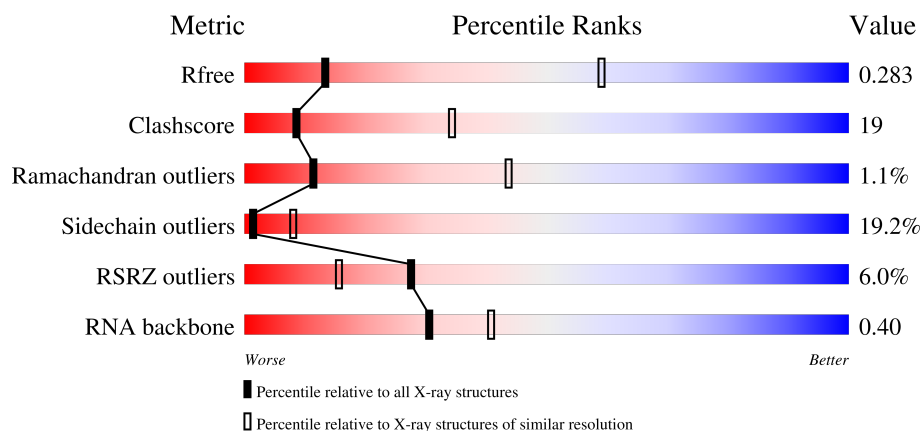
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.54 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	1008 (3.58-3.50)
Clashscore	190562	1062 (3.58-3.50)
Ramachandran outliers	187476	1033 (3.58-3.50)
Sidechain outliers	187428	1034 (3.58-3.50)
RSRZ outliers	180081	1007 (3.58-3.50)
RNA backbone	3983	1006 (4.02-3.06)

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	A	275	
2	B	211	
3	C	205	
4	D	180	

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Mol	Chain	Length	Quality of chain
5	E	185	
6	G	174	
7	H	134	
8	I	156	
9	J	141	
10	K	116	
11	L	114	
12	M	165	
13	N	118	
14	O	100	
15	P	137	
16	Q	95	
17	R	115	
18	S	237	
19	T	91	
20	U	81	
21	V	67	
22	W	55	
23	Z	60	
24	1	55	
25	2	47	
26	3	65	
27	X	2880	
28	Y	124	

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
29	MG	X	2904	-	-	-	X
29	MG	X	2914	-	-	-	X
29	MG	X	2915	-	-	-	X
29	MG	X	2916	-	-	-	X
29	MG	X	2918	-	-	-	X
29	MG	X	2926	-	-	-	X
29	MG	X	2935	-	-	-	X
29	MG	X	2943	-	-	-	X
29	MG	X	2965	-	-	-	X

2 Entry composition [i](#)

There are 30 unique types of molecules in this entry. The entry contains 84117 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 protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	260	Total	C	N	O	S	0	0	0
			1987	1235	399	350	3			

- Molecule 2 is a protein called 50S ribosomal protein L3.

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

- Molecule 3 is a protein called 50S ribosomal protein L4.

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

- Molecule 4 is a protein called 50S ribosomal protein L5.

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

- Molecule 5 is a protein called 50S ribosomal protein L6.

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

- Molecule 6 is a protein called 50S ribosomal protein L13.

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

- Molecule 7 is a protein called 50S ribosomal protein L14.

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

- Molecule 8 is a protein called 50S ribosomal protein L15.

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

- Molecule 9 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	J	136	Total	C	N	O	S	0	0	0
			1090	696	202	185	7			

- Molecule 10 is a protein called 50S ribosomal protein L17.

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

- Molecule 11 is a protein called 50S ribosomal protein L18.

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

- Molecule 12 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	M	108	Total	C	N	O		0	0	0
			871	543	172	156				

- Molecule 13 is a protein called 50S ribosomal protein L20.

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

- Molecule 14 is a protein called 50S ribosomal protein L21.

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

- Molecule 15 is a protein called 50S ribosomal protein L22,50S ribosomal protein L22.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	P	130	Total	C	N	O	S		
			1038	655	205	176	2	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	110	VAL	-	linker	UNP Q9RXJ7
P	111	PRO	-	linker	UNP Q9RXJ7
P	112	ARG	-	linker	UNP Q9RXJ7

- Molecule 16 is a protein called 50S ribosomal protein L23.

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

- Molecule 17 is a protein called 50S ribosomal protein L24.

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

- Molecule 18 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	S	175	Total	C	N	O	S		
			1345	849	236	254	6	0	0

- Molecule 19 is a protein called 50S ribosomal protein L27.

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

- Molecule 20 is a protein called 50S ribosomal protein L28.

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

- Molecule 21 is a protein called 50S ribosomal protein L29.

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

- Molecule 22 is a protein called 50S ribosomal protein L30.

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

- Molecule 23 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	Z	56	Total	C	N	O	S			
			443	272	91	75	5	0	0	0

- Molecule 24 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	1	53	Total	C	N	O	S			
			431	274	80	76	1	0	0	0

- Molecule 25 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	2	46	Total	C	N	O	S			
			383	230	91	60	2	0	0	0

- Molecule 26 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	3	59	Total	C	N	O	S			
			462	290	95	73	4	0	0	0

- Molecule 27 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	X	2680	Total	C	N	O	P	0	0	0
			57533	25663	10626	18564	2680			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	1526	U	UNK	conflict	GB 11612676

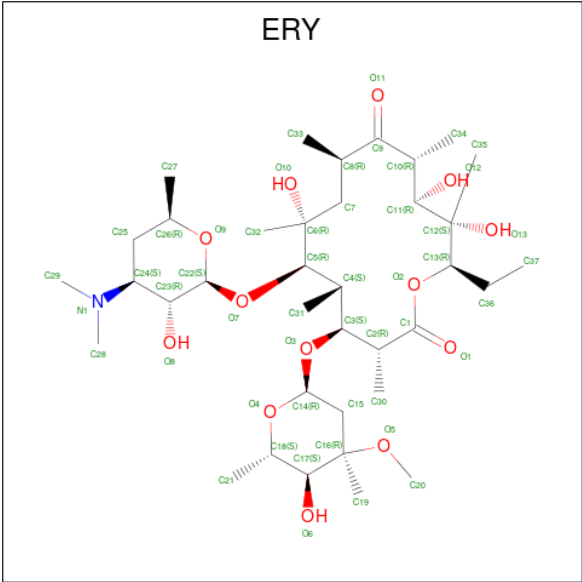
- Molecule 28 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	Y	122	Total	C	N	O	P	0	0	0
			2601	1161	476	842	122			

- Molecule 29 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
29	A	1	Total	Mg	0	0
			1	1		
29	B	1	Total	Mg	0	0
			1	1		
29	K	2	Total	Mg	0	0
			2	2		
29	M	2	Total	Mg	0	0
			2	2		
29	X	64	Total	Mg	0	0
			64	64		

- Molecule 30 is ERYTHROMYCIN A (CCD ID: ERY) (formula: C₃₇H₆₇NO₁₃).

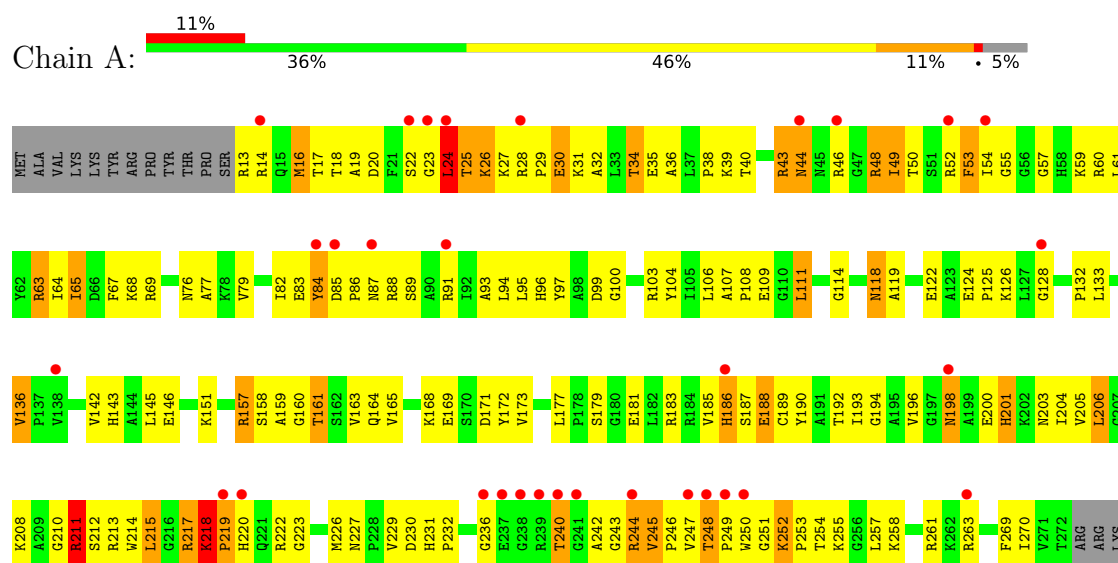


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
30	X	1	Total	C	N	O	0	0
			51	37	1	13		

