



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 05:42 PM GMT

PDB ID : 4IOC  
Title : Crystal structure of compound 4f bound to large ribosomal subunit (50S) from *Deinococcus radiodurans*  
Authors : Han, S.; Marr, E.S.  
Deposited on : 2013-01-07  
Resolution : 3.60 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

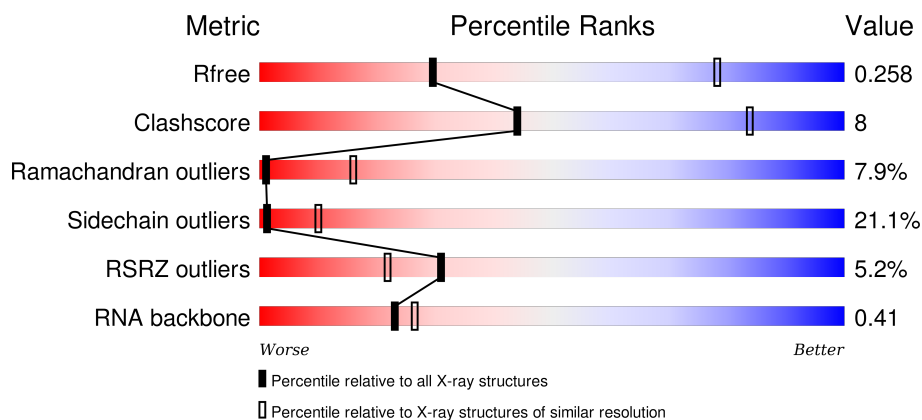
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

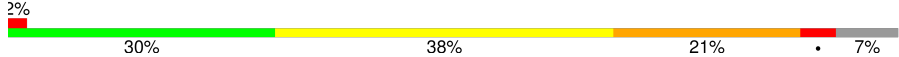
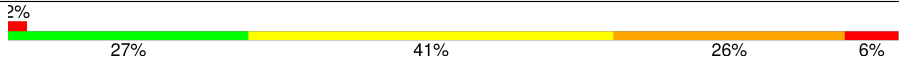
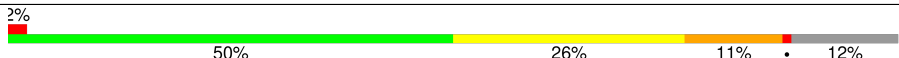
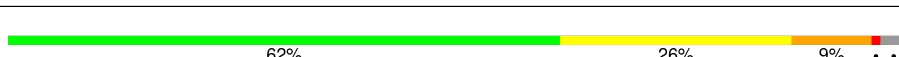
The reported resolution of this entry is 3.60 Å.

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))
$R_{free}$	91344	1408 (3.80-3.40)
Clashscore	102246	1010 (3.74-3.46)
Ramachandran outliers	100387	1007 (3.76-3.44)
Sidechain outliers	100360	1007 (3.76-3.44)
RSRZ outliers	91569	1003 (3.78-3.42)
RNA backbone	2183	1058 (4.40-2.80)

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. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	X	2880	
2	Y	123	
3	A	274	
4	B	211	

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Mol	Chain	Length	Quality of chain
5	C	205	
6	D	180	
7	E	185	
8	F	144	
9	G	174	
10	H	134	
11	I	156	
12	J	141	
13	K	116	
14	L	114	
15	M	166	
16	N	118	
17	O	100	
18	P	134	
19	Q	95	
20	R	115	
21	S	237	
22	T	91	
23	U	81	
24	V	67	
25	W	55	
26	Z	60	
27	1	55	
28	2	47	
29	3	66	

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Mol	Chain	Length	Quality of chain
30	4	37	<div> <div>68%</div> <div>70%</div> <div>27%</div> </div>

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
31	MG	X	2901	-	-	-	X
31	MG	X	2907	-	-	-	X
31	MG	X	2914	-	-	-	X
31	MG	X	2915	-	-	-	X
31	MG	X	2917	-	-	-	X
31	MG	X	2922	-	-	-	X
31	MG	X	2924	-	-	-	X
31	MG	X	2926	-	-	-	X
31	MG	Y	202	-	-	-	X

## 2 Entry composition

There are 32 unique types of molecules in this entry. The entry contains 83877 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	X	2686	Total	C	N	O	P	0	0	0
			57651	25718	10642	18606	2685			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	Y	122	Total	C	N	O	P	0	0	0
			2598	1161	476	840	121			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	240	Total	C	N	O	S	0	0	0
			1826	1137	366	321	2			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	C	197	Total	C	N	O	S	0	0	0
			1506	935	287	282	2			

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

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

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

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

- Molecule 8 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	F	71	Total	C	N	O	S	0	0	0
			503	310	91	99	3			

- Molecule 9 is a protein called 50S ribosomal protein L13.

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

- Molecule 10 is a protein called 50S ribosomal protein L14.

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

- Molecule 11 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	I	141	Total	C	N	O	0	0	0
			1067	655	216	196			

- Molecule 12 is a protein called 50S ribosomal protein L16.

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

- Molecule 13 is a protein called 50S ribosomal protein L17.

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

- Molecule 14 is a protein called 50S ribosomal protein L18.

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

- Molecule 15 is a protein called 50S ribosomal protein L19.

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

- Molecule 16 is a protein called 50S ribosomal protein L20.

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

- Molecule 17 is a protein called 50S ribosomal protein L21.

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

- Molecule 18 is a protein called 50S ribosomal protein L22.

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

- Molecule 19 is a protein called 50S ribosomal protein L23.

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

- Molecule 20 is a protein called 50S ribosomal protein L24.

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

- Molecule 21 is a protein called 50S ribosomal protein L25.

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

- Molecule 22 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	T	84	Total	C	N	O	S	0	0	0
			625	393	122	109	1			

- Molecule 23 is a protein called 50S ribosomal protein L28.

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

- Molecule 24 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	V	66	Total	C	N	O	S	0	0	0
			533	327	107	96	3			

- Molecule 25 is a protein called 50S ribosomal protein L30.

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

- Molecule 26 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	Z	58	Total	C	N	O	S	0	0	0
			457	281	94	77	5			

- Molecule 27 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
27	1	53	Total C	0	0	53
			53 53			

- Molecule 28 is a protein called 50S ribosomal protein L34.



