



wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 10:59 AM GMT

PDB ID : 4KD0
Title : 70S Ribosome translocation intermediate GDPNP-I containing elongation factor EFG/GDPNP, MRNA, AND TRNA BOUND IN THE pe^*/E STATE. THIS ENTRY CONTAINS THE 30S RIBOSOMAL SUBUNIT B. THE 50S SUBUNIT B CAN BE FOUND IN 4KD2. MOLECULE A IN THE SAME ASYMMETRIC UNIT IS DEPOSITED AS 4KCY (30S) AND 4KCZ (50S)
Authors : Zhou, J.; Lancaster, L.; Donohue, J.P.; Noller, H.F.
Deposited on : 2013-04-24
Resolution : 3.50 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

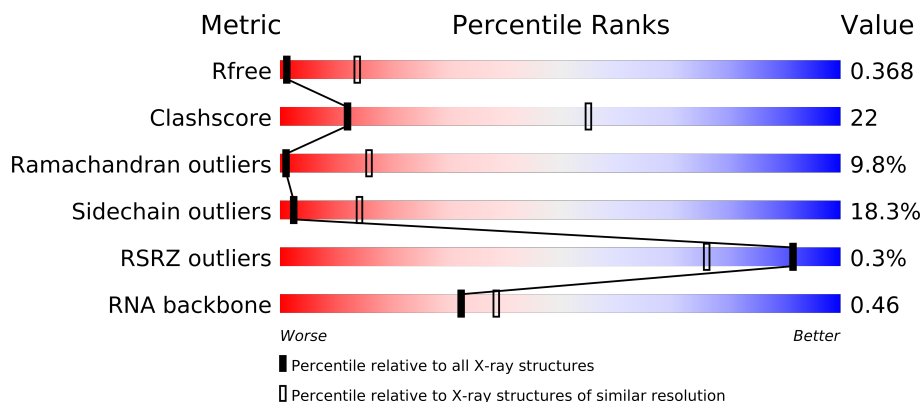
The following versions of software and data (see [references](#)) were used in the production of this report:

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 3.50 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.



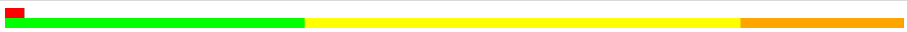
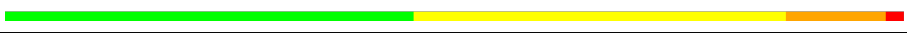
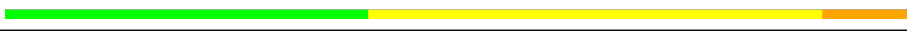

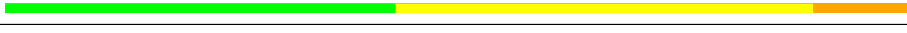


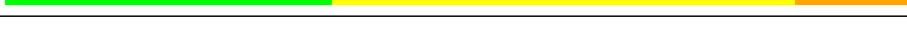

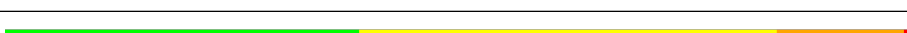
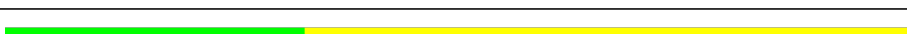

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	1243 (3.70-3.30)
Clashscore	79885	1039 (3.66-3.34)
Ramachandran outliers	78287	1000 (3.66-3.34)
Sidechain outliers	78261	1000 (3.66-3.34)
RSRZ outliers	66119	1243 (3.70-3.30)
RNA backbone	1838	1007 (4.22-2.76)

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. 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	B	235	
2	C	207	
3	D	208	
4	E	151	
5	F	101	
6	G	155	
7	H	138	
8	I	127	
9	J	99	
10	K	119	
11	L	125	
12	M	125	

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Mol	Chain	Length	Quality of chain
13	N	60	
14	O	88	
15	P	84	
16	Q	100	
17	R	70	
18	S	79	
19	T	99	
20	A	1511	
21	W	77	
22	V	23	
23	Y	687	
24	U	6	

2 Entry composition

There are 26 unique types of molecules in this entry. The entry contains 59087 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 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	235	Total	C	N	O	S	0	0	0
			1910	1218	342	345	5			

- Molecule 2 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	207	Total	C	N	O	S	0	0	0
			1621	1022	315	283	1			

- Molecule 3 is a protein called 30S ribosomal protein S4.

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

- Molecule 4 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	151	Total	C	N	O	S	0	0	0
			1156	729	218	205	4			

- Molecule 5 is a protein called 30S ribosomal protein S6.

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

- Molecule 6 is a protein called 30S ribosomal protein S7.

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

- Molecule 7 is a protein called 30S ribosomal protein S8.

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

- Molecule 8 is a protein called 30S ribosomal protein S9.

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

- Molecule 9 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	J	99	Total	C	N	O	S	0	0	0
			802	504	157	140	1			

- Molecule 10 is a protein called 30S ribosomal protein S11.

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

- Molecule 11 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	L	125	Total	C	N	O	S	0	0	0
			976	614	196	165	1			

- Molecule 12 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	M	125	Total	C	N	O	S	0	0	0
			997	617	207	171	2			

- Molecule 13 is a protein called 30S ribosomal protein S14 type Z.

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

- Molecule 14 is a protein called 30S ribosomal protein S15.

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

- Molecule 15 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	P	84	Total	C	N	O	S	0	0	0
			706	446	140	119	1			

- Molecule 16 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	Q	100	Total	C	N	O	S	0	0	0
			835	534	156	143	2			

- Molecule 17 is a protein called 30S ribosomal protein S18.

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

- Molecule 18 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	S	79	Total	C	N	O	S	0	0	0
			634	405	115	112	2			

- Molecule 19 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	T	99	Total	C	N	O	S	0	0	0
			762	469	162	129	2			

- Molecule 20 is a RNA chain called ribosomal RNA 16S.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	A	1511	Total	C	N	O	P	0	0	0
			32474	14455	6015	10494	1510			

- Molecule 21 is a RNA chain called transfer RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	W	77	Total	C	N	O	P	0	0	0
			1635	732	291	536	76			

- Molecule 22 is a RNA chain called messenger RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	V	23	Total	C	N	O	P	0	0	0
			503	227	106	148	22			

- Molecule 23 is a protein called Elongation factor G.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	Y	687	Total	C	N	O	S	0	0	0
			5380	3414	922	1024	20			

