



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2018 – 06:38 pm GMT

PDB ID : 3CC7
Title : Structure of Anisomycin resistant 50S Ribosomal Subunit: 23S rRNA mutation C2487U
Authors : Blaha, G.; Gurel, G.
Deposited on : 2008-02-25
Resolution : 2.70 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix) : 1.13
EDS : trunk30967
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30967

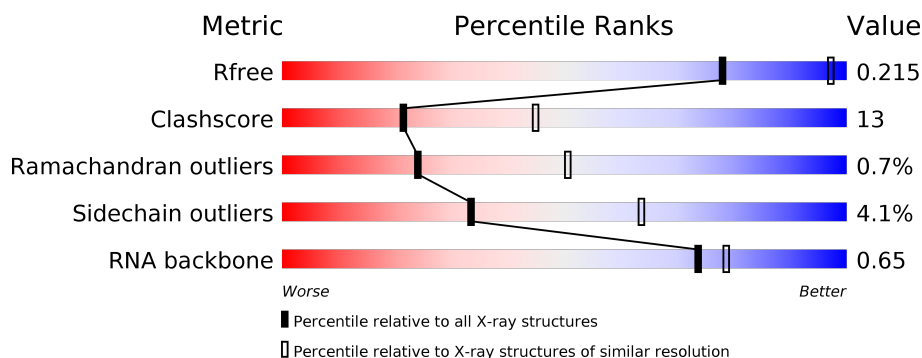
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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.



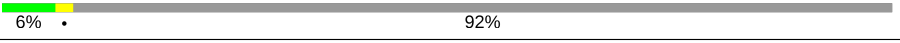















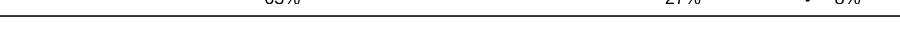
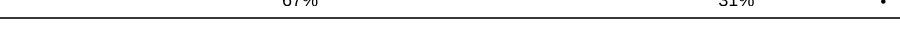
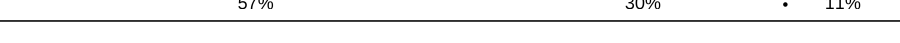
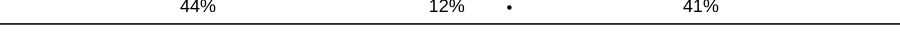
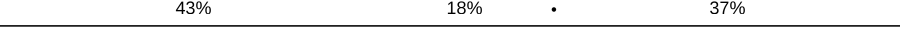
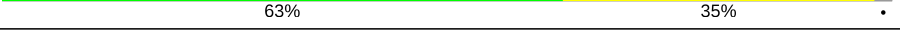



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	111664	2449 (2.70-2.70)
Clashscore	122126	2756 (2.70-2.70)
Ramachandran outliers	120053	2716 (2.70-2.70)
Sidechain outliers	120020	2716 (2.70-2.70)
RNA backbone	2636	1009 (3.00-2.40)

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	240	70% 26% ...
2	B	338	65% 32% .
3	C	246	74% 22% .
4	D	177	49% 28% . 21%
5	E	178	79% 17% ..
6	F	120	75% 23% ..

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Mol	Chain	Length	Quality of chain
7	G	348	
8	H	177	
9	I	162	
10	J	145	
11	K	132	
12	L	165	
13	M	196	
14	N	187	
15	O	116	
16	P	149	
17	Q	96	
18	R	155	
19	S	85	
20	T	120	
21	U	67	
22	V	71	
23	W	154	
24	X	92	
25	Y	241	
26	Z	116	
27	1	57	
28	2	50	
29	3	92	
30	0	2923	
31	9	122	

2 Entry composition

There are 38 unique types of molecules in this entry. The entry contains 99122 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 L2P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	237	Total	C	N	O	S	0	0	0
			1753	1072	352	324	5			

- Molecule 2 is a protein called 50S ribosomal protein L3P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	337	Total	C	N	O	S	0	0	0
			2625	1616	493	511	5			

- Molecule 3 is a protein called 50S ribosomal protein L4P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	246	Total	C	N	O	S	0	0	0
			1860	1130	345	384	1			

- Molecule 4 is a protein called 50S ribosomal protein L5P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	140	Total	C	N	O	S	0	0	0
			1094	685	195	210	4			

- Molecule 5 is a protein called 50S ribosomal protein L6P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	172	Total	C	N	O	S	0	0	0
			1357	840	224	289	4			

- Molecule 6 is a protein called 50S ribosomal protein L7Ae.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	119	Total	C	N	O	S	0	0	0
			890	551	141	197	1			

- Molecule 7 is a protein called 50S ribosomal protein L10E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	29	Total	C	N	O	S	0	0	0
			240	149	39	51	1			

- Molecule 8 is a protein called 50S ribosomal protein L10e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	160	Total	C	N	O	S	0	0	0
			1282	798	240	238	6			

- Molecule 9 is a protein called 50S ribosomal protein L11P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	70	Total	C	N	O	S	0	0	0
			519	323	81	114	1			

- Molecule 10 is a protein called 50S ribosomal protein L13P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	142	Total	C	N	O	S	0	0	0
			1120	696	199	222	3			

- Molecule 11 is a protein called 50S ribosomal protein L14P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	132	Total	C	N	O	S	0	0	0
			994	609	189	192	4			

- Molecule 12 is a protein called 50S ribosomal protein L15P.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
12	L	145	Total	C	N	O	0	0	0
			1118	670	222	226			

- Molecule 13 is a protein called 50S ribosomal protein L15e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	194	Total	C	N	O	S	0	0	0
			1558	943	333	281	1			

- Molecule 14 is a protein called 50S ribosomal protein L18P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	186	Total	C	N	O	S	0	0	0
			1445	895	262	286	2			

- Molecule 15 is a protein called 50S ribosomal protein L18e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	O	115	Total	C	N	O		0	0	0
			865	529	161	175				