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
28	2	46	Total C 46 46	0	0	46

- Molecule 29 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
29	3	63	Total C 63 63	0	0	63

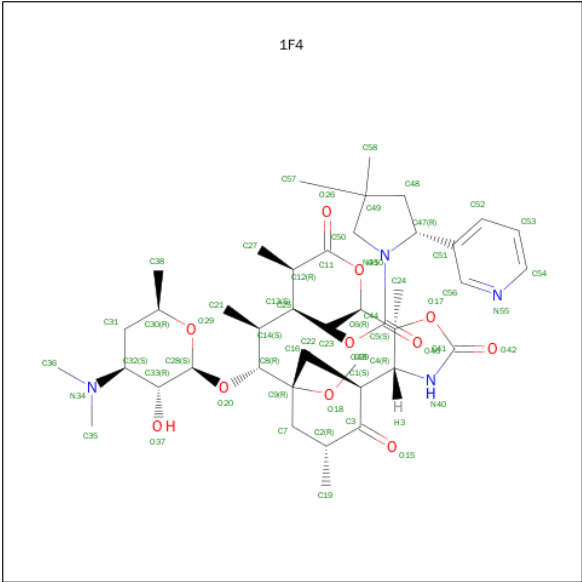
- Molecule 30 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
30	4	37	Total C N O S 297 179 66 47 5	0	0	0

- Molecule 31 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
31	X	28	Total Mg 28 28	0	0
31	Y	6	Total Mg 6 6	0	0
31	M	1	Total Mg 1 1	0	0

- Molecule 32 is (3AS,4R,7R,8S,9S,10R,11R,13R,15S,15AR)-4-ETHYL-11-METHOXY-3A,7,9,11,13,15-HEXAMETHYL-2,6,14-TRIOXO-10-{[3,4,6-TRIDEOXY-3-(DIMETHYLAMINO)-BETA-D-XYLO-HEXOPYRANOSYL]OXY}TETRADECAHYDRO-2H-OXACYCLO TETRADECINO[4,3-D][1,3]OXAZOL-8-YL (2R)-4,4-DIMETHYL-2-(PYRIDIN-3-YL)PYRROLIDINE-1-CARBOXYLATE (three-letter code: 1F4) (formula: C<sub>43</sub>H<sub>68</sub>N<sub>4</sub>O<sub>11</sub>).

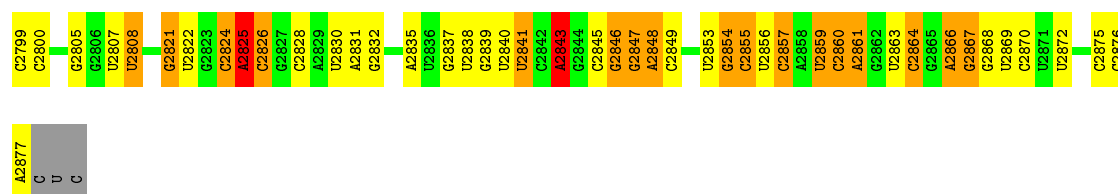


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
32	X	1	Total	C	N	O	0	0
			58	43	4	11		

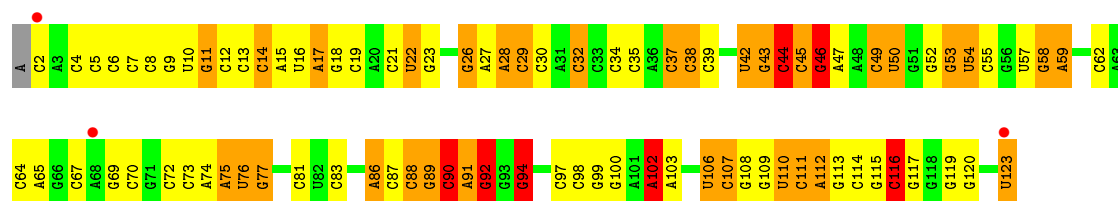


U1710	A1561	G1488	C1343	A1275	G1200	A1126	G1064	A994	U919	G854	U789	C723
C1711	G1562	C1489	C1344	U1276	G1201	C1127	G1067	A995	A922	G858	A790	C724
G1712	U1563	G1490	G1345	G1277	U1202	A1128	A1068	C996	A923	U859	G793	C725
A1643	G1346	G1491	C1346	A1278	A1203	A1129	G1069	C997	G926	U860	A794	A7726
U1647	A1567	G1495	G1347	G1279	A1208	G1130	G1070	C998	U925	C863	A795	U727
C1648	C1570	G1496	A1349	A1281	G1209	C1132	U1071	A999	C926	C864	A796	G728
U1651	G1571	C1497	A1350	A1282	C1211	G1133	U1072	G1000	C927	A865	A797	G729
C1723	C1572	G1498	A1353	C1283	U1217	C1134	G1074	A1001	G931	U866	G798	C730
G1724	A1573	G1499	A1354	G1284	G1210	C1135	U1075	C1002	G932	G867	G799	A731
C1725	C1574	U1500	A1355	A1285	C1212	G1136	G1076	C1003	U800	U868	U732	C733
U1729	G1575	U1505	G1356	U1286	U1218	A1137	U1077	C1006	G933	C869	A801	G738
G1730	C1576	C1506	U1357	A1287	C1219	A1138	U1078	A1007	G934	C870	A802	G739
C1731	U1507	A1508	C1358	A1288	G1220	A1139	G1079	G1008	C935	U871	C803	A740
U1732	C1509	G1493	G1359	A1289	C1221	A1140	U1080	C1009	G937	U872	C804	G741
C1733	A1510	G1494	C1360	U1291	G1223	U1141	A1081	U1010	C938	U873	A806	G742
G1734	A1511	G1495	C1361	G1294	A1224	C1142	G1082	A1020	C939	A874	A807	A743
C1735	U1513	G1496	A1366	G1295	G1225	U1144	C1083	G1014	G940	G875	C808	C744
G1736	C1514	A1437	A1367	C1229	C1229	C1145	A1084	U1015	U941	A876	C809	C745
U1737	U1515	G1438	G1368	C1230	C1230	G1146	G1085	C1016	U942	G877	U810	G746
G1738	A1516	G1439	G1371	U1303	A1231	G1147	C1086	C1017	U943	C878	C812	C749
A1667	C1517	G1441	A1372	G1305	U1232	G1149	A1088	U1019	U944	A879	G813	C750
G1668	C1518	A1441	G1373	U1306	A1233	C1150	A1089	A1021	U946	U881	G814	C751
A1669	G1519	G1443	G1374	U1307	C1234	U1151	C1090	A1022	C947	C882	A815	G752
G1670	U1520	C1437	C1375	C1308	C1235	C1152	C1091	A1023	G951	A883	U816	U753
U1671	G1521	U1446	C1378	G1309	G1236	A1153	U1093	U1023	U952	C884	A817	C754
C1744	C1522	U1447	A1379	C1310	A1237	C1154	U1094	G1024	G953	A885	C818	C755
G1745	C1523	U1448	C1380	G1312	G1238	U1159	C1095	U1028	U954	A886	C819	C756
A1746	C1524	U1449	G1381	U1313	U1241	C1160	A1096	G1029	G955	C889	G822	U757
C1749	U1525	U1454	G1382	A1314	U1244	U1161	A1097	U1030	G956	U890	U823	C758
A1750	A1526	C1455	G1383	C1315	U1245	A1162	G1098	C1031	G957	G	U824	U760
U1678	G1527	C1456	C1384	G1316	G1246	C1163	A1099	A1032	G958	G	C825	G761
G1679	C1528	A1457	G1385	G1317	G1247	A1167	G1100	G1033	C959	G	U826	A762
U1680	G1529	A1458	C1386	A1318	U1247	G1168	U1101	U1034	U960	G	C827	A763
A1681	U1530	U1459	A1387	C1319	G1248	C1169	G1102	G1035	G961	G	C828	A764
G1682	C1531	G1460	G1387	A1320	G1249	C1169	C1103	G1036	G967	G	C829	C765
U1683	A1532	C1461	C1388	A1321	A1250	U1172	G1104	U1037	C968	C	C830	U768
G1684	G1533	U1465	C1389	U1324	C1251	G1173	A1105	U1038	U969	U	C831	C769
A1685	A1534	C1466	A1390	U1325	G1252	U1173	A1106	A1039	U970	A	A833	U770
C1686	U1539	U1467	U1391	U1326	G1253	C1181	U1108	A1040	C971	C	A834	C771
U1687	C1540	A1468	G1393	U1327	G1254	U1182	A1109	U1044	C972	A	U837	A774
U1689	A1541	U1469	G1394	C1327	A1255	C1183	C1111	G1045	U973	G	A838	U775
G1690	G1542	C1470	A1395	C1328	U1257	G1184	C1112	C1049	U974	C	U839	G776
U1770	U1543	G1471	C1396	U1329	U1257	C1185	U1113	C975	C976	U	U840	A777
A1771	G1544	C1472	A1397	G1330	C1261	G1186	C1114	U1051	C977	U	C841	G778
C1772	U1545	U1473	G1398	G1331	U1262	A1187	C1115	G1052	U978	A	A842	U779
G1773	U1546	A1474	C1399	G1332	G1263	A1188	U1116	C1053	U979	C	G843	U780
A1694	U1548	U1475	U1403	G1333	C1264	G1189	C1117	A1054	G980	C	U844	G781
U1695	C1549	C1476	C1404	A1334	G1265	C1190	G1118	C1055	U981	C	U845	U782
A1699	G1550	U1477	A1405	G1336	G1266	G1191	C1119	U1056	G982	C	A846	G783
C1775	U1551	C1478	A1406	G1337	A1267	A1192	G1121	A1057	G983	C	U847	U784
A1776	C1552	G1479	G1407	G1338	U1268	G1193	U1121	G1058	A984	C	C850	U785
G1777	G1553	U1480	A1408	U1339	G1269	U1194	A1122	A1059	G985	C	C851	U786
C1778	U1554	U1481	U1409	C1340	C1270	C1198	G1123	C1060	U990	C	U852	A787
U1705	G1559	U1482	U1410	G1341	C1271	U1199	G1125				C853	G788
A1706		C1487	U1411	U1342								
C1707												
U1709												