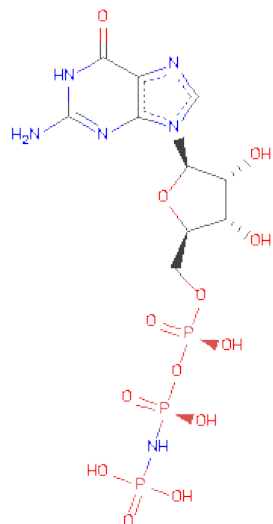
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Y	129	LYS	HIS	CONFLICT	UNP Q72I01
Y	226	ASN	HIS	CONFLICT	UNP Q72I01

- Molecule 24 is a protein called VIOMYCIN.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
24	U	6	Total	C	N	O	0	0	0
			48	25	13	10			

- Molecule 25 is PHOSPHOAMINOPHOSPHONICACID-GUANYLATE ESTER (three-letter code: GNP) (formula: C₁₀H₁₇N₆O₁₃P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
25	Y	1	32	10	6	13	3	0	0

- Molecule 26 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

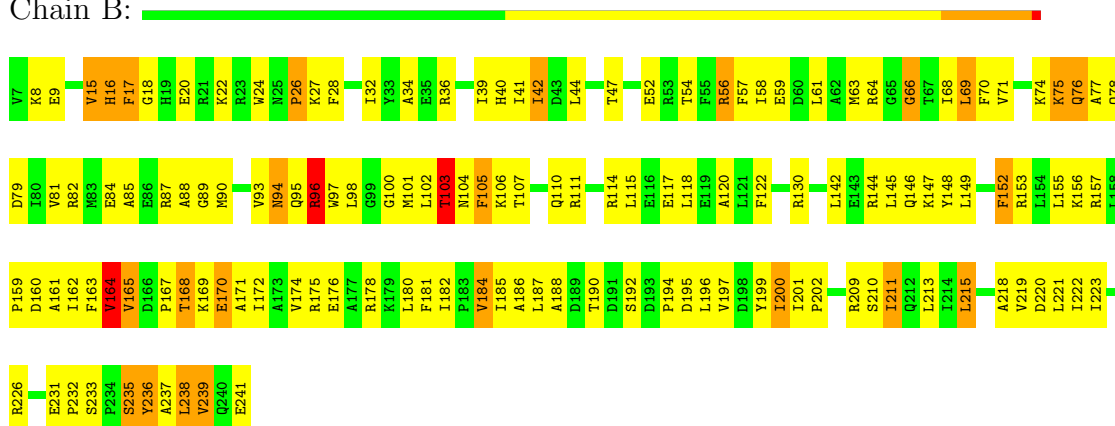
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
26	Y	1	1	1	0	0

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.

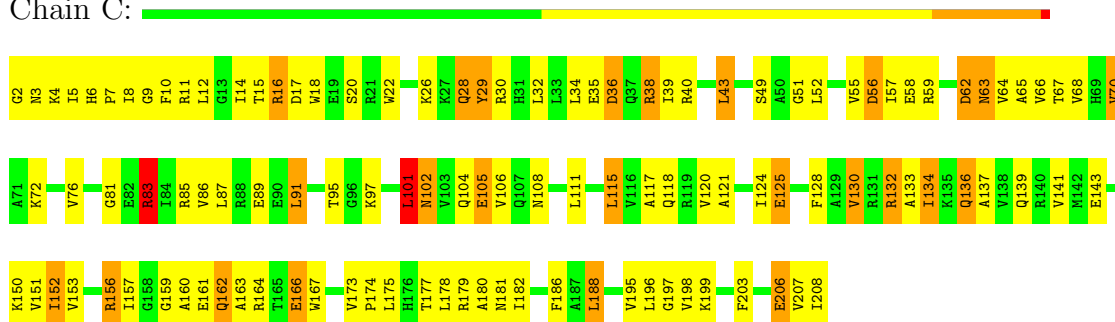
• Molecule 1: 30S ribosomal protein S2

Chain B:



• Molecule 2: 30S ribosomal protein S3

Chain C:



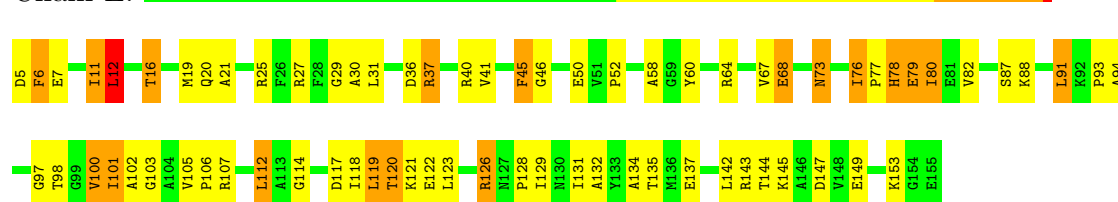
• Molecule 3: 30S ribosomal protein S4

Chain D:



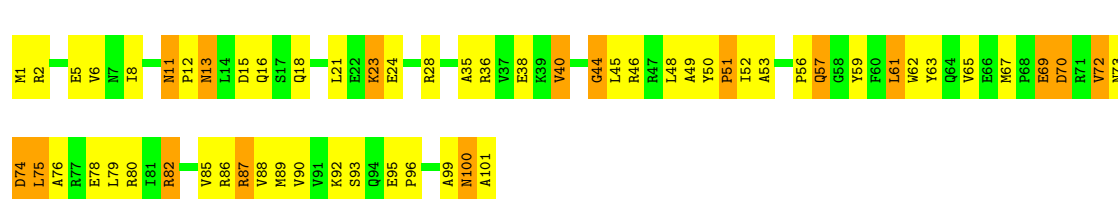
- Molecule 4: 30S ribosomal protein S5

Chain E:



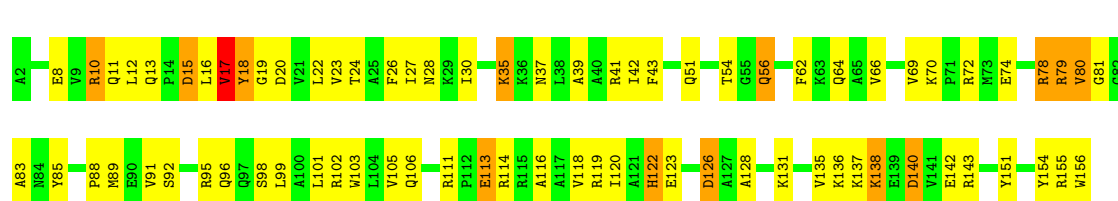
- Molecule 5: 30S ribosomal protein S6

Chain F:



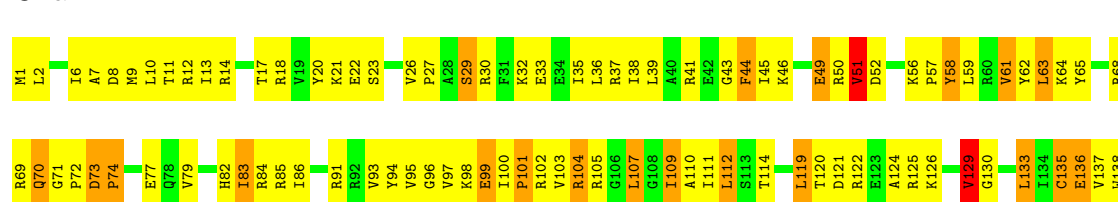
- Molecule 6: 30S ribosomal protein S7

Chain G:



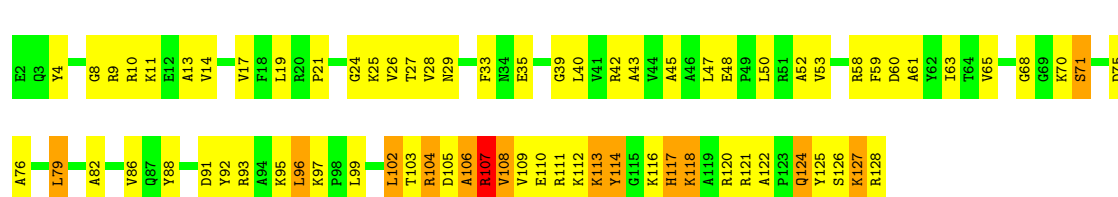
- Molecule 7: 30S ribosomal protein S8

Chain H:



- Molecule 8: 30S ribosomal protein S9

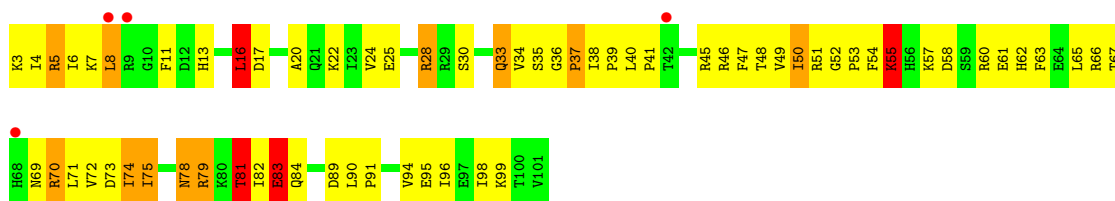
Chain I:



- Molecule 9: 30S ribosomal protein S10

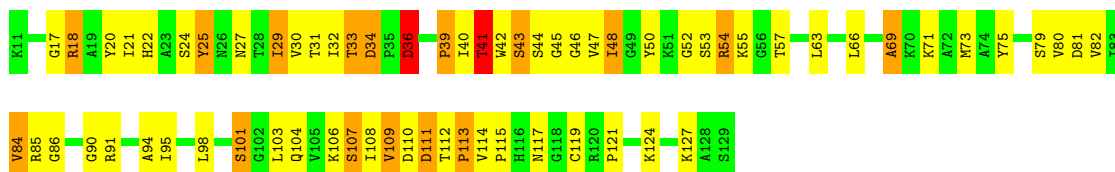
Chain J:





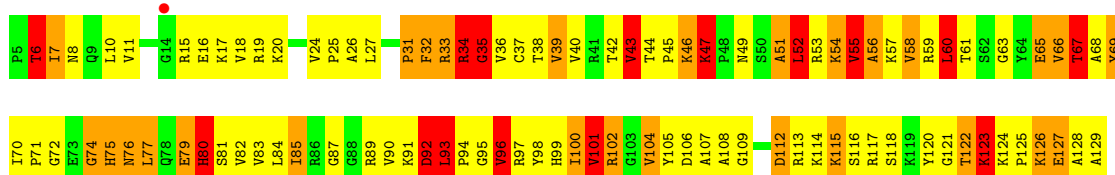
• Molecule 10: 30S ribosomal protein S11

Chain K:



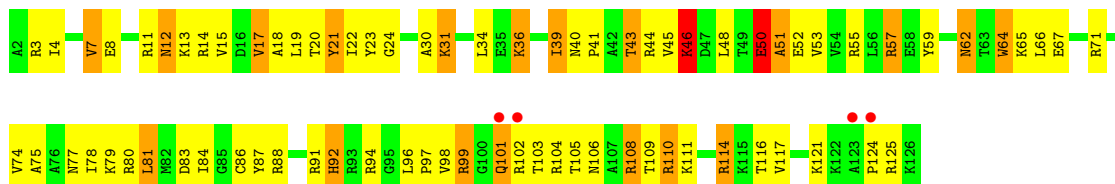
• Molecule 11: 30S ribosomal protein S12

Chain L:



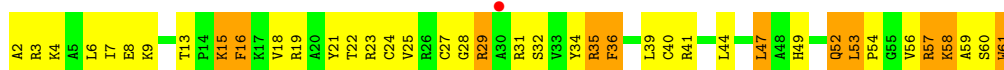
• Molecule 12: 30S ribosomal protein S13

Chain M:



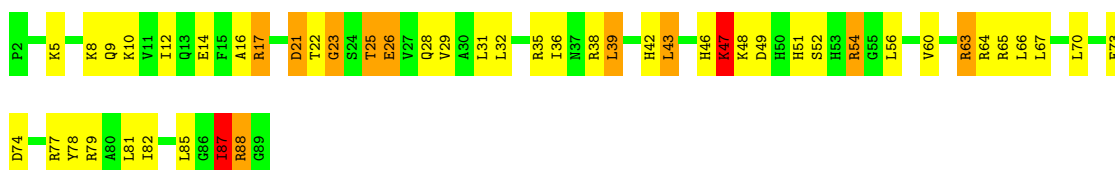
• Molecule 13: 30S ribosomal protein S14 type Z

Chain N:



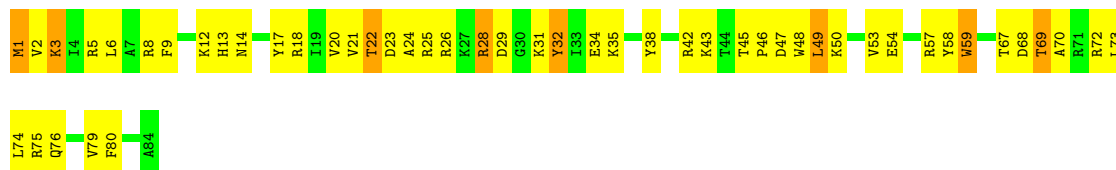
• Molecule 14: 30S ribosomal protein S15

Chain O:



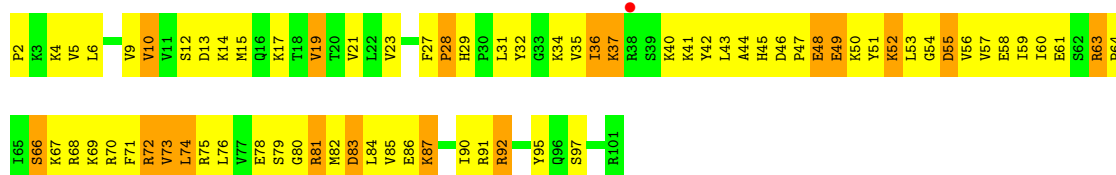
- Molecule 15: 30S ribosomal protein S16

Chain P:



- Molecule 16: 30S ribosomal protein S17

Chain Q:

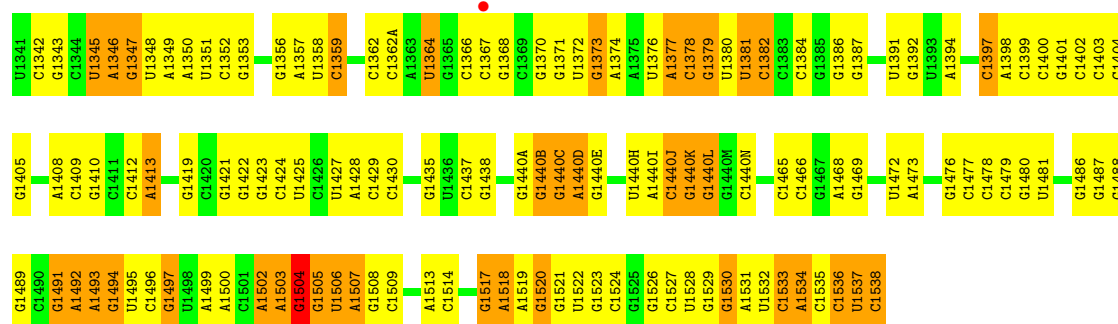


- Molecule 17: 30S ribosomal protein S18

Chain R:

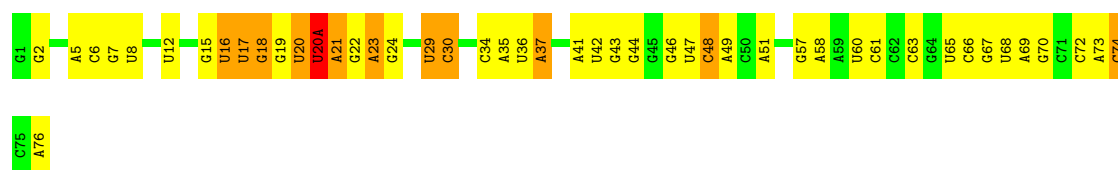


U1276	U1277	U1278	U1279	U1280	U1281	U1282	U1283	U1284	U1285	U1286	U1287	U1288	U1289	U1290	U1291	U1292	U1293	U1294	U1295	U1296	U1297	U1298	U1299	U1300	U1301	U1302	U1303	U1304	U1305	U1306	U1307	U1308	U1309	U1310	U1311	U1312	U1313	U1314	U1315	U1316	U1317	U1318	U1319	U1320	U1321	U1322	U1323	U1324	U1325	U1326	U1327	U1328	U1329	U1330	U1331	U1332	U1333	U1334	U1335	U1336	U1337	U1338	U1339	U1340																																																																																																																																																																																																																																																																																								
U1212	U1213	U1214	U1215	U1216	U1217	U1218	U1219	U1220	U1221	U1222	U1223	U1224	U1225	U1226	U1227	U1228	U1229	U1230	U1231	U1232	U1233	U1234	U1235	U1236	U1237	U1238	U1239	U1240	U1241	U1242	U1243	U1244	U1245	U1246	U1247	U1248	U1249	U1250	U1251	U1252	U1253	U1254	U1255	U1256	U1257	U1258	U1259	U1260	U1261	U1262	U1263	U1264	U1265	U1266	U1267	U1268	U1269	U1270	U1271	U1272	U1273	U1274																																																																																																																																																																																																																																																																																										
A1130	G1131	G1132	G1133	G1134	G1135	G1136	G1137	G1138	G1139	G1140	G1141	G1142	G1143	G1144	G1145	G1146	G1147	G1148	G1149	G1150	G1151	G1152	G1153	G1154	G1155	G1156	G1157	G1158	G1159	G1160	G1161	G1162	G1163	G1164	G1165	G1166	G1167	G1168	G1169	G1170	G1171	G1172	G1173	G1174	G1175	G1176	G1177	G1178	G1179	G1180	G1181	G1182	G1183	G1184	G1185	G1186	G1187	G1188	G1189	G1190	G1191	G1192	G1193	G1194	G1195	G1196	G1197	G1198	G1199	G1200	G1201	G1202	G1203	G1204	G1205	G1206	G1207	G1208	G1209	G1210	G1211																																																																																																																																																																																																																																																																							
C1045	C1046	C1047	C1048	C1049	C1050	C1051	C1052	C1053	C1054	C1055	C1056	C1057	C1058	C1059	C1060	C1061	C1062	C1063	C1064	C1065	C1066	C1067	C1068	C1069	C1070	C1071	C1072	C1073	C1074	C1075	C1076	C1077	C1078	C1079	C1080	C1081	C1082	C1083	C1084	C1085	C1086	C1087	C1088	C1089	C1090	C1091	C1092	C1093	C1094	C1095	C1096	C1097	C1098	C1099	C1100	C1101	C1102	C1103	C1104	C1105	C1106	C1107	C1108	C1109	C1110	C1111	C1112	C1113	C1114	C1115	C1116	C1117	C1118	C1119	C1120	C1121	C1122	C1123	C1124																																																																																																																																																																																																																																																																									
A977	A978	A979	A980	A981	A982	A983	A984	A985	A986	A987	A988	A989	A990	A991	A992	A993	A994	A995	A996	A997	A998	A999	A1000	A1001	A1002	A1003	A1004	A1005	A1006	A1007	A1008	A1009	A1010	A1011	A1012	A1013	A1014	A1015	A1016	A1017	A1018	A1019	A1020	A1021	A1022	A1023	A1024	A1025	A1026	A1027	A1028	A1029	A1030	A1031	A1032	A1033	A1034	A1035	A1036	A1037	A1038	A1039	A1040	A1041	A1042	A1043	A1044																																																																																																																																																																																																																																																																																					
U833	U834	U835	U836	U837	U838	U839	U840	U841	U842	U843	U844	U845	U846	U847	U848	U849	U850	U851	U852	U853	U854	U855	U856	U857	U858	U859	U860	U861	U862	U863	U864	U865	U866	U867	U868	U869	U870	U871	U872	U873	U874	U875	U876	U877	U878	U879	U880	U881	U882	U883	U884	U885	U886	U887	U888	U889	U890	U891	U892	U893	U894	U895	U896	U897	U898	U899	U900	U901	U902	U903	U904	U905	U906	U907																																																																																																																																																																																																																																																																														
C680	C681	C682	C683	C684	C685	C686	C687	C688	C689	C690	C691	C692	C693	C694	C695	C696	C697	C698	C699	C700	C701	C702	C703	C704	C705	C706	C707	C708	C709	C710	C711	C712	C713	C714	C715	C716	C717	C718	C719	C720	C721	C722	C723	C724	C725	C726	C727	C728	C729	C730	C731	C732	C733	C734	C735	C736	C737	C738	C739	C740	C741	C742	C743	C744	C745	C746	C747	C748	C749	C750	C751	C752	C753	C754	C755	C756																																																																																																																																																																																																																																																																												
U600	U601	U602	U603	U604	U605	U606	U607	U608	U609	U610	U611	U612	U613	U614	U615	U616	U617	U618	U619	U620	U621	U622	U623	U624	U625	U626	U627	U628	U629	U630	U631	U632	U633	U634	U635	U636	U637	U638	U639	U640	U641	U642	U643	U644	U645	U646	U647	U648	U649	U650	U651	U652	U653	U654	U655	U656	U657	U658	U659	U660	U661	U662	U663	U664	U665	U666	U667	U668	U669	U670	U671	U672	U673	U674	U675	U676	U677	U678	U679	U680	U681	U682	U683	U684	U685	U686	U687	U688	U689	U690	U691	U692	U693	U694	U695	U696	U697	U698	U699	U700	U701	U702	U703	U704	U705	U706	U707	U708	U709	U710	U711	U712	U713	U714	U715	U716	U717	U718	U719	U720	U721	U722	U723	U724	U725	U726	U727	U728	U729	U730	U731	U732	U733	U734	U735	U736	U737	U738	U739	U740	U741	U742	U743	U744	U745	U746	U747	U748	U749	U750	U751	U752	U753	U754	U755	U756																																																																																																																																																																																												
U531	U532	U533	U534	U535	U536	U537	U538	U539	U540	U541	U542	U543	U544	U545	U546	U547	U548	U549	U550	U551	U552	U553	U554	U555	U556	U557	U558	U559	U560	U561	U562	U563	U564	U565	U566	U567	U568	U569	U570	U571	U572	U573	U574	U575	U576	U577	U578	U579	U580	U581	U582	U583	U584	U585	U586	U587	U588	U589	U590	U591	U592	U593	U594	U595	U596	U597	U598	U599																																																																																																																																																																																																																																																																																				
A441	A442	A443	A444	A445	A446	A447	A448	A449	A450	A451	A452	A453	A454	A455	A456	A457	A458	A459	A460	A461	A462	A463	A464	A465	A466	A467	A468	A469	A470	A471	A472	A473	A474	A475	A476	A477	A478	A479	A480	A481	A482	A483	A484	A485	A486	A487	A488	A489	A490	A491	A492	A493	A494	A495	A496	A497	A498	A499	A500	A501	A502	A503	A504	A505	A506	A507	A508	A509	A510	A511	A512	A513	A514	A515	A516	A517	A518	A519	A520	A521	A522	A523	A524	A525	A526	A527	A528	A529	A530																																																																																																																																																																																																																																																															
U284	U285	U286	U287	U288	U289	U290	U291	U292	U293	U294	U295	U296	U297	U298	U299	U300	U301	U302	U303	U304	U305	U306	U307	U308	U309	U310	U311	U312	U313	U314	U315	U316	U317	U318	U319	U320	U321	U322	U323	U324	U325	U326	U327	U328	U329	U330	U331	U332	U333	U334	U335	U336	U337	U338	U339	U340	U341	U342	U343	U344	U345	U346	U347	U348	U349	U350	U351	U352	U353	U354	U355	U356	U357	U358	U359	U360	U361	U362																																																																																																																																																																																																																																																																										
C218	C219	C220	C221	C222	C223	C224	C225	C226	C227	C228	C229	C230	C231	C232	C233	C234	C235	C236	C237	C238	C239	C240	C241	C242	C243	C244	C245	C246	C247	C248	C249	C250	C251	C252	C253	C254	C255	C256	C257	C258	C259	C260	C261	C262	C263	C264	C265	C266	C267	C268	C269	C270	C271	C272	C273	C274	C275	C276	C277	C278	C279	C280	C281	C282	C283	C284	C285	C286	C287	C288	C289	C290	C291	C292	C293																																																																																																																																																																																																																																																																													
U186I	U186J	U186K	U186L	U186M	U186N	U186O	U186P	U186Q	U186R	U186S	U186T	U186U	U186V	U186W	U186X	U186Y	U186Z	U186AA	U186AB	U186AC	U186AD	U186AE	U186AF	U186AG	U186AH	U186AI	U186AJ	U186AK	U186AL	U186AM	U186AN	U186AO	U186AP	U186AQ	U186AR	U186AS	U186AT	U186AU	U186AV	U186AW	U186AX	U186AY	U186AZ	U186BA	U186BB	U186BC	U186BD	U186BE	U186BF	U186BG	U186BH	U186BI	U186BJ	U186BK	U186BL	U186BM	U186BN	U186BO	U186BP	U186BQ	U186BR	U186BS	U186BT	U186BU	U186BV	U186BW	U186BX	U186BY	U186BZ	U186CA	U186CB	U186CC	U186CD	U186CE	U186CF	U186CG	U186CH	U186CI	U186CJ	U186CK	U186CL	U186CM	U186CN	U186CO	U186CP	U186CQ	U186CR	U186CS	U186CT	U186CU	U186CV	U186CW	U186CX	U186CY	U186CZ	U186DA	U186DB	U186DC	U186DD	U186DE	U186DF	U186DG	U186DH	U186DI	U186DJ	U186DK	U186DL	U186DM	U186DN	U186DO	U186DP	U186DQ	U186DR	U186DS	U186DT	U186DU	U186DV	U186DW	U186DX	U186DY	U186DZ	U186EA	U186EB	U186EC	U186ED	U186EE	U186EF	U186EG	U186EH	U186EI	U186EJ	U186EK	U186EL	U186EM	U186EN	U186EO	U186EP	U186EQ	U186ER	U186ES	U186ET	U186EU	U186EV	U186EW	U186EX	U186EY	U186EZ	U186FA	U186FB	U186FC	U186FD	U186FE	U186FF	U186FG	U186FH	U186FI	U186FJ	U186FK	U186FL	U186FM	U186FN	U186FO	U186FP	U186FQ	U186FR	U186FS	U186FT	U186FU	U186FV	U186FW	U186FX	U186FY	U186FZ	U186GA	U186GB	U186GC	U186GD	U186GE	U186GF	U186GG	U186GH	U186GI	U186GJ	U186GK	U186GL	U186GM	U186GN	U186GO	U186GP	U186GQ	U186GR	U186GS	U186GT	U186GU	U186GV	U186GW	U186GX	U186GY	U186GZ	U186HA	U186HB	U186HC	U186HD	U186HE	U186HF	U186HG	U186HH	U186HI	U186HJ	U186HK	U186HL	U186HM	U186HN	U186HO	U186HP	U186HQ	U186HR	U186HS	U186HT	U186HU	U186HV	U186HW	U186HX	U186HY	U186HZ	U186IA	U186IB	U186IC	U186ID	U186IE	U186IF	U186IG	U186IH	U186II	U186IJ	U186IK	U186IL	U186IM	U186IN	U186IO	U186IP	U186IQ	U186IR	U186IS	U186IT	U186IU	U186IV	U186IW	U186IX	U186IY	U186IZ	U186JA	U186JB	U186JC	U186JD	U186JE	U186JF	U186JG	U186JH	U186JI	U186JJ	U186JK	U186JL	U186JM	U186JN	U186JO	U186JP	U186JQ	U186JR	U186JS	U186JT	U186JU	U186JV	U186JW	U186JX	U186JY	U186JZ	U186KA	U186KB	U186KC	U186KD	U186KE	U186KF	U186KG	U186KH	U186KI	U186KJ	U186KK	U186KL	U186KM	U186KN	U186KO	U186KP	U186KQ	U186KR	U186KS	U186KT	U186KU	U186KV	U186KW	U186KX	U186KY	U186KZ	U186LA	U186LB	U186LC	U186LD	U186LE	U186LF	U186LG	U186LH	U186LI	U186LJ	U186LK	U186LL	U186LM	U186LN	U186LO	U186LP	U186LQ	U186LR	U186LS	U186LT	U186LU	U186LV	U186LW	U186LX	U186LY	U186LZ	U186MA	U186MB	U186MC	U186MD	U186ME	U186MF	U186MG	U186MH	U186MI	U186MJ	U186MK	U186ML	U186MN	U186MO	U186