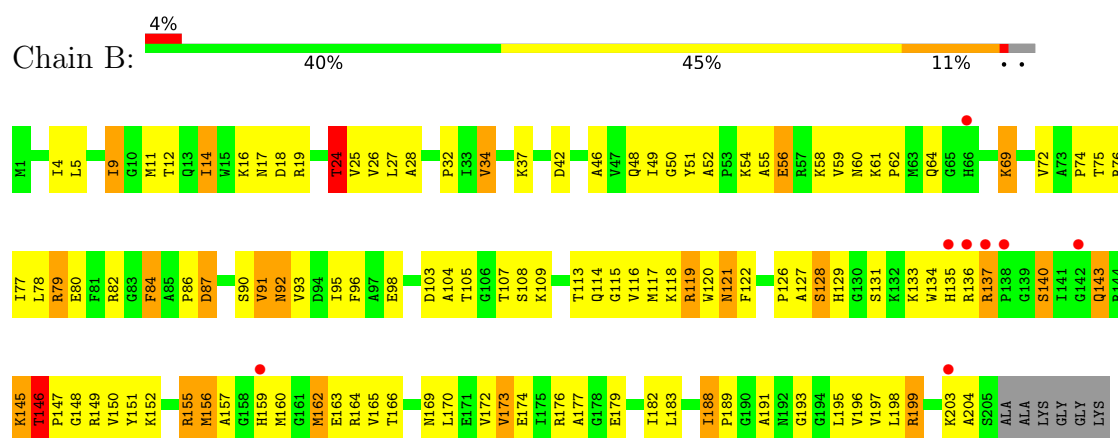
3 Residue-property plots

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 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.

• Molecule 1: 50S ribosomal protein L2

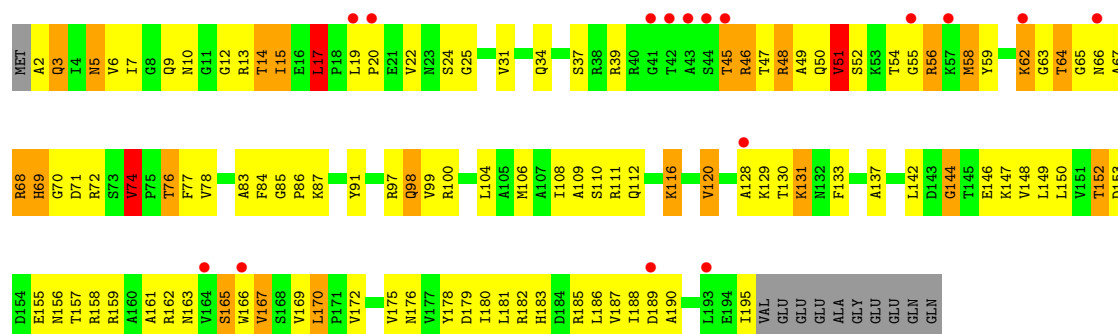


• Molecule 2: 50S ribosomal protein L3

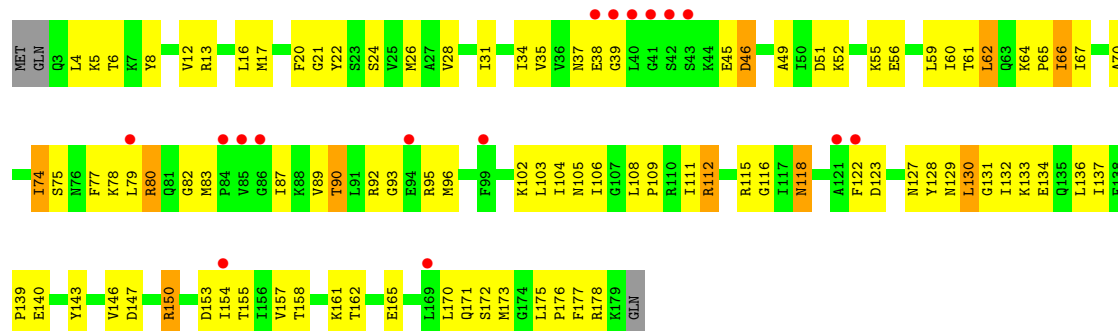
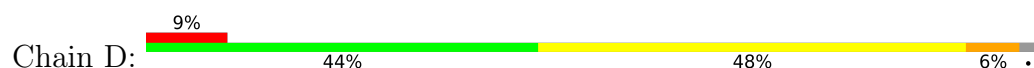


• Molecule 3: 50S ribosomal protein L4

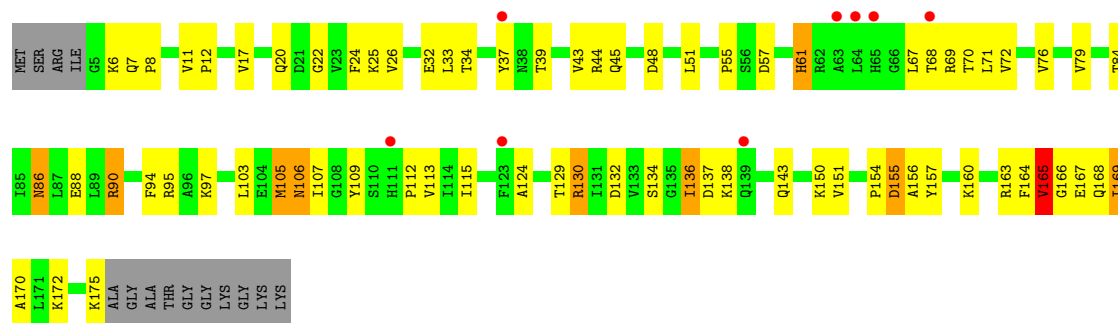




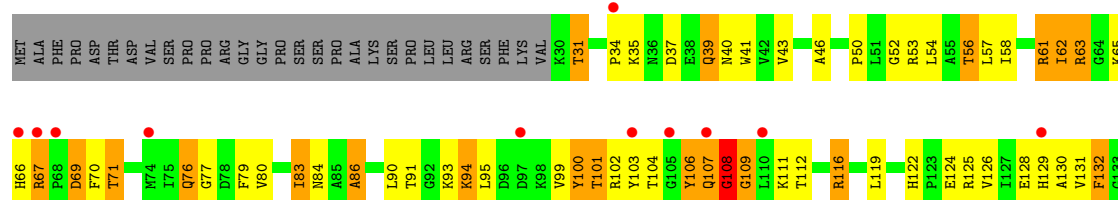
• Molecule 4: 50S ribosomal protein L5



• Molecule 5: 50S ribosomal protein L6

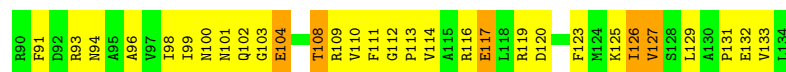
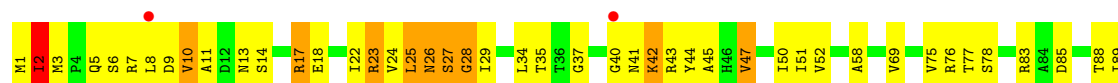
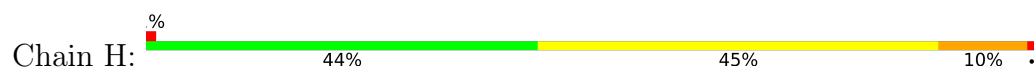


• Molecule 6: 50S ribosomal protein L13

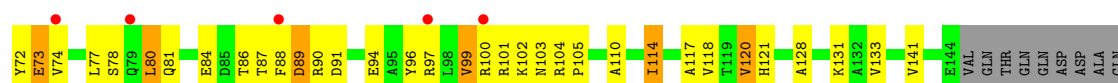
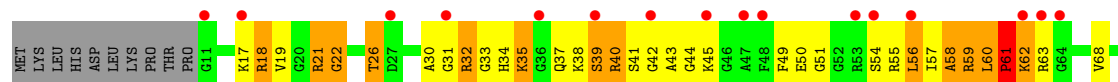
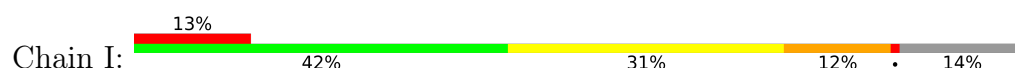




