



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 05:05 am GMT

PDB ID : 1JZY
Title : Structural Basis for the Interaction of Antibiotics with the Peptidyl Transferase Center in Eubacteria
Authors : Schlutzen, F.; Zarivach, R.; Harms, J.; Bashan, A.; Tocilj, A.; Albrecht, R.; Yonath, A.; Franceschi, F.
Deposited on : 2001-09-17
Resolution : 3.50 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

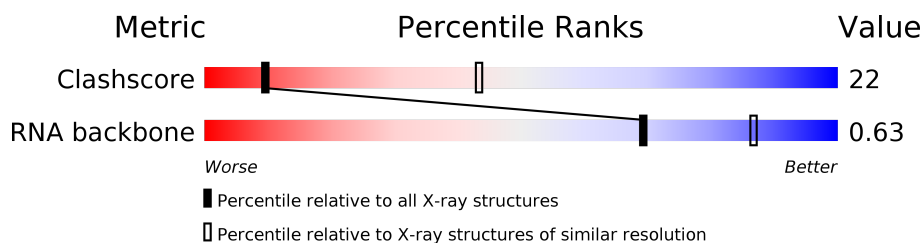
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 Å.

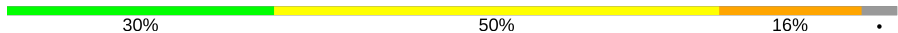
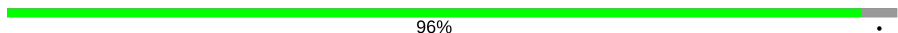
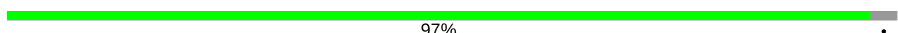

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	112137	1322 (3.60-3.40)
RNA backbone	2435	1024 (4.10-2.86)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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.

Note EDS was not executed.

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

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
5	ERY	A	2881	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 59970 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 rRNA.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 2 is a protein called Ribosomal Protein L4.

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

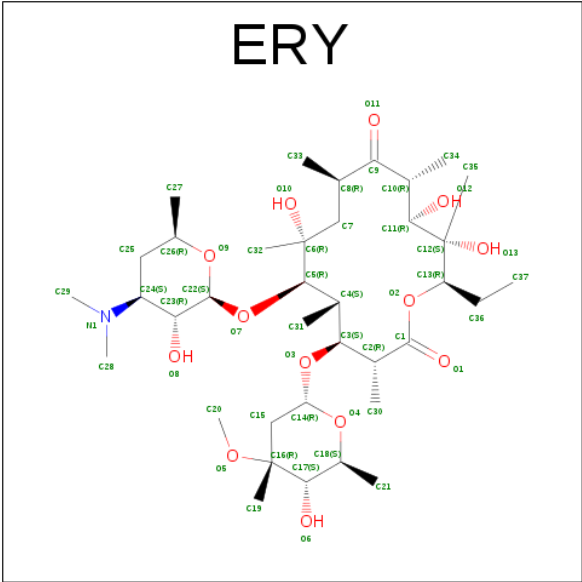
- Molecule 3 is a protein called Ribosomal Protein L22.

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

- Molecule 4 is a protein called Ribosomal Protein L32.

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

- Molecule 5 is ERYTHROMYCIN A (three-letter code: ERY) (formula: C₃₇H₆₇NO₁₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			51	37	1	13		