• Molecule 21: transfer RNA

Chain W:



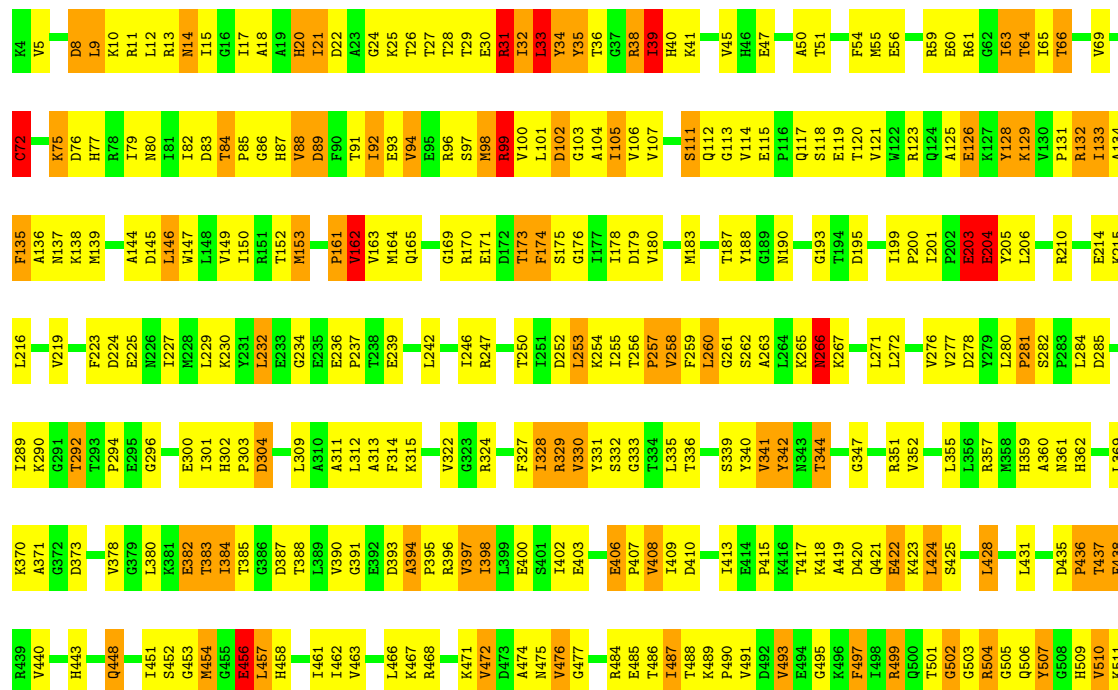
• Molecule 22: messenger RNA

Chain V:



• Molecule 23: Elongation factor G

Chain Y:





● Molecule 24: VIOMYCIN

Chain U:



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	306.01Å 673.49Å 351.98Å 90.00° 92.69° 90.00°	Depositor
Resolution (Å)	40.00 – 3.50 131.34 – 3.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-3.50) 74.9 (131.34-3.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.30 (at 3.49Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.262 , 0.309 0.366 , 0.368	Depositor DCC
R_{free} test set	38207 reflections (4.99%)	DCC
Wilson B-factor (Å ²)	80.5	Xtriage
Anisotropy	0.125	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 271.9	EDS
Estimated twinning fraction	0.247 for h,-k,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.26$, $\langle L^2 \rangle = 0.11$	Xtriage
Outliers	0 of 765681 reflections	Xtriage
F_o, F_c correlation	0.59	EDS
Total number of atoms	59087	wwPDB-VP
Average B, all atoms (Å ²)	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.50% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities 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: GNP, DPP, MG, KBE, UAL, 5OH

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	B	0.40	0/1945	0.69	1/2621 (0.0%)
2	C	0.33	0/1645	0.58	1/2216 (0.0%)
3	D	0.34	0/1733	0.61	0/2318
4	E	0.34	0/1172	0.63	1/1576 (0.1%)
5	F	0.35	0/856	0.64	1/1154 (0.1%)
6	G	0.35	0/1276	0.58	0/1709
7	H	0.33	0/1136	0.57	0/1527
8	I	0.36	0/1029	0.61	1/1378 (0.1%)
9	J	0.33	0/815	0.65	1/1095 (0.1%)
10	K	0.37	0/900	0.63	0/1213
11	L	0.47	0/992	0.88	4/1327 (0.3%)
12	M	0.32	0/1008	0.58	0/1347
13	N	0.35	0/501	0.57	0/664
14	O	0.35	0/745	0.59	0/992
15	P	0.33	0/722	0.56	0/970
16	Q	0.42	0/848	0.71	0/1131
17	R	0.31	0/579	0.57	0/768
18	S	0.31	0/647	0.56	0/870
19	T	0.37	0/764	0.62	0/1006
20	A	0.38	0/36351	0.95	35/56736 (0.1%)
21	W	0.41	1/1827 (0.1%)	1.06	9/2845 (0.3%)
22	V	0.95	3/568 (0.5%)	1.74	19/886 (2.1%)
23	Y	0.52	7/5481 (0.1%)	0.76	12/7418 (0.2%)
24	U	1.06	0/11	1.28	0/13
All	All	0.40	11/63551 (0.0%)	0.87	85/93780 (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
1	B	0	1
11	L	0	1
23	Y	0	8
All	All	0	10

