



wwPDB X-ray Structure Validation Summary Report ⓘ

May 28, 2020 – 08:33 pm BST

PDB ID : 1N36
Title : Structure of the *Thermus thermophilus* 30S ribosomal subunit in the presence of crystallographically disordered codon and near-cognate transfer RNA anticodon stem-loop mismatched at the second codon position
Authors : Ogle, J.M.; Murphy IV, F.V.; Tarry, M.J.; Ramakrishnan, V.
Deposited on : 2002-10-25
Resolution : 3.65 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
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

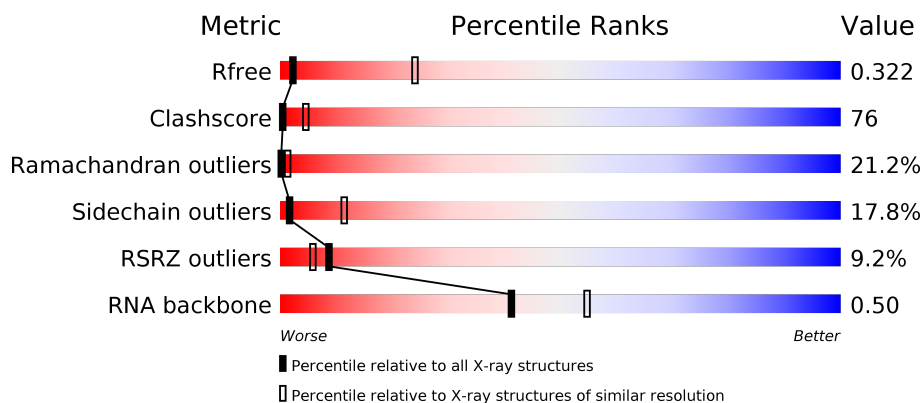
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.65 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}	130704	1557 (3.82-3.50)
Clashscore	141614	1037 (3.80-3.52)
Ramachandran outliers	138981	1004 (3.80-3.52)
Sidechain outliers	138945	1002 (3.80-3.52)
RSRZ outliers	127900	1441 (3.82-3.50)
RNA backbone	3102	1024 (4.30-3.00)

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

Mol	Chain	Length	Quality of chain
1	A	1522	<div> <div>11%</div> <div> <div></div> <div>9%</div> <div>70%</div> <div>18%</div> <div>••</div> </div> </div>
2	B	256	<div> <div>%</div> <div> <div></div> <div>8%</div> <div>55%</div> <div>23%</div> <div>5%</div> <div>9%</div> </div> </div>
3	C	239	<div> <div>8%</div> <div> <div></div> <div>6%</div> <div>49%</div> <div>29%</div> <div>•</div> <div>14%</div> </div> </div>
4	D	208	<div> <div>3%</div> <div> <div></div> <div>12%</div> <div>57%</div> <div>25%</div> <div>6%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
5	E	161	
6	F	101	
7	G	155	
8	H	138	
9	I	128	
10	J	104	
11	K	129	
12	L	135	
13	M	126	
14	N	60	
15	O	88	
16	P	88	
17	Q	104	
18	R	88	
19	S	92	
20	T	106	
21	V	26	

2 Entry composition

There are 22 unique types of molecules in this entry. The entry contains 51680 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 16S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1513	Total	C	N	O	P	22	0	0
			32508	14472	6016	10509	1511			

- Molecule 2 is a protein called 30S RIBOSOMAL PROTEIN S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	234	Total	C	N	O	S	0	0	0
			1900	1213	341	341	5			

- Molecule 3 is a protein called 30S RIBOSOMAL PROTEIN S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	206	Total	C	N	O	S	0	0	0
			1612	1016	314	281	1			

- Molecule 4 is a protein called 30S RIBOSOMAL PROTEIN S4.

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

- Molecule 5 is a protein called 30S RIBOSOMAL PROTEIN S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	150	Total	C	N	O	S	0	0	0
			1146	724	217	201	4			

- Molecule 6 is a protein called 30S RIBOSOMAL PROTEIN S6.

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

- Molecule 7 is a protein called 30S RIBOSOMAL PROTEIN S7.

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

- Molecule 8 is a protein called 30S RIBOSOMAL PROTEIN S8.

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

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	25	ASP	GLU	CONFLICT	UNP Q5SHQ2
H	37	ARG	LYS	CONFLICT	UNP Q5SHQ2
H	52	ASP	GLU	CONFLICT	UNP Q5SHQ2
H	61	VAL	ILE	CONFLICT	UNP Q5SHQ2
H	62	TYR	HIS	CONFLICT	UNP Q5SHQ2
H	81	HIS	LYS	CONFLICT	UNP Q5SHQ2
H	88	LYS	ARG	CONFLICT	UNP Q5SHQ2
H	115	SER	PRO	CONFLICT	UNP Q5SHQ2

- Molecule 9 is a protein called 30S RIBOSOMAL PROTEIN S9.

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

- Molecule 10 is a protein called 30S RIBOSOMAL PROTEIN S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	98	Total	C	N	O	S	0	0	0
			792	498	156	137	1			

- Molecule 11 is a protein called 30S RIBOSOMAL PROTEIN S11.

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

- Molecule 12 is a protein called 30S RIBOSOMAL PROTEIN S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	124	Total	C	N	O	S	0	0	0
			970	611	195	163	1			

- Molecule 13 is a protein called 30S RIBOSOMAL PROTEIN S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	118	Total	C	N	O	S	0	0	0
			937	579	193	163	2			

- Molecule 14 is a protein called 30S RIBOSOMAL PROTEIN S14.

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

- Molecule 15 is a protein called 30S RIBOSOMAL PROTEIN S15.

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

- Molecule 16 is a protein called 30S RIBOSOMAL PROTEIN S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	P	83	Total	C	N	O	S	0	0	0
			700	443	139	117	1			

- Molecule 17 is a protein called 30S RIBOSOMAL PROTEIN S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Q	104	Total	C	N	O	S	0	0	0
			857	547	161	147	2			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	50	LYS	ARG	CONFLICT	UNP Q5SHP7
Q	53	LEU	VAL	CONFLICT	UNP Q5SHP7
Q	62	SER	ALA	CONFLICT	UNP Q5SHP7
Q	79	SER	GLU	CONFLICT	UNP Q5SHP7
Q	82	MET	LEU	CONFLICT	UNP Q5SHP7
Q	90	ILE	VAL	CONFLICT	UNP Q5SHP7

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Chain	Residue	Modelled	Actual	Comment	Reference
Q	96	GLN	ALA	CONFLICT	UNP Q5SHP7

- Molecule 18 is a protein called 30S RIBOSOMAL PROTEIN S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	R	73	Total	C	N	O	0	0	0
			597	380	118	99			

- Molecule 19 is a protein called 30S RIBOSOMAL PROTEIN S19.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
19	S	80	Total	C	N	O S	0	0	0
			647	414	119	112 2			

- Molecule 20 is a protein called 30S RIBOSOMAL PROTEIN S20.