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

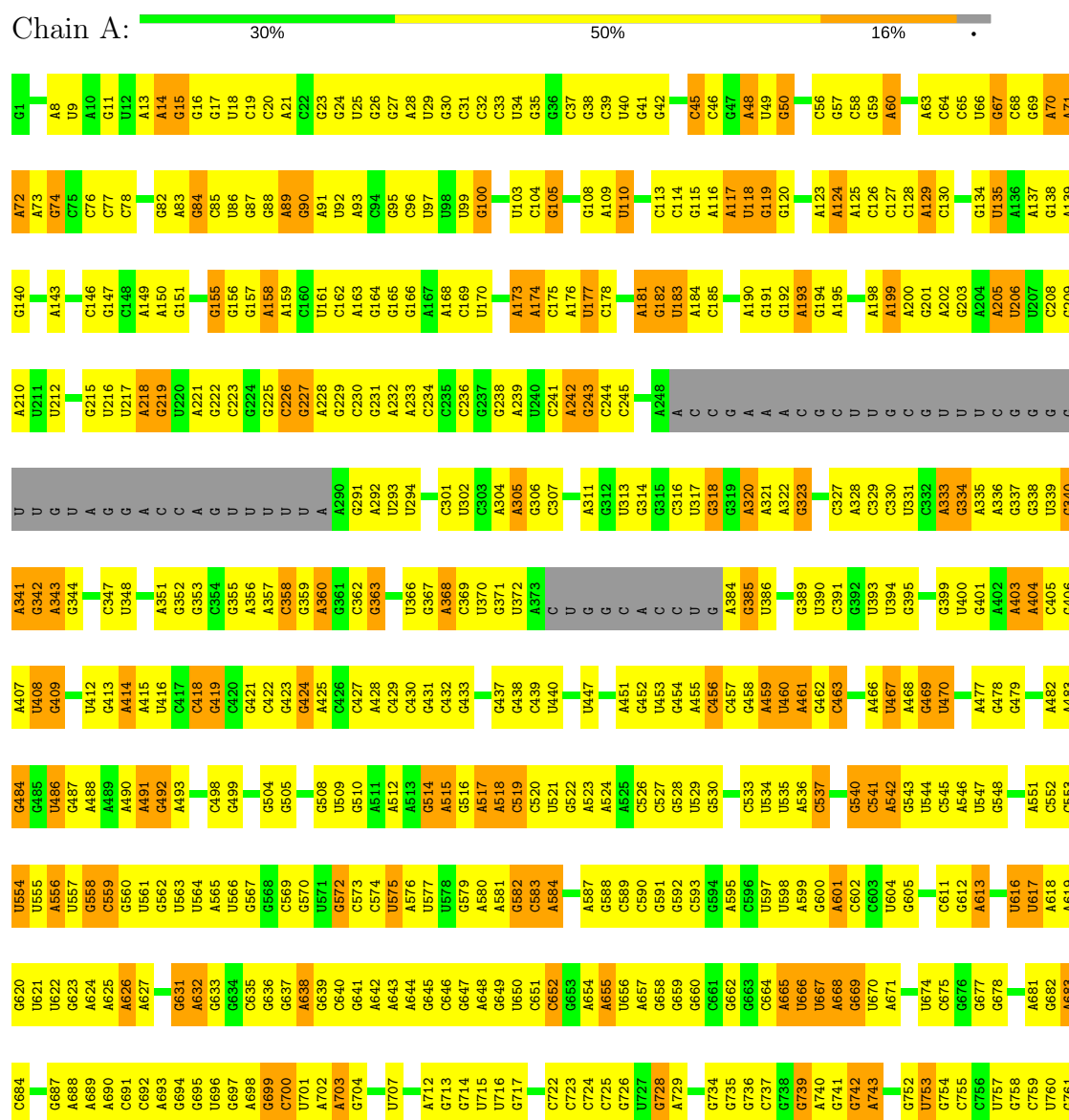
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	2	Total	Mg	0	0
			2	2		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

Note EDS was not executed.