- Molecule 16 is a protein called 50S ribosomal protein L19e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	P	143	Total	C	N	O		0	0	0
			1136	683	229	224				

- Molecule 17 is a protein called 50S ribosomal protein L21e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Q	95	Total	C	N	O		0	0	0
			735	450	141	144				

- Molecule 18 is a protein called 50S ribosomal protein L22P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	R	150	Total	C	N	O	S	0	0	0
			1149	713	209	223	4			

- Molecule 19 is a protein called 50S ribosomal protein L23P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	S	81	Total	C	N	O	S	0	0	0
			641	389	111	138	3			

- Molecule 20 is a protein called 50S ribosomal protein L24P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	T	119	Total	C	N	O		0	0	0
			950	568	180	202				

- Molecule 21 is a protein called 50S ribosomal protein L24e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	U	53	Total	C	N	O	S	0	0	0
			410	244	75	86	5			

- Molecule 22 is a protein called 50S ribosomal protein L29P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	V	65	Total	C	N	O	S	0	0	0
			499	304	94	100	1			

- Molecule 23 is a protein called 50S ribosomal protein L30P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	W	154	Total	C	N	O	S	0	0	0
			1196	737	209	244	6			

- Molecule 24 is a protein called 50S ribosomal protein L31e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	X	82	Total	C	N	O	S	0	0	0
			654	402	129	122	1			

- Molecule 25 is a protein called 50S ribosomal protein L32e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	Y	142	Total	C	N	O		0	0	0
			1130	686	228	216				

- Molecule 26 is a protein called 50S ribosomal protein L37Ae.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	Z	73	Total	C	N	O	S	0	0	0
			573	343	113	112	5			

- Molecule 27 is a protein called 50S ribosomal protein L37e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	1	56	Total	C	N	O	S	0	0	0
			431	258	86	83	4			

- Molecule 28 is a protein called 50S ribosomal protein L39e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	2	46	Total	C	N	O	S	0	0	0
			396	239	89	67	1			

- Molecule 29 is a protein called 50S ribosomal protein L44E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	3	92	Total	C	N	O	S	0	0	0
			755	458	153	137	7			

- Molecule 30 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	0	2754	Total	C	N	O	P	0	0	0
			59020	26349	10872	19054	2745			

- Molecule 31 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	9	122	Total	C	N	O	P	0	0	0
			2599	1160	471	847	121			

- Molecule 32 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
32	0	85	Total	Mg	0	0
			85	85		
32	9	1	Total	Mg	0	0
			1	1		
32	K	1	Total	Mg	0	0
			1	1		
32	B	2	Total	Mg	0	0
			2	2		
32	A	2	Total	Mg	0	0
			2	2		
32	T	1	Total	Mg	0	0
			1	1		
32	Y	1	Total	Mg	0	0
			1	1		

- Molecule 33 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	0	10	Total 10	Cl 10	0	0
33	J	3	Total 3	Cl 3	0	0
33	B	1	Total 1	Cl 1	0	0
33	A	1	Total 1	Cl 1	0	0
33	N	1	Total 1	Cl 1	0	0
33	O	1	Total 1	Cl 1	0	0
33	R	1	Total 1	Cl 1	0	0
33	Y	1	Total 1	Cl 1	0	0
33	L	1	Total 1	Cl 1	0	0
33	3	1	Total 1	Cl 1	0	0
33	M	1	Total 1	Cl 1	0	0

- Molecule 34 is STRONTIUM ION (three-letter code: SR) (formula: Sr).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	0	93	Total 93	Sr 93	0	0
34	J	1	Total 1	Sr 1	0	0
34	1	2	Total 2	Sr 2	0	0
34	B	2	Total 2	Sr 2	0	0
34	3	2	Total 2	Sr 2	0	0
34	A	3	Total 3	Sr 3	0	0
34	R	1	Total 1	Sr 1	0	0
34	9	2	Total 2	Sr 2	0	0
34	S	1	Total 1	Sr 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	F	1	Total	Sr	0	0
			1	1		

- Molecule 35 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	0	66	Total	Na	0	0
			66	66		
35	J	1	Total	Na	0	0
			1	1		
35	Q	1	Total	Na	0	0
			1	1		
35	C	1	Total	Na	0	0
			1	1		
35	R	2	Total	Na	0	0
			2	2		
35	9	2	Total	Na	0	0
			2	2		
35	S	1	Total	Na	0	0
			1	1		
35	M	1	Total	Na	0	0
			1	1		

- Molecule 36 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	O	1	Total	Cd	0	0
			1	1		
36	Z	1	Total	Cd	0	0
			1	1		
36	1	1	Total	Cd	0	0
			1	1		
36	3	1	Total	Cd	0	0
			1	1		
36	U	1	Total	Cd	0	0
			1	1		

- Molecule 37 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	0	2	Total	K	0	0
			2	2		

- Molecule 38 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
38	A	111	Total O 111 111	0	0
38	B	153	Total O 153 153	0	0
38	C	165	Total O 165 165	0	0
38	D	46	Total O 46 46	0	0
38	E	44	Total O 44 44	0	0
38	F	23	Total O 23 23	0	0
38	G	19	Total O 19 19	0	0
38	H	71	Total O 71 71	0	0
38	I	10	Total O 10 10	0	0
38	J	54	Total O 54 54	0	0
38	K	56	Total O 56 56	0	0
38	L	80	Total O 80 80	0	0
38	M	130	Total O 130 130	0	0
38	N	59	Total O 59 59	0	0
38	O	41	Total O 41 41	0	0
38	P	61	Total O 61 61	0	0
38	Q	51	Total O 51 51	0	0
38	R	78	Total O 78 78	0	0
38	S	33	Total O 33 33	0	0
38	T	37	Total O 37 37	0	0
38	U	25	Total O 25 25	0	0