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	V	24	Total	C	N	O	0	0	0
			208	128	50	30			

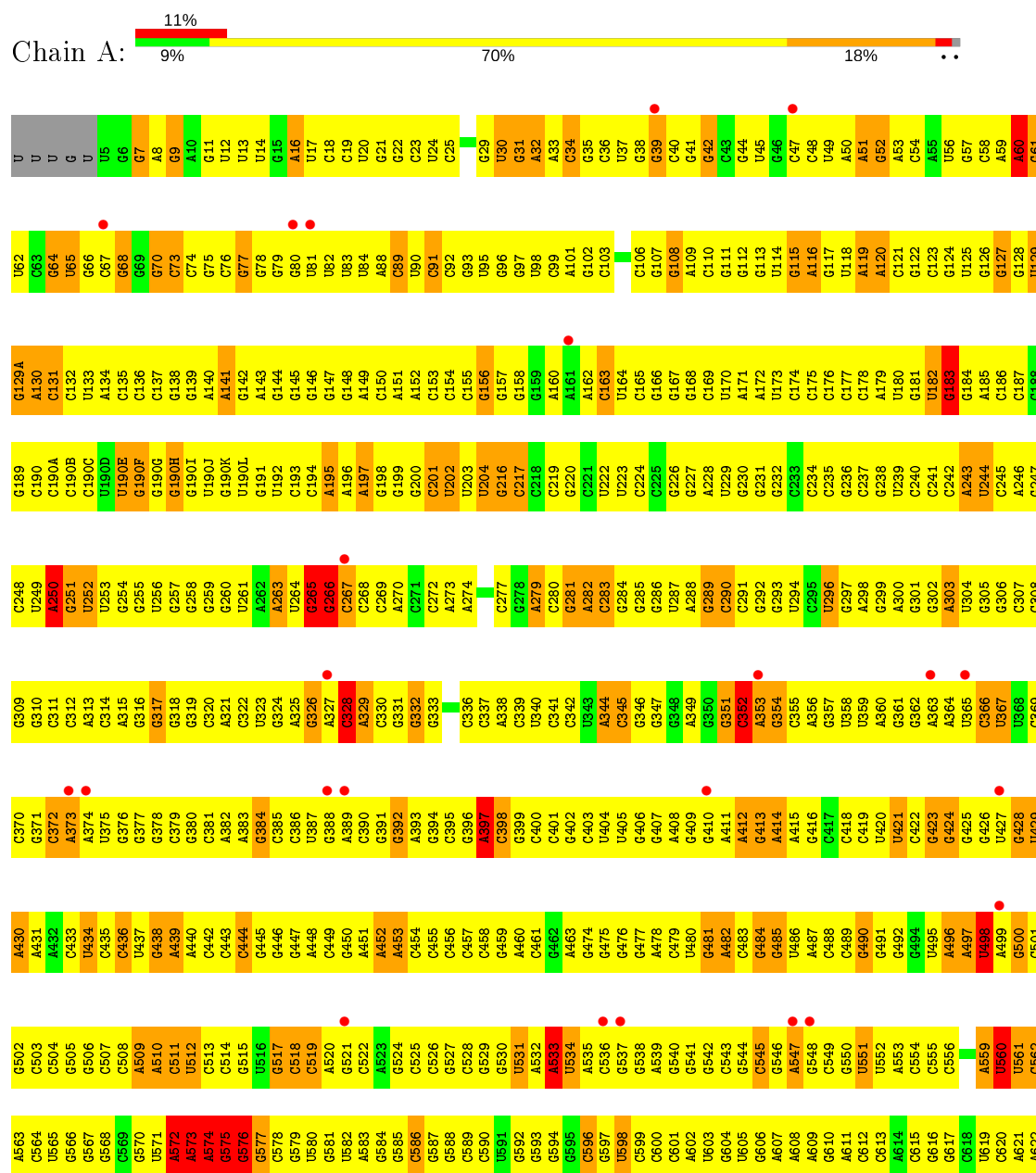
- Molecule 22 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