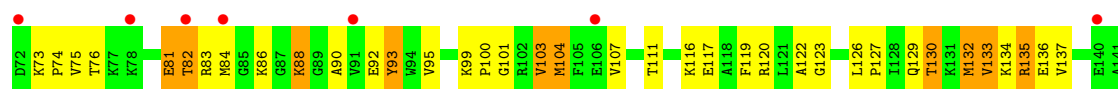
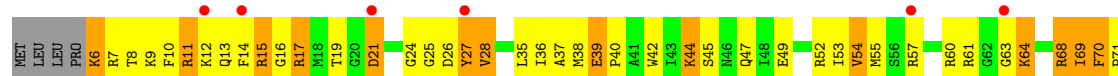
• Molecule 7: 50S ribosomal protein L14



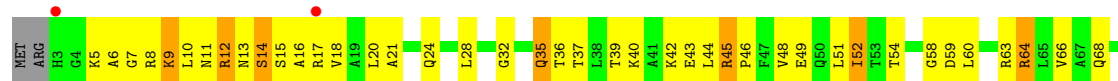
• Molecule 8: 50S ribosomal protein L15



• Molecule 9: 50S ribosomal protein L16

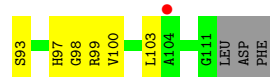
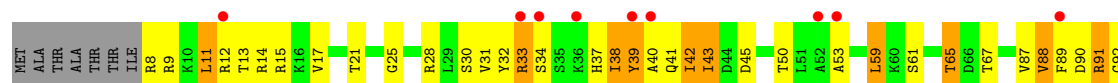


• Molecule 10: 50S ribosomal protein L17

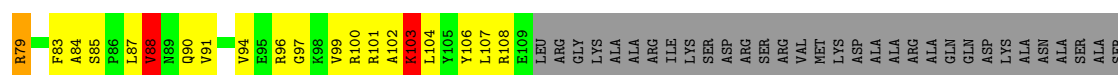
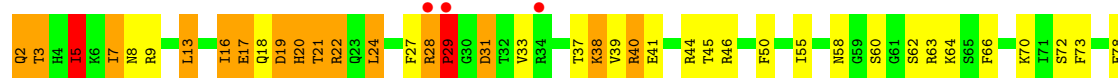
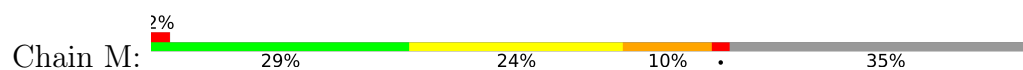




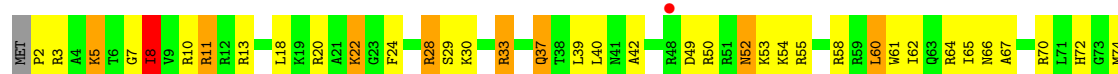
- Molecule 11: 50S ribosomal protein L18



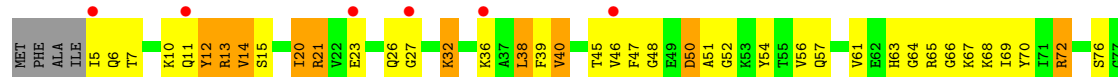
- Molecule 12: 50S ribosomal protein L19



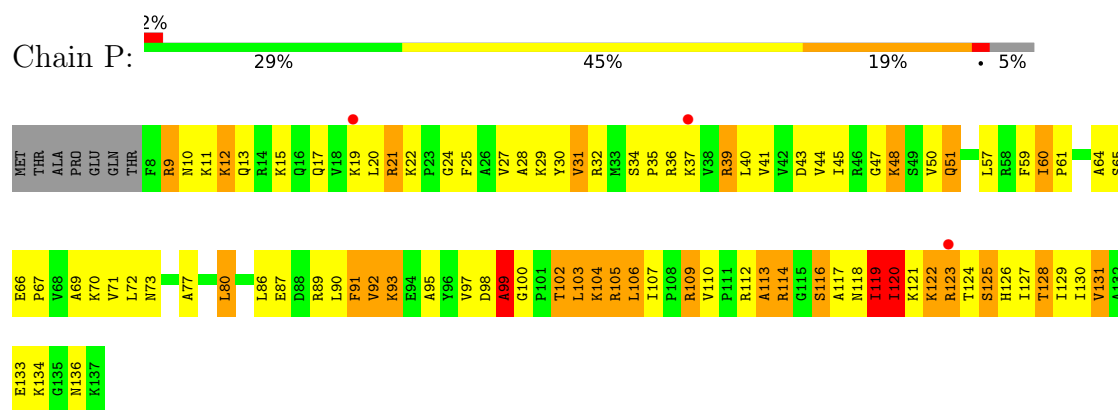
- Molecule 13: 50S ribosomal protein L20



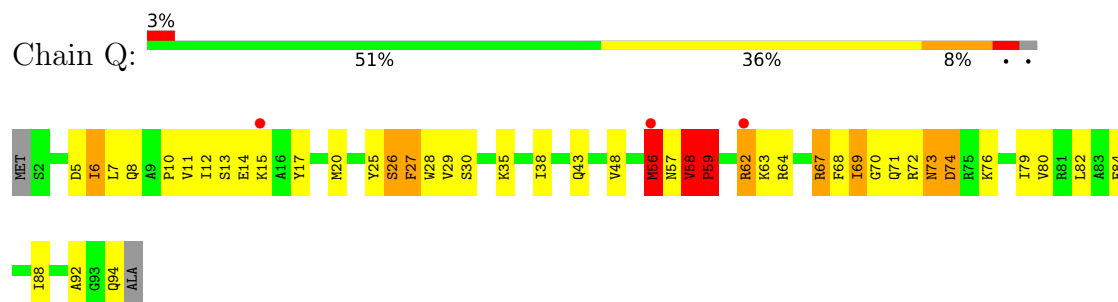
- Molecule 14: 50S ribosomal protein L21



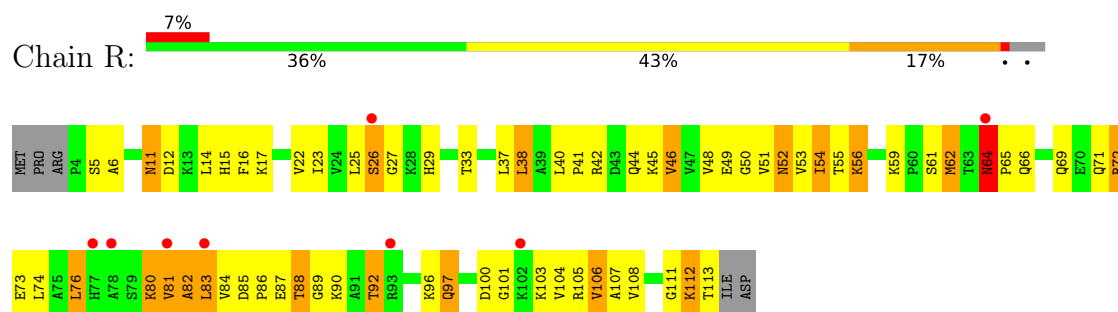
- Molecule 15: 50S ribosomal protein L22, 50S ribosomal protein L22



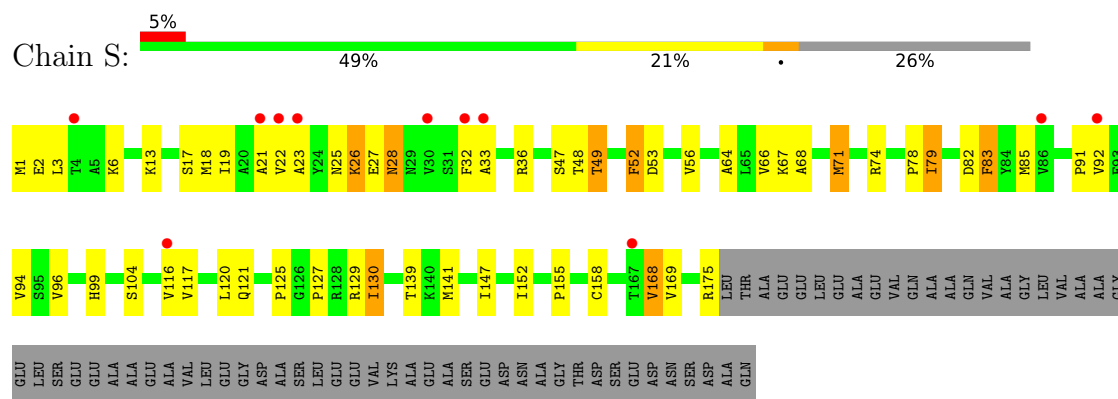
• Molecule 16: 50S ribosomal protein L23