• Molecule 1: 23S rRNA



A1821	U1748	C1674	U1601	G1465	U1392	G1323	U1176	A1107	A1040	U969	U	C828	A763
C1824	G1749	C1675	G1602	C1466	A1397	G1324	U1177	U1108	G1041	U969	A	C829	A763
C1825	A1750	C1676	A1603	U1467	A1397	U1325	C1178	A1109	U1044	A970	C	C830	A764
C1826	A1751	C1677	A1604	U1468	A1398	U1326	C1179	G1110	U1044	A971	C	C831	A765
C1827	U1752	C1678	C1606	G1470	C1399	C1327	C1183	C1111	U1045	G972	A	A832	A766
C1828	U1753	C1679	A1607	U1471	A1400	C1328	A1187	C1112	U1046	G973	G	A833	A767
C1829	G1754	C1680	A1607	U1472	G1401	U1329	A1188	C1113	U1047	U974	C	A834	U768
C1830	G1755	A1681	U1608	U1473	G1402	G1330	A1189	G1118	U1048	G975	U	A838	G772
C1831	G1756	A1682	U1608	U1474	U1403	G1333	A1189	U1119	U1049	G976	U	U839	G773
C1832	C1757	G1683	U1612	U1475	C1404	G1266	C1190	U1119	U1050	G977	A	U840	A774
C1833	C1758	G1684	U1613	G1476	A1405	A1334	C1191	G1120	C1054	U978	C910	G841	U775
C1834	A1759	A1685	G1613	U1477	U1409	G1337	A1192	G1121	A1055	U979	C911	A842	U776
C1835	G1760	C1686	C1614	U1480	U1410	G1338	G1193	A1122	U1056	G980	A911	G843	G776
C1836	G1761	C1687	G1617	U1481	U1411	U1339	U1194	G1123	A1057	C981	A912	G844	A777
A1840	G1762	U1688	G1618	U1482	C1412	C1340	U1195	U1124	U1058	G982	A913	G845	G778
A1841	C1763	U1689	U1619	G1484	C1412	G1341	U1196	G1125	A1059	G983	C914	G846	G779
A1851	A1764	U1690	A1619	U1485	C1415	U1342	U1197	A1126	U1060	A984	C915	C850	U784
A1852	C1765	G1691	C1623	U1486	C1416	U1343	U1198	G1127	A1061	G985	A918	U851	U785
A1853	G1766	C1692	A1624	U1487	A1417	C1344	U1199	G1128	U1062	G986	U919	U852	U786
A1854	C1767	A1693	A1625	U1488	C1417	C1345	G1200	A1129	A1063	A994	U919	U853	U787
A1855	U1768	A1694	A1626	U1489	C1418	U1346	G1201	A1130	A1064	A995	U919	U854	A788
A1856	U1769	U1695	A1627	U1490	C1419	C1347	U1202	A1131	G1065	A996	A922	U855	G789
A1857	U1770	U1696	C1627	U1491	U1421	U1348	G1203	C1134	A1066	C997	A923	U856	A790
A1858	A1771	C1698	U1697	U1492	C1422	U1349	G1204	C1135	G1067	C998	C924	U857	G791
A1859	C1772	A1699	U1698	U1493	U1423	A1349	G1205	G1136	U1070	A999	U925	U858	U792
A1860	C1773	U1703	A1631	U1494	G1425	G1350	U1206	A1137	U1071	G1000	C926	U859	G793
A1861	A1774	C1704	A1632	U1495	G1426	G1351	U1207	A1138	G1072	A1001	C927	U860	A794
A1862	U1775	G1704	C1633	U1496	G1427	G1352	U1208	A1139	U1073	A999	G928	G861	A795
A1863	A1776	U1710	A1634	U1497	G1428	U1353	U1209	A1140	G1074	C1003	A929	U862	A796
A1864	C1777	C1711	C1640	U1498	A1429	A1354	U1210	A1141	C1075	A1004	A930	U863	A797
