



# wwPDB X-ray Structure Validation Summary Report

Feb 27, 2014 – 03:41 PM GMT

PDB ID : 4ABR  
Title : COMPLEX OF SMPB, A TMRNA FRAGMENT AND EF-TU-GDP-KIRROMYCIN WITH THE 70S RIBOSOME  
Authors : Neubauer, C.; Gillet, R.; Kelley, A.C.; Ramakrishnan, V.  
Deposited on : 2011-12-10  
Resolution : 3.10 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

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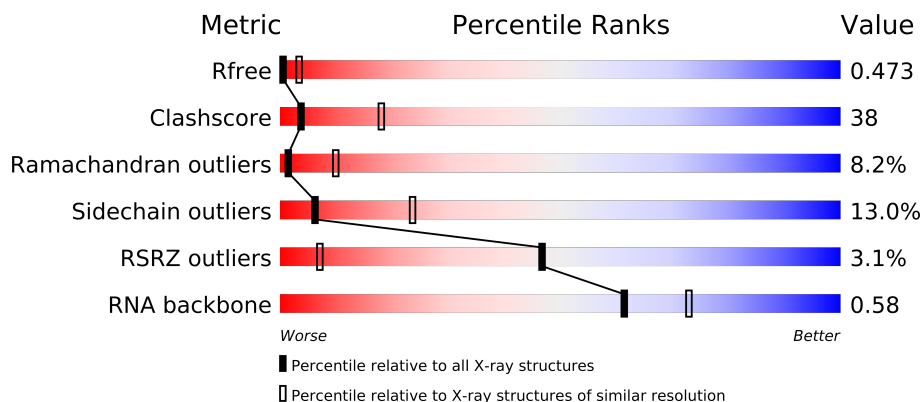
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 3.10 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))
$R_{free}$	66092	1007 (3.18-3.02)
Clashscore	79885	1078 (3.16-3.04)
Ramachandran outliers	78287	1044 (3.16-3.04)
Sidechain outliers	78261	1044 (3.16-3.04)
RSRZ outliers	66119	1008 (3.18-3.02)
RNA backbone	1838	1047 (3.60-2.60)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	2	144	
2	A	1522	
3	B	256	
4	C	239	
5	D	209	
6	E	162	
7	F	101	
8	G	156	
9	H	138	
10	I	128	
11	J	105	
12	K	129	

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Mol	Chain	Length	Quality of chain
13	L	135	
14	M	126	
15	N	61	
16	O	89	
17	P	88	
18	Q	105	
19	R	88	
20	S	93	
21	T	106	
22	U	27	
23	V	77	
23	W	77	
24	X	19	
25	Y	90	
26	Z	405	

## 2 Entry composition

There are 30 unique types of molecules in this entry. The entry contains 60380 atoms, of which 0 are hydrogen and 0 are deuterium.

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 SMALL PROTEIN B SMPB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	2	144	Total	C	N	O	S	0	0	0
			1184	754	219	210	1			

- Molecule 2 is a RNA chain called 16S RRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	1504	Total	C	N	O	P	0	0	0
			32330	14391	5994	10442	1503			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1489	A	G	CONFLICT	GB NC_006461
A	1490	A	C	CONFLICT	GB NC_006461

- Molecule 3 is a protein called 30S RIBOSOMAL PROTEIN S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	B	235	Total	C	N	O	S	0	0	1
			1901	1213	342	341	5			

- Molecule 4 is a protein called 30S RIBOSOMAL PROTEIN S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	C	207	Total	C	N	O	S	0	0	1
			1613	1016	315	281	1			

- Molecule 5 is a protein called 30S RIBOSOMAL PROTEIN S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	D	208	Total	C	N	O	S	0	0	0
			1703	1066	339	291	7			

- Molecule 6 is a protein called 30S RIBOSOMAL PROTEIN S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	E	151	Total	C	N	O	S	0	0	1
			1147	724	218	201	4			

- Molecule 7 is a protein called 30S RIBOSOMAL PROTEIN S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	F	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			

- Molecule 8 is a protein called 30S RIBOSOMAL PROTEIN S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	G	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			

- Molecule 9 is a protein called 30S RIBOSOMAL PROTEIN S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	H	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			

- Molecule 10 is a protein called 30S RIBOSOMAL PROTEIN S9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	I	127	Total	C	N	O	S	0	0	0
			1011	639	198	174				

- Molecule 11 is a protein called 30S RIBOSOMAL PROTEIN S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	J	99	Total	C	N	O	S	0	0	1
			795	499	157	138	1			

- Molecule 12 is a protein called 30S RIBOSOMAL PROTEIN S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	K	119	Total	C	N	O	S	0	0	0
			885	549	168	165	3			

- Molecule 13 is a protein called 30S RIBOSOMAL PROTEIN S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	L	125	Total	C	N	O	S	0	0	1
			971	611	196	163	1			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	1	MET	-	EXPRESSION TAG	UNP Q5SHN3
L	2	VAL	-	EXPRESSION TAG	UNP Q5SHN3
L	3	ALA	-	EXPRESSION TAG	UNP Q5SHN3
L	4	LEU	-	EXPRESSION TAG	UNP Q5SHN3

- Molecule 14 is a protein called 30S RIBOSOMAL PROTEIN S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	M	125	Total	C	N	O	S	0	0	1
			988	611	206	169	2			

- Molecule 15 is a protein called 30S RIBOSOMAL PROTEIN S14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	N	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			

- Molecule 16 is a protein called 30S RIBOSOMAL PROTEIN S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	O	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			

- Molecule 17 is a protein called 30S RIBOSOMAL PROTEIN S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	P	84	Total	C	N	O	S	0	0	1
			701	443	140	117	1			

- Molecule 18 is a protein called 30S RIBOSOMAL PROTEIN S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	Q	100	Total	C	N	O	S	0	0	1
			824	528	152	142	2			

- Molecule 19 is a protein called 30S RIBOSOMAL PROTEIN S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
19	R	70	Total	C	N	O	0	0	0
			574	367	112	95			

- Molecule 20 is a protein called 30S RIBOSOMAL PROTEIN S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	S	79	Total	C	N	O	S	0	0	1
			630	403	115	110	2			

- Molecule 21 is a protein called 30S RIBOSOMAL PROTEIN S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	T	99	Total	C	N	O	S	0	0	0
			763	470	162	129	2			

- Molecule 22 is a protein called 30S RIBOSOMAL PROTEIN THX.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
22	U	25	Total	C	N	O	0	0	1
			209	128	51	30			

- Molecule 23 is a RNA chain called E-SITE TRNA FMET OR P-SITE TRNA FMET.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	V	77	Total	C	N	O	P	0	0	0
			1640	732	297	535	76			
23	W	77	Total	C	N	O	P	0	0	0
			1640	732	297	535	76			

- Molecule 24 is a RNA chain called MRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	X	5	Total	C	N	O	P	0	0	0
			104	48	19	33	4			