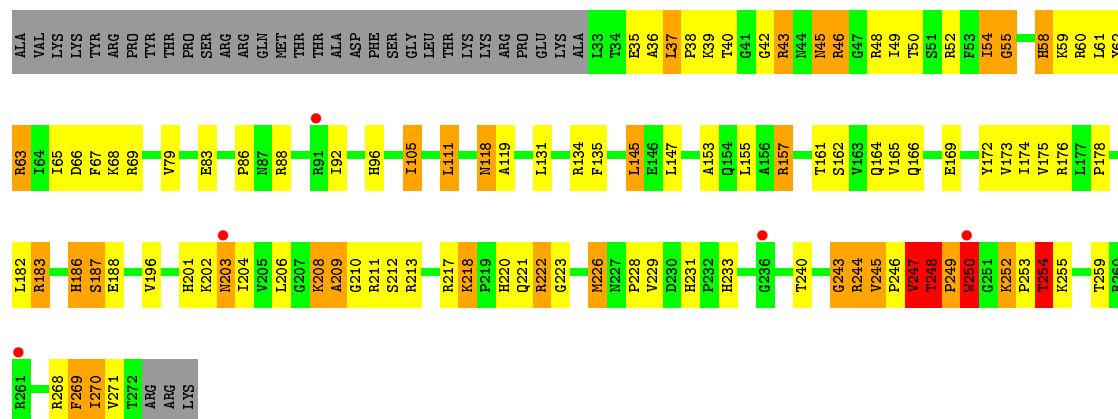




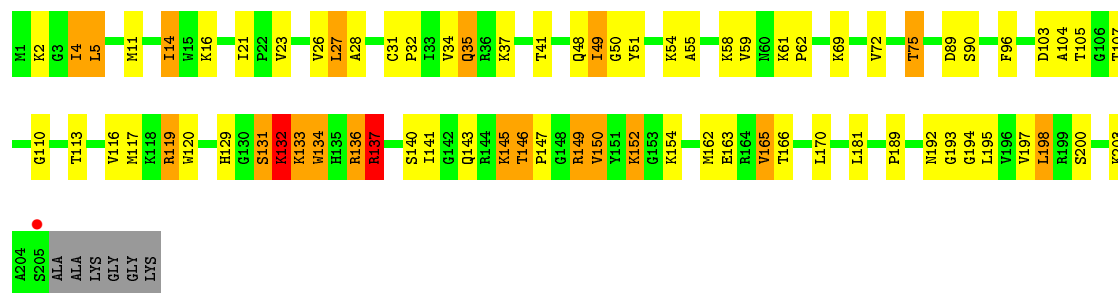
- Molecule 2: 5S ribosomal RNA



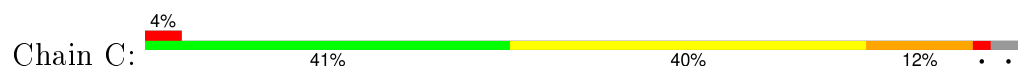
- Molecule 3: 50S ribosomal protein L2

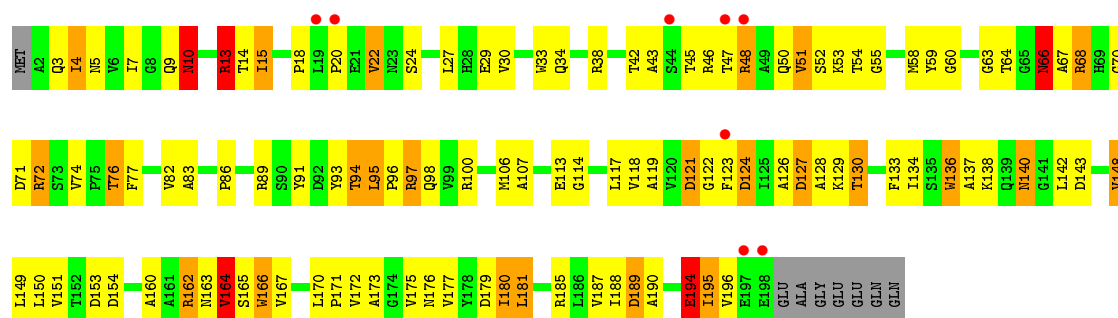


- Molecule 4: 50S ribosomal protein L3

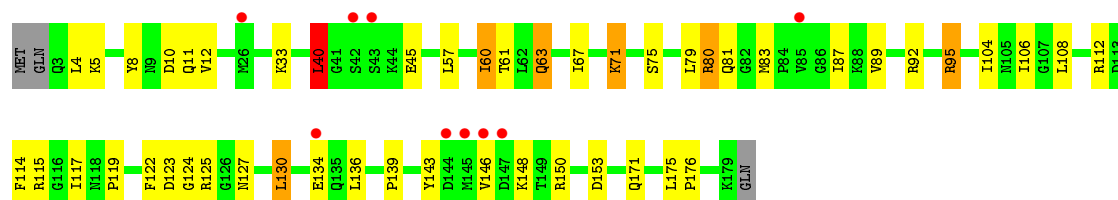


- Molecule 5: 50S ribosomal protein L4

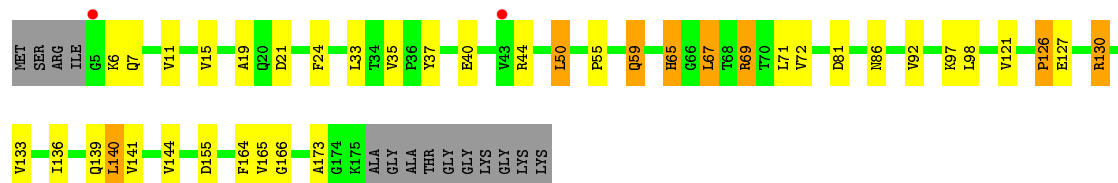




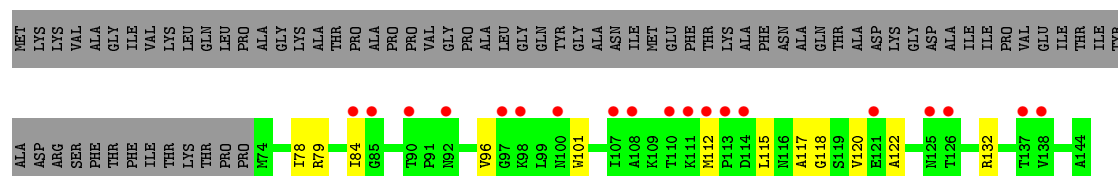
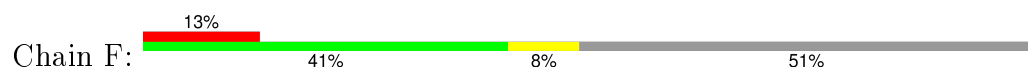