• Molecule 17: 50S ribosomal protein L24

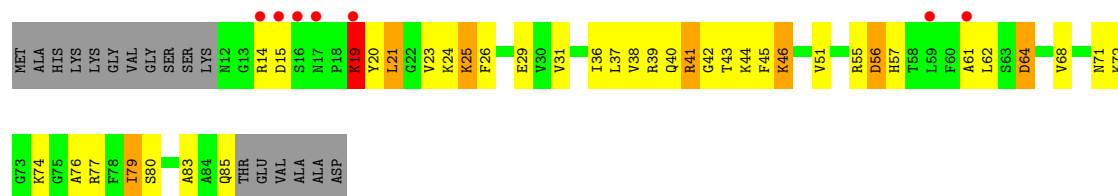


• Molecule 18: 50S ribosomal protein L25

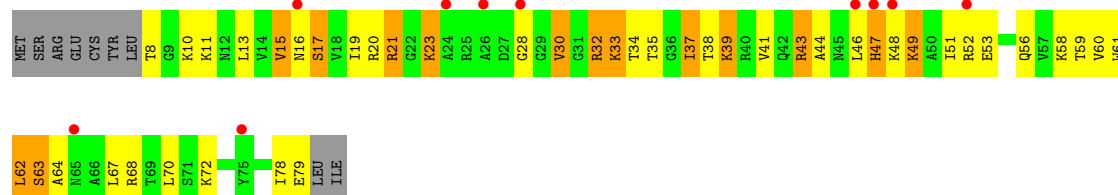


• Molecule 19: 50S ribosomal protein L27

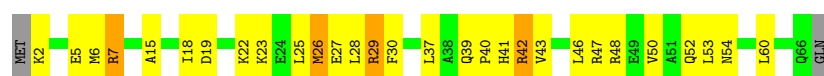




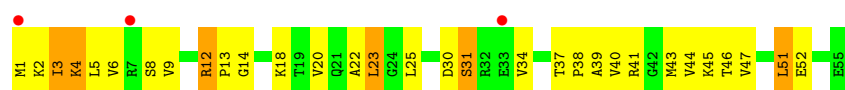
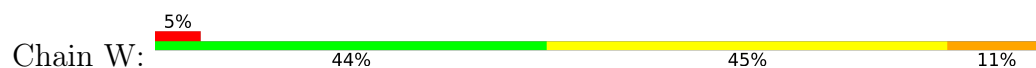
• Molecule 20: 50S ribosomal protein L28