- Molecule 25 is a RNA chain called TMRNA DELA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	Y	62	Total	C	N	O	P	0	0	0
			1306	582	233	430	61			

- Molecule 26 is a protein called ELONGATION FACTOR TU.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	Z	378	Total	C	N	O	S	0	0	1
			2929	1854	510	553	12			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Z	181	GLU	GLN	CONFLICT	UNP Q5SHN6
Z	184	LYS	ARG	CONFLICT	UNP Q5SHN6
Z	189	LYS	ARG	CONFLICT	UNP Q5SHN6
Z	264	LYS	ARG	CONFLICT	UNP Q5SHN6
Z	288	LEU	VAL	CONFLICT	UNP Q5SHN6
Z	322	ILE	VAL	CONFLICT	UNP Q5SHN6
Z	336	THR	SER	CONFLICT	UNP Q5SHN6
Z	354	ARG	GLN	CONFLICT	UNP Q5SHN6
Z	357	GLN	PRO	CONFLICT	UNP Q5SHN6

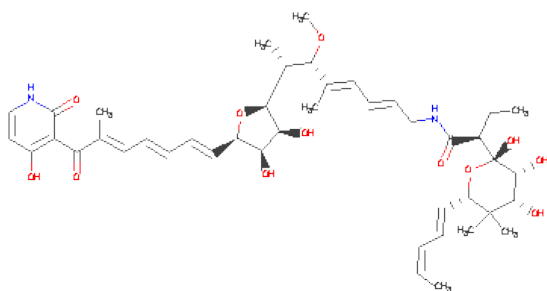
- Molecule 27 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
27	Z	2	Total	Mg	0	0
			2	2		

- Molecule 28 is ZINC ION (three-letter code: ZN) (formula: Zn).

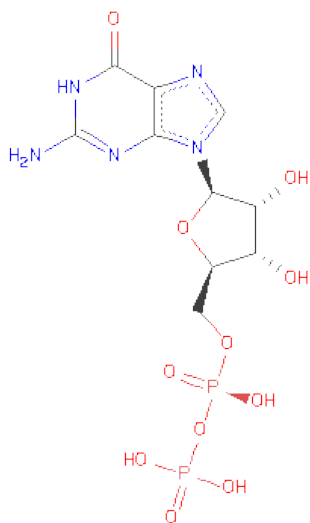
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
28	Y	1	Total	Zn	0	0
			1	1		
28	D	1	Total	Zn	0	0
			1	1		
28	N	1	Total	Zn	0	0
			1	1		

- Molecule 29 is KIRROMYCIN (three-letter code: KIR) (formula: C<sub>43</sub>H<sub>60</sub>N<sub>2</sub>O<sub>12</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
29	Z	1	Total	C	N	O	0	0
			57	43	2	12		

- Molecule 30 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula:  $C_{10}H_{15}N_5O_{11}P_2$ ).

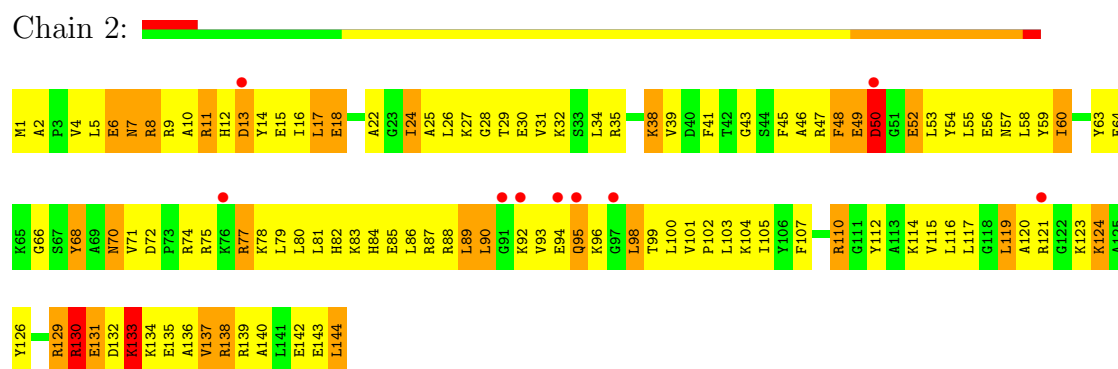


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
30	Z	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