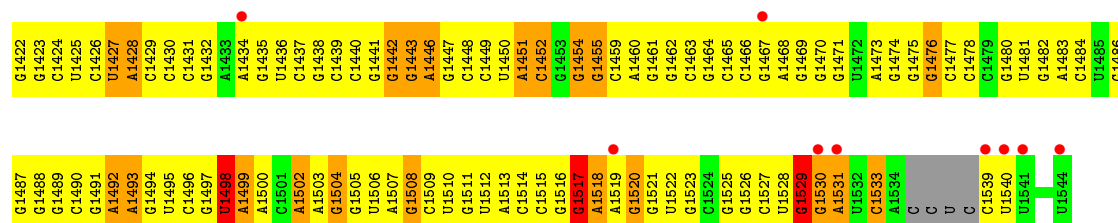
3 Residue-property plots

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

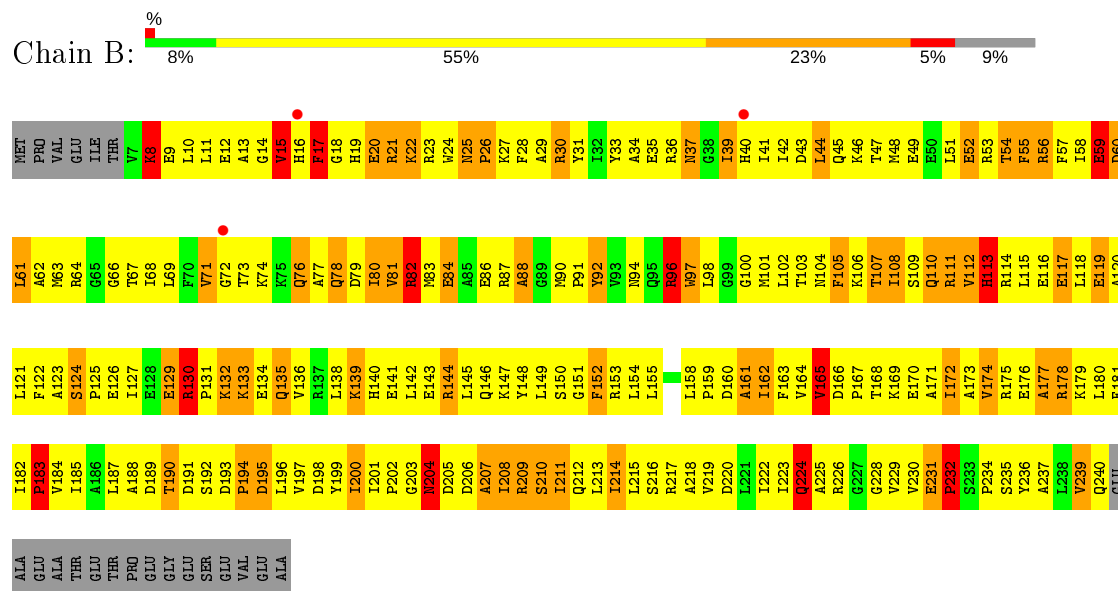
• Molecule 1: 16S RIBOSOMAL RNA



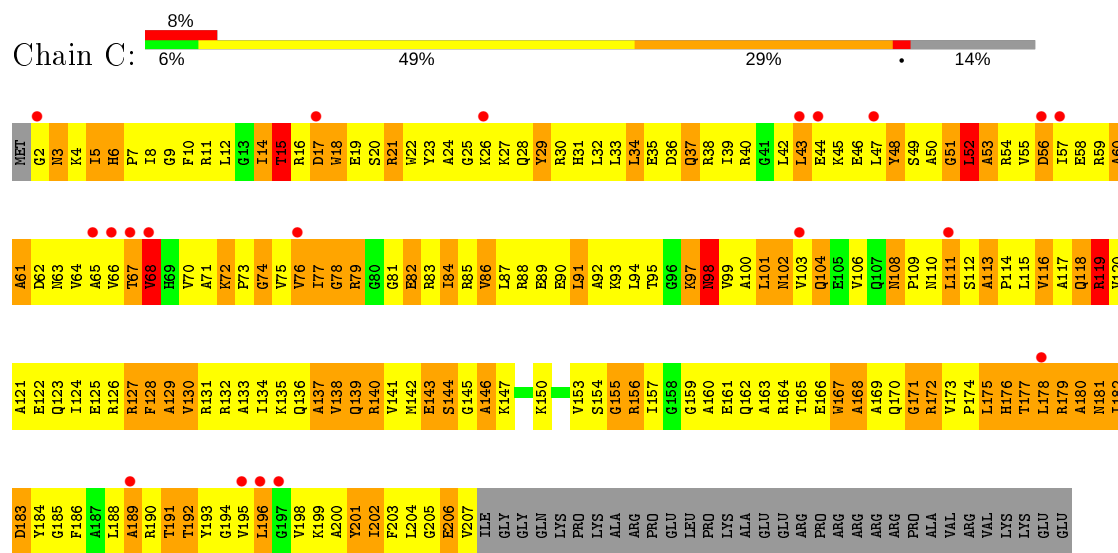
A1360	A1299	A1239	A1179	C1116	U1056	U997	A937	C875	G809	C749	U866	C623
A1361	A1300	C1240	A1180	G1117	G1057	G998	A938	G876	C810	G749	A687	C624
C1361A	U1301	C1241	A1181	C1118	G1058	C999	G939	C877	C811	U751	G888	C625
C1362	U1302	C1242	G1182	C1119	C1059	U1000	C940	G878	C812	G752	C899	
A1363	A1303	C1243	A1183	G1120	C1060	U1001	G941	C879	U813	A753	G890	
C1364	C1304	C1244	G1184	U1121	G1061	G1002	G942	C880	A814	C754	G891	
C1365	C1305	A1245	G1185	U1122	U1062	G1003	U943	G881	A815	G755		
C1366	A1306	C1246	G1186	A1123	C1063	G1003A	G944	C882	A816	C756	A694	
C1367	U1307	U1247	G1187	G1124	A1004	A1004	G945	C883	C817	U757	A695	
C1368			A1188	U1125	U1065	A1005	A946	U884	G818	G758	A696	
C1369	G1310	C1249	C1189	U1126	C1066	U1006	G947	G885	A819	A759	U697	
C1370	G1311	A1250	G1190	G1127	A1067	C1007	C948	G886	U820	G760		
C1371	G1312	A1251	A1191	C1128	G1068	C1008	A949	G887	G821	G761	C701	
C1372	U1313	A1252	C1129	C1069	U1069	G1011	U950		C822	G762	A702	
C1373	C1314	G1253	G1193	A1130	U1070	U1012	G951	U891	C823	G763	G703	
A1374	U1315	C1254	A1374	G1131	C1071	U1013	U952	A892	C824	C764	A704	
A1375	C1316	G1255	C1195	C1132	U1072	G1013	G953	C893	G825	G765	U705	
U1376	C1317	A1256	U1196	G1133	U1073	A1014	G954	G894	C826	A766	A706	
A1377	A1318	U1257	G1197	G1134	U1074	A1015	U955	G895	U827	A767	C707	
C1378	A1319	G1258	G1198	U1135	C1075	A1016	U956	C896	A828	A768	C708	
C1379	C1320	C1259	U1199	C1136	U1076	G1017	U957	C897	G829	G769	G709	
A1380	C1321	C1260	C1200	U1137	G1077	C1018	G958	C898	G830	C770	G710	
U1381	A1261	A1261	A1201	G1138	U1078	C1019	A959	C899	U831	G771	G711	
C1382	G1323	C1262	G1202	G1139	U1079	U1020	U960	A900	C832	U772	A712	
C1383	C1324	C1263	C1203	C1140	A1080	G1021	U961	A901	U833	G773	G713	
C1384	C1325	C1264	A1204	C1141	G1081	C1022	C962	G902	C834	G774	G714	
C1385	G1265	G1265	U1205	G1142	G1082	G1023	G963	G903	U835	G775	A715	
C1386		G1266	G1206	G1143	U1083	G1024	A964	C904	G836	A776	A716	
		C1267	G1207	G1144	U1084	U1025	A965	U905	G837	A777	C717	
U1390	A1329	A1268	C1208	C1145	U1085	G1026	G966	G906	G838	G778	G718	
U1391	C1330	A1269	C1209	A1146	U1086	C1027	C967	A907	U839	C779	C719	
C1392	G1331	C1270	C1210	C1147	G1087	U1028	A968	A908	C840	A780	C720	
U1393	A1332	G1271	U1211	U1148	C1088	C1029	A969	A909	U841	A781	G721	
A1394	A1333	G1272	U1212	C1149	G1089	C1030	C970	C910	C848	A782	A722	
C1395	G1334	G1273	C1213	U1150	U1090	G1030A	G971	U911	C849	C783	U723	
A1396	C1335	G1274	A1214	A1151	U1091	C972	C972	G912	U850	C784	G724	
C1397	C1336	A1275	G1215	A1152	A1092	G1030B	G973	A913	G851	G785	G725	
A1398	G1337	C1276	C1216	G1153	A1093	A1030D	A974	A914	G852	A786	C726	
C1399	G1338	C1277	C1217	G1154	G1094	A975	A975	A915	G853	A787	G727	
A1400	C1400	U1278	G1218	G1155	U1095	G1096	G976	G916	G854	U788	A728	
C1401	A1340	A1279	U1219	C1156	C1096	G1036	A977	G917	G855	U789	A729	
C1402	U1341	A1280	G1220	A1157	C1097	C1037	A787	A918	C856	A790	G730	
C1403	C1342	U1281	G1221	C1158	C1098	U1038	C979	A919	C857	G791	G731	
C1404	G1343	C1282	C1222	U1159	G1099	C1039	C980	U920	G858	A792	C732	
C1405	C1344	G1283	C1223	G1160	C1100	U1040	U981	U921	G859	G670	A733	
U1406	U1345	C1284	G1224	A1161	A1101	A1041	U982	G922	A860	A794	G734	
C1407	A1346	A1285	A1225	C1162	A1102	G1042	A983	A923	G861	C795	C735	
A1408	C1347	A1286	C1226	G1163	C1103	C1043	C984	G924	C862	C796	C736	
C1348	U1348	A1287	A1227	G1164	G1104	A1044	C985	G925	U863	C797	A737	
C1409	A1288	C1288	C1228		A1105	C1045	A986	G926	A864	G798	C738	
C1410	A1349	A1289	A1229	A1168	G1106	A1046	G987	G927	A865	G799	C739	
C1411	C1350	C1290	C1230	A1169	C1107	G1047	G988	G928	C866	G800	U740	
C1412	U1351	G1291	G1231	G1171	C1108	G1048	C989	G929	G867	U801	G741	
C1413	C1352	G1291	C1231	C1172	C1109	U1049	C990	G930	C868	A802	G742	
U1414	G1353	U1292	U1232	C1173	A1110	G1050	C991	C931	C869	G803	G743	
G1415	C1354	G1293	G1233	G1173	A1111	C1051	U992	C932	U870	G681	C744	
	C1355	C1294	C1234	G1174	A1112	G1052	U993	G933	U871	C805	C745	
A1418	C1356	G1295	U1235	G1175	C1113	U1053	A994	C934	A872	C806	A746	
A1419	A1357	C1296	A1236	A1176	G1114	G1054	C995	G935	A873	G807	C747	
C1420	C1358	C1297	C1237	G1177	C1115	A1055	C996	G936	C874	C989	C748	
A1421	U1359	C1298	A1238	C1178	C1116	U1056	C997	G937	A874	A808	C749	