• Molecule 21: 50S ribosomal protein L29



• Molecule 22: 50S ribosomal protein L30



• Molecule 23: 50S ribosomal protein L32



• Molecule 24: 50S ribosomal protein L33

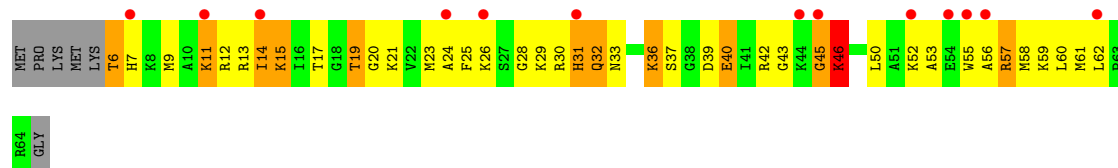


• Molecule 25: 50S ribosomal protein L34

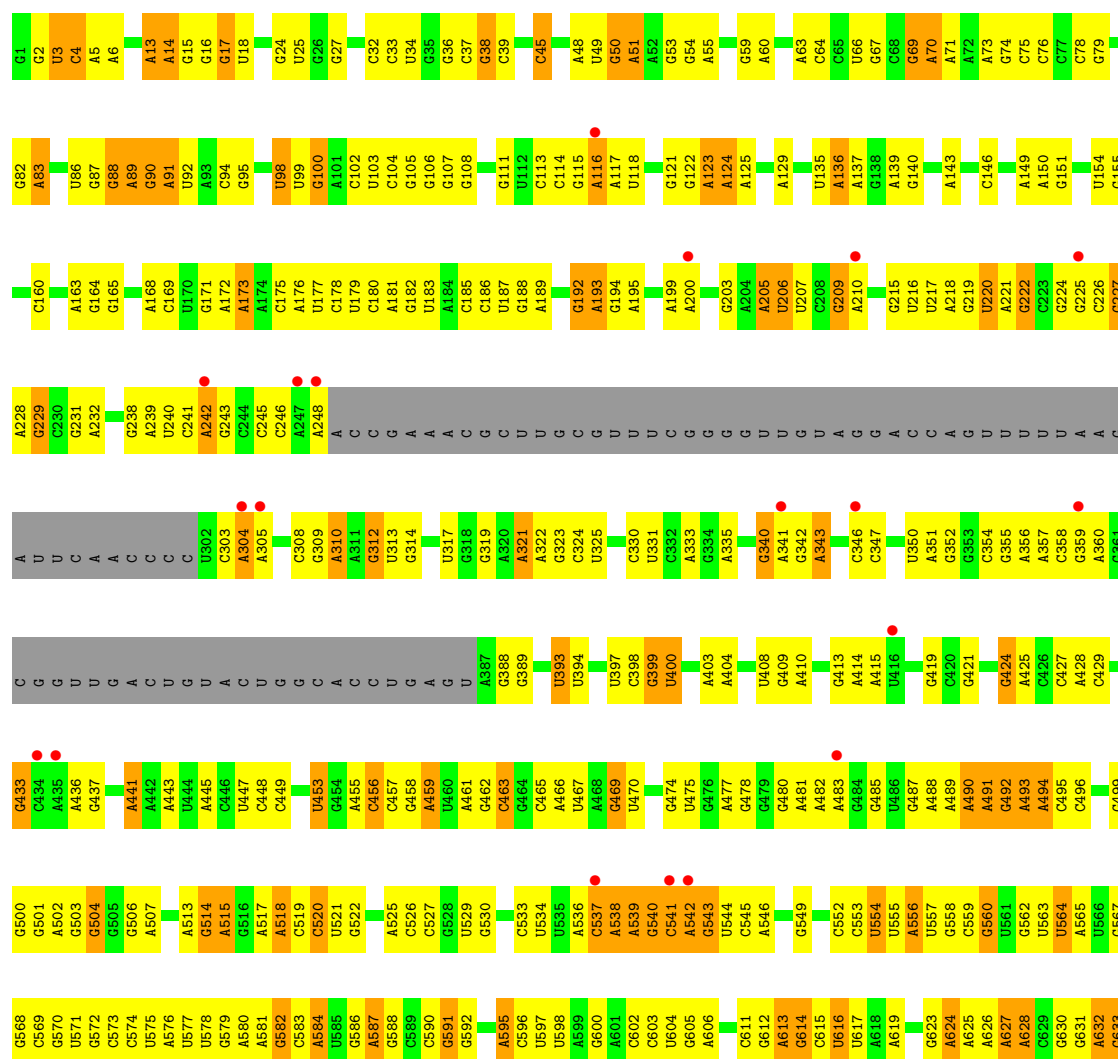




• Molecule 26: 50S ribosomal protein L35

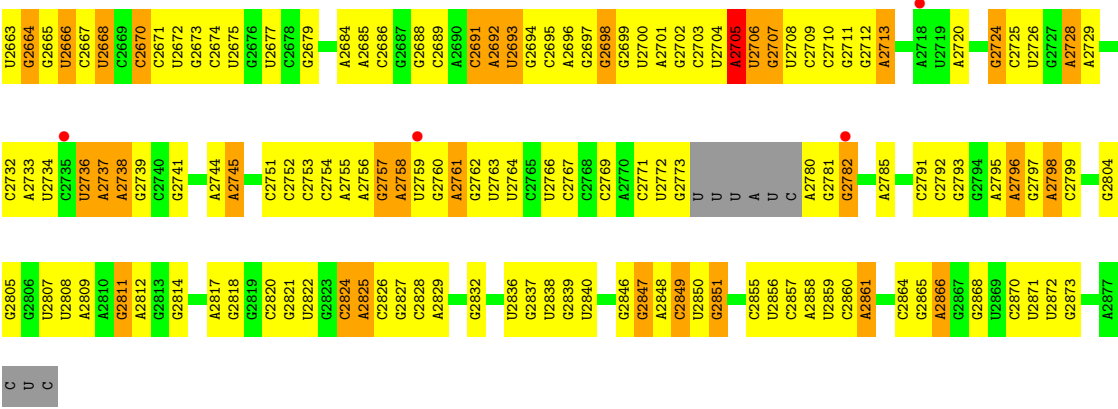


• Molecule 27: 23S ribosomal RNA

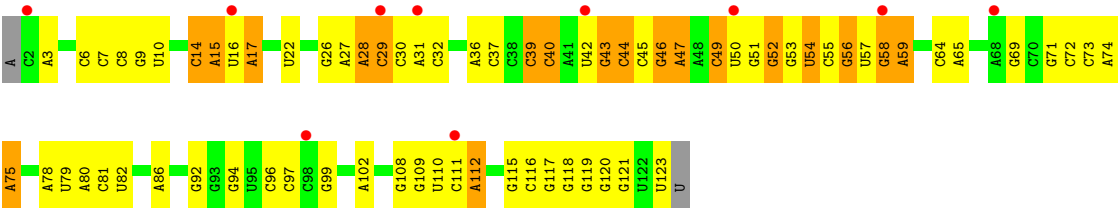


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A1597	U1505	G1435	U1365	A1287	U1217	G1142	G1069	A999	A929	G943	G772	C700	C635
C1598	A1506	G1436	A1366	A1288	C1218	C1145	U1071	G1000	A930	G844	A774	U701	G636
G1599	G1508	G1438	A1367	A1289	C1219	U1070	U1070	A1001	G931	U845	G773	G702	A637
U1600	G1514	G1439	G1291	G1291	G1220	G1147	G1073	U1005	G834	A846	U784	G704	A638
U1601	G1514	G1440	U1370	G1296	G1223	G1148	G1074	U1006	G935	U852	G787	C705	C640
U1602	A1603	A1441	U1371	G1296	A1224	G1149	A1080	C1006	C955	U853	A787	C711	G641
A1604	C1517	G1442	A1372	A1289	G1225	C1150	A1081	A1007	A936	G854	G788	G712	A642
U1607	G1518	G1443	G1373	A1290	A1226	U1151	G1082	U1010	G938	U857	A790	G713	G645
U1608	G1519	C1444	G1374	U1301	A1227	C1152	C1083	A1011	G939	G858	G791	G717	G646
U1609	C1524	A1448	A1378	C1302	G1228	A1154	C1084	U1014	G940	U859	U792	G717	G647
G1609	A1525	U1451	A1379	C1302	C1229	G1155	G1085	U1015	U941	C863	G793	C721	A648
A1610	U1526	U1452	C1380	C1310	C1230	U1159	C1086	U1016	U942	C864	A794	C721	G649
C1614	C1528	A1453	G1382	C1311	C1231	U1160	C1087	C1017	U943	C865	A795	C721	G650
C1615	C1531	U1454	G1383	U1313	G1236	U1161	A1088	C1018	G945	A865	A796	C725	C651
C1616	U1532	C1455	A1314	A1288	G1237	A1162	C1089	U1019	G946	U871	G798	U727	G652
G1617	G1533	C1456	C1385	A1315	A1289	C1163	U1093	A1020	C947	U872	C799	U728	G653
C1623	U1534	U1459	A1386	G1316	A1299	G1165	A1095	A1021	C948	G873	U800	A729	A654
A1624	G1539	C1461	C1388	G1317	G1240	A1166	A1096	U1022	U951	G874	A801	C730	A655
A1625	U1540	C1462	A1321	U1247	U1248	A1167	A1097	U1023	G952	A875	A802	A731	A656
A1626	G1541	U1465	G1322	G1249	G1250	A1171	A1098	U1026	U953	G877	C803	G732	G658
G1629	U1551	C1466	G1323	G1251	A1255	U1172	A1099	C1027	G955	C878	C804	G733	G659
A1630	C1552	U1467	U1325	C1252	C1256	U1173	U1101	U1030	A956	A879	A806	G734	G660
C1632	G1553	A1468	U1326	A1257	U1257	G1174	U1102	U1031	U957	G883	A807	G735	G661
G1633	U1554	U1469	C1327	U1261	A1265	A1175	C1103	U1032	G958	C884	C808	G736	G662
A1634	A1555	C1470	G1328	U1262	C1266	U1182	G1104	A1033	C959	A891	U810	G737	G663
G1635	U1556	U1473	U1329	U1267	U1267	C1183	U1105	G1033	U960	G	G811	G739	A665
G1636	U1557	A1474	G1330	C1268	G1268	U1184	U1106	U1034	G961	G	G812	G742	U666
U1637	G1562	U1475	G1331	C1269	G1269	C1185	U1107	G1035	C962	G	A813	A743	A668
C1640	U1563	G1476	A1334	U1269	U1275	U1186	U1108	G1036	G963	G	C814	G744	G669
C1641	U1564	C1477	A1335	U1270	A1276	A1187	U1109	U1037	A964	G	C815	C745	U670
G1642	U1567	U1478	G1336	U1271	U1277	A1188	C1111	A1040	A866	C	A817	G746	A671
A1643	A1568	G1479	G1337	C1284	G1284	G1189	U1112	G1041	G967	C	C818	A747	C672
G1644	U1569	U1480	U1410	G1285	G1285	C1113	C1114	G1042	C967	U	C819	A748	G673
U1645	C1570	U1481	C1411	G1286	G1286	U1114	A1115	A1043	U969	A	U820	C749	U674
G1646	U1571	U1482	C1412	U1287	G1287	U1115	U1116	U1044	A970	C	A821	C750	C675
U1647	C1572	G1483	U1342	U1288	U1288	U1195	U1117	G1045	A971	C	C825	C751	G676
C1648	U1573	U1484	C1343	G1289	G1289	U1196	C1120	U1046	C972	A	U824	G752	G677
U1651	A1574	U1485	C1344	C1270	C1270	U1197	G1121	U1051	U973	G	U825	U753	G682
G1652	C1575	C1489	C1347	G1273	G1273	G1200	G1122	C976	C976	C	C826	G754	A683
C1653	A1580	U1490	C1348	C1274	C1274	G1201	G1123	U	C977	U	C827	G755	A684
A1654	C1581	A1493	C1349	A1275	A1275	U1202	U1124	C1053	U978	U	C828	G758	C684
U1655	U1586	U1494	G1350	U1276	U1276	A1203	U1125	A1054	A979	A	C829	C759	U685
G1659	G1583	G1495	G1351	U1277	U1277	G1204	G1126	A1055	C980	C	G830	U760	G686
C1661	U1586	C1496	A1352	U1278	U1278	G1205	G1127	U1056	G981	C	A832	G761	G687
G1662	C1588	U1498	A1353	U1279	U1279	G1206	G1128	A1057	C982	A911	A762	A762	A690
U1663	U1589	G1499	A1354	U1280	U1280	G1207	G1133	U1058	C983	C914	A763	A764	C692
C1664	A1592	C1501	U1357	U1281	U1281	G1209	C1134	A1059	G984	U835	A765	A765	A693
C1665	U1592	G1502	U1358	A1282	A1282	C1210	A1137	A1061	G985	G920	U836	U766	G694
		U1502	G1359	C1283	C1283	U1211	A1138	A1065	A992	A922	U837	G767	G695
		G1503	A1433	A1285	A1285	U1212	A1139	C993	C993	A923	U838	U768	U696
						U1213	A1140	G1067	A994	C924	U839	U770	A698