A1865	U1778	G1712	U1641	U1499	A1430	A1355	U1211	U1142	U1076	U1005	G931	U864	G798
A1866	A1762	C1713	G1642	U1500	U1431	G1356	U1212	A1143	U1077	C1006	G932	U865	G799
A1867	U1767	A1714	U1645	U1501	G1432	U1357	G1213	A1144	A1078	A1007	G933	U866	U800
A1868	C1768	G1716	U1646	U1502	U1433	C1358	A1215	C1145	U1079	U868	A801	U867	A802
A1869	U1769	A1717	C1648	U1504	U1434	G1359	U1216	A1080	A1080	C934	G934	C869	C803
A1870	G1790	U1722	U1651	U1505	G1435	U1364	C1218	A1081	A1081	A1012	C937	C870	C804
A1871	C1791	U1723	G1652	U1506	A1437	U1365	G1219	G1149	C1082	G1013	G938	U871	C805
A1872	C1792	C1724	C1653	U1507	G1438	A1366	C1220	C1150	C1083	G1014	C939	G872	G806
A1873	C1793	C1725	A1654	U1508	G1439	A1367	C1221	U1151	A1084	U1015	G940	U873	A807
A1874	A1794	C1726	A1655	U1509	A1440	G1368	G1222	C1152	G1085	C1016	U941	A874	C808
A1875	C1795	C1727	U1656	A1510	A1441	U1369	G1223	A1153	C1086	U1019	U942	G875	C809
A1876	U1796	C1728	U1657	A1511	G1442	U1370	A1224	A1154	C1087	A1020	A944	A876	U810
A1877	C1801	A1729	A1658	A1512	G1443	G1371	U1225	G1155	C1088	A1021	G945	G877	C811
A1878	U1802	C1729	U1659	U1513	C1444	A1372	A1226	C1160	C1089	A1022	C948	C878	G812
A1879	G1803	G1730	U1660	U1514	A1445	G1373	U1227	U1161	C1090	A1023	C948	C879	A813
A1880	C1804	U1733	C1661	U1515	U1446	G1374	A1228	A1162	C1091	G1024	G949	C880	A814
A1881	U1805	G1734	U1662	U1516	U1447	U1375	C1234	C1163	U1093	U1025	G950	A886	A815
A1882	C1806	C1735	G1663	U1517	G1450	G1376	G1240	C1164	A1096	G1028	G951	G887	U816
A1883	U1807	U1736	U1664	U1518	C1451	C1380	G1241	G1165	A1097	C1029	G952	G888	A817
A1884	C1808	C1737	C1665	U1519	U1452	G1381	G1242	A1166	C1098	U1030	G953	C889	G818
A1885	U1809	U1738	U1666	U1520	A1453	G1382	U1243	A1167	A1099	C1031	U954	U890	C819
A1886	U1810	C1739	A1667	C1524	C1454	C1383	U1244	U1170	G1099	A1032	G955	A891	U820
A1887	A1811	U1738	U1668	U1525	C1455	G1384	G1245	C1168	G1100	G1033	A956	G892	A821
A1888	U1812	U1739	U1669	U1526	A1456	C1385	U1246	U1171	U1101	U1034	G957	G893	G822
A1889	A1813	G1742	U1670	U1527	A1457	C1386	G1249	A1171	G1102	G1035	G958	G	U823
A1890	C1809	C1743	U1671	G1527	A1458	A1387	A1250	U1172	C1103	G1036	C959	G	U824
A1891	U1814	U1746	A1672	U1528	U1459	G1387	G1251	U1173	G1104	U1037	U960	G	C825
A1892	U1815	G1747	C1673	C1529	G1460	A1391	G1252	G1174	U1105	U1038	U961	G	U826
A1893	U1816	U1748	U1674	U1530	U1600		G1253	A1175	A1106	A1039	A964	C	C827