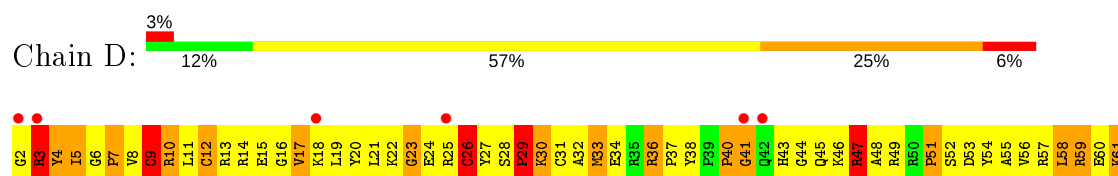
• Molecule 2: 30S RIBOSOMAL PROTEIN S2

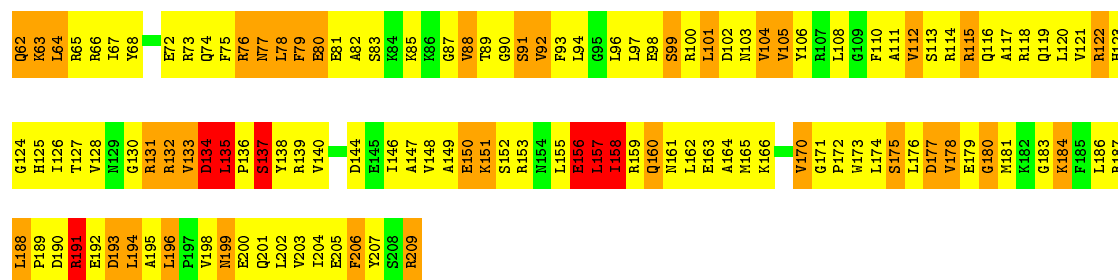


• Molecule 3: 30S RIBOSOMAL PROTEIN S3

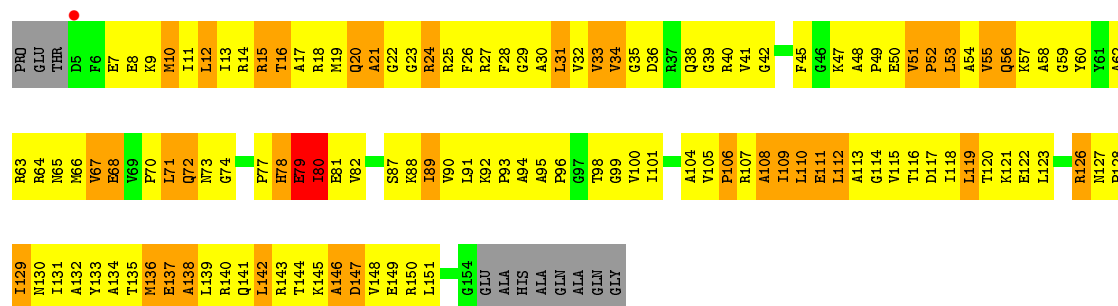
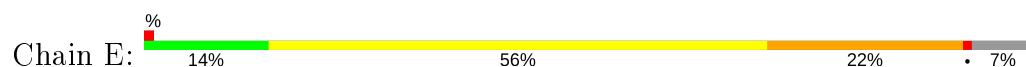