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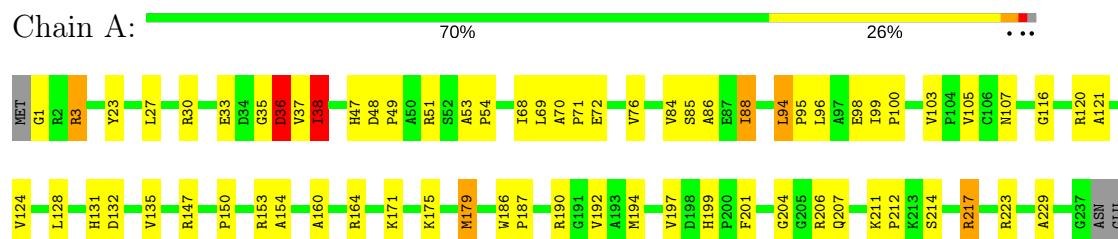
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	V	11	Total 11	O 11	0	0
38	W	63	Total 63	O 63	0	0
38	X	28	Total 28	O 28	0	0
38	Y	91	Total 91	O 91	0	0
38	Z	28	Total 28	O 28	0	0
38	1	52	Total 52	O 52	0	0
38	2	37	Total 37	O 37	0	0
38	3	68	Total 68	O 68	0	0
38	0	5951	Total 5951	O 5951	0	0
38	9	147	Total 147	O 147	0	0

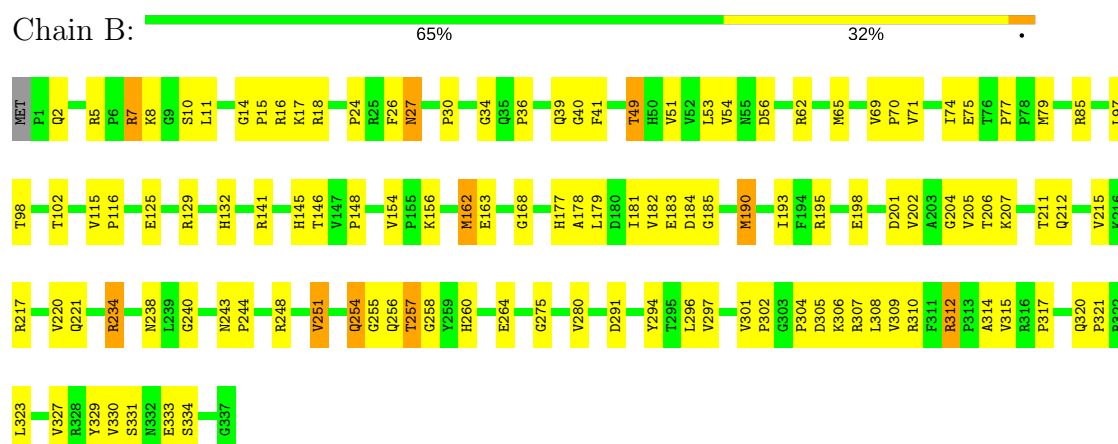
3 Residue-property plots [i](#)

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. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

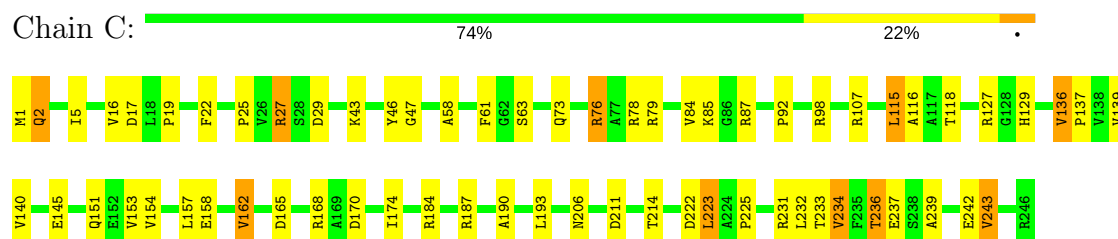
• Molecule 1: 50S ribosomal protein L2P



• Molecule 2: 50S ribosomal protein L3P



• Molecule 3: 50S ribosomal protein L4P

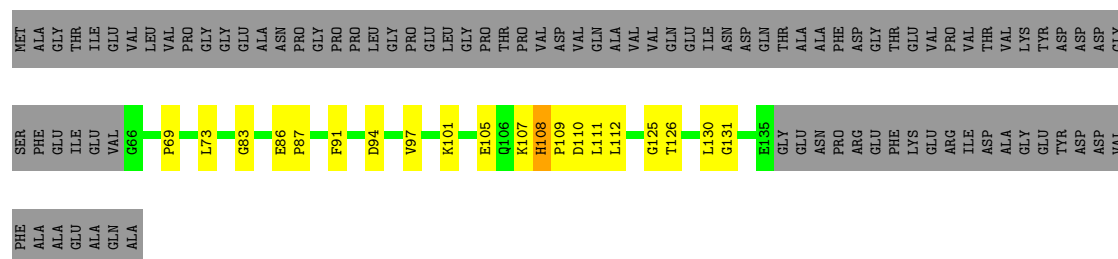


• Molecule 4: 50S ribosomal protein L5P

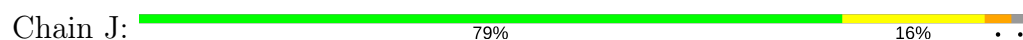




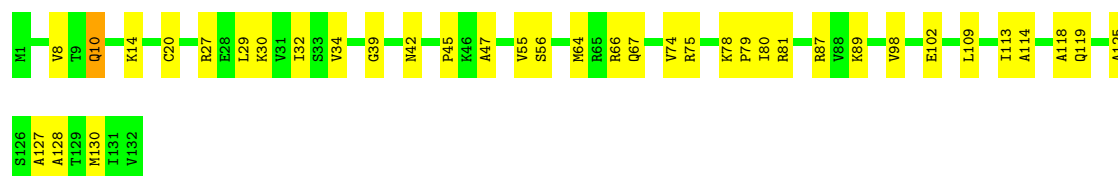
- Molecule 9: 50S ribosomal protein L11P