- Molecule 6: 50S ribosomal protein L5



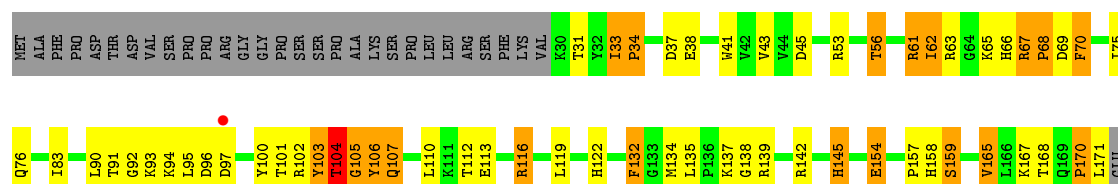
- Molecule 7: 50S ribosomal protein L6



- Molecule 8: 50S ribosomal protein L11

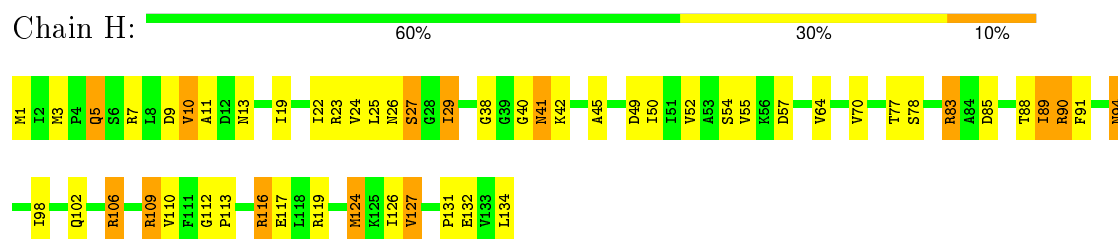


- Molecule 9: 50S ribosomal protein L13

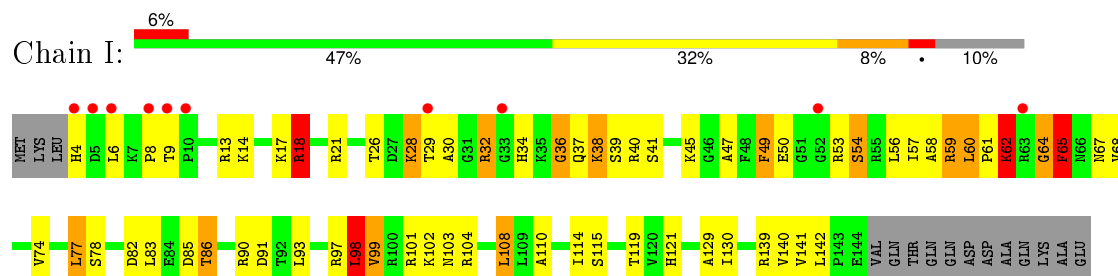


VAL  
LYS

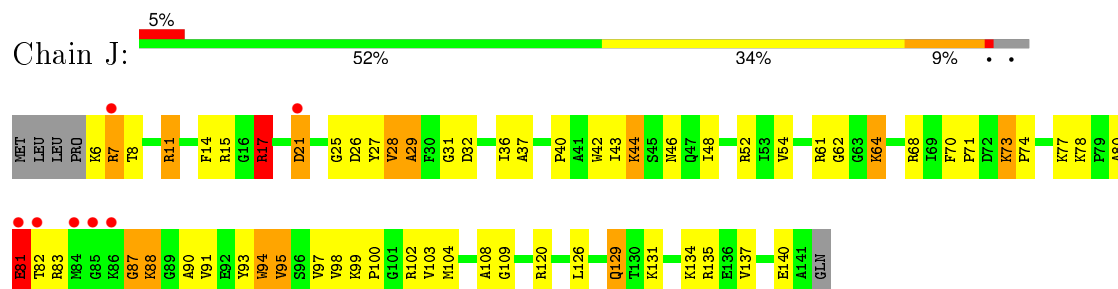
- Molecule 10: 50S ribosomal protein L14



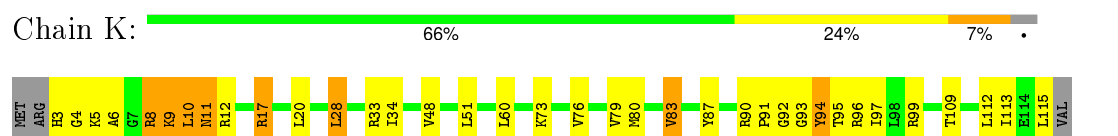
- Molecule 11: 50S ribosomal protein L15