• Molecule 28: 5S ribosomal RNA



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	170.09Å 411.59Å 695.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.99 – 3.54 19.99 – 3.54	Depositor EDS
% Data completeness (in resolution range)	90.4 (19.99-3.54) 89.9 (19.99-3.54)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.02 (at 3.48Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.234 , 0.282 0.235 , 0.283	Depositor DCC
R_{free} test set	13640 reflections (4.55%)	wwPDB-VP
Wilson B-factor (Å ²)	100.0	Xtriage
Anisotropy	0.674	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.18 , 26.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	84117	wwPDB-VP
Average B, all atoms (Å ²)	93.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.27% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ERY, 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	A	0.60	0/2025	1.24	23/2726 (0.8%)
2	B	0.72	0/1567	1.14	6/2105 (0.3%)
3	C	0.61	0/1504	1.17	16/2036 (0.8%)
4	D	0.38	0/1419	0.89	2/1903 (0.1%)
5	E	0.40	0/1308	0.91	1/1771 (0.1%)
6	G	0.61	0/1138	1.24	14/1539 (0.9%)
7	H	0.79	1/1007 (0.1%)	1.21	8/1352 (0.6%)
8	I	0.63	0/1022	1.26	11/1366 (0.8%)
9	J	0.70	1/1113 (0.1%)	1.29	18/1486 (1.2%)
10	K	0.87	1/886 (0.1%)	1.30	8/1188 (0.7%)
11	L	0.46	0/785	0.93	1/1048 (0.1%)
12	M	0.86	0/884	1.33	8/1186 (0.7%)
13	N	0.55	0/994	1.06	6/1323 (0.5%)
14	O	0.52	0/750	1.07	8/1000 (0.8%)
15	P	0.78	0/1052	1.24	13/1409 (0.9%)
16	Q	0.57	0/737	1.21	8/988 (0.8%)
17	R	0.59	0/835	1.20	12/1121 (1.1%)
18	S	0.44	0/1370	0.93	1/1862 (0.1%)
19	T	0.55	0/563	1.13	4/747 (0.5%)
20	U	0.61	0/556	1.11	3/741 (0.4%)
21	V	0.36	0/529	0.91	2/704 (0.3%)
22	W	0.51	0/426	1.02	2/568 (0.4%)
23	Z	0.71	0/455	1.33	3/611 (0.5%)
24	1	0.56	0/438	1.19	5/583 (0.9%)
25	2	0.60	0/387	1.31	3/509 (0.6%)
26	3	0.65	0/468	1.36	6/614 (1.0%)
27	X	0.34	0/64429	0.55	3/100499 (0.0%)
28	Y	0.23	0/2907	0.42	0/4529
All	All	0.43	3/91554 (0.0%)	0.73	195/137514 (0.1%)

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
2	B	0	1
6	G	0	1
7	H	0	1
8	I	0	3
10	K	0	2
16	Q	0	1
17	R	0	1
19	T	0	1
20	U	0	1
23	Z	0	1
25	2	0	1
26	3	0	1
All	All	0	15

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	K	52	ILE	CA-CB	6.65	1.62	1.54
7	H	2	ILE	CA-CB	-5.75	1.46	1.54
9	J	19	THR	CA-C	5.41	1.58	1.52

The worst 5 of 195 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	K	92	GLY	N-CA-C	-12.79	95.74	110.96
25	2	38	GLY	N-CA-C	-11.94	96.42	111.70
6	G	106	TYR	N-CA-C	-11.74	90.24	109.96
1	A	245	VAL	CA-C-N	11.63	134.38	119.84
1	A	245	VAL	C-N-CA	11.63	134.38	119.84

There are no chirality outliers.

5 of 15 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	146	THR	Peptide
6	G	108	GLY	Peptide
7	H	26	ASN	Peptide
8	I	35	LYS	Peptide
8	I	40	ARG	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1987	0	2056	145	0
2	B	1539	0	1600	115	0
3	C	1481	0	1504	101	0
4	D	1400	0	1481	61	0
5	E	1286	0	1336	54	0
6	G	1114	0	1144	75	0
7	H	997	0	1046	57	0
8	I	1011	0	1047	74	0
9	J	1090	0	1125	64	0
10	K	878	0	930	47	0
11	L	779	0	820	36	0
12	M	871	0	894	61	0
13	N	978	0	1020	54	0
14	O	741	0	756	52	0
15	P	1038	0	1125	87	0
16	Q	726	0	753	35	0
17	R	825	0	881	54	0
18	S	1345	0	1372	42	0
19	T	556	0	579	30	0
20	U	552	0	604	36	0
21	V	525	0	546	21	0
22	W	424	0	470	18	0
23	Z	443	0	444	27	0
24	1	431	0	456	30	0
25	2	383	0	414	26	0
26	3	462	0	506	54	0
27	X	57533	0	28987	1345	0
28	Y	2601	0	1327	65	0
29	A	1	0	0	0	0
29	B	1	0	0	0	0
29	K	2	0	0	0	0
29	M	2	0	0	0	0
29	X	64	0	0	0	0
30	X	51	0	67	9	0
All	All	84117	0	55290	2511	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 19.

The worst 5 of 2511 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)
2:B:116:VAL:HG22	2:B:136:ARG:HG3	1.32	1.11
23:Z:19:ARG:NH2	27:X:1277:G:OP1	1.90	1.04
13:N:66:ASN:HB3	13:N:76:TYR:HB2	1.46	0.97
27:X:854:G:H1	27:X:948:C:H42	1.04	0.96
7:H:40:GLY:HA3	27:X:2545:A:H61	1.29	0.95

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	
1	A	258/275 (94%)	221 (86%)	34 (13%)	3 (1%)	10	42
2	B	203/211 (96%)	178 (88%)	24 (12%)	1 (0%)	24	58
3	C	192/205 (94%)	164 (85%)	26 (14%)	2 (1%)	12	45
4	D	175/180 (97%)	155 (89%)	19 (11%)	1 (1%)	21	55
5	E	169/185 (91%)	157 (93%)	11 (6%)	1 (1%)	21	55
6	G	140/174 (80%)	127 (91%)	13 (9%)	0	100	100
7	H	132/134 (98%)	120 (91%)	11 (8%)	1 (1%)	16	50
8	I	132/156 (85%)	102 (77%)	26 (20%)	4 (3%)	3	25
9	J	134/141 (95%)	113 (84%)	21 (16%)	0	100	100
10	K	111/116 (96%)	102 (92%)	8 (7%)	1 (1%)	14	47
11	L	102/114 (90%)	86 (84%)	16 (16%)	0	100	100
12	M	106/165 (64%)	99 (93%)	6 (6%)	1 (1%)	14	47
13	N	115/118 (98%)	103 (90%)	10 (9%)	2 (2%)	7	35

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	O	92/100 (92%)	82 (89%)	10 (11%)	0	100	100
15	P	128/137 (93%)	109 (85%)	15 (12%)	4 (3%)	3	24
16	Q	91/95 (96%)	76 (84%)	12 (13%)	3 (3%)	3	23
17	R	108/115 (94%)	91 (84%)	16 (15%)	1 (1%)	14	47
18	S	173/237 (73%)	154 (89%)	19 (11%)	0	100	100
19	T	72/91 (79%)	62 (86%)	9 (12%)	1 (1%)	9	38
20	U	70/81 (86%)	52 (74%)	14 (20%)	4 (6%)	1	13
21	V	63/67 (94%)	58 (92%)	5 (8%)	0	100	100
22	W	53/55 (96%)	48 (91%)	5 (9%)	0	100	100
23	Z	54/60 (90%)	48 (89%)	6 (11%)	0	100	100
24	1	51/55 (93%)	38 (74%)	10 (20%)	3 (6%)	1	12
25	2	44/47 (94%)	41 (93%)	3 (7%)	0	100	100
26	3	57/65 (88%)	46 (81%)	10 (18%)	1 (2%)	6	34
All	All	3025/3379 (90%)	2632 (87%)	359 (12%)	34 (1%)	11	44

5 of 34 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
15	P	120	ILE
16	Q	6	ILE
16	Q	69	ILE
1	A	24	LEU
1	A	25	THR

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	
1	A	202/216 (94%)	161 (80%)	41 (20%)	1	7
2	B	155/157 (99%)	123 (79%)	32 (21%)	1	7
3	C	154/163 (94%)	126 (82%)	28 (18%)	2	10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	D	153/156 (98%)	138 (90%)	15 (10%)	7	30
5	E	136/144 (94%)	117 (86%)	19 (14%)	3	19
6	G	118/146 (81%)	94 (80%)	24 (20%)	1	7
7	H	103/103 (100%)	83 (81%)	20 (19%)	1	8
8	I	101/121 (84%)	83 (82%)	18 (18%)	2	10
9	J	110/115 (96%)	86 (78%)	24 (22%)	1	6
10	K	90/93 (97%)	72 (80%)	18 (20%)	1	7
11	L	74/82 (90%)	56 (76%)	18 (24%)	1	4
12	M	94/133 (71%)	70 (74%)	24 (26%)	0	3
13	N	96/97 (99%)	77 (80%)	19 (20%)	1	8
14	O	75/79 (95%)	58 (77%)	17 (23%)	1	5
15	P	112/118 (95%)	84 (75%)	28 (25%)	0	4
16	Q	75/76 (99%)	62 (83%)	13 (17%)	2	12
17	R	91/96 (95%)	72 (79%)	19 (21%)	1	6
18	S	149/192 (78%)	137 (92%)	12 (8%)	11	35
19	T	55/67 (82%)	43 (78%)	12 (22%)	1	6
20	U	57/66 (86%)	43 (75%)	14 (25%)	1	4
21	V	53/55 (96%)	46 (87%)	7 (13%)	4	21
22	W	48/48 (100%)	37 (77%)	11 (23%)	1	5
23	Z	50/53 (94%)	42 (84%)	8 (16%)	2	14
24	1	46/48 (96%)	33 (72%)	13 (28%)	0	3
25	2	39/40 (98%)	27 (69%)	12 (31%)	0	2
26	3	46/51 (90%)	36 (78%)	10 (22%)	1	6
All	All	2482/2715 (91%)	2006 (81%)	476 (19%)	1	8