• Molecule 4: 30S RIBOSOMAL PROTEIN S4

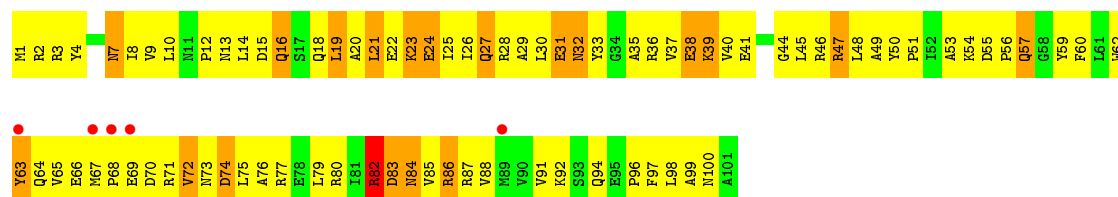




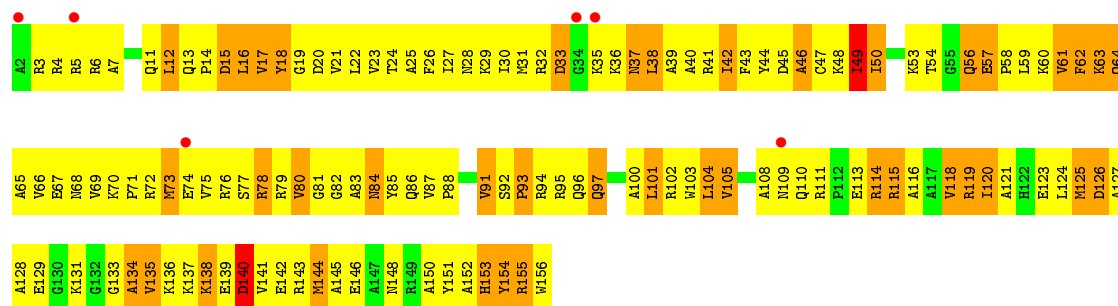
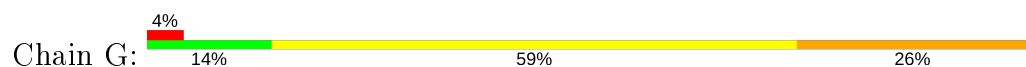
- Molecule 5: 30S RIBOSOMAL PROTEIN S5