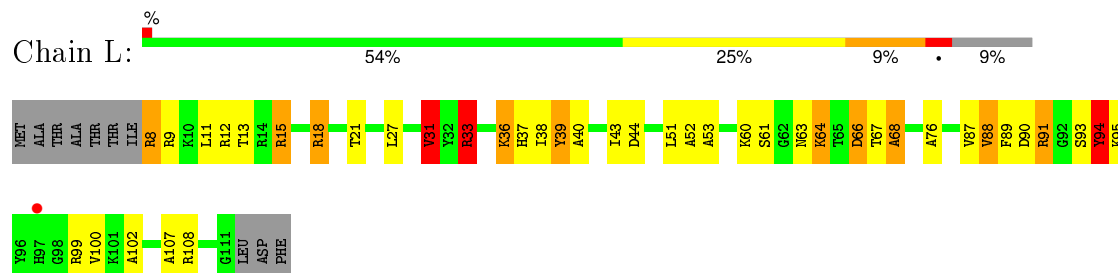
- Molecule 12: 50S ribosomal protein L16



- Molecule 13: 50S ribosomal protein L17

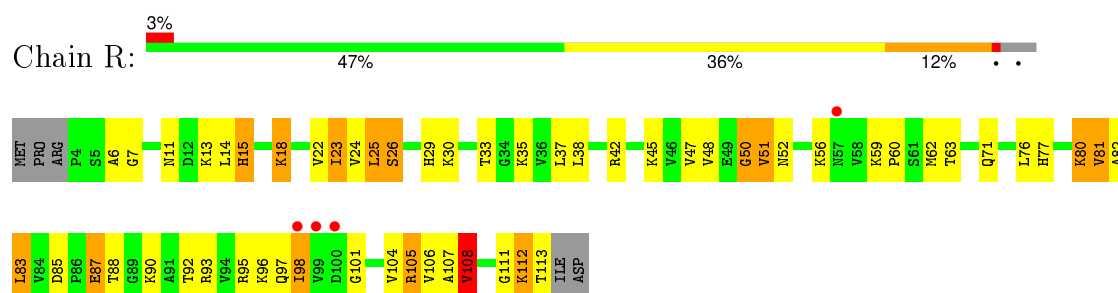


- Molecule 14: 50S ribosomal protein L18

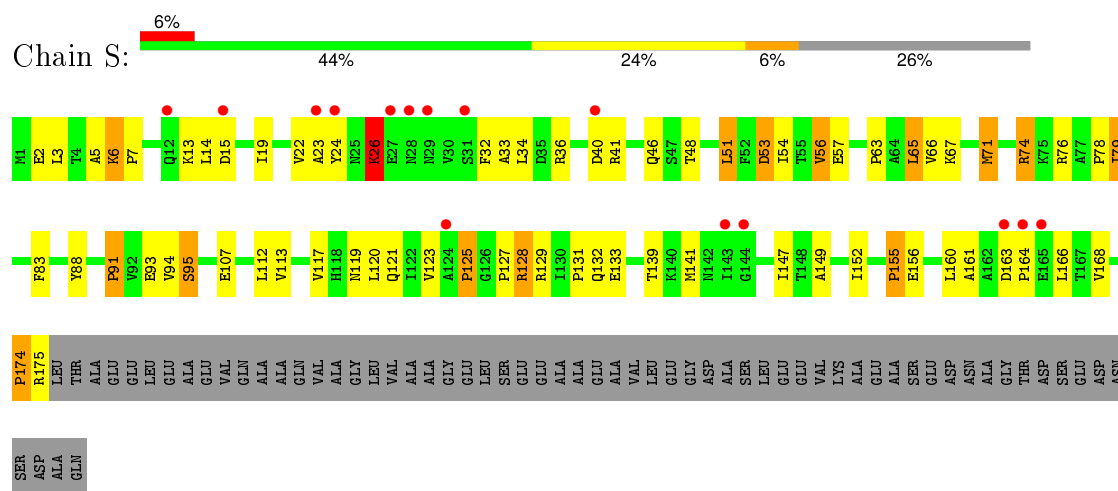




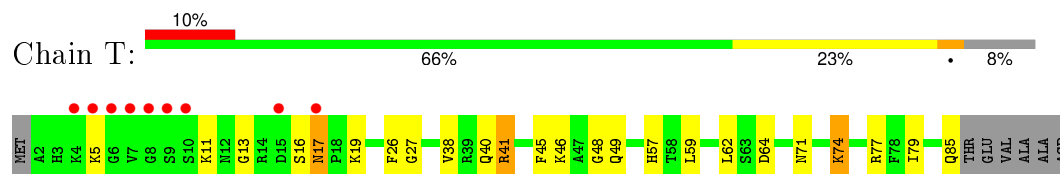




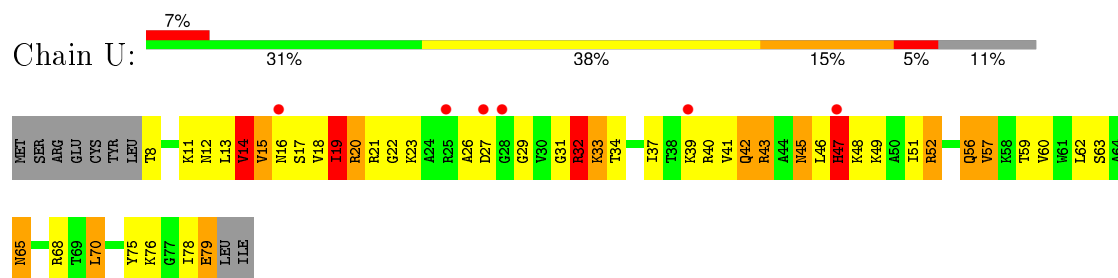
- Molecule 21: 50S ribosomal protein L25



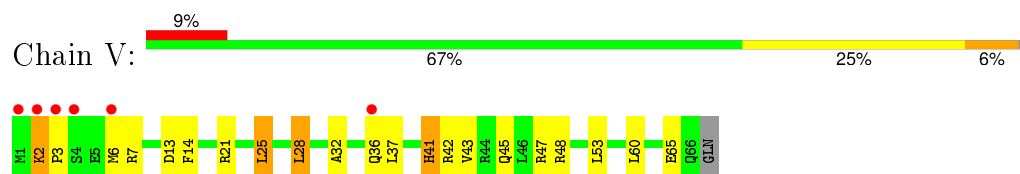
- Molecule 22: 50S ribosomal protein L27



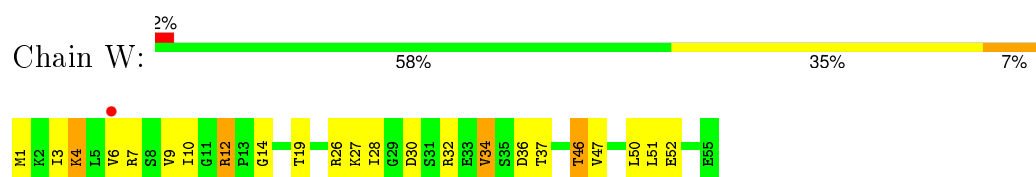
- Molecule 23: 50S ribosomal protein L28



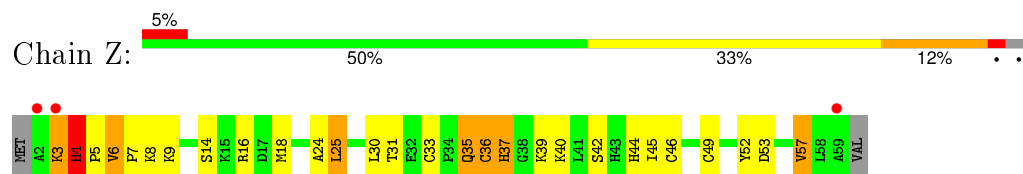
- Molecule 24: 50S ribosomal protein L29