U2853	G2854	C2855	A2858	U2859	C2860	A2861	G2862	G2865	U2866	G2867	U2868	C2870	U2871	A2874	C2875	G2876	C2877	U2878	C2879	G2880	C2881	U2882	C2883	U2884	U2885	C2886	U2887	C2888	U2889	C2890	U2891	C2892	U2893	C2894	U2895	C2896	U2897	C2898	U2899	C2900	U2901	C2902	U2903	C2904	U2905	C2906	U2907	C2908	U2909	C2910	U2911	C2912	U2913	C2914	U2915	C2916	U2917	C2918	U2919	C2920	U2921	C2922	U2923	C2924	U2925	C2926	U2927	C2928	U2929	C2930	U2931	C2932	U2933	C2934	U2935	C2936	U2937	C2938	U2939	C2940	U2941	C2942	U2943	C2944	U2945	C2946	U2947	C2948	U2949	C2950	U2951	C2952	U2953	C2954	U2955	C2956	U2957	C2958	U2959	C2960	U2961	C2962	U2963	C2964	U2965	C2966	U2967	C2968	U2969	C2970	U2971	C2972	U2973	C2974	U2975	C2976	U2977	C2978	U2979	C2980	U2981	C2982	U2983	C2984	U2985	C2986	U2987	C2988	U2989	C2990	U2991	C2992	U2993	C2994	U2995	C2996	U2997	C2998	U2999	C3000	U3001	C3002	U3003	C3004	U3005	C3006	U3007	C3008	U3009	C3010	U3011	C3012	U3013	C3014	U3015	C3016	U3017	C3018	U3019	C3020	U3021	C3022	U3023	C3024	U3025	C3026	U3027	C3028	U3029	C3030	U3031	C3032	U3033	C3034	U3035	C3036	U3037	C3038	U3039	C3040	U3041	C3042	U3043	C3044	U3045	C3046	U3047	C3048	U3049	C3050	U3051	C3052	U3053	C3054	U3055	C3056	U3057	C3058	U3059	C3060	U3061	C3062	U3063	C3064	U3065	C3066	U3067	C3068	U3069	C3070	U3071	C3072	U3073	C3074	U3075	C3076	U3077	C3078	U3079	C3080	U3081	C3082	U3083	C3084	U3085	C3086	U3087	C3088	U3089	C3090	U3091	C3092	U3093	C3094	U3095	C3096	U3097	C3098	U3099	C3100	U3101	C3102	U3103	C3104	U3105	C3106	U3107	C3108	U3109	C3110	U3111	C3112	U3113	C3114	U3115	C3116	U3117	C3118	U3119	C3120	U3121	C3122	U3123	C3124	U3125	C3126	U3127	C3128	U3129	C3130	U3131	C3132	U3133	C3134	U3135	C3136	U3137	C3138	U3139	C3140	U3141	C3142	U3143	C3144	U3145	C3146	U3147	C3148	U3149	C3150	U3151	C3152	U3153	C3154	U3155	C3156	U3157	C3158	U3159	C3160	U3161	C3162	U3163	C3164	U3165	C3166	U3167	C3168	U3169	C3170	U3171	C3172	U3173	C3174	U3175	C3176	U3177	C3178	U3179	C3180	U3181	C3182	U3183	C3184	U3185	C3186	U3187	C3188	U3189	C3190	U3191	C3192	U3193	C3194	U3195	C3196	U3197	C3198	U3199	C3200	U3201	C3202	U3203	C3204	U3205	C3206	U3207	C3208	U3209	C3210	U3211	C3212	U3213	C3214	U3215	C3216	U3217	C3218	U3219	C3220	U3221	C3222	U3223	C3224	U3225	C3226	U3227	C3228	U3229	C3230	U3231	C3232	U3233	C3234	U3235	C3236	U3237	C3238	U3239	C3240	U3241	C3242	U3243	C3244	U3245	C3246	U3247	C3248	U3249	C3250	U3251	C3252	U3253	C3254	U3255	C3256	U3257	C3258	U3259	C3260	U3261	C3262	U3263	C3264	U3265	C3266	U3267	C3268	U3269	C3270	U3271	C3272	U3273	C3274	U3275	C3276	U3277	C3278	U3279	C3280	U3281	C3282	U3283	C3284	U3285	C3286	U3287	C3288	U3289	C3290	U3291	C3292	U3293	C3294	U3295	C3296	U3297	C3298	U3299	C3300	U3301	C3302	U3303	C3304	U3305	C3306	U3307	C3308	U3309	C3310	U3311	C3312	U3313	C3314	U3315	C3316	U3317	C3318	U3319	C3320	U3321	C3322	U3323	C3324	U3325	C3326	U3327	C3328	U3329	C3330	U3331	C3332	U3333	C3334	U3335	C3336	U3337	C3338	U3339	C3340	U3341	C3342	U3343	C3344	U3345	C3346	U3347	C3348	U3349	C3350	U3351	C3352	U3353	C3354	U3355	C3356	U3357	C3358	U3359	C3360	U3361	C3362	U3363	C3364	U3365	C3366	U3367	C3368	U3369	C3370	U3371	C3372	U3373	C3374	U3375	C3376	U3377	C3378	U3379	C3380	U3381	C3382	U3383	C3384	U3385	C3386	U3387	C3388	U3389	C3390	U3391	C3392	U3393	C3394	U3395	C3396	U3397	C3398	U3399	C3400	U3401	C3402	U3403	C3404	U3405	C3406	U3407	C3408	U3409	C3410	U3411	C3412	U3413	C3414	U3415	C3416	U3417	C3418	U3419	C3420	U3421	C3422	U3423	C3424	U3425	C3426	U3427	U3428	U3429	