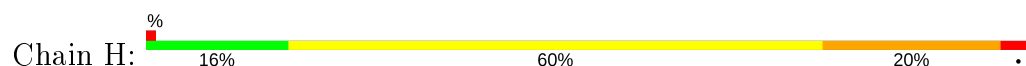
- Molecule 6: 30S RIBOSOMAL PROTEIN S6

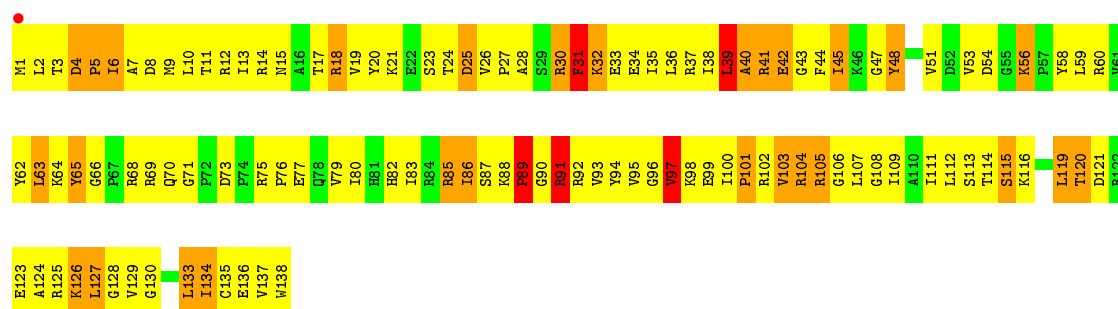


• Molecule 7: 30S RIBOSOMAL PROTEIN S7

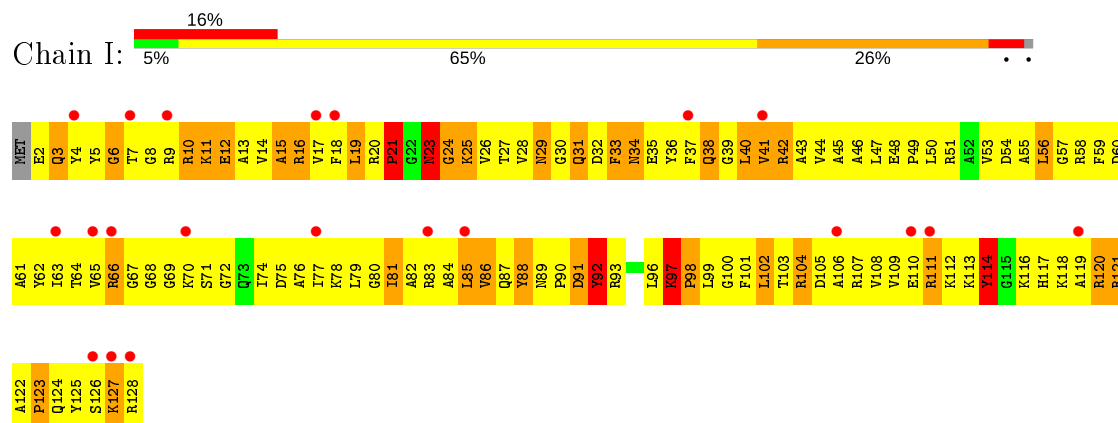


● Molecule 8: 30S RIBOSOMAL PROTEIN S8

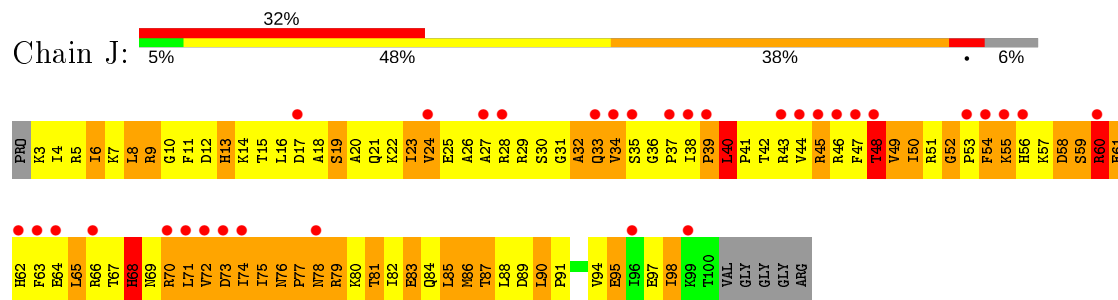




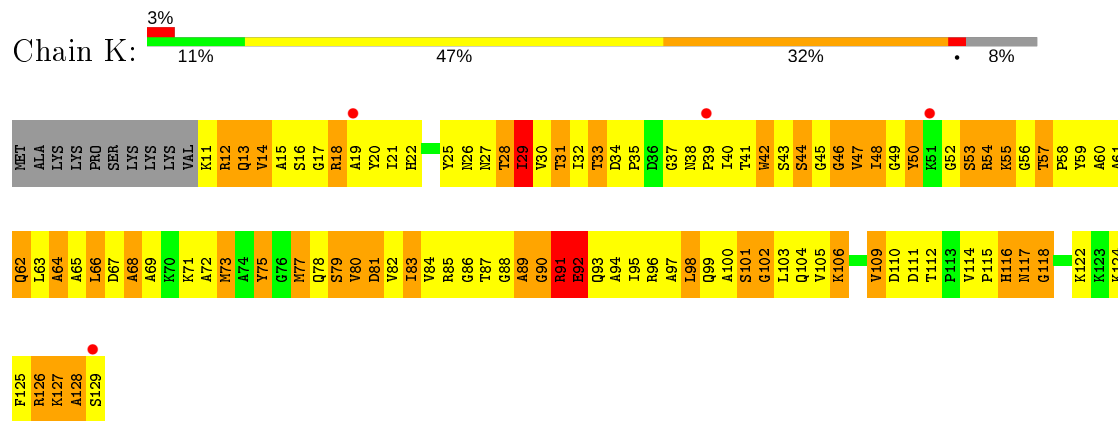
• Molecule 9: 30S RIBOSOMAL PROTEIN S9



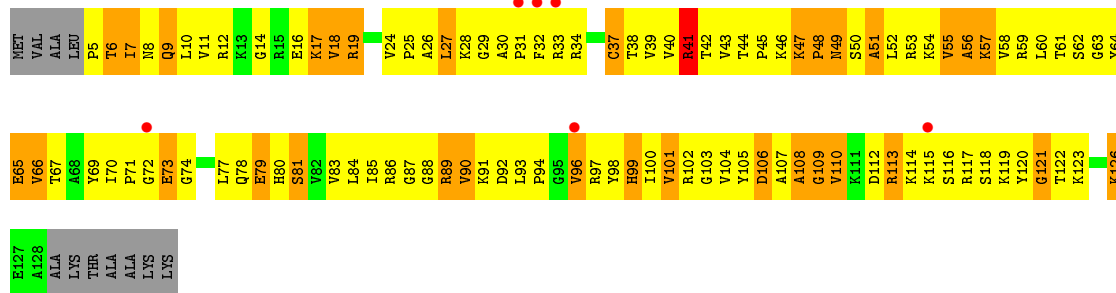
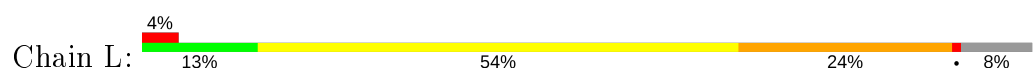
• Molecule 10: 30S RIBOSOMAL PROTEIN S10



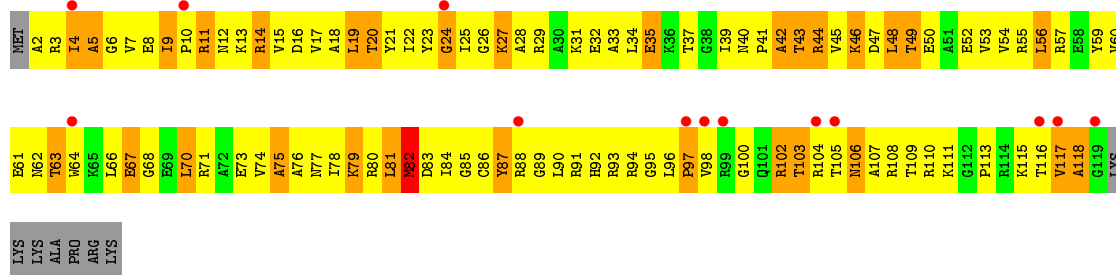
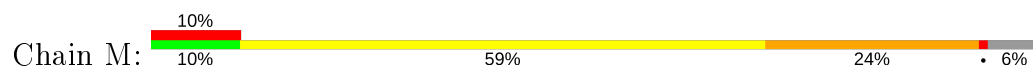
• Molecule 11: 30S RIBOSOMAL PROTEIN S11



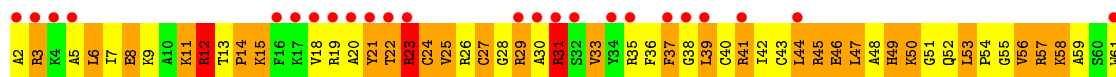
• Molecule 12: 30S RIBOSOMAL PROTEIN S12



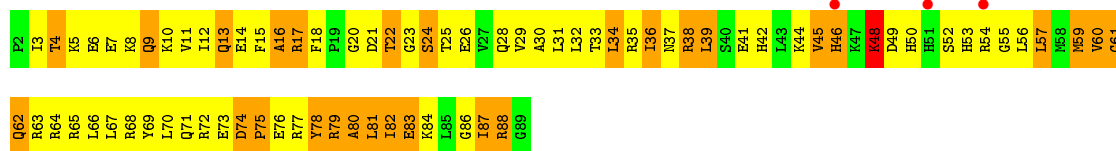
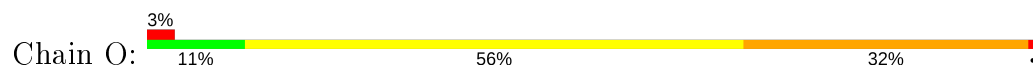
• Molecule 13: 30S RIBOSOMAL PROTEIN S13



• Molecule 14: 30S RIBOSOMAL PROTEIN S14

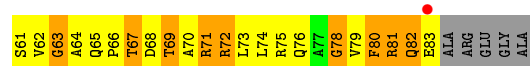


• Molecule 15: 30S RIBOSOMAL PROTEIN S15

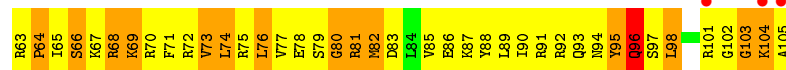
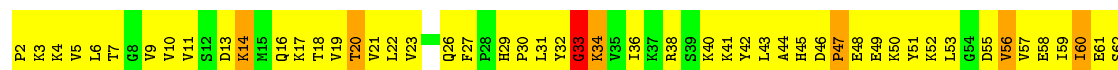
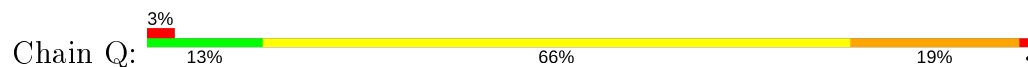