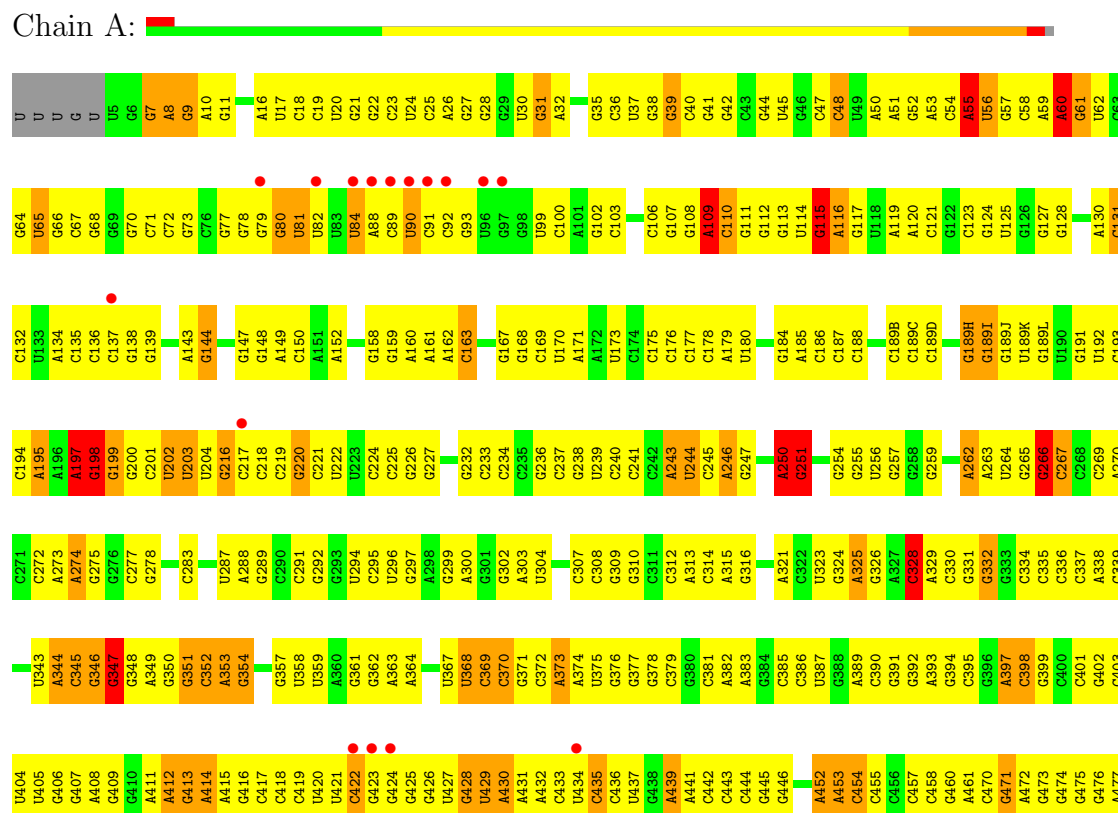
### 3 Residue-property plots

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

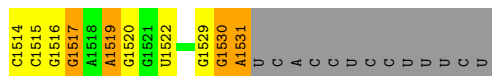
#### • Molecule 1: SMALL PROTEIN B SMPB



#### • Molecule 2: 16S RRNA

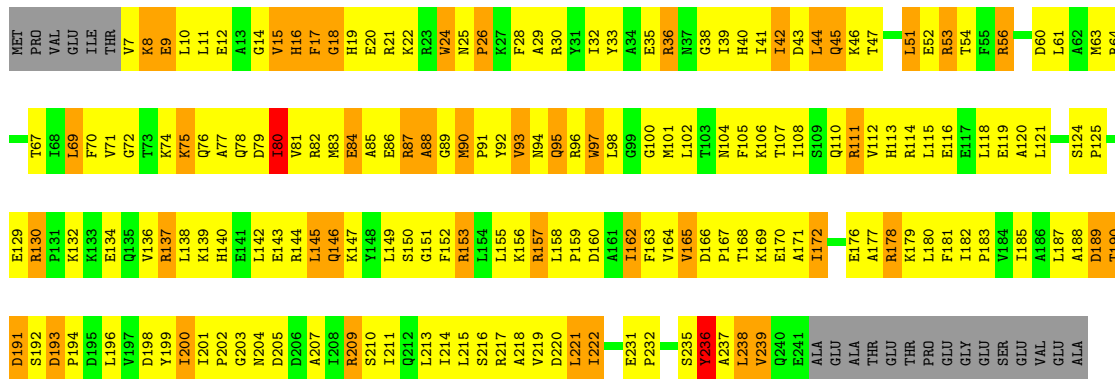


C1437	G1438	C1439	G1440	G1441	G1442	G1442A	G1442B	G1443	A1447	G1452	G1456	G1457	G1458	G1459	A1460	G1461	G1462	G1469	G1470	A1473	G1474	G1475	G1476	C1477	C1478	C1479	G1480	G1481	C1484	C1485	G1486	G1487	C1488	C1489	G1490	G1491	G1492	A1495	A1496	U1498	A1499	G1500	C1501	G1502	C1503	C1504	G1505	G1506	C1507	C1508	A1509	A1510	C1511	U1512	C1513	U1516	U1517	C1518	C1519	C1520	G1521	C1522	A1523	C1524	C1525	C1526	G1527	G1530	U1531	A1532	U1534	A1535	A1536	G1537	A1538	A1539	C1540	G1541	G1542	C1543	G1544																																
C545	G546	A547	G548	C549	G550	U551	U552	C556	C557	G558	G559	G560	U561	C562	G566	A572	A573	A574	A575	G576	G577	U580	G581	G585	C586	C590	U591	G592	G593	G594	G595	G596	C597	U603	G604	U605	G606	A607	A608	C609	G610	G611	G612	C613	U619	C620	G621	G622	G623	C624	G625	U626	G627	G628	G629	G630	A632	G633	C634	G635	U636	G637	G638	G639	G640	U641	C642	C643	C644	C645	U646	C647	U648	G649	G650	U653	A654	C655	C656	G657	G658	U659	G660	G661	A662	G663	U664	A665	G666	G667	G668	G671	U672	G673	G674	A675	U676	U677	C910	U678	C911	U679	G681	G682	G685	U686							
A687	G688	G689	U690	G691	U692	U697	G698	C701	A632	G633	A702	G633	A704	U705	A800	A781	C707	G638	C708	G709	A640	U641	A572	A573	A574	A575	G576	G577	U580	G581	G585	C586	C590	U591	G592	G593	G594	G595	G596	C597	U603	G604	U605	G606	A607	A608	C609	G610	G611	G612	C613	U619	C620	G621	G622	G623	C624	G625	U626	G627	G628	G629	G630	A632	G633	C634	G635	U636	G637	G638	G639	G640	U641	C642	C643	C644	C645	U646	C647	U648	G649	G650	U653	A654	C655	C656	G657	G658	U659	G660	G661	A662	G663	U664	A665	G666	G667	G668	G671	U672	G673	G674	A675	U676	U677	C910	U678	C911	U679	G681	G682	G685	U686
C762	G763	G764	G765	A766	G769	C770	U772	C776	G777	A778	G779	A780	A781	C707	G638	C708	G709	A640	U641	A572	A573	A574	A575	G576	G577	U580	G581	G585	C586	C590	U591	G592	G593	G594	G595	G596	C597	U603	G604	U605	G606	A607	A608	C609	G610	G611	G612	C613	U619	C620	G621	G622	G623	C624	G625	U626	G627	G628	G629	G630	A632	G633	C634	G635	U636	G637	G638	G639	G640	U641	C642	C643	C644	C645	U646	C647	U648	G649	G650	U653	A654	C655	C656	G657	G658	U659	G660	G661	A662	G663	U664	A665	G666	G667	G668	G671	U672	G673	G674	A675	U676	U677	C910	U678	C911	U679	G681	G682	G685	U686			
G838	U839	C840	U841	C848	C849	U850	G851	G852	G853	G854	C857	G858	A859	C860	G861	A864	A865	C866	G867	C868	C869	A872	C875	A792	G793	A794	C797	G798	G799	G800	U801	A802	G803	C808	G809	A891	A892	C893	G894	G895	C896	C899	A900	A901	C902	G903	C904	A909	C910	U911	C912	A913	G914	A915																																																											
G916	G917	A918	U919	C948	U920	G921	G922	A923	C924	G925	G926	G927	G928	C929	C930	C931	C934	A835	C936	A937	A938	G939	C940	G941	G942	G943	G944	G945	G946	G947	G948	A949	U950	G951	U952	G953	G954	U955	U956	U957	A958	A959	U960	C961	G962	G963	A964	A965	G966	C967	A968	A969	C970	G971	G972	G973	A974	A975	G976	A977																																																					
A978	C979	U980	U981	U982	U983	U984	U985	U986	U987	U988	U989	U990	U991	U992	U993	U994	U995	U996	A1001	G1001A	G1002	G1003	A1004	C1007	G1008	G1009	G1010	G1011	G1012	G1013	A1014	A1015	A1016	G1017	G1018	C1019	U1020	G1023	U1024	U1025	G1026	U1027	C1028	C1029	C1030	A1030A	G1031	G1032	G1033	G1034	G1035	G1036	C1037	U1038	C1039	U1040																																																									
A1041	G1042	A1046	G1047	G1048	U1049	G1050	G1051	U1052	G1053	U1054	A1055	U1056	G1057	G1058	C1059	G1060	G1061	U1062	G1063	G1064	U1065	C1066	U1070	C1075	U1076	G1077	A1080	G1081	G1082	U1090	U1091	G1094	U1095	C1096	C1097	G1098	G1099	C1100	A1101	A1102	C1103	G1104	A1105	G1106	C1107	G1108	A1111	C1112	C1113	C1114	A1116																																																														
G1117	C1118	C1119	U1120	U1121	U1122	A1123	G1124	U1125	U1126	U1127	C1128	U1129	A1130	G1131	G1132	U1133	U1134	U1135	U1136	U1137	G1138	C1139	C1140	C1141	G1142	G1143	G1144	C1145	A1146	C1147	U1148	C1149	U1150	A1151	A1152	C1153	G1154	G1155	G1156	A1157	C1158	U1159	G1160	C1161	C1162	C1163	C1164	C1165	G1166	A1168	A1169	C1170	C1171	C1172	G1173	U1174	G1175	A1176	A1179																																																						
A1180	G1181	G1184	G1187	C1188	G1189	G1190	A1191	C1192	G1193	U1194	U1195	U1196	U1197	U1198	U1199	C1200	A1201	G1202	C1203	A1204	U1205	G1206	U1211	U1212	A1213	C1214	G1215	G1216	C1217	C1218	U1219	A1220	G1221	G1222	A1225	C1226	A1227	C1228	A1229	C1230	G1231	U1232	G1233	C1234	U1235	A1236	C1237	A1238	A1239	C1240	G1241	C1242	C1243	C1244	A1245																																																										
C1246	U1247	C1248	C1249	A1250	C1251	A1252	G1253	C1254	G1255	A1256	U1257	G1258	C1259	C1260	A1261	C1262	C1263	C1264	G1265	G1266	A1269	C1270	G1271	G1276	C1277	U1278	A1279	A1280	U1281	C1282	C1283	C1284	A1285	A1286	A1287	A1288	A1289	G1290	G1291	U1292	G1293	G1294	G1295	C1296	A1299	G1300	U1301	U1302	C1303	C1304	G1305	G1306	U1307	U1308	G1309	G1310																																																									
G1311	G1312	U1313	C1314	U1315	C1316	C1317	A1318	C1319	C1320	C1321	C1322	G1323	A1324	C1325	C1326	C1327	C1328	A1329	U1330	G1331	A1332	A1333	G1334	G1335	C1342	G1343	C1344	U1345	A1346	G1347	U1348	A1349	A1350	U1351	C1352	G1353	C1354	G1355	G1356	A1357	U1358	G1359	A1360	G1361	C1362	C1363	A1363A	U1364	G1365	C1366	C1367	G1368	C1369	G1370	G1371	A1372	G1373	U1374	A1375																																																						
A1376	U1377	C1378	G1379	U1380	U1381	C1382	C1383	C1384	G1385	G1386	G1387	C1388	C1389	U1390	U1391	C1392	U1393	A1394	C1395	A1396	C1397	A1398	C1399	C1400	G1401	C1402	C1403	C1404	G1405	C1406	C1407	A1408	C1409	G1410	C1411	C1412	A1413	U1414	G1415	G1416	G1417	A1418	G1419	G1422	U1425	C1426	A1428	C1429	A1507	C1430	G1431	C1432	G1433	A1434	U1512	A1513																																																									
A1497	U1498	A1499	A1500	C1501	A1502	A1503	G1504	G1505	U1506	A1507	C1508	C1509	U1510	U1511	U1512	A1513																																																																																																	