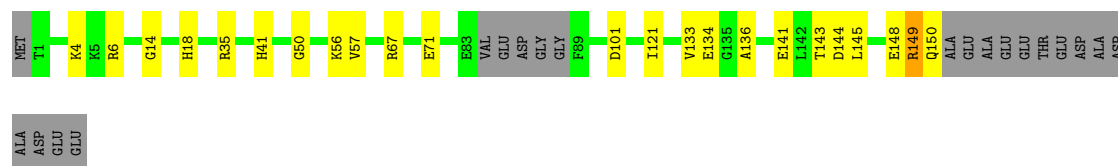
- Molecule 10: 50S ribosomal protein L13P



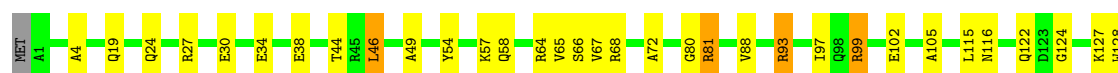
- Molecule 11: 50S ribosomal protein L14P

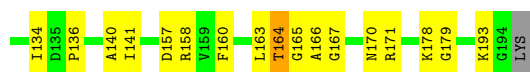


- Molecule 12: 50S ribosomal protein L15P



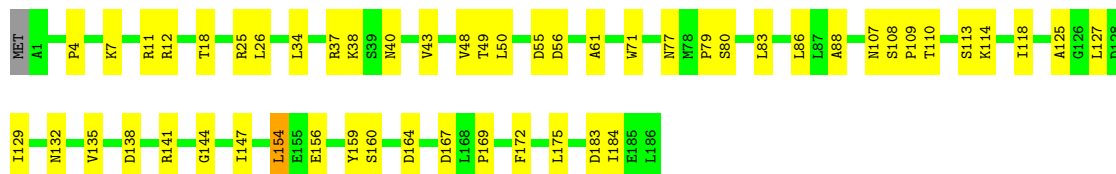
- Molecule 13: 50S ribosomal protein L15e





- Molecule 14: 50S ribosomal protein L18P

Chain N: 72% 27% ..



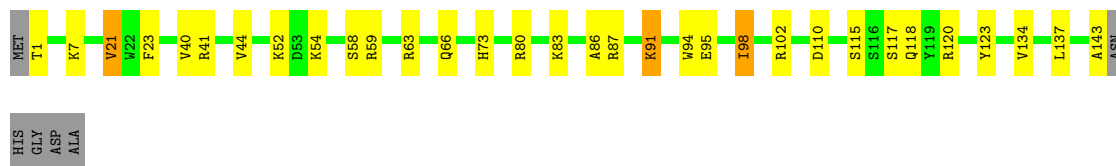
- Molecule 15: 50S ribosomal protein L18e

Chain O: 80% 18% ..



- Molecule 16: 50S ribosomal protein L19e

Chain P: 74% 19% • •



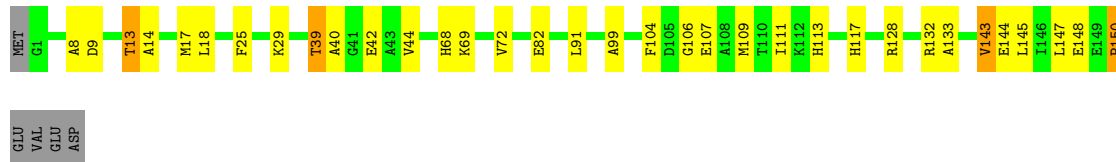
- Molecule 17: 50S ribosomal protein L21e

Chain Q: 83% 16% •



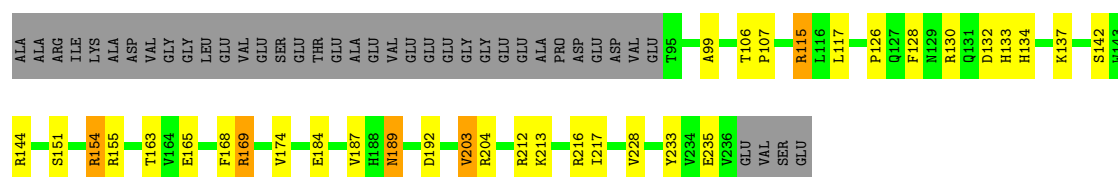
- Molecule 18: 50S ribosomal protein L22P