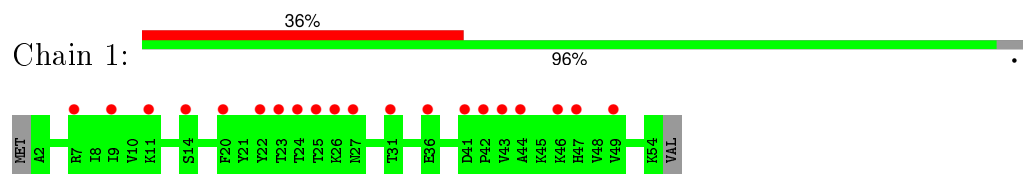
- Molecule 25: 50S ribosomal protein L30



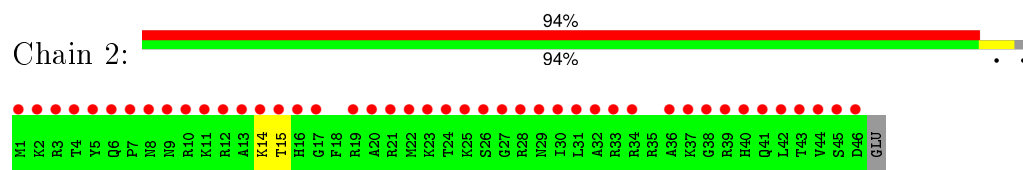
- Molecule 26: 50S ribosomal protein L32



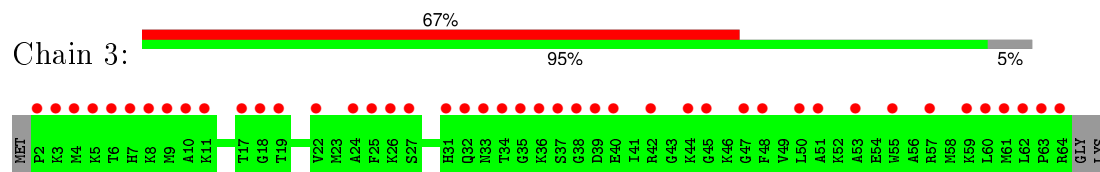
- Molecule 27: 50S ribosomal protein L33



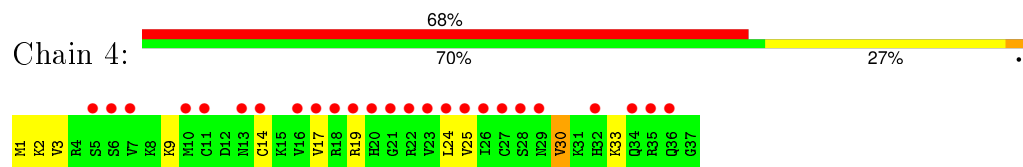
- Molecule 28: 50S ribosomal protein L34



- Molecule 29: 50S ribosomal protein L35



- Molecule 30: 50S ribosomal protein L36



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	169.64Å 408.49Å 692.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.60 30.11 – 3.61	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-3.60) 88.4 (30.11-3.61)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.33 (at 3.65Å)	Xtriage
Refinement program	autobuster	Depositor
R, $R_{free}$	0.198 , 0.239 0.215 , 0.258	Depositor DCC
$R_{free}$ test set	12232 reflections (5.30%)	DCC
Wilson B-factor (Å <sup>2</sup> )	129.2	Xtriage
Anisotropy	0.611	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.22 , 93.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 242941 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	83877	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	107.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.08% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 1F4, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	X	1.02	36/64561 (0.1%)	1.86	1991/100708 (2.0%)
2	Y	1.22	2/2904 (0.1%)	1.83	99/4525 (2.2%)
3	A	0.58	0/1862	0.93	4/2510 (0.2%)
4	B	0.55	0/1567	0.88	1/2105 (0.0%)
5	C	0.62	0/1529	0.96	0/2070
6	D	0.46	0/1419	0.68	0/1903
7	E	0.47	0/1308	0.71	0/1771
8	F	0.50	0/508	0.67	0/683
9	G	0.58	0/1138	0.92	2/1539 (0.1%)
10	H	0.53	0/1007	0.84	0/1352
11	I	0.67	0/1081	1.06	2/1448 (0.1%)
12	J	0.86	0/1113	0.96	1/1486 (0.1%)
13	K	0.66	0/886	0.92	0/1188
14	L	0.52	0/785	0.93	0/1048
15	M	0.59	0/884	1.00	2/1186 (0.2%)
16	N	0.53	0/994	0.79	0/1323
17	O	0.52	0/750	0.96	1/1000 (0.1%)
18	P	0.57	0/1027	0.88	0/1373
19	Q	0.56	0/737	0.99	2/988 (0.2%)
20	R	0.59	0/835	1.02	0/1121
21	S	0.61	0/1370	0.76	0/1862
22	T	0.54	0/633	0.88	0/838
23	U	0.71	0/556	1.08	2/741 (0.3%)
24	V	0.52	0/537	0.73	0/714
25	W	0.51	0/426	0.81	0/568
26	Z	0.62	0/469	0.98	0/629
30	4	0.49	0/298	0.73	0/390
All	All	0.94	38/91184 (0.0%)	1.68	2107/137069 (1.5%)

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	X	0	3

The worst 5 of 38 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	559	C	C3'-O3'	8.19	1.53	1.42
1	X	655	A	C3'-O3'	7.84	1.53	1.42
1	X	774	A	C5-C4	7.25	1.43	1.38
1	X	699	G	N9-C4	-6.97	1.32	1.38
1	X	1688	U	C2-N3	6.58	1.42	1.37

The worst 5 of 2107 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1288	A	C1'-O4'-C4'	-30.77	85.29	109.90
1	X	1019	U	P-O3'-C3'	19.01	142.51	119.70
1	X	1288	A	C5'-C4'-O4'	18.79	131.64	109.10
1	X	774	A	N1-C6-N6	17.73	129.24	118.60
1	X	559	C	O4'-C1'-N1	17.43	122.14	108.20

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	X	1251	G	Sidechain
1	X	699	G	Sidechain
1	X	967	G	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	X	57651	0	29049	535	0
2	Y	2598	0	1328	22	0
3	A	1826	0	1885	83	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	1539	0	1600	57	0
5	C	1506	0	1525	57	0
6	D	1400	0	1481	17	0
7	E	1286	0	1336	10	0
8	F	503	0	520	5	0
9	G	1114	0	1144	46	0
10	H	997	0	1046	30	0
11	I	1067	0	1103	39	0
12	J	1090	0	1125	31	0
13	K	878	0	930	24	0
14	L	779	0	820	19	0
15	M	871	0	894	25	0
16	N	978	0	1020	33	0
17	O	741	0	756	24	0
18	P	1014	0	1096	23	0
19	Q	726	0	753	11	0
20	R	825	0	881	26	0
21	S	1345	0	1372	30	0
22	T	625	0	655	11	0
23	U	552	0	604	31	0
24	V	533	0	558	7	0
25	W	424	0	470	15	0
26	Z	457	0	462	20	0
27	1	53	0	0	0	0
28	2	46	0	0	1	0
29	3	63	0	0	0	0
30	4	297	0	330	4	0
31	M	1	0	0	0	0
31	X	28	0	0	0	0
31	Y	6	0	0	0	0
32	X	58	0	67	19	0
All	All	83877	0	54810	1080	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 8.