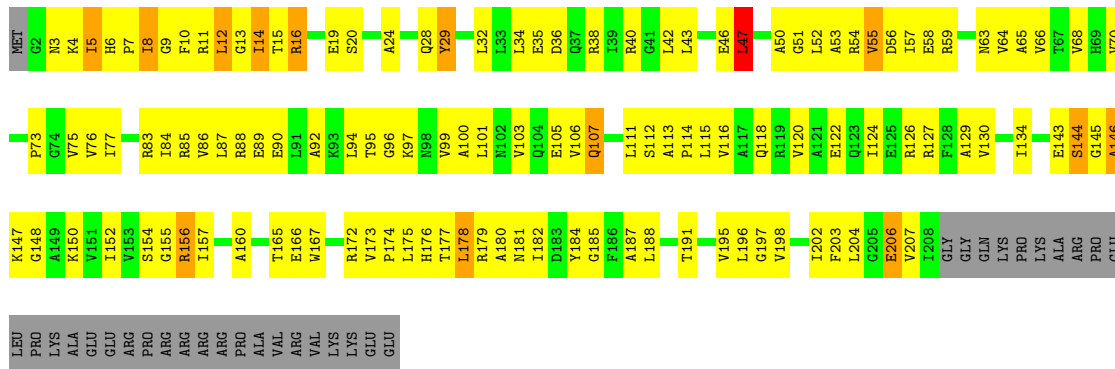
● Molecule 3: 30S RIBOSOMAL PROTEIN S2

Chain B:



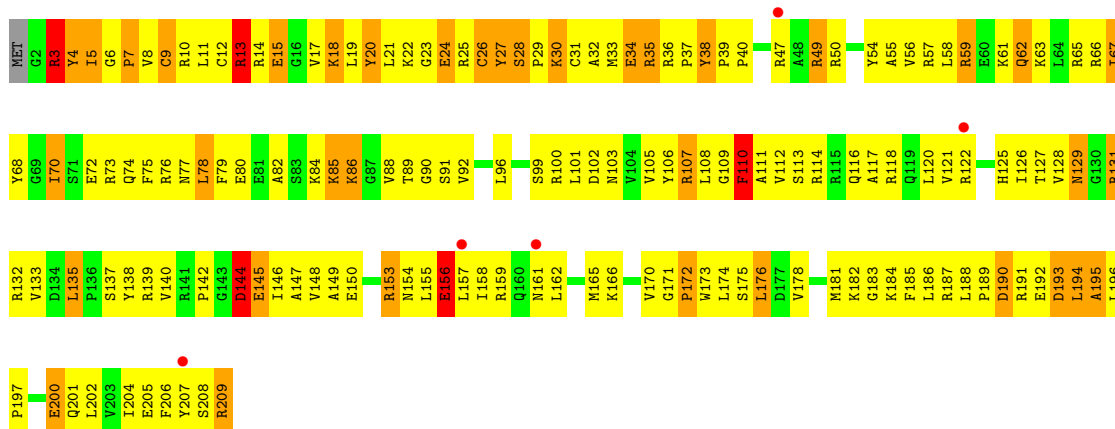
- Molecule 4: 30S RIBOSOMAL PROTEIN S3

Chain C:



- Molecule 5: 30S RIBOSOMAL PROTEIN S4

Chain D:



- Molecule 6: 30S RIBOSOMAL PROTEIN S5

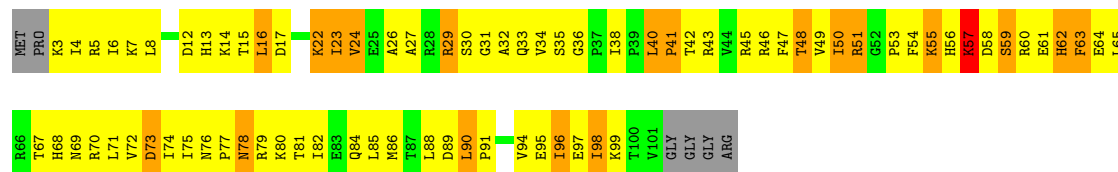
## Chain E:





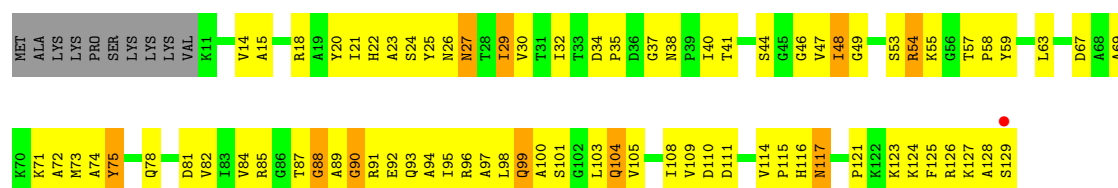
• Molecule 11: 30S RIBOSOMAL PROTEIN S10

Chain J:



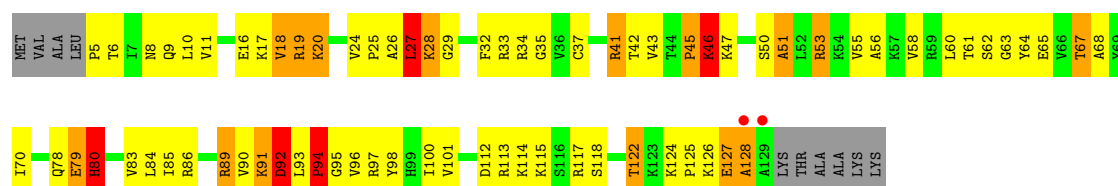
• Molecule 12: 30S RIBOSOMAL PROTEIN S11

Chain K:



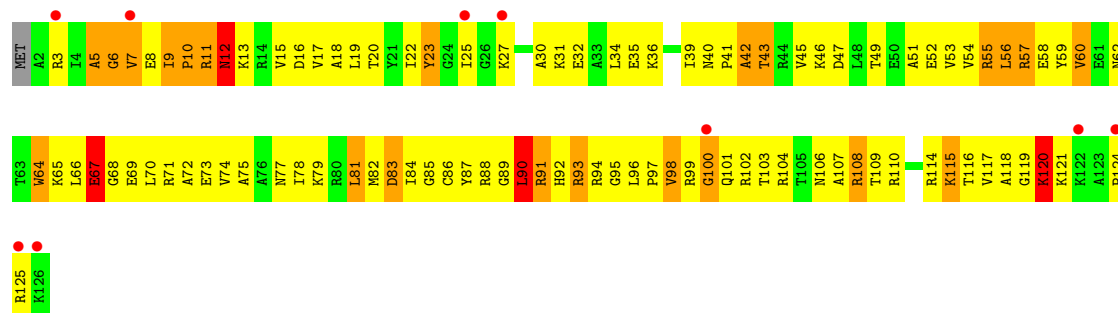
• Molecule 13: 30S RIBOSOMAL PROTEIN S12

Chain L:



• Molecule 14: 30S RIBOSOMAL PROTEIN S13

Chain M:



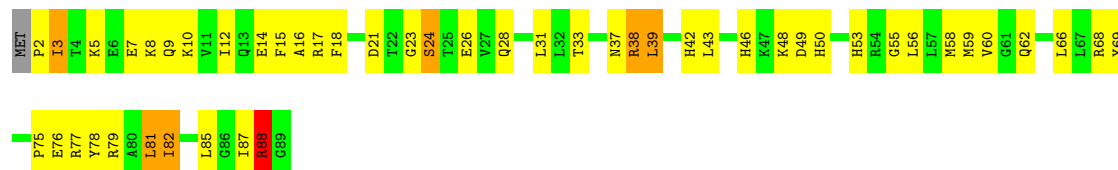
• Molecule 15: 30S RIBOSOMAL PROTEIN S14

Chain N:



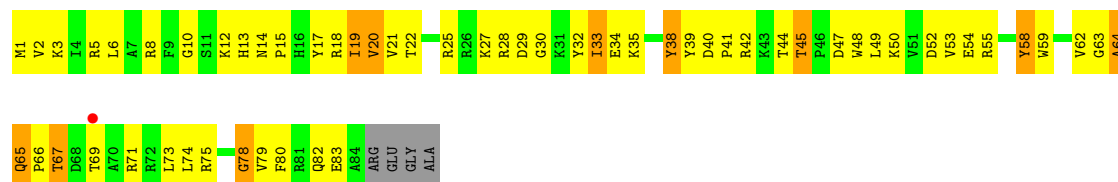
- Molecule 16: 30S RIBOSOMAL PROTEIN S15

Chain O:



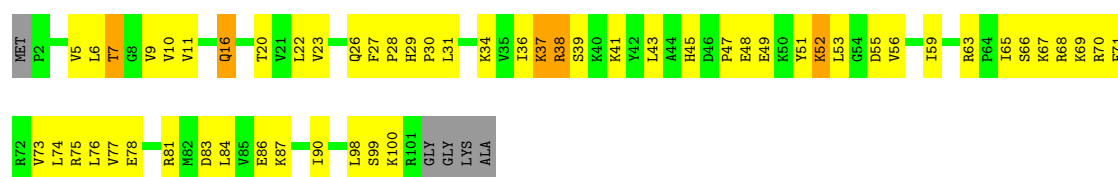
- Molecule 17: 30S RIBOSOMAL PROTEIN S16

Chain P:



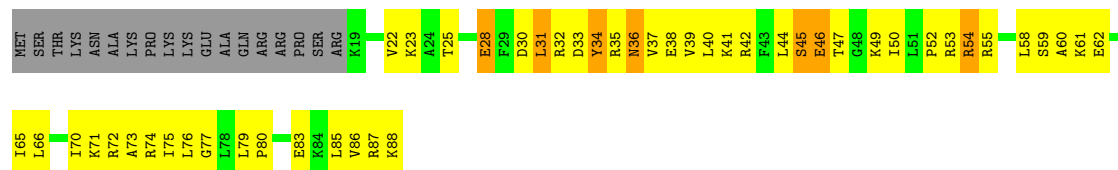
- Molecule 18: 30S RIBOSOMAL PROTEIN S17