5 of 476 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
10	K	51	LEU
24	1	20	PHE
13	N	22	LYS
23	Z	29	ASN
26	3	46	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 82 such sidechains are listed below:

Mol	Chain	Res	Type
15	P	118	ASN
18	S	118	HIS
16	Q	44	GLN
17	R	32	GLN
20	U	54	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
27	X	2673/2880 (92%)	640 (23%)	40 (1%)
28	Y	121/124 (97%)	29 (23%)	1 (0%)
All	All	2794/3004 (93%)	669 (23%)	41 (1%)

5 of 669 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
27	X	3	U
27	X	4	C
27	X	13	A
27	X	14	A
27	X	17	G

5 of 41 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
27	X	2204	A
27	X	2705	A
27	X	2299	A
27	X	2404	A
27	X	2756	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 oligosaccharides in this entry.

5.6 Ligand geometry

Of 71 ligands modelled in this entry, 70 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
30	ERY	X	2902	-	53,53,53	0.88	1 (1%)	82,82,82	1.31	8 (9%)

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
30	ERY	X	2902	-	-	4/72/107/107	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	X	2902	ERY	O2-C13	2.17	1.50	1.46

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	X	2902	ERY	O8-C23-C22	-2.56	103.96	110.08
30	X	2902	ERY	C2-C3-C4	-2.42	105.94	112.91
30	X	2902	ERY	C30-C2-C1	-2.31	103.83	108.97
30	X	2902	ERY	C16-C15-C14	-2.21	111.25	114.99
30	X	2902	ERY	C13-O2-C1	-2.20	114.36	118.20

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
30	X	2902	ERY	C15-C14-O3-C3
30	X	2902	ERY	O4-C14-O3-C3

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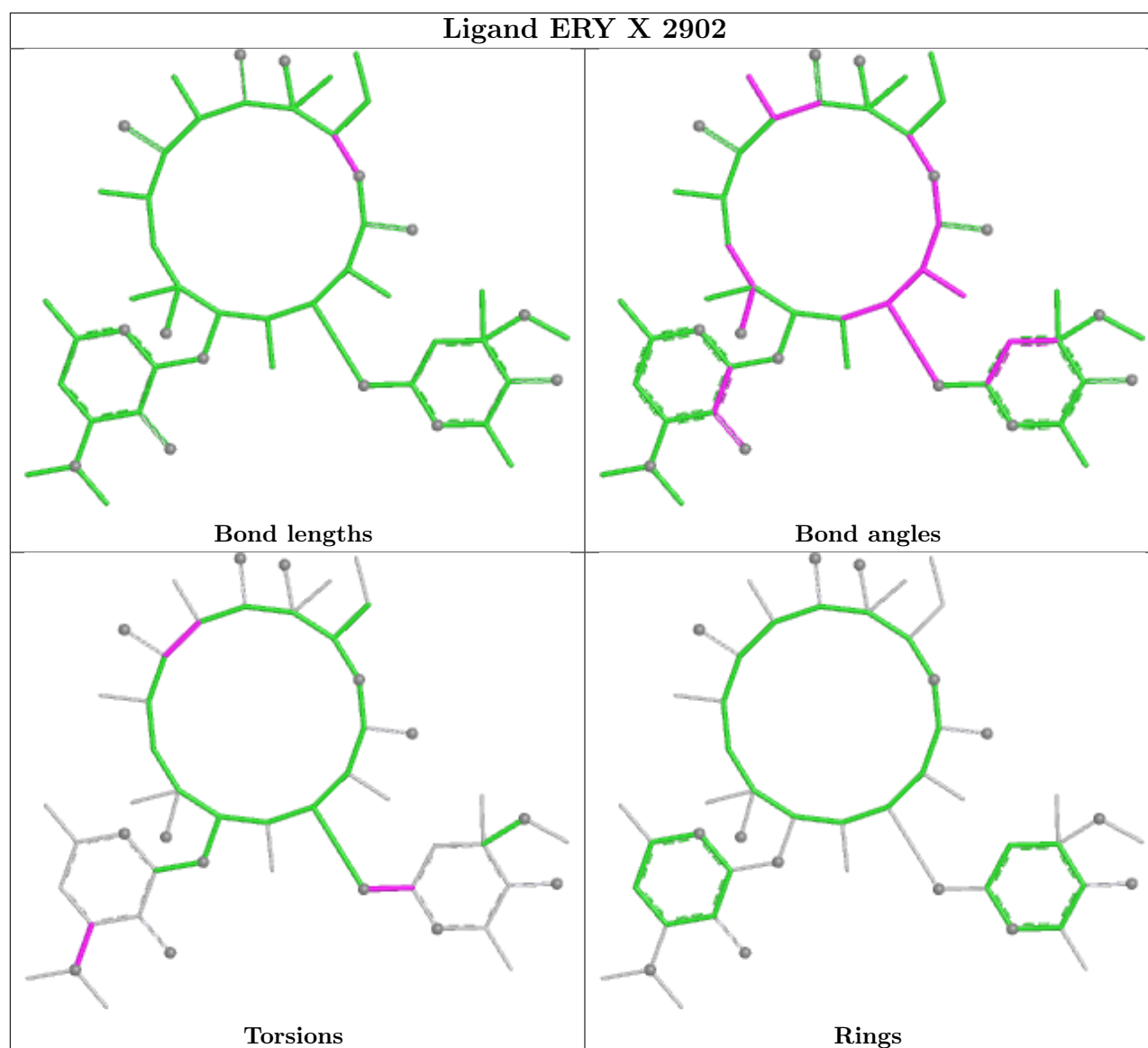
Mol	Chain	Res	Type	Atoms
30	X	2902	ERY	C25-C24-N1-C28
30	X	2902	ERY	C34-C10-C9-O11

There are no ring outliers.

1 monomer is involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	X	2902	ERY	9	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	A	260/275 (94%)	0.68	31 (11%) 9 6	48, 104, 163, 221	0
2	B	205/211 (97%)	0.10	8 (3%) 43 22	27, 50, 107, 233	0
3	C	194/205 (94%)	0.34	16 (8%) 17 11	39, 102, 180, 292	0
4	D	177/180 (98%)	0.56	16 (9%) 15 9	114, 175, 232, 282	0
5	E	171/185 (92%)	0.20	8 (4%) 36 18	57, 131, 192, 243	0
6	G	142/174 (81%)	0.60	16 (11%) 10 6	38, 77, 160, 339	0
7	H	134/134 (100%)	0.01	2 (1%) 72 43	33, 45, 87, 135	0
8	I	134/156 (85%)	0.90	21 (15%) 5 4	55, 126, 192, 315	0
9	J	136/141 (96%)	0.59	13 (9%) 13 8	56, 94, 163, 214	0
10	K	113/116 (97%)	-0.07	3 (2%) 56 30	27, 32, 67, 100	0
11	L	104/114 (91%)	0.84	10 (9%) 13 8	130, 161, 200, 243	0
12	M	108/165 (65%)	0.14	3 (2%) 55 30	30, 43, 95, 242	0
13	N	117/118 (99%)	0.28	4 (3%) 48 26	41, 76, 133, 232	0
14	O	94/100 (94%)	0.38	6 (6%) 25 15	52, 94, 178, 204	0
15	P	130/137 (94%)	0.04	3 (2%) 61 34	33, 51, 147, 188	0
16	Q	93/95 (97%)	0.11	3 (3%) 50 27	49, 94, 162, 192	0
17	R	110/115 (95%)	0.66	8 (7%) 21 13	65, 100, 189, 259	0
18	S	175/237 (73%)	0.36	11 (6%) 26 15	93, 144, 224, 285	0
19	T	74/91 (81%)	0.63	7 (9%) 14 8	72, 112, 158, 228	0
20	U	72/81 (88%)	0.91	10 (13%) 6 5	75, 119, 185, 238	0
21	V	65/67 (97%)	-0.06	0 100 100	76, 115, 164, 208	0
22	W	55/55 (100%)	-0.02	3 (5%) 30 16	72, 91, 128, 190	0
23	Z	56/60 (93%)	0.23	2 (3%) 46 24	32, 40, 80, 152	0
24	1	53/55 (96%)	1.22	12 (22%) 2 2	102, 129, 217, 266	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	2	46/47 (97%)	0.57	5 (10%) 10 7	38, 67, 122, 169	0
26	3	59/65 (90%)	1.16	13 (22%) 2 2	80, 100, 172, 278	0
27	X	2680/2880 (93%)	0.27	111 (4%) 41 21	26, 76, 186, 299	0
28	Y	122/124 (98%)	0.70	10 (8%) 17 11	74, 153, 190, 332	0
All	All	5879/6383 (92%)	0.36	355 (6%) 27 15	26, 89, 188, 339	0