• Molecule 16: 30S RIBOSOMAL PROTEIN S16

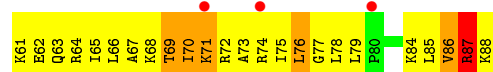




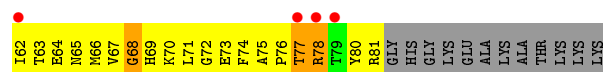
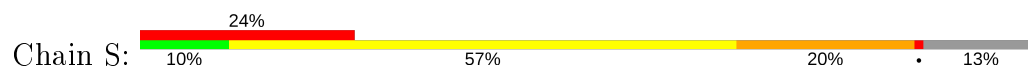
• Molecule 17: 30S RIBOSOMAL PROTEIN S17



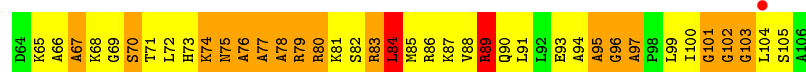
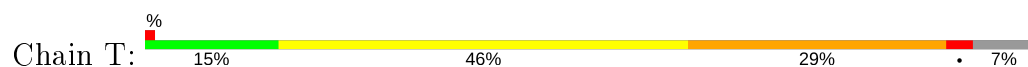
• Molecule 18: 30S RIBOSOMAL PROTEIN S18



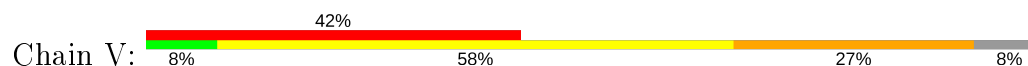
• Molecule 19: 30S RIBOSOMAL PROTEIN S19



• Molecule 20: 30S RIBOSOMAL PROTEIN S20



• Molecule 21: 30S RIBOSOMAL PROTEIN THX



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	402.84Å 402.84Å 174.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	141.42 – 3.65 148.66 – 3.64	Depositor EDS
% Data completeness (in resolution range)	92.6 (141.42-3.65) 89.6 (148.66-3.64)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.14	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.44 (at 3.67Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.260 , 0.324 0.259 , 0.322	Depositor DCC
R_{free} test set	7116 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	107.1	Xtriage
Anisotropy	0.426	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.22 , 121.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	51680	wwPDB-VP
Average B, all atoms (Å ²)	93.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.54% 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:
ZN

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	0.64	4/36387 (0.0%)	0.78	27/56789 (0.0%)
2	B	0.47	0/1935	0.79	0/2609
3	C	0.46	0/1636	0.77	0/2205
4	D	0.49	0/1733	0.70	0/2318
5	E	0.61	0/1162	0.88	2/1564 (0.1%)
6	F	0.42	0/856	0.72	0/1154
7	G	0.44	0/1276	0.77	1/1709 (0.1%)
8	H	0.65	0/1136	0.87	1/1527 (0.1%)
9	I	0.45	0/1029	0.73	0/1378
10	J	0.47	0/805	0.86	0/1082
11	K	0.49	0/900	0.81	0/1213
12	L	0.51	0/986	0.87	0/1320
13	M	0.40	0/947	0.73	0/1270
14	N	0.46	0/501	0.75	1/664 (0.2%)
15	O	0.51	0/745	0.74	0/992
16	P	0.58	0/716	0.88	1/963 (0.1%)
17	Q	0.58	0/870	0.90	2/1159 (0.2%)
18	R	0.45	0/603	0.75	0/799
19	S	0.47	0/661	0.82	0/890
20	T	0.48	0/765	0.79	0/1007
21	V	0.48	0/212	0.66	0/277
All	All	0.59	4/55861 (0.0%)	0.78	35/82889 (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
1	A	1	63
8	H	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
All	All	1	64

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	858	G	C5-C6	-6.65	1.35	1.42
1	A	1508	G	C5-C6	-5.12	1.37	1.42
1	A	574	A	C5-C6	-5.04	1.36	1.41
1	A	821	G	C5-C6	-5.03	1.37	1.42

The worst 5 of 35 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	290	C	N1-C1'-C2'	-8.80	102.33	112.00
1	A	1498	U	C2'-C3'-O3'	8.73	128.71	109.50
1	A	575	G	C2'-C3'-O3'	7.82	126.70	109.50
1	A	60	A	C2'-C3'-O3'	7.67	126.37	109.50
1	A	1454	G	N9-C1'-C2'	-7.34	103.92	112.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	1498	U	C3'

5 of 64 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	127	G	Sidechain
1	A	129	U	Sidechain
1	A	156	G	Sidechain
1	A	183	G	Sidechain
1	A	77	G	Sidechain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	32508	0	16414	2582	0
2	B	1900	0	1951	415	0
3	C	1612	0	1677	503	0
4	D	1703	0	1764	410	0
5	E	1146	0	1207	238	0
6	F	843	0	857	150	0
7	G	1257	0	1296	278	0
8	H	1116	0	1177	221	0
9	I	1011	0	1043	277	0
10	J	792	0	835	283	0
11	K	885	0	904	167	0
12	L	970	0	1057	204	0
13	M	937	0	995	225	0
14	N	492	0	532	165	0
15	O	734	0	771	150	0
16	P	700	0	720	199	0
17	Q	857	0	930	177	0
18	R	597	0	668	137	0
19	S	647	0	673	182	0
20	T	763	0	861	206	0
21	V	208	0	221	52	0
22	D	1	0	0	0	0
22	N	1	0	0	0	0
All	All	51680	0	36553	6732	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 76.

The worst 5 of 6732 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:158:ILE:H	4:D:158:ILE:CD1	1.57	1.15
1:A:243:A:H4'	1:A:244:U:H5'	1.22	1.12
4:D:176:LEU:HG	4:D:177:ASP:H	0.96	1.12
1:A:1250:A:H4'	9:I:68:GLY:HA2	1.31	1.12
1:A:1347:G:N2	1:A:1373:G:H2'	1.65	1.12