C3432	U3433	U3434	U3437	U3438	U3439	U3440	U3441	U3442	U3443	U3444	U3445	U3446	U3449	U3450	U3454	U3455	U3456	U3457	U3458	U3459	U3460	U3463	U3464	U3465	U3466	U3467	U3468	U3469	U3470	U3471	U3472	U3473	U3474	U3475	U3476	U3477	U3478	U3479	U3480	U3481	U3482	U3483	U3484	U3485	U3486	U3487	U3488	U3489	U3490	U3491	U3492	U3493	U3494	U3495	U3496	U3497	U3498	U3499	U3500	U3501	U3502	U3503	U3504	U3505	U3506	U3507	U3508	U3509	U3510	U3515	U3516	U3517	U3518	U3519	U3520	U3521	U3522	U3523	U3524	U3525	U3526	U3527	U3528	U3529	U3530	U3531	U3532	U3533	U3534	U3535	U3536	U3537	U3538	U3539	U3540	U3541	U3542	U3543	U3544	U3545	U3546	U3547	U3548	U3549	U3550	U3551	U3552	U3553	U3554	U3555	U3556	U3557	U3558	U3559	U3560	U3561	U3562	U3563	U3564	U3565	U3566	U3567	U3568	U3569	U3570	U3571	U3572	U3573	U3574	U3575	U3576	U3577	U3578	U3579	U3580	U3581	U3582	U3583	U3584	U3585	U3586	U3587	U3588	U3589	U3590	U3591	U3592	U3593	U3594	U3595	U3596	U3597	U3598	U3599	U3600	U3601	U3602	U3603	U3604	U3605	U3606	U3607	U3608	U3609	U3610	U3611	U3612	U3613	U3614	U3615	U3616	U3617	U3618	U3619	U3620	U3621	U3622	U3623	U3624	U3625	U3626	U3627	U3628	U3629	U3630	U3631	U3632	U3633	U3634	U3635	U3636	U3637	U3638	U3639	U3640	U3641	U3642	U3643	U3644	U3645	U3646	U3647	U3648	U3649	U3650	U3651	U3652	U3653	U3654	U3655	U3656	U3657	U3658	U3659	U3660	U3661	U3662	U3663	U3664	U3665	U3666	U3667	U3668	U3669	U3670	U3671	U3672	U3673	U3674	U3675	U3676	U3677	U3678	U3679	U3680	U3681	U3682	U3683	U3684	U3685	U3686	U3687	U3688	U3689	U3690	U3691	U3692	U3693	U3694	U3695	U3696	U3697	U3698	U3699	U3700	U3701	U3702	U3703	U3704	U3705	U3706	U3707	U3708	U3709	U3710	U3711	U3712	U3713	U3714	U3715	U3716	U3717	U3718	U3719	U3720	U3721	U3722	U3723	U3724	U3725	U3726	U3727	U3728	U3729	U3730	U3731	U3732	U3733	U3734	U3735	U3736	U3737	U3738	U3739	U3740	U3741	U3742	U3743	U3744	U3745	U3746	U3747	U3748	U3749	U3750	U3751	U3752	U3753	U3754	U3755	U3756	U3757	U3758	U3759	U3760	U3761	U3762	U3763	U3764	U3765	U3766	U3767	U3768	U3769	U3770	U3771	U3772	U3773	U3774	U3775	U3776	U3777	U3778	U3779	U3780	U3781	U3782	U3783	U3784	U3785	U3786	U3787	U3788	U3789	U3790	U3791	U3792	U3793	U3794	U3795	U3796	U3797	U3798	U3799	U3800	U3801	U3802	U3803	U3804	U3805	U3806	U3807	U3808	U3809	U3810	U3811	U3812	U3813	U3814	U3815	U3816	U3817	U3818	U3819	U3820	U3821	U3822	U3823	U3824	U3825	U3826	U3827	U3828	U3829	U3830	U3831	U3832	U3833	U3834	U3835	U3836	U3837	U3838	U3839	U3840	U3841	U3842	U3843	U3844	U3845	U3846	U3847	U3848	U3849	U3850	U3851	U3852	U3853	U3854	U3855	U3856	U3857	U3858	U3859	U3860	U3861	U3862	U3863	U3864	U3865	U3866	U3867	U3868	U3869	U3870	U3871	U3872	U3873	U3874	U3875	U3876	U3877	U3878	U3879	U3880	U3881	U3882	U3883	U3884	U3885	U3886	U3887	U3888	U3889	U3890	U3891	U3892	U3893	U3894	U3895	U3896	U3897	U3898	U3899	U3900	U3901	U3902	U3903	U3904	U3905	U3906	U3907	U3908	U3909	U3910	U3911	U3912	U3913	U3914	U3915	U3916	U3917	U3918	U3919	U3920	U3921	U3922	U3923	U3924	U3925	U3926	U3927	U3928	U3929	U3930	U3931	U3932	U3933	U3934	U3935	U3936	U3937	U3938	U3939	U3940	U3941	U3942	U3943	U3944	U3945	U3946	U3947	U3948	U3949	U3950	U3951	U3952	U3953	U3954	U3955	U3956	U3957	U3958	U3959	U3960	U3961	U3962	U3963	U3964	U3965	U3966	U3967	U3968	U3969	U3970	U3971	U3972	U3973	U3974	U3975	U3976	U3977	U3978	U3979	U3980	U3981	U3982	U3983	U3984	U3985	U3986	U3987	U3988	U3989	U3990	U3991	U3992	U3993	U3994	U3995	U3996	U3997	U3998	U3999	U4000
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• Molecule 2: Ribosomal Protein L4