The worst 5 of 1080 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)
4:B:117:MET:SD	4:B:117:MET:CE	2.02	1.47
9:G:100:TYR:HB2	9:G:116:ARG:NH1	1.69	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:G:33:ILE:HB	9:G:34:PRO:HD3	1.38	1.03
1:X:558:G:H4'	1:X:559:C:H5'	1.40	1.02
1:X:1448:A:H61	1:X:1574:A:H61	1.09	1.00

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	A	238/274 (87%)	173 (73%)	47 (20%)	18 (8%)	1	17
4	B	203/211 (96%)	173 (85%)	25 (12%)	5 (2%)	7	48
5	C	195/205 (95%)	127 (65%)	40 (20%)	28 (14%)	0	5
6	D	175/180 (97%)	142 (81%)	26 (15%)	7 (4%)	4	35
7	E	169/185 (91%)	134 (79%)	26 (15%)	9 (5%)	2	27
8	F	69/144 (48%)	57 (83%)	9 (13%)	3 (4%)	3	33
9	G	140/174 (80%)	99 (71%)	26 (19%)	15 (11%)	0	10
10	H	132/134 (98%)	117 (89%)	12 (9%)	3 (2%)	8	50
11	I	139/156 (89%)	81 (58%)	39 (28%)	19 (14%)	0	6
12	J	134/141 (95%)	98 (73%)	24 (18%)	12 (9%)	1	13
13	K	111/116 (96%)	92 (83%)	13 (12%)	6 (5%)	2	27
14	L	102/114 (90%)	75 (74%)	15 (15%)	12 (12%)	0	8
15	M	106/166 (64%)	90 (85%)	10 (9%)	6 (6%)	2	25
16	N	115/118 (98%)	91 (79%)	17 (15%)	7 (6%)	2	24
17	O	92/100 (92%)	66 (72%)	13 (14%)	13 (14%)	0	5
18	P	125/134 (93%)	104 (83%)	17 (14%)	4 (3%)	5	42
19	Q	91/95 (96%)	63 (69%)	16 (18%)	12 (13%)	0	6

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	R	108/115 (94%)	65 (60%)	26 (24%)	17 (16%)	0	4
21	S	173/237 (73%)	135 (78%)	27 (16%)	11 (6%)	2	23
22	T	82/91 (90%)	65 (79%)	12 (15%)	5 (6%)	2	24
23	U	70/81 (86%)	41 (59%)	15 (21%)	14 (20%)	0	2
24	V	64/67 (96%)	57 (89%)	5 (8%)	2 (3%)	5	43
25	W	53/55 (96%)	47 (89%)	5 (9%)	1 (2%)	10	53
26	Z	56/60 (93%)	45 (80%)	6 (11%)	5 (9%)	1	13
30	4	35/37 (95%)	23 (66%)	11 (31%)	1 (3%)	6	44
All	All	2977/3390 (88%)	2260 (76%)	482 (16%)	235 (8%)	1	16

5 of 235 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	45	ASN
3	A	209	ALA
3	A	217	ARG
3	A	248	THR
3	A	249	PRO

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	A	185/215 (86%)	145 (78%)	40 (22%)	1	9
4	B	155/157 (99%)	119 (77%)	36 (23%)	1	7
5	C	157/163 (96%)	112 (71%)	45 (29%)	0	4
6	D	153/156 (98%)	130 (85%)	23 (15%)	3	25
7	E	136/144 (94%)	115 (85%)	21 (15%)	3	23
8	F	51/107 (48%)	49 (96%)	2 (4%)	39	77
9	G	118/146 (81%)	94 (80%)	24 (20%)	1	11
10	H	103/103 (100%)	80 (78%)	23 (22%)	1	8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	I	108/121 (89%)	79 (73%)	29 (27%)	0	4
12	J	110/115 (96%)	89 (81%)	21 (19%)	2	12
13	K	90/93 (97%)	76 (84%)	14 (16%)	3	23
14	L	74/82 (90%)	51 (69%)	23 (31%)	0	3
15	M	94/134 (70%)	71 (76%)	23 (24%)	1	6
16	N	96/97 (99%)	76 (79%)	20 (21%)	1	10
17	O	75/79 (95%)	56 (75%)	19 (25%)	1	6
18	P	109/115 (95%)	91 (84%)	18 (16%)	3	19
19	Q	75/76 (99%)	60 (80%)	15 (20%)	1	11
20	R	91/96 (95%)	75 (82%)	16 (18%)	2	16
21	S	149/192 (78%)	117 (78%)	32 (22%)	1	9
22	T	62/67 (92%)	53 (86%)	9 (14%)	4	26
23	U	57/66 (86%)	33 (58%)	24 (42%)	0	1
24	V	54/55 (98%)	43 (80%)	11 (20%)	1	11
25	W	48/48 (100%)	37 (77%)	11 (23%)	1	8
26	Z	51/53 (96%)	41 (80%)	10 (20%)	1	12
30	4	35/35 (100%)	29 (83%)	6 (17%)	2	18
All	All	2436/2715 (90%)	1921 (79%)	515 (21%)	1	10

5 of 515 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	I	77	LEU
14	L	43	ILE
23	U	78	ILE
11	I	99	VAL
12	J	131	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 61 such sidechains are listed below:

Mol	Chain	Res	Type
15	M	58	ASN
17	O	79	GLN
25	W	54	GLN
15	M	90	GLN

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Mol	Chain	Res	Type
16	N	66	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	X	2683/2880 (93%)	701 (26%)	250 (9%)
2	Y	121/123 (98%)	41 (33%)	12 (9%)
All	All	2804/3003 (93%)	742 (26%)	262 (9%)

5 of 742 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	X	2	G
1	X	7	G
1	X	13	A
1	X	14	A
1	X	15	G

5 of 262 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	X	1186	G
1	X	1475	U
1	X	2807	U
1	X	1250	A
1	X	1357	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 ⓘ

Of 36 ligands modelled in this entry, 35 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	$\# Z  > 2$
32	1F4	X	2929	-	60,62,62	1.24	4 (6%)	82,95,95	2.85	37 (45%)

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	1F4	X	2929	-	-	0/74/119/119	1/5/5/5

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	X	2929	1F4	O46-C44	2.10	1.24	1.21
32	X	2929	1F4	C22-C9	2.57	1.58	1.52
32	X	2929	1F4	C52-C51	3.33	1.44	1.39
32	X	2929	1F4	C41-N40	4.13	1.39	1.33

The worst 5 of 37 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	X	2929	1F4	C5-O17-C41	-11.29	99.90	109.28
32	X	2929	1F4	C58-C49-C50	-5.36	104.57	110.59
32	X	2929	1F4	C4-N40-C41	-5.32	106.10	112.55
32	X	2929	1F4	C22-C9-C7	-4.56	103.00	111.05
32	X	2929	1F4	C9-C7-C2	-4.43	108.70	116.09

There are no chirality outliers.