Chain R: 75% 19% • •

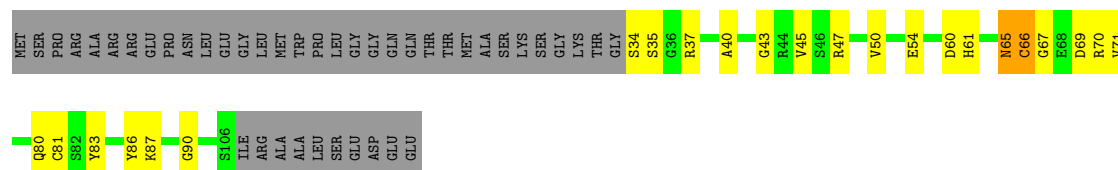


- Molecule 19: 50S ribosomal protein L23P

Chain S: 76% 18% 5%



- Molecule 26: 50S ribosomal protein L37Ae



- Molecule 27: 50S ribosomal protein L37e



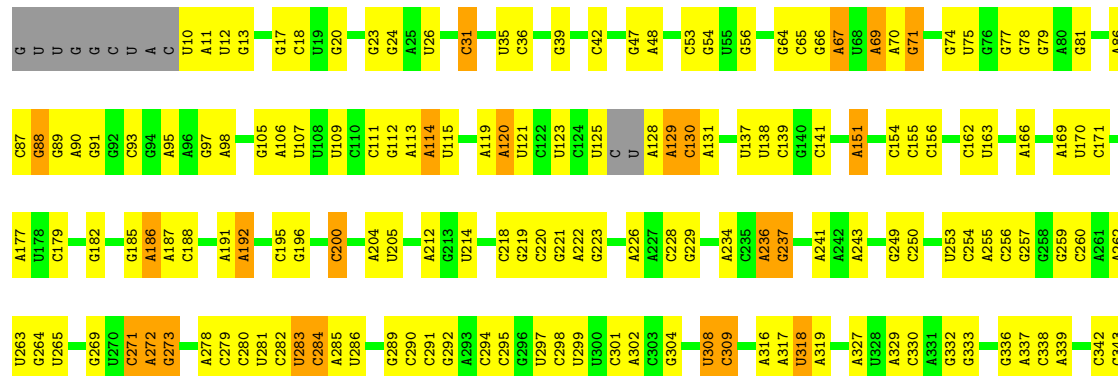
- Molecule 28: 50S ribosomal protein L39e



- Molecule 29: 50S ribosomal protein L44E



- Molecule 30: 23S ribosomal RNA



G1820	G1723	U1625	G1520	U1418	A1321	U1234	C1156	G1045	C963	G871	G775	G657	A532	C440	C344
U1724	U1725	A1626	A1521	C1420	G1322	G1235	C1157	C1051	G968	U872	U776	A660	G537	A441	G345
C1826	C1725	G1627	A1522	C1421	G1323	A1236	G1158	G1052	G969	A875	U777	G661	C538	A442	U346
A1829	G1730	A1632	U1524	C1423	G1328	C1238	A1161	G1053	U970	A876	A790	C667	G539	C444	A347
C1834	A1732	C1633	G1525	A1427	A1320	G1239	G1162	G1055	G	A878	A791	C668	U445	U445	G350
U1835	A1733	G1634	A1526	A1428	A1331	A1242	G1163	U1056	U	A792	G792	C669	C541	A446	G358
A1836	C1734	U1635	A1527	U1432	G1332	C1243	U1164	A1057	C	A793	U793	C670	A542	A447	C363
G1837	C1735	U1636	G1528	G1433	C1333	U1244	A1166	A1058	C	U883	U794	A671	G544	A448	U364
U1838	U1741	A1641	G1535	A1434	C1334	C1245	G1167	C1060	C	A886	A796	C672	G545	C450	G365
A1839	U1742	C1643	U1536	U1435	C1335	A1246	C1168	C1063	G	A882	A797	C677	G553	C451	G366
A1840	C1750	U1645	C1536	C1436	U1336	A1249	U1169	G1063	C	G892	U797	C678	A453	C452	G367
C1841	G1751	U1646	U1544	U1440	G1339	U1249	U1170	U1066	U	G898	G800	C681	U454	C453	G368
A1842	G1752	C1654	C1545	G1441	G1340	C1250	A1171	A1067	C	A682	U801	G682	U559	C369	G369
A1845	A1755	U1655	G1546	A1442	G1341	C1251	A1172	G1071	C	G902	A806	G683	U560	A455	U370
U1846	G1756	A1656	A1547	G1443	C1342	C1253	A1173	G1072	A	U903	A807	G684	G564	G458	U371
C1853	U1757	A1657	U1548	G1444	C1343	A1260	A1174	A1073	G	U904	A808	G685	U567	C461	A372
C1856	C1763	G1668	G1552	U1445	C1343	G1261	G1175	G1074	A	C905	G809	A686	C567	A462	G373
A1857	G1764	A1670	C1553	U1446	U1352	A1262	C1176	A1075	G	C906	A812	C687	U582	A466	A378
G1863	U1765	G1666	G1554	C1451	C1353	C1262	U1180	A1076	G	A907	C813	A688	C583	C467	A380
G1867	G1766	A1667	G1555	G1456	G1360	U1266	A1181	A1078	A	A912	C814	G689	U584	U468	G381
G1868	C1767	U1668	G1556	U1457	C1366	G1267	C1182	C1080	U	C920	C815	G690	C588	U470	U382
C1873	G1768	G1669	G1557	C1458	C1376	C1268	C1183	A1081	C	G921	C816	C691	C594	C383	A383
A1874	C1769	A1671	C1558	U1459	C1377	G1269	U1185	A1086	G	A922	A818	U701	C595	G482	G379
G1877	U1773	U1672	U1559	G1460	A1372	A1271	U1187	A1087	C	A923	C819	G702	C596	A484	U392
C1878	G1774	C1673	C1562	C1474	A1375	A1278	A1188	A1088	A	A926	U821	C703	A602	A485	G393
A1879	A1778	A1674	C1565	U1477	C1378	U1279	U1189	A1090	A	U932	C822	C705	A603	U495	U396
U1880	C1779	C1675	C1566	U1478	G1378	A1280	A1192	A1097	C999	U932	U825	C706	A604	C487	A397
G1881	G1782	A1680	C1567	G1481	C1384	U1285	A1193	A1098	U1001	C933	U826	G711	C605	U488	C399
C1882	A1783	G1681	C1568	U1482	G1385	A1286	A1194	G1099	A1005	C936	G834	U714	C613	A498	C400
U1883	U1784	C1682	G1569	A1486	G1387	U1288	U1198	U1109	A1006	G941	U835	U	U614	C401	C402
A1884	C1787	A1683	G1574	U1487	C1387	C1289	A1199	G1110	U1007	U942	G836	G716	U619	A407	A408
U1885	U1788	G1684	C1574	U1488	G1391	G1290	A1200	U1116	C1008	A943	U840	C717	A620	G506	A409
A1886	U1789	C1685	C1575	A1494	A1392	U1293	C1201	A1117	U1009	U944	A841	C718	G621	A507	C412
U1887	C1790	U1686	G1576	C1495	C1393	A1294	A1202	A1118	C1010	U945	C842	G724	G522	A508	G413
C1888	U1791	C1687	U1577	U1500	C1396	G1296	G1203	G1119	A1013	C946	A843	C725	U623	A509	C414
A1889	G1795	A1688	U1578	U1501	G1397	U1298	U1205	U1120	C1014	U947	A844	C729	A629	U510	U511
U1890	A1796	C1689	C1579	U1502	G1398	U1299	A1207	U1130	U1016	U949	A846	C741	A632	G512	G417
G1891	C1797	U1689	U1580	U1503	A1399	G1300	C1208	G1131	G950	C847	C848	G742	A632	A513	C418
U1892	U1798	A1690	U1504	A1504	A1406	U1304	C1209	A1132	A951	C952	C849	G743	A635	G514	A419
C1893	A1799	G1691	U1505	U1505	A1407	U1305	G1210	G1135	C1023	G953	C853	G744	G636	U517	U420
U1894	C1799	C1692	C1506	U1506	U1408	G1306	G1211	U1136	C1025	U954	C854	G745	C637	G518	C421
A1895	U1800	A1693	U1507	C1507	G1409	A1307	C1212	G1137	U1029	A955	C855	A746	C638	C424	C424
C1896	G1787	C1694	U1508	U1511	G1410	A1308	C1213	G1138	A1032	G958	A857	C759	A639	A521	U425
U1897	U1788	C1695	C1509	U1512	A1414	G1311	A1215	U1149	U1039	C959	U858	C760	G644	U522	C427
G1898	U1789	A1696	G1510	U1515	G1415	G1312	G1216	A1150	G1039	G960	C868	C761	U645	G523	G437
C1899	C1790	U1697	C1511	U1516	A1416	A1313	C1229	G1151	C1044	A961	C869	C764	G656	A524	A437
U1900	U1791	C1698	U1512	U1517	G1417	U1314	A1230	C1151			G870	G765		G531	