The worst 5 of 355 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
8	I	54	SER	14.5
19	T	16	SER	11.8
6	G	129	HIS	10.2
9	J	21	ASP	9.1
1	A	236	GLY	8.3

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
29	MG	X	2916	1/1	0.46	0.76	41,41,41,41	0
29	MG	X	2915	1/1	0.54	0.51	63,63,63,63	0
29	MG	X	2943	1/1	0.56	0.45	42,42,42,42	0
29	MG	X	2935	1/1	0.59	0.47	34,34,34,34	0
29	MG	X	2919	1/1	0.62	0.24	62,62,62,62	0
29	MG	A	301	1/1	0.65	0.34	54,54,54,54	0
29	MG	X	2914	1/1	0.66	0.46	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
29	MG	X	2918	1/1	0.72	0.82	43,43,43,43	0
29	MG	K	202	1/1	0.73	0.37	27,27,27,27	0
29	MG	X	2910	1/1	0.74	0.35	56,56,56,56	0
29	MG	X	2904	1/1	0.75	0.52	32,32,32,32	0
29	MG	X	2926	1/1	0.75	0.84	44,44,44,44	0
29	MG	X	2965	1/1	0.79	0.83	43,43,43,43	0
29	MG	X	2956	1/1	0.80	0.25	27,27,27,27	0
29	MG	X	2942	1/1	0.80	0.33	46,46,46,46	0
29	MG	X	2950	1/1	0.81	0.51	32,32,32,32	0
29	MG	X	2952	1/1	0.81	0.29	29,29,29,29	0
29	MG	X	2908	1/1	0.81	0.36	32,32,32,32	0
29	MG	X	2925	1/1	0.81	0.54	31,31,31,31	0
29	MG	X	2958	1/1	0.82	0.24	44,44,44,44	0
29	MG	X	2941	1/1	0.83	0.25	38,38,38,38	0
29	MG	X	2960	1/1	0.83	0.37	61,61,61,61	0
29	MG	X	2920	1/1	0.83	0.29	52,52,52,52	0
29	MG	X	2944	1/1	0.84	0.29	35,35,35,35	0
29	MG	M	201	1/1	0.85	0.16	35,35,35,35	0
29	MG	X	2955	1/1	0.85	0.39	30,30,30,30	0
29	MG	X	2905	1/1	0.85	0.24	31,31,31,31	0
29	MG	X	2930	1/1	0.85	0.61	29,29,29,29	0
29	MG	X	2923	1/1	0.85	0.27	40,40,40,40	0
29	MG	X	2936	1/1	0.85	0.40	45,45,45,45	0
29	MG	X	2901	1/1	0.86	0.43	69,69,69,69	0
29	MG	X	2921	1/1	0.86	0.27	28,28,28,28	0
29	MG	X	2957	1/1	0.86	0.58	52,52,52,52	0
29	MG	X	2946	1/1	0.86	0.73	46,46,46,46	0
29	MG	X	2927	1/1	0.86	0.35	29,29,29,29	0
29	MG	B	301	1/1	0.86	0.23	34,34,34,34	0
29	MG	X	2962	1/1	0.87	0.08	69,69,69,69	0
29	MG	X	2949	1/1	0.88	0.41	42,42,42,42	0
29	MG	X	2903	1/1	0.88	0.72	30,30,30,30	0
29	MG	X	2911	1/1	0.88	0.56	56,56,56,56	0
29	MG	X	2938	1/1	0.88	0.40	31,31,31,31	0
29	MG	X	2913	1/1	0.88	0.65	43,43,43,43	0
29	MG	X	2954	1/1	0.89	0.43	45,45,45,45	0
29	MG	X	2940	1/1	0.89	0.25	36,36,36,36	0
29	MG	K	201	1/1	0.89	0.27	27,27,27,27	0
29	MG	X	2963	1/1	0.89	0.20	56,56,56,56	0
29	MG	X	2917	1/1	0.89	0.53	40,40,40,40	0
29	MG	X	2931	1/1	0.90	1.06	46,46,46,46	0
29	MG	M	202	1/1	0.91	0.15	35,35,35,35	0

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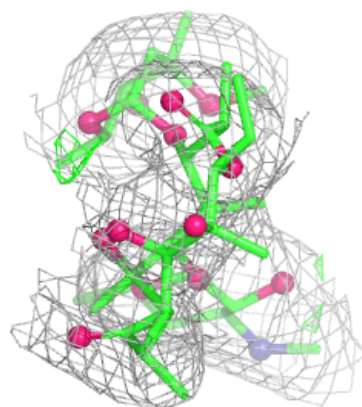
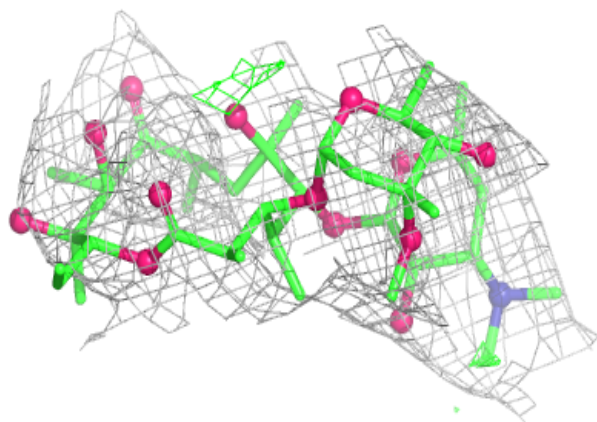
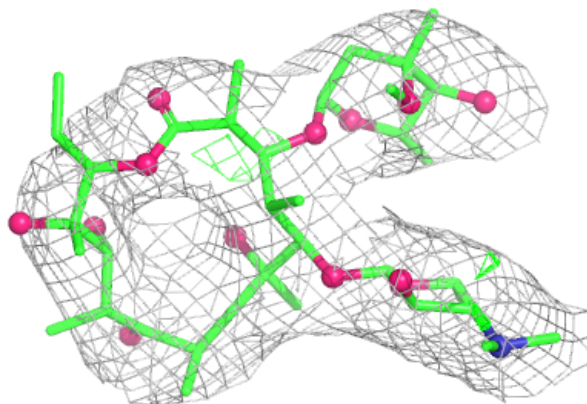
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
29	MG	X	2959	1/1	0.91	0.41	41,41,41,41	0
29	MG	X	2906	1/1	0.91	0.67	28,28,28,28	0
29	MG	X	2947	1/1	0.92	0.19	34,34,34,34	0
29	MG	X	2922	1/1	0.92	0.18	29,29,29,29	0
29	MG	X	2928	1/1	0.92	0.25	55,55,55,55	0
29	MG	X	2951	1/1	0.92	0.72	32,32,32,32	0
29	MG	X	2932	1/1	0.92	0.26	37,37,37,37	0
29	MG	X	2939	1/1	0.93	0.29	50,50,50,50	0
29	MG	X	2909	1/1	0.93	0.41	28,28,28,28	0
29	MG	X	2945	1/1	0.94	0.28	38,38,38,38	0
29	MG	X	2953	1/1	0.94	0.48	56,56,56,56	0
29	MG	X	2937	1/1	0.94	0.61	44,44,44,44	0
29	MG	X	2961	1/1	0.95	0.85	56,56,56,56	0
29	MG	X	2933	1/1	0.95	0.93	36,36,36,36	0
29	MG	X	2934	1/1	0.95	0.50	29,29,29,29	0
29	MG	X	2964	1/1	0.95	0.27	28,28,28,28	0
29	MG	X	2907	1/1	0.95	0.39	28,28,28,28	0
30	ERY	X	2902	51/51	0.95	0.10	31,34,36,36	0
29	MG	X	2912	1/1	0.96	0.18	27,27,27,27	0
29	MG	X	2924	1/1	0.96	0.46	38,38,38,38	0
29	MG	X	2948	1/1	0.96	0.18	34,34,34,34	0
29	MG	X	2929	1/1	0.97	0.10	30,30,30,30	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.

Electron density around ERY X 2902:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.