Chain Q:



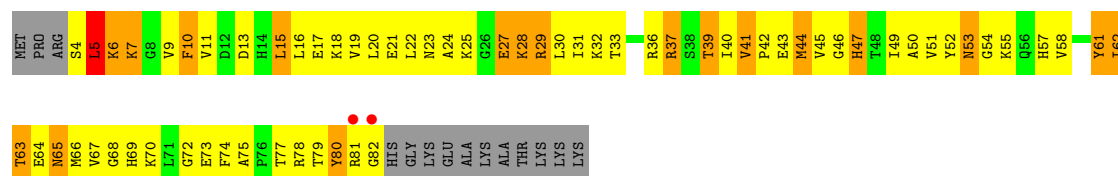
- Molecule 19: 30S RIBOSOMAL PROTEIN S18

Chain R:



- Molecule 20: 30S RIBOSOMAL PROTEIN S19

Chain S:



- Molecule 21: 30S RIBOSOMAL PROTEIN S20

Chain T:



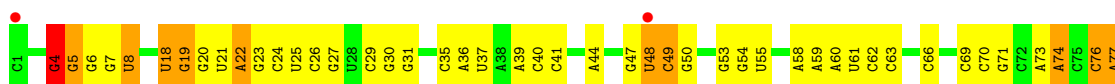
● Molecule 22: 30S RIBOSOMAL PROTEIN THX

Chain U:



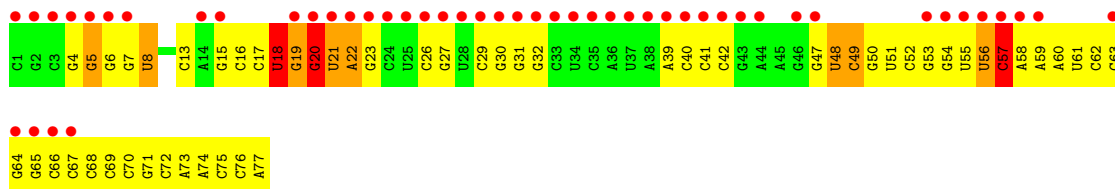
- Molecule 23: E-SITE TRNA FMET OR P-SITE TRNA FMET

Chain V:



- Molecule 23: E-SITE TRNA FMET OR P-SITE TRNA FMET

Chain W:



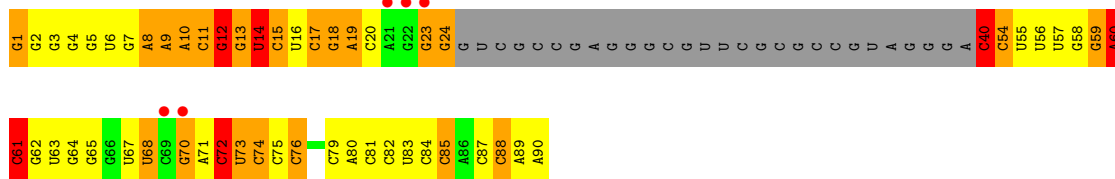
- Molecule 24: mRNA

Chain X:



- Molecule 25: TMRNA DELA

Chain Y:



• Molecule 26: ELONGATION FACTOR TU

Chain Z:



T347	D348	V349	V352	V353	R354	L355	P356	V359	E360	M361	V362	M363	P365	D366	N367	V368	T369	F370	T371	V372	E373	L374	K375	K376	P377	V378	A379	L380	E381	E382	G383	L384	R385	I388	R393	T394	V395	G396	A397	G398	V399	V400	T401	K402	T403	L404	E405										
A282	G283	D284	N285	V286	G287	L288	L289	L290	R291	G292	V293	S294	R295	V298	E299	R300	G301	Q302	V303	L304	P307	T310	T311	P312	H313	T314	A315	F316	E317	A318	Y321	I322	L323	K324	K325	E326	E327	G328	G329	R330	H331	T332	G333	F334	F335	T336	G337	Y338	R339	P340	Q341	F342	R345	T346			
D218	K219	F220	F221	L222	M223	P224	V225	E226	D227	V228	F229	T230	I231	T232	G233	R234	G235	T236	V237	A238	T239	G240	R241	I242	E243	R244	V247	K248	V249	G250	D251	V252	E254	I255	V256	G257	T262	R263	K264	T265	V266	V267	T268	G269	V270	E271	H272	H273	R274	K275	T276	L277	Q278	E279	G280	I281	
M113	P114	Q115	T116	H119	I120	L121	L122	A123	R124	Q125	V126	P129	Y130	I131	V132	V133	F134	M135	D139	M140	V141	D142	D143	P144	E145	L146	L147	D148	E180	E181	M182	H183	K184	M185	P186	K187	T188	M193	E194	W195	V196	D197	K198	I199	L202	L206	D207	E208	Y209	T210	P211	T212	T213	V214	R215	D216	V217
A73	K74	H75	H76	Y77	S78	H79	Y80	D81	C82	P83	G84	H85	A86	D87	Y88	I89	K90	N91	A96	A97	Q98	M99	D100	G101	A102	M113	P114	Q115	T116	H119	I120	L121	L122	A123	R124	Q125	V126	P129	Y130	I131	V132	V133	F134	M135	D139	M140	V141	D142	D143	P144	E145	L146	L147	D148			

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	202.17Å 290.76Å 250.65Å 90.00° 97.63° 90.00°	Depositor
Resolution (Å)	50.00 – 3.10 49.68 – 3.10	Depositor EDS
% Data completeness (in resolution range)	97.7 (50.00-3.10) 97.4 (49.68-3.10)	Depositor EDS
$R_{merge}$	0.24	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.94 (at 3.12Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.230 , 0.270 0.466 , 0.473	Depositor DCC
$R_{free}$ test set	24439 reflections (4.85%)	DCC
Wilson B-factor (Å <sup>2</sup> )	44.8	Xtriage
Anisotropy	0.304	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 39.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 503945 reflections	Xtriage
$F_o, F_c$ correlation	0.44	EDS
Total number of atoms	60380	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.67% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GDP, KIR, ZN, 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	2	0.49	0/1203	0.71	1/1606 (0.1%)
2	A	0.48	1/36192 (0.0%)	0.78	39/56489 (0.1%)
3	B	0.46	0/1936	0.72	0/2611
4	C	0.43	0/1637	0.69	0/2207
5	D	0.40	0/1733	0.68	0/2318
6	E	0.49	0/1163	0.72	0/1566
7	F	0.43	0/856	0.68	1/1154 (0.1%)
8	G	0.36	0/1276	0.61	0/1709
9	H	0.45	0/1136	0.75	0/1527
10	I	0.41	0/1029	0.67	0/1378
11	J	0.42	0/808	0.69	0/1087
12	K	0.39	0/900	0.65	0/1213
13	L	0.45	0/987	0.74	0/1322
14	M	0.38	0/999	0.71	0/1338
15	N	0.45	0/501	0.75	0/664
16	O	0.45	0/745	0.70	0/992
17	P	0.42	0/717	0.65	0/965
18	Q	0.42	0/837	0.67	0/1119
19	R	0.42	0/579	0.70	0/768
20	S	0.45	0/643	0.67	1/867 (0.1%)
21	T	0.37	0/765	0.65	0/1007
22	U	0.48	0/213	0.63	0/279
23	V	0.45	0/1832	0.79	1/2855 (0.0%)
23	W	0.45	0/1832	0.81	3/2855 (0.1%)
24	X	0.71	0/116	0.89	0/179
25	Y	0.82	5/1455 (0.3%)	0.97	5/2258 (0.2%)
26	Z	0.42	0/2986	0.69	0/4050
All	All	0.47	6/65076 (0.0%)	0.76	51/96383 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is

detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	A	4	40
23	V	0	1
23	W	0	3
25	Y	0	3
All	All	4	47