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	Y	502	GLY	C-O	18.54	1.53	1.23
22	V	16	A	O3'-P	-10.50	1.48	1.61
23	Y	504	ARG	C-N	8.54	1.48	1.33
21	W	37	A	O3'-P	-8.36	1.51	1.61
22	V	15	A	N9-C4	-7.84	1.33	1.37

The worst 5 of 85 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	W	37	A	P-O3'-C3'	19.49	143.09	119.70
22	V	16	A	P-O3'-C3'	18.93	142.41	119.70
23	Y	502	GLY	O-C-N	-12.85	101.35	123.20
23	Y	502	GLY	CA-C-N	12.59	141.38	116.20
23	Y	502	GLY	C-N-CA	11.35	146.14	122.30

There are no chirality outliers.

5 of 10 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	163	PHE	Peptide
11	L	32	PHE	Peptide
23	Y	31	ARG	Peptide
23	Y	32	ILE	Peptide
23	Y	34	TYR	Peptide

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	B	1910	0	1957	98	0
2	C	1621	0	1688	67	0
3	D	1703	0	1763	120	0
4	E	1156	0	1213	54	0
5	F	843	0	857	38	0
6	G	1257	0	1296	61	0
7	H	1116	0	1177	73	0
8	I	1011	0	1043	54	0
9	J	802	0	849	61	0
10	K	885	0	904	61	0
11	L	976	0	1062	113	0
12	M	997	0	1072	72	0
13	N	492	0	529	35	0
14	O	734	0	771	42	0
15	P	706	0	725	39	0
16	Q	835	0	906	63	0
17	R	574	0	644	36	0
18	S	634	0	655	32	0
19	T	762	0	859	32	0
20	A	32474	0	16393	843	0
21	W	1635	0	831	52	0
22	V	503	0	252	34	0
23	Y	5380	0	5435	341	0
24	U	48	0	39	8	0
25	Y	32	0	13	32	0
26	Y	1	0	0	0	0
All	All	59087	0	42933	2172	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 22.

The worst 5 of 2172 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
21:W:37:A:C2	22:V:16:A:C2	1.85	1.57
23:Y:138:LYS:HE2	25:Y:701:GNP:C4	1.55	1.33
23:Y:138:LYS:HG2	25:Y:701:GNP:C6	1.57	1.31
23:Y:30:GLU:O	23:Y:33:LEU:N	1.69	1.24
23:Y:137:ASN:ND2	23:Y:263:ALA:H	1.45	1.15

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	B	233/235 (99%)	174 (75%)	36 (16%)	23 (10%)	1	15
2	C	205/207 (99%)	152 (74%)	34 (17%)	19 (9%)	1	18
3	D	206/208 (99%)	149 (72%)	46 (22%)	11 (5%)	3	35
4	E	149/151 (99%)	116 (78%)	24 (16%)	9 (6%)	2	31
5	F	99/101 (98%)	81 (82%)	7 (7%)	11 (11%)	1	13
6	G	153/155 (99%)	119 (78%)	27 (18%)	7 (5%)	4	39
7	H	136/138 (99%)	102 (75%)	21 (15%)	13 (10%)	1	17
8	I	125/127 (98%)	92 (74%)	25 (20%)	8 (6%)	2	29
9	J	97/99 (98%)	71 (73%)	16 (16%)	10 (10%)	1	14
10	K	117/119 (98%)	78 (67%)	26 (22%)	13 (11%)	1	13
11	L	123/125 (98%)	39 (32%)	44 (36%)	40 (32%)	0	0
12	M	123/125 (98%)	91 (74%)	18 (15%)	14 (11%)	1	12
13	N	58/60 (97%)	40 (69%)	14 (24%)	4 (7%)	2	27
14	O	86/88 (98%)	66 (77%)	15 (17%)	5 (6%)	3	32
15	P	82/84 (98%)	59 (72%)	18 (22%)	5 (6%)	2	30
16	Q	98/100 (98%)	68 (69%)	20 (20%)	10 (10%)	1	14
17	R	68/70 (97%)	52 (76%)	10 (15%)	6 (9%)	1	19
18	S	77/79 (98%)	56 (73%)	12 (16%)	9 (12%)	1	12
19	T	97/99 (98%)	75 (77%)	14 (14%)	8 (8%)	1	21
23	Y	685/687 (100%)	457 (67%)	156 (23%)	72 (10%)	1	14
24	U	2/6 (33%)	1 (50%)	1 (50%)	0	100	100
All	All	3019/3063 (99%)	2138 (71%)	584 (19%)	297 (10%)	1	16

5 of 297 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	17	PHE

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Mol	Chain	Res	Type
1	B	66	GLY
1	B	75	LYS
1	B	76	GLN
1	B	96	ARG

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	B	203/203 (100%)	177 (87%)	26 (13%)	6	33
2	C	161/161 (100%)	122 (76%)	39 (24%)	1	6
3	D	180/180 (100%)	142 (79%)	38 (21%)	1	9
4	E	116/116 (100%)	95 (82%)	21 (18%)	2	15
5	F	90/90 (100%)	74 (82%)	16 (18%)	2	16
6	G	126/126 (100%)	112 (89%)	14 (11%)	9	42
7	H	119/119 (100%)	91 (76%)	28 (24%)	1	7
8	I	98/98 (100%)	77 (79%)	21 (21%)	1	9
9	J	89/89 (100%)	66 (74%)	23 (26%)	1	5
10	K	90/90 (100%)	72 (80%)	18 (20%)	2	11
11	L	104/104 (100%)	77 (74%)	27 (26%)	1	5
12	M	100/100 (100%)	86 (86%)	14 (14%)	5	28
13	N	49/49 (100%)	35 (71%)	14 (29%)	0	4
14	O	79/79 (100%)	66 (84%)	13 (16%)	3	20
15	P	72/72 (100%)	61 (85%)	11 (15%)	4	25
16	Q	95/95 (100%)	80 (84%)	15 (16%)	4	23
17	R	61/61 (100%)	53 (87%)	8 (13%)	6	32
18	S	69/69 (100%)	52 (75%)	17 (25%)	1	6
19	T	76/76 (100%)	68 (90%)	8 (10%)	10	46
23	Y	579/579 (100%)	483 (83%)	96 (17%)	3	19
24	U	2/2 (100%)	2 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2558/2558 (100%)	2091 (82%)	467 (18%)	2 14