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	
2	B	232/256 (91%)	104 (45%)	70 (30%)	58 (25%)	0	0
3	C	204/239 (85%)	95 (47%)	59 (29%)	50 (24%)	0	0
4	D	206/208 (99%)	94 (46%)	62 (30%)	50 (24%)	0	0
5	E	148/161 (92%)	86 (58%)	38 (26%)	24 (16%)	0	3
6	F	99/101 (98%)	72 (73%)	15 (15%)	12 (12%)	0	5
7	G	153/155 (99%)	78 (51%)	45 (29%)	30 (20%)	0	1
8	H	136/138 (99%)	81 (60%)	32 (24%)	23 (17%)	0	2
9	I	125/128 (98%)	66 (53%)	38 (30%)	21 (17%)	0	2
10	J	96/104 (92%)	54 (56%)	19 (20%)	23 (24%)	0	0
11	K	117/129 (91%)	53 (45%)	33 (28%)	31 (26%)	0	0
12	L	122/135 (90%)	65 (53%)	28 (23%)	29 (24%)	0	0
13	M	116/126 (92%)	67 (58%)	28 (24%)	21 (18%)	0	1
14	N	58/60 (97%)	25 (43%)	19 (33%)	14 (24%)	0	0
15	O	86/88 (98%)	44 (51%)	23 (27%)	19 (22%)	0	1
16	P	81/88 (92%)	41 (51%)	18 (22%)	22 (27%)	0	0
17	Q	102/104 (98%)	66 (65%)	25 (24%)	11 (11%)	0	6
18	R	71/88 (81%)	38 (54%)	16 (22%)	17 (24%)	0	0
19	S	78/92 (85%)	43 (55%)	24 (31%)	11 (14%)	0	3
20	T	97/106 (92%)	31 (32%)	36 (37%)	30 (31%)	0	0
21	V	22/26 (85%)	14 (64%)	7 (32%)	1 (4%)	2	23
All	All	2349/2532 (93%)	1217 (52%)	635 (27%)	497 (21%)	0	1

5 of 497 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	15	VAL

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Mol	Chain	Res	Type
2	B	17	PHE
2	B	39	ILE
2	B	78	GLN
2	B	82	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	
2	B	202/220 (92%)	163 (81%)	39 (19%)	1	9
3	C	160/188 (85%)	127 (79%)	33 (21%)	1	7
4	D	180/180 (100%)	147 (82%)	33 (18%)	1	10
5	E	115/122 (94%)	98 (85%)	17 (15%)	3	18
6	F	90/90 (100%)	79 (88%)	11 (12%)	5	24
7	G	126/126 (100%)	105 (83%)	21 (17%)	2	14
8	H	119/119 (100%)	103 (87%)	16 (13%)	4	21
9	I	98/99 (99%)	71 (72%)	27 (28%)	0	3
10	J	87/91 (96%)	63 (72%)	24 (28%)	0	3
11	K	90/99 (91%)	73 (81%)	17 (19%)	1	9
12	L	104/111 (94%)	90 (86%)	14 (14%)	4	21
13	M	94/101 (93%)	80 (85%)	14 (15%)	3	17
14	N	49/49 (100%)	31 (63%)	18 (37%)	0	0
15	O	79/79 (100%)	68 (86%)	11 (14%)	3	20
16	P	72/74 (97%)	59 (82%)	13 (18%)	1	10
17	Q	96/96 (100%)	82 (85%)	14 (15%)	3	18
18	R	64/77 (83%)	55 (86%)	9 (14%)	3	19
19	S	71/79 (90%)	62 (87%)	9 (13%)	4	23
20	T	76/82 (93%)	68 (90%)	8 (10%)	7	30
21	V	19/21 (90%)	13 (68%)	6 (32%)	0	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1991/2103 (95%)	1637 (82%)	354 (18%)	2 11

5 of 354 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	H	65	TYR
10	J	8	LEU
18	R	53	ARG
8	H	97	VAL
9	I	34	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 66 such sidechains are listed below:

Mol	Chain	Res	Type
6	F	32	ASN
7	G	148	ASN
17	Q	94	ASN
6	F	57	GLN
7	G	11	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1511/1522 (99%)	253 (16%)	62 (4%)

5 of 253 RNA backbone outliers are listed below:

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

5 of 62 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	559	A
1	A	792	A
1	A	1346	A

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Mol	Chain	Res	Type
1	A	687	A
1	A	913	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 2 ligands modelled in this entry, 2 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 ⓘ

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	A	1512/1522 (99%)	0.83	169 (11%) 5 3	12, 87, 171, 195	0
2	B	234/256 (91%)	-0.14	3 (1%) 77 65	21, 87, 149, 181	0
3	C	206/239 (86%)	0.38	20 (9%) 7 5	31, 115, 164, 182	0
4	D	208/208 (100%)	0.04	6 (2%) 51 37	15, 83, 140, 189	0
5	E	150/161 (93%)	0.01	1 (0%) 87 80	4, 55, 110, 132	0
6	F	101/101 (100%)	0.12	5 (4%) 28 20	32, 111, 151, 174	0
7	G	155/155 (100%)	-0.16	6 (3%) 39 27	27, 116, 156, 189	0
8	H	138/138 (100%)	-0.07	1 (0%) 87 80	0, 45, 102, 156	0
9	I	127/128 (99%)	0.66	21 (16%) 1 1	30, 120, 164, 186	0
10	J	98/104 (94%)	1.32	33 (33%) 0 0	43, 122, 168, 183	0
11	K	119/129 (92%)	0.17	4 (3%) 45 33	21, 87, 147, 195	0
12	L	124/135 (91%)	0.13	6 (4%) 30 21	2, 77, 127, 154	0
13	M	118/126 (93%)	0.47	13 (11%) 5 4	45, 118, 163, 195	0
14	N	60/60 (100%)	1.98	24 (40%) 0 0	50, 118, 171, 186	0
15	O	88/88 (100%)	-0.10	3 (3%) 45 33	23, 79, 143, 195	0
16	P	83/88 (94%)	0.06	2 (2%) 59 45	0, 60, 119, 138	0
17	Q	104/104 (100%)	-0.06	3 (2%) 51 37	8, 59, 132, 195	0
18	R	73/88 (82%)	-0.04	3 (4%) 37 26	3, 81, 147, 182	0
19	S	80/92 (86%)	1.33	22 (27%) 0 0	49, 124, 178, 181	0
20	T	99/106 (93%)	-0.33	1 (1%) 82 72	10, 66, 124, 141	0
21	V	24/26 (92%)	2.00	11 (45%) 0 0	84, 114, 145, 180	0
All	All	3901/4054 (96%)	0.46	357 (9%) 9 6	0, 90, 162, 195	0

The worst 5 of 357 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
14	N	4	LYS	10.9
19	S	3	ARG	8.4
17	Q	105	ALA	7.9
4	D	42	GLN	7.8
21	V	24	ARG	7.3

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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. 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	RSCC	RSR	B-factors(\AA^2)	Q<0.9
22	ZN	N	307	1/1	0.97	0.10	74,74,74,74	0
22	ZN	D	306	1/1	0.97	0.45	74,74,74,74	0

6.5 Other polymers [i](#)

There are no such residues in this entry.