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	Y	12	G	C2-N2	-13.61	1.21	1.34
25	Y	40	C	OP3-P	-6.93	1.52	1.61
25	Y	1	G	OP3-P	-6.81	1.52	1.61
25	Y	12	G	N9-C4	5.51	1.42	1.38
25	Y	12	G	N3-C4	5.17	1.39	1.35

The worst 5 of 51 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	115	G	C2'-C3'-O3'	9.61	130.64	109.50
2	A	966	G	N9-C1'-C2'	-9.47	101.58	112.00
2	A	1498	U	C2'-C3'-O3'	9.43	130.25	109.50
2	A	575	G	C2'-C3'-O3'	8.98	129.25	109.50
23	V	4	G	N9-C1'-C2'	-8.74	102.39	112.00

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	115	G	C3'
2	A	1399	C	C3'
2	A	1498	U	C3'
2	A	1504	G	C3'

5 of 47 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	197	A	Sidechain
2	A	198	G	Sidechain
2	A	245	C	Sidechain
2	A	250	A	Sidechain
2	A	251	G	Sidechain

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2	1184	0	1235	205	0
2	A	32330	0	16318	1284	0
3	B	1901	0	1951	255	0
4	C	1613	0	1677	152	0
5	D	1703	0	1764	264	0
6	E	1147	0	1207	135	0
7	F	843	0	857	69	0
8	G	1257	0	1296	103	0
9	H	1116	0	1177	77	0
10	I	1011	0	1043	156	0
11	J	795	0	840	176	0
12	K	885	0	904	83	0
13	L	971	0	1057	105	0
14	M	988	0	1059	166	0
15	N	492	0	529	90	0
16	O	734	0	771	61	0
17	P	701	0	720	70	0
18	Q	824	0	891	54	0
19	R	574	0	644	62	0
20	S	630	0	652	103	0
21	T	763	0	861	83	0
22	U	209	0	221	14	0
23	V	1640	0	837	40	0
23	W	1640	0	837	74	0
24	X	104	0	55	4	0
25	Y	1306	0	663	82	0
26	Z	2929	0	2941	340	0
27	Z	2	0	0	0	0
28	D	1	0	0	0	0
28	N	1	0	0	0	0
28	Y	1	0	0	0	0
29	Z	57	0	58	7	0
30	Z	28	0	12	2	0
All	All	60380	0	43077	3966	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 38.

The worst 5 of 3966 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:D:20:TYR:HA	5:D:26:CYS:SG	1.82	1.19
1:2:129:ARG:HA	2:A:1397:C:H42	1.06	1.15
26:Z:101:GLY:HA3	26:Z:210:ILE:HD11	1.25	1.14
26:Z:315:LYS:HB2	26:Z:405:GLU:HG2	1.30	1.13
14:M:12:ASN:HD21	14:M:46:LYS:HB2	1.14	1.10

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	2	142/144 (99%)	124 (87%)	14 (10%)	4 (3%)	8	39
3	B	233/256 (91%)	153 (66%)	55 (24%)	25 (11%)	1	5
4	C	205/239 (86%)	141 (69%)	49 (24%)	15 (7%)	2	12
5	D	206/209 (99%)	126 (61%)	52 (25%)	28 (14%)	0	2
6	E	149/162 (92%)	121 (81%)	21 (14%)	7 (5%)	4	23
7	F	99/101 (98%)	80 (81%)	14 (14%)	5 (5%)	3	22
8	G	153/156 (98%)	109 (71%)	34 (22%)	10 (6%)	2	15
9	H	136/138 (99%)	120 (88%)	14 (10%)	2 (2%)	15	57
10	I	125/128 (98%)	73 (58%)	33 (26%)	19 (15%)	0	1
11	J	97/105 (92%)	69 (71%)	18 (19%)	10 (10%)	1	6
12	K	117/129 (91%)	87 (74%)	21 (18%)	9 (8%)	1	11
13	L	123/135 (91%)	84 (68%)	23 (19%)	16 (13%)	0	3
14	M	123/126 (98%)	76 (62%)	28 (23%)	19 (15%)	0	1
15	N	58/61 (95%)	43 (74%)	5 (9%)	10 (17%)	0	0
16	O	86/89 (97%)	67 (78%)	16 (19%)	3 (4%)	6	32

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	P	82/88 (93%)	53 (65%)	23 (28%)	6 (7%)	2	12
18	Q	98/105 (93%)	76 (78%)	20 (20%)	2 (2%)	11	49
19	R	68/88 (77%)	53 (78%)	10 (15%)	5 (7%)	2	11
20	S	77/93 (83%)	53 (69%)	14 (18%)	10 (13%)	0	3
21	T	97/106 (92%)	72 (74%)	17 (18%)	8 (8%)	1	10
22	U	23/27 (85%)	11 (48%)	10 (44%)	2 (9%)	1	9
26	Z	374/405 (92%)	295 (79%)	58 (16%)	21 (6%)	3	19
All	All	2871/3090 (93%)	2086 (73%)	549 (19%)	236 (8%)	1	10

5 of 236 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	2	133	LYS
3	B	15	VAL
3	B	18	GLY
3	B	75	LYS
3	B	97	TRP