There are no torsion outliers.

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
32	X	2929	1F4	C1-C11-C12-C13-C14-C2-C3-C4-C5-C6-C7-C8-C9-O10

1 monomer is involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	X	2929	1F4	19	0

## 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](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	X	2686/2880 (93%)	-0.09	66 (2%) 61 46	43, 92, 197, 276	0
2	Y	122/123 (99%)	-0.08	3 (2%) 61 46	83, 135, 170, 191	0
3	A	240/274 (87%)	-0.18	5 (2%) 67 52	68, 115, 146, 172	0
4	B	205/211 (97%)	-0.32	1 (0%) 91 86	45, 73, 105, 154	0
5	C	197/205 (96%)	-0.12	8 (4%) 41 29	57, 114, 154, 187	0
6	D	177/180 (98%)	-0.15	9 (5%) 32 22	146, 183, 216, 227	0
7	E	171/185 (92%)	-0.49	2 (1%) 81 69	92, 143, 192, 206	0
8	F	71/144 (49%)	1.56	19 (26%) 1 1	211, 236, 252, 257	0
9	G	142/174 (81%)	-0.29	1 (0%) 89 81	72, 97, 144, 161	0
10	H	134/134 (100%)	-0.38	0 100 100	50, 70, 97, 121	0
11	I	141/156 (90%)	0.33	10 (7%) 19 12	67, 129, 174, 204	0
12	J	136/141 (96%)	0.27	7 (5%) 32 22	74, 103, 149, 184	0
13	K	113/116 (97%)	-0.35	0 100 100	35, 60, 79, 91	0
14	L	104/114 (91%)	-0.12	1 (0%) 84 73	98, 134, 156, 168	0
15	M	108/166 (65%)	-0.58	0 100 100	50, 73, 111, 145	0
16	N	117/118 (99%)	-0.40	0 100 100	59, 90, 128, 159	0
17	O	94/100 (94%)	-0.27	2 (2%) 67 52	66, 115, 157, 173	0
18	P	127/134 (94%)	-0.47	0 100 100	50, 68, 107, 158	0
19	Q	93/95 (97%)	-0.22	2 (2%) 65 50	73, 106, 162, 195	0
20	R	110/115 (95%)	-0.14	4 (3%) 46 33	88, 117, 170, 178	0
21	S	175/237 (73%)	0.38	15 (8%) 13 10	121, 155, 175, 190	0
22	T	84/91 (92%)	0.49	9 (10%) 8 6	79, 107, 186, 200	0
23	U	72/81 (88%)	0.08	6 (8%) 14 10	92, 128, 153, 161	0
24	V	66/67 (98%)	0.05	6 (9%) 11 8	100, 132, 211, 216	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
25	W	55/55 (100%)	-0.45	1 (1%) 71 58	80, 98, 126, 152	0
26	Z	58/60 (96%)	-0.14	3 (5%) 31 22	49, 70, 105, 114	0
27	1	53/55 (96%)	2.48	20 (37%) 0 0	8, 32, 62, 93	0
28	2	46/47 (97%)	5.87	44 (95%) 0 0	3, 15, 38, 59	0
29	3	63/66 (95%)	3.42	44 (69%) 0 0	3, 25, 40, 61	0
30	4	37/37 (100%)	4.00	25 (67%) 0 0	228, 254, 266, 269	0
All	All	5997/6561 (91%)	0.03	313 (5%) 31 22	3, 100, 196, 276	0

The worst 5 of 313 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
27	1	7	ARG	18.6
28	2	27	GLY	13.6
22	T	9	SER	13.0
30	4	25	VAL	12.8
28	2	8	ASN	12.5

## 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, 95<sup>th</sup> 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
31	MG	X	2926	1/1	0.79	1.78	49.42	45,45,45,45	0
31	MG	X	2917	1/1	0.94	1.09	36.65	55,55,55,55	0
31	MG	X	2924	1/1	0.79	1.09	25.25	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
31	MG	X	2907	1/1	0.97	0.81	22.51	51,51,51,51	0
31	MG	Y	202	1/1	0.88	1.43	21.89	88,88,88,88	0
31	MG	X	2901	1/1	0.53	0.69	19.73	50,50,50,50	0
31	MG	X	2915	1/1	0.85	0.73	16.42	57,57,57,57	0
31	MG	X	2922	1/1	0.95	0.86	12.18	44,44,44,44	0
31	MG	X	2914	1/1	0.96	0.64	4.42	27,27,27,27	0
32	1F4	X	2929	58/58	0.96	0.21	-0.27	20,20,20,20	0
31	MG	X	2925	1/1	0.97	0.27	-	122,122,122,122	0
31	MG	X	2927	1/1	0.68	0.53	-	64,64,64,64	0
31	MG	M	201	1/1	0.98	1.39	-	23,23,23,23	0
31	MG	X	2902	1/1	0.93	0.31	-	94,94,94,94	0
31	MG	X	2910	1/1	0.99	0.69	-	41,41,41,41	0
31	MG	Y	201	1/1	0.93	0.46	-	98,98,98,98	0
31	MG	X	2921	1/1	0.91	0.70	-	80,80,80,80	0
31	MG	X	2913	1/1	0.37	1.00	-	60,60,60,60	0
31	MG	Y	204	1/1	0.34	0.97	-	86,86,86,86	0
31	MG	X	2920	1/1	0.54	0.46	-	113,113,113,113	0
31	MG	X	2928	1/1	0.56	0.81	-	61,61,61,61	0
31	MG	X	2916	1/1	0.86	1.18	-	37,37,37,37	0
31	MG	Y	203	1/1	0.81	0.89	-	59,59,59,59	0
31	MG	X	2903	1/1	0.45	0.63	-	89,89,89,89	0
31	MG	X	2906	1/1	0.94	0.95	-	58,58,58,58	0
31	MG	X	2919	1/1	0.92	0.92	-	30,30,30,30	0
31	MG	X	2905	1/1	0.89	0.49	-	65,65,65,65	0
31	MG	Y	205	1/1	0.92	0.40	-	82,82,82,82	0
31	MG	X	2923	1/1	0.96	0.34	-	34,34,34,34	0
31	MG	X	2909	1/1	0.33	0.62	-	97,97,97,97	0
31	MG	X	2908	1/1	0.82	2.34	-	37,37,37,37	0
31	MG	Y	206	1/1	0.84	0.29	-	78,78,78,78	0
31	MG	X	2911	1/1	0.77	0.39	-	68,68,68,68	0
31	MG	X	2904	1/1	0.92	0.30	-	110,110,110,110	0
31	MG	X	2918	1/1	0.84	1.24	-	42,42,42,42	0
31	MG	X	2912	1/1	0.70	0.58	-	71,71,71,71	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.