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	212.83Å 299.90Å 576.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.83 – 2.70 85.81 – 2.41	Depositor EDS
% Data completeness (in resolution range)	92.7 (49.83-2.70) 90.8 (85.81-2.41)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.00 (at 2.40Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.184 , 0.226 0.174 , 0.215	Depositor DCC
R_{free} test set	6547 reflections (0.98%)	wwPDB-VP
Wilson B-factor (Å ²)	47.5	Xtriage
Anisotropy	0.113	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 67.2	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	0.89	EDS
Total number of atoms	99122	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.48% 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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, OMG, CL, SR, NA, K, CD, OMU, UR3, 1MA, PSU

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	0.32	0/1786	0.64	0/2408
2	B	0.32	0/2690	0.65	0/3652
3	C	0.36	0/1885	0.62	0/2552
4	D	0.31	0/1111	0.55	0/1498
5	E	0.32	0/1382	0.56	0/1880
6	F	0.32	0/901	0.57	0/1224
7	G	0.31	0/241	0.48	0/324
8	H	0.32	0/1302	0.63	0/1743
9	I	0.29	0/526	0.51	0/716
10	J	0.35	0/1136	0.59	0/1530
11	K	0.33	0/1004	0.65	0/1351
12	L	0.33	0/1130	0.63	0/1509
13	M	0.34	0/1582	0.62	0/2116
14	N	0.29	0/1474	0.61	0/1999
15	O	0.34	0/874	0.59	1/1181 (0.1%)
16	P	0.32	0/1147	0.52	0/1528
17	Q	0.35	0/749	0.68	0/1005
18	R	1.26	7/1172 (0.6%)	1.11	6/1578 (0.4%)
19	S	0.31	0/648	0.57	0/875
20	T	0.33	0/958	0.62	1/1289 (0.1%)
21	U	0.34	0/417	0.55	0/562
22	V	0.31	0/502	0.52	0/675
23	W	0.34	0/1219	0.64	0/1655
24	X	0.34	0/664	0.58	0/895
25	Y	0.36	0/1146	0.60	0/1536
26	Z	0.35	0/584	0.60	0/781
27	1	0.37	0/438	0.61	0/578
28	2	0.34	0/401	0.55	0/529
29	3	0.36	0/771	0.57	0/1024
30	0	0.36	0/65957	0.68	17/102867 (0.0%)
31	9	0.32	0/2904	0.68	1/4526 (0.0%)
All	All	0.38	7/98701 (0.0%)	0.67	26/147586 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
18	R	1	0
30	0	0	42
31	9	0	1
All	All	1	43

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	R	150	PRO	CB-CG	27.34	2.86	1.50
18	R	150	PRO	CA-C	-18.21	1.16	1.52
18	R	150	PRO	CG-CD	13.97	1.96	1.50
18	R	150	PRO	C-O	11.88	1.47	1.23
18	R	150	PRO	N-CA	11.28	1.66	1.47

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	R	150	PRO	CB-CA-C	-22.47	55.83	112.00
18	R	150	PRO	N-CA-C	-19.39	61.69	112.10
18	R	150	PRO	CA-N-CD	12.31	128.94	111.70
18	R	150	PRO	N-CA-CB	10.98	116.48	103.30
18	R	150	PRO	CA-C-O	-8.51	99.77	120.20