### 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	2	120/120 (100%)	81 (68%)	39 (32%)	0	0
3	B	202/220 (92%)	172 (85%)	30 (15%)	4	17
4	C	160/188 (85%)	149 (93%)	11 (7%)	22	62
5	D	180/181 (99%)	152 (84%)	28 (16%)	4	14
6	E	115/123 (94%)	99 (86%)	16 (14%)	5	21
7	F	90/90 (100%)	76 (84%)	14 (16%)	4	14
8	G	126/127 (99%)	115 (91%)	11 (9%)	15	49
9	H	119/119 (100%)	108 (91%)	11 (9%)	13	45
10	I	98/99 (99%)	87 (89%)	11 (11%)	9	33
11	J	88/92 (96%)	74 (84%)	14 (16%)	4	13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	K	90/99 (91%)	84 (93%)	6 (7%)	23	63
13	L	104/111 (94%)	91 (88%)	13 (12%)	7	25
14	M	99/101 (98%)	84 (85%)	15 (15%)	4	16
15	N	49/50 (98%)	41 (84%)	8 (16%)	3	12
16	O	79/80 (99%)	72 (91%)	7 (9%)	14	47
17	P	72/74 (97%)	64 (89%)	8 (11%)	9	33
18	Q	94/97 (97%)	89 (95%)	5 (5%)	32	72
19	R	61/77 (79%)	56 (92%)	5 (8%)	17	53
20	S	69/80 (86%)	57 (83%)	12 (17%)	3	11
21	T	76/82 (93%)	68 (90%)	8 (10%)	10	35
22	U	19/22 (86%)	16 (84%)	3 (16%)	4	14
26	Z	316/338 (94%)	275 (87%)	41 (13%)	6	23
All	All	2426/2570 (94%)	2110 (87%)	316 (13%)	6	23

5 of 316 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	G	77	SER
11	J	51	ARG
26	Z	218	ASP
8	G	144	MET
10	I	10	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 65 such sidechains are listed below:

Mol	Chain	Res	Type
8	G	148	ASN
11	J	78	ASN
26	Z	19	HIS
9	H	82	HIS
10	I	124	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	A	1503/1522 (98%)	248 (16%)	56 (3%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
23	V	76/77 (98%)	12 (15%)	2 (2%)
23	W	76/77 (98%)	11 (14%)	2 (2%)
24	X	4/19 (21%)	1 (25%)	0
25	Y	60/90 (66%)	22 (36%)	13 (21%)
All	All	1719/1785 (96%)	294 (17%)	73 (4%)

5 of 294 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	A	8	A
2	A	9	G
2	A	31	G
2	A	32	A
2	A	39	G

5 of 73 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	A	983	A
2	A	1139	G
25	Y	23	G
2	A	1053	G
2	A	1157	A

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 7 ligands modelled in this entry, 5 are monoatomic - leaving 2 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	$\# Z  > 2$
29	KIR	Z	1406	-	59,59,59	3.53	22 (37%)	82,84,84	2.13	22 (26%)
30	GDP	Z	1407	27	30,30,30	1.32	3 (10%)	44,47,47	2.51	9 (20%)

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
29	KIR	Z	1406	-	-	0/53/98/98	0/3/3/3
30	GDP	Z	1407	27	-	0/16/32/32	0/1/3/3

The worst 5 of 25 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	Z	1406	KIR	O18-C17	-12.54	1.24	1.44
29	Z	1406	KIR	O30-C30	-12.10	1.16	1.42
29	Z	1406	KIR	O34-C33	-11.32	1.28	1.44
29	Z	1406	KIR	C45-C28	5.65	1.61	1.54
29	Z	1406	KIR	C5-C4	4.84	1.48	1.39

The worst 5 of 31 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	Z	1407	GDP	C6-C5-N7	-12.71	132.43	134.14
29	Z	1406	KIR	C3-C2-N1	8.86	122.86	115.40
29	Z	1406	KIR	O29-C29-O34	-5.89	100.64	110.22
29	Z	1406	KIR	C4-C3-C7	5.27	133.90	119.37
29	Z	1406	KIR	C45-C28-C27	4.84	111.63	108.10

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	2	144/144 (100%)	0.55	9 (6%) 19 3	49, 78, 118, 124	0
2	A	1504/1522 (98%)	0.36	40 (2%) 52 8	14, 52, 128, 187	0
3	B	235/256 (91%)	-0.00	0 100 100	27, 51, 114, 128	0
4	C	207/239 (86%)	0.04	0 100 100	36, 59, 86, 96	0
5	D	208/209 (99%)	0.40	5 (2%) 56 9	47, 74, 111, 116	0
6	E	151/162 (93%)	-0.12	0 100 100	23, 40, 70, 92	0
7	F	101/101 (100%)	-0.05	0 100 100	33, 56, 71, 95	0
8	G	155/156 (99%)	0.29	5 (3%) 45 7	52, 75, 107, 129	0
9	H	138/138 (100%)	0.00	2 (1%) 72 17	17, 36, 54, 67	0
10	I	127/128 (99%)	0.31	1 (0%) 83 28	46, 82, 107, 111	0
11	J	99/105 (94%)	0.20	0 100 100	42, 82, 119, 122	0
12	K	119/129 (92%)	0.13	1 (0%) 83 28	26, 56, 90, 107	0
13	L	125/135 (92%)	0.21	2 (1%) 68 15	24, 50, 69, 112	0
14	M	125/126 (99%)	0.33	9 (7%) 15 2	42, 80, 107, 139	0
15	N	60/61 (98%)	0.11	1 (1%) 67 15	38, 48, 70, 77	0
16	O	88/89 (98%)	-0.08	0 100 100	22, 41, 64, 69	0
17	P	84/88 (95%)	0.19	1 (1%) 75 20	39, 58, 77, 102	0
18	Q	100/105 (95%)	0.03	0 100 100	27, 47, 68, 73	0
19	R	70/88 (79%)	-0.19	0 100 100	28, 46, 71, 79	0
20	S	79/93 (84%)	0.24	2 (2%) 54 9	55, 73, 101, 111	0
21	T	99/106 (93%)	0.14	0 100 100	46, 65, 101, 104	0
22	U	25/27 (92%)	0.46	0 100 100	52, 65, 83, 84	0
23	V	77/77 (100%)	0.21	2 (2%) 53 8	36, 57, 97, 104	0
23	W	77/77 (100%)	3.09	49 (63%) 0 0	95, 192, 197, 199	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
24	X	5/19 (26%)	0.24	0 100 100	34, 36, 69, 80	0
25	Y	62/90 (68%)	0.89	5 (8%) 12 2	55, 85, 125, 136	0
26	Z	378/405 (93%)	0.10	8 (2%) 60 11	23, 56, 92, 124	0
All	All	4642/4875 (95%)	0.27	142 (3%) 47 7	14, 59, 114, 199	0

The worst 5 of 142 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
23	W	35	C	15.2
23	W	34	U	8.3
23	W	42	C	8.3
23	W	36	A	8.2
2	A	422	C	7.8

## 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
28	ZN	D	1001	1/1	0.14	-	59,59,59,59	0
30	GDP	Z	1407	28/28	0.16	-	36,43,44,45	0
29	KIR	Z	1406	57/57	0.40	-	101,117,134,134	0
28	ZN	N	1001	1/1	0.07	-	51,51,51,51	0
27	MG	Z	1002	1/1	0.25	-	10,10,10,10	0
27	MG	Z	1001	1/1	0.18	-	25,25,25,25	0
28	ZN	Y	1001	1/1	0.08	-	58,58,58,58	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.