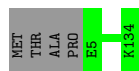
Chain K:

96%

MET	A2	E198	GLU	ALA	GLY	GLU	GLU	GLN
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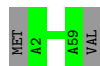
- Molecule 3: Ribosomal Protein L22

Chain L:  97% .



- Molecule 4: Ribosomal Protein L32

Chain M:  97% .



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	169.20Å 410.00Å 695.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.50	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-3.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS, REFMAC	Depositor
R, R_{free}	0.268 , 0.301	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	59970	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

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: MG, ERY

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.23	0/66661	0.66	3/103976 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	1746	A	C2'-C3'-O3'	6.01	123.32	113.70
1	A	777	A	C2'-C3'-O3'	5.45	122.42	113.70
1	A	2588	U	C2'-C3'-O3'	5.12	121.89	113.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	59532	0	30004	1926	0
2	K	197	0	0	0	0
3	L	130	0	0	0	0
4	M	58	0	0	0	0
5	A	51	0	67	22	0
6	A	2	0	0	0	0
All	All	59970	0	30071	1944	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 22.

The worst 5 of 1944 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)
1:A:1747:G:H4'	1:A:1749:G:H1'	1.30	1.12
1:A:2668:U:H4'	1:A:2669:C:H5'	1.33	1.11
1:A:940:G:H3'	1:A:941:U:H5''	1.34	1.09
1:A:367:G:H2'	1:A:368:A:H5''	1.34	1.08
1:A:1199:U:H3'	1:A:1200:G:H5''	1.35	1.06

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	A	2765/2880 (96%)	561 (20%)	0

5 of 561 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	13	A
1	A	14	A
1	A	15	G
1	A	23	G
1	A	45	C

There are no RNA pucker outliers to report.

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	ERY	A	2881	-	53,53,53	1.53	11 (20%)	82,82,82	3.01	43 (52%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	ERY	A	2881	-	-	1/72/107/107	1/3/3/3

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	2881	ERY	O2-C13	-3.16	1.40	1.46
5	A	2881	ERY	C19-C16	-2.16	1.47	1.52
5	A	2881	ERY	C12-C13	2.03	1.58	1.54
5	A	2881	ERY	C2-C1	2.03	1.56	1.51
5	A	2881	ERY	C32-C6	2.10	1.56	1.52

The worst 5 of 43 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	2881	ERY	O5-C16-C19	-7.29	98.23	110.96
5	A	2881	ERY	O5-C16-C15	-5.07	104.47	112.95
5	A	2881	ERY	C27-C26-C25	-5.06	105.28	113.39
5	A	2881	ERY	C15-C16-C17	-5.00	98.21	107.69
5	A	2881	ERY	C20-O5-C16	-4.83	107.13	117.63

There are no chirality outliers.

All (1) torsion outliers are listed below:

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

All (1) ring outliers are listed below:

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

1 monomer is involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	2881	ERY	22	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](#)

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.