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
18	R	150	PRO	CA

5 of 43 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
30	0	221	G	Sidechain
30	0	26	U	Sidechain
30	0	396	U	Sidechain
30	0	458	G	Sidechain
30	0	48	A	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	A	1753	0	1766	75	0
2	B	2625	0	2533	92	0
3	C	1860	0	1813	57	0
4	D	1094	0	1085	40	0
5	E	1357	0	1266	23	0
6	F	890	0	843	26	0
7	G	240	0	231	7	0
8	H	1282	0	1292	37	0
9	I	519	0	500	15	0
10	J	1120	0	1098	30	0
11	K	994	0	1027	36	0
12	L	1118	0	1076	22	0
13	M	1558	0	1573	42	0
14	N	1445	0	1401	45	0
15	O	865	0	873	15	0
16	P	1136	0	1123	28	0
17	Q	735	0	729	14	0
18	R	1149	0	1122	34	0
19	S	641	0	605	11	0
20	T	950	0	924	19	0
21	U	410	0	364	19	0
22	V	499	0	511	17	0
23	W	1196	0	1137	55	0
24	X	654	0	653	24	0
25	Y	1130	0	1133	36	0
26	Z	573	0	531	16	0
27	1	431	0	426	22	0
28	2	396	0	413	19	0
29	3	755	0	728	20	0
30	0	59020	0	29806	1142	0
31	9	2599	0	1325	101	0
32	0	85	0	0	0	0
32	9	1	0	0	0	0
32	A	2	0	0	0	0
32	B	2	0	0	0	0
32	K	1	0	0	0	0
32	T	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	Y	1	0	0	0	0
33	0	10	0	0	2	0
33	3	1	0	0	0	0
33	A	1	0	0	0	0
33	B	1	0	0	0	0
33	J	3	0	0	0	0
33	L	1	0	0	0	0
33	M	1	0	0	0	0
33	N	1	0	0	1	0
33	O	1	0	0	0	0
33	R	1	0	0	0	0
33	Y	1	0	0	0	0
34	0	93	0	0	0	0
34	1	2	0	0	0	0
34	3	2	0	0	0	0
34	9	2	0	0	0	0
34	A	3	0	0	0	0
34	B	2	0	0	0	0
34	F	1	0	0	0	0
34	J	1	0	0	0	0
34	R	1	0	0	0	0
34	S	1	0	0	0	0
35	0	66	0	0	0	0
35	9	2	0	0	0	0
35	C	1	0	0	0	0
35	J	1	0	0	0	0
35	M	1	0	0	0	0
35	Q	1	0	0	0	0
35	R	2	0	0	0	0
35	S	1	0	0	0	0
36	1	1	0	0	0	0
36	3	1	0	0	0	0
36	O	1	0	0	0	0
36	U	1	0	0	0	0
36	Z	1	0	0	0	0
37	0	2	0	0	0	0
38	0	5951	0	0	153	0
38	1	52	0	0	3	0
38	2	37	0	0	2	0
38	3	68	0	0	5	0
38	9	147	0	0	8	0
38	A	111	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	B	153	0	0	14	0
38	C	165	0	0	11	0
38	D	46	0	0	2	0
38	E	44	0	0	2	0
38	F	23	0	0	1	0
38	G	19	0	0	0	0
38	H	71	0	0	6	0
38	I	10	0	0	2	0
38	J	54	0	0	1	0
38	K	56	0	0	3	0
38	L	80	0	0	6	0
38	M	130	0	0	5	0
38	N	59	0	0	5	0
38	O	41	0	0	3	0
38	P	61	0	0	1	0
38	Q	51	0	0	2	0
38	R	78	0	0	3	0
38	S	33	0	0	2	0
38	T	37	0	0	2	0
38	U	25	0	0	3	0
38	V	11	0	0	0	0
38	W	63	0	0	4	0
38	X	28	0	0	1	0
38	Y	91	0	0	6	0
38	Z	28	0	0	3	0
All	All	99122	0	59907	1937	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 13.

The worst 5 of 1937 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)
18:R:150:PRO:CG	18:R:150:PRO:CD	1.96	1.44
30:0:1160:G:C5'	30:0:1161:A:H5'	1.81	1.10
31:9:56:A:H2'	31:9:57:A:H5''	1.33	1.08
30:0:871:G:C8	30:0:871:G:H5'	1.87	1.07
18:R:150:PRO:CG	18:R:150:PRO:C	2.22	1.07

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	235/240 (98%)	212 (90%)	18 (8%)	5 (2%)	8	20
2	B	335/338 (99%)	306 (91%)	26 (8%)	3 (1%)	19	44
3	C	244/246 (99%)	228 (93%)	16 (7%)	0	100	100
4	D	134/177 (76%)	112 (84%)	19 (14%)	3 (2%)	7	19
5	E	170/178 (96%)	161 (95%)	9 (5%)	0	100	100
6	F	117/120 (98%)	107 (92%)	9 (8%)	1 (1%)	19	44
7	G	25/348 (7%)	24 (96%)	1 (4%)	0	100	100
8	H	156/177 (88%)	149 (96%)	6 (4%)	1 (1%)	27	54
9	I	68/162 (42%)	55 (81%)	10 (15%)	3 (4%)	3	6
10	J	140/145 (97%)	131 (94%)	9 (6%)	0	100	100
11	K	130/132 (98%)	125 (96%)	5 (4%)	0	100	100
12	L	141/165 (86%)	127 (90%)	13 (9%)	1 (1%)	24	50
13	M	192/196 (98%)	182 (95%)	9 (5%)	1 (0%)	31	58
14	N	184/187 (98%)	168 (91%)	13 (7%)	3 (2%)	11	27
15	O	113/116 (97%)	109 (96%)	4 (4%)	0	100	100
16	P	141/149 (95%)	141 (100%)	0	0	100	100
17	Q	93/96 (97%)	88 (95%)	5 (5%)	0	100	100
18	R	148/155 (96%)	140 (95%)	8 (5%)	0	100	100
19	S	79/85 (93%)	78 (99%)	1 (1%)	0	100	100
20	T	117/120 (98%)	110 (94%)	6 (5%)	1 (1%)	19	44
21	U	51/67 (76%)	47 (92%)	4 (8%)	0	100	100
22	V	63/71 (89%)	60 (95%)	2 (3%)	1 (2%)	11	27
23	W	152/154 (99%)	148 (97%)	4 (3%)	0	100	100
24	X	80/92 (87%)	73 (91%)	6 (8%)	1 (1%)	13	33
25	Y	140/241 (58%)	138 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	Z	71/116 (61%)	61 (86%)	8 (11%)	2 (3%)	5	13
27	1	54/57 (95%)	51 (94%)	3 (6%)	0	100	100
28	2	42/50 (84%)	41 (98%)	1 (2%)	0	100	100
29	3	90/92 (98%)	86 (96%)	3 (3%)	1 (1%)	16	38
All	All	3705/4472 (83%)	3458 (93%)	220 (6%)	27 (1%)	24	50