5 of 467 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
9	J	47	PHE
11	L	77	LEU
23	Y	451	ILE
9	J	70	ARG
10	K	75	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
10	K	116	HIS
12	M	92	HIS
23	Y	40	HIS
10	K	27	ASN
19	T	18	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
20	A	1511/1511 (100%)	310 (20%)	16 (1%)
21	W	76/77 (98%)	19 (25%)	1 (1%)
22	V	22/23 (95%)	9 (40%)	3 (13%)
All	All	1609/1611 (99%)	338 (21%)	20 (1%)

5 of 338 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
20	A	6	G
20	A	8	A
20	A	9	G
20	A	10	A
20	A	13	U

5 of 20 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
20	A	992	U
20	A	1064	G
21	W	20(A)	U
20	A	705	U
20	A	748	C

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

4 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	$\# Z > 2$
24	KBE	U	1	24	8,8,9	8.13	1 (12%)	6,8,10	0.58	0
24	DPP	U	2	24	5,5,6	6.82	1 (20%)	3,5,7	2.64	2 (66%)
24	UAL	U	5	24	7,8,9	1.30	1 (14%)	6,9,11	1.36	1 (16%)
24	5OH	U	6	24	12,12,13	6.61	3 (25%)	13,16,18	0.84	0

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
24	KBE	U	1	24	-	0/6/7/8	0/0/0/0
24	DPP	U	2	24	-	0/2/4/6	0/0/0/0
24	UAL	U	5	24	-	0/3/7/9	0/0/0/0
24	5OH	U	6	24	-	0/2/18/20	0/1/1/1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	U	1	KBE	O-C	22.95	1.27	1.11
24	U	6	5OH	O-C	22.13	1.26	1.11
24	U	2	DPP	O-C	15.12	1.21	1.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	U	6	5OH	CQ-NP	5.15	1.40	1.34
24	U	6	5OH	CQ-NR	2.37	1.40	1.32

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	U	2	DPP	C-CA-N	-3.74	110.10	113.83
24	U	2	DPP	CB-CA-N	-2.18	104.19	111.50
24	U	5	UAL	CB-CA-N	2.06	127.80	123.24

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 2 ligands modelled in this entry, 1 is 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	$\# Z > 2$
25	GNP	Y	701	26	34,34,34	1.72	6 (17%)	50,54,54	5.62	14 (28%)

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
25	GNP	Y	701	26	-	0/18/38/38	0/1/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	Y	701	GNP	PG-O1G	6.08	1.53	1.46
25	Y	701	GNP	PB-N3B	-4.55	1.60	1.64
25	Y	701	GNP	PA-O3A	-2.77	1.54	1.59
25	Y	701	GNP	PA-O2A	-2.18	1.45	1.55
25	Y	701	GNP	PB-O3A	-2.17	1.56	1.59

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	Y	701	GNP	C6-C5-N7	-37.53	129.09	134.14
25	Y	701	GNP	PA-O3A-PB	-4.63	115.98	131.81
25	Y	701	GNP	C2-N3-C4	-3.71	109.89	115.09
25	Y	701	GNP	C4-C5-N7	3.63	112.63	109.52
25	Y	701	GNP	C4'-O4'-C1'	-3.59	105.85	109.75

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	B	235/235 (100%)	-0.38	0 100 100	34, 86, 153, 201	0
2	C	207/207 (100%)	-0.25	0 100 100	23, 75, 130, 190	0
3	D	208/208 (100%)	-0.23	1 (0%) 88 64	23, 85, 142, 184	0
4	E	151/151 (100%)	-0.04	0 100 100	14, 58, 106, 151	0
5	F	101/101 (100%)	-0.25	0 100 100	29, 61, 123, 148	0
6	G	155/155 (100%)	-0.33	0 100 100	38, 82, 137, 180	0
7	H	138/138 (100%)	-0.24	0 100 100	25, 75, 121, 155	0
8	I	127/127 (100%)	-0.09	0 100 100	0, 84, 149, 220	0
9	J	99/99 (100%)	0.19	4 (4%) 36 16	31, 75, 127, 166	0
10	K	119/119 (100%)	-0.19	0 100 100	38, 72, 133, 151	0
11	L	125/125 (100%)	-0.11	1 (0%) 83 53	29, 69, 136, 170	0
12	M	125/125 (100%)	-0.09	4 (3%) 45 21	53, 100, 158, 223	0
13	N	60/60 (100%)	0.23	1 (1%) 67 34	39, 69, 117, 135	0
14	O	88/88 (100%)	-0.30	0 100 100	25, 68, 119, 170	0
15	P	84/84 (100%)	-0.10	0 100 100	52, 81, 127, 153	0
16	Q	100/100 (100%)	-0.01	1 (1%) 79 47	0, 68, 126, 150	0
17	R	70/70 (100%)	-0.23	0 100 100	39, 63, 113, 155	0
18	S	79/79 (100%)	-0.15	0 100 100	44, 99, 145, 189	0
19	T	99/99 (100%)	-0.13	0 100 100	0, 79, 131, 166	0
20	A	1511/1511 (100%)	-0.11	3 (0%) 93 80	18, 70, 157, 272	0
21	W	77/77 (100%)	-0.49	0 100 100	39, 101, 193, 240	0
22	V	23/23 (100%)	-0.21	0 100 100	41, 118, 186, 216	0
23	Y	687/687 (100%)	-0.27	0 100 100	40, 92, 149, 204	0
24	U	2/6 (33%)	-0.22	0 100 100	119, 119, 119, 119	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
All	All	4670/4674 (99%)	-0.17	15 (0%) 91 76	0, 77, 148, 272	0

The worst 5 of 15 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
20	A	1257	U	5.9
12	M	102	ARG	4.6
16	Q	38	ARG	3.9
9	J	8	LEU	2.9
12	M	101	GLN	2.7

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

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
24	DPP	U	2	6/7	0.16	-	118,118,118,118	0
24	UAL	U	5	9/10	0.15	-	118,118,118,118	0
24	KBE	U	1	9/10	0.19	-	118,118,118,118	0
24	5OH	U	6	12/13	0.13	-	99,101,102,102	0

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
25	GNP	Y	701	32/32	0.14	-	58,71,81,83	0
26	MG	Y	702	1/1	0.10	-	135,135,135,135	0

6.5 Other polymers ⓘ

There are no such residues in this entry.