5 of 27 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	27	LEU
1	A	37	VAL
14	N	154	LEU
14	N	183	ASP
14	N	184	ILE

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	179/182 (98%)	171 (96%)	8 (4%)	30	60
2	B	282/283 (100%)	265 (94%)	17 (6%)	21	46
3	C	193/193 (100%)	178 (92%)	15 (8%)	14	32
4	D	117/148 (79%)	109 (93%)	8 (7%)	17	40
5	E	152/156 (97%)	147 (97%)	5 (3%)	41	71
6	F	93/94 (99%)	93 (100%)	0	100	100
7	G	27/282 (10%)	26 (96%)	1 (4%)	37	67
8	H	134/145 (92%)	127 (95%)	7 (5%)	25	53
9	I	58/130 (45%)	57 (98%)	1 (2%)	63	87
10	J	118/121 (98%)	112 (95%)	6 (5%)	26	54
11	K	106/106 (100%)	103 (97%)	3 (3%)	47	77
12	L	113/127 (89%)	111 (98%)	2 (2%)	62	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	M	158/160 (99%)	150 (95%)	8 (5%)	26	54
14	N	149/150 (99%)	144 (97%)	5 (3%)	40	71
15	O	93/94 (99%)	91 (98%)	2 (2%)	55	83
16	P	113/117 (97%)	108 (96%)	5 (4%)	31	60
17	Q	79/80 (99%)	77 (98%)	2 (2%)	50	80
18	R	117/122 (96%)	113 (97%)	4 (3%)	40	71
19	S	71/74 (96%)	70 (99%)	1 (1%)	69	89
20	T	105/106 (99%)	99 (94%)	6 (6%)	23	48
21	U	44/53 (83%)	43 (98%)	1 (2%)	53	82
22	V	51/57 (90%)	50 (98%)	1 (2%)	58	84
23	W	130/130 (100%)	126 (97%)	4 (3%)	43	73
24	X	66/74 (89%)	60 (91%)	6 (9%)	10	24
25	Y	120/196 (61%)	114 (95%)	6 (5%)	27	55
26	Z	60/94 (64%)	59 (98%)	1 (2%)	63	87
27	1	46/47 (98%)	46 (100%)	0	100	100
28	2	42/46 (91%)	41 (98%)	1 (2%)	52	81
29	3	79/79 (100%)	77 (98%)	2 (2%)	50	80
All	All	3095/3646 (85%)	2967 (96%)	128 (4%)	33	63

5 of 128 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	H	91	ARG
12	L	35	ARG
25	Y	115	ARG
8	H	169	GLU
10	J	107	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 75 such sidechains are listed below:

Mol	Chain	Res	Type
13	M	58	GLN
16	P	73	HIS
27	1	16	HIS
13	M	137	ASN

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Mol	Chain	Res	Type
14	N	107	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
30	0	2745/2923 (93%)	239 (8%)	32 (1%)
31	9	121/122 (99%)	16 (13%)	1 (0%)
All	All	2866/3045 (94%)	255 (8%)	33 (1%)

5 of 255 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
30	0	31	C
30	0	67	A
30	0	69	A
30	0	70	A
30	0	71	G

5 of 33 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
30	0	1352	A
30	0	1684	A
30	0	2761	A
30	0	1377	C
30	0	1474	C

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

5 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	OMU	0	2587	30	14,22,23	1.00	1 (7%)	18,31,34	3.65	2 (11%)
30	OMG	0	2588	30	19,26,27	1.08	2 (10%)	22,38,41	2.43	4 (18%)
30	UR3	0	2619	30	13,22,23	0.70	0	15,32,35	0.69	0
30	PSU	0	2621	30	16,21,22	1.67	3 (18%)	20,30,33	5.44	4 (20%)
30	1MA	0	628	30,35	16,25,26	0.97	1 (6%)	12,37,40	1.29	1 (8%)

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	OMU	0	2587	30	-	0/5/27/28	0/2/2/2
30	OMG	0	2588	30	-	0/5/27/28	0/3/3/3
30	UR3	0	2619	30	-	0/3/25/26	0/2/2/2
30	PSU	0	2621	30	-	0/7/25/26	0/2/2/2
30	1MA	0	628	30,35	-	0/3/25/26	0/3/3/3

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	0	2621	PSU	C5-C1'	-5.08	1.47	1.52
30	0	2588	OMG	C8-N7	-2.11	1.30	1.34
30	0	2587	OMU	C4-N3	2.54	1.37	1.33
30	0	2621	PSU	C2-N1	2.58	1.43	1.38
30	0	628	1MA	C6-N6	2.73	1.33	1.27

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	0	2621	PSU	N1-C2-N3	-17.45	114.39	128.41
30	0	2588	OMG	C5-C6-N1	-8.19	111.82	123.47
30	0	2621	PSU	C5-C4-N3	-8.16	114.84	125.36
30	0	628	1MA	C2-N3-C4	-3.87	110.60	116.51
30	0	2587	OMU	C5-C4-N3	-3.62	114.77	123.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	0	2587	OMU	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 305 ligands modelled in this entry, 305 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.