



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 29, 2020 – 02:00 PM BST

PDB ID : 1N34
Title : Structure of the *Thermus thermophilus* 30S ribosomal subunit in the presence of codon and crystallographically disordered near-cognate transfer rna anticodon stem-loop mismatched at the first codon position
Authors : Ogle, J.M.; Murphy IV, F.V.; Tarry, M.J.; Ramakrishnan, V.
Deposited on : 2002-10-25
Resolution : 3.80 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	:	2.13
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)	:	2.13

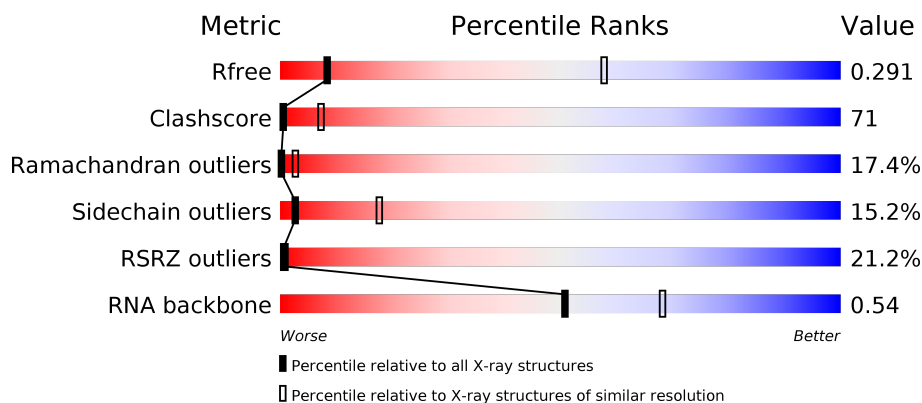
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.80 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	1212 (4.00-3.60)
Clashscore	141614	1288 (4.00-3.60)
Ramachandran outliers	138981	1243 (4.00-3.60)
Sidechain outliers	138945	1237 (4.00-3.60)
RSRZ outliers	127900	1121 (4.00-3.60)
RNA backbone	3102	1036 (4.60-3.00)

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>38%</div> <div> <div>10%</div> <div>72%</div> <div>17%</div> <div>••</div> </div> </div>
2	Z	6	<div> <div>17%</div> <div>50%</div> <div>33%</div> </div>
3	B	256	<div> <div>2%</div> <div>8%</div> <div>58%</div> <div>24%</div> <div>•</div> <div>9%</div> </div>
4	C	239	<div> <div>15%</div> <div>11%</div> <div>51%</div> <div>23%</div> <div>•</div> <div>14%</div> </div>

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Mol	Chain	Length	Quality of chain
5	D	208	
6	E	161	
7	F	101	
8	G	155	
9	H	138	
10	I	128	
11	J	104	
12	K	129	
13	L	135	
14	M	126	
15	N	60	
16	O	88	
17	P	88	
18	Q	104	
19	R	88	
20	S	92	
21	T	106	
22	V	26	

2 Entry composition [i](#)

There are 23 unique types of molecules in this entry. The entry contains 51757 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	42	0	0
			32508	14472	6016	10509	1511			

- Molecule 2 is a RNA chain called A-SITE MESSENGER RNA FRAGMENT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	Z	4	Total	C	N	O	P	0	0	0
			77	36	8	30	3			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	C	206	Total	C	N	O	S	0	0	0
			1612	1016	314	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	150	Total	C	N	O	S	0	0	0
			1146	724	217	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			

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 10 is a protein called 30S RIBOSOMAL PROTEIN S9.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	I	127	Total	C	N	O	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	98	Total	C	N	O	S	0	0	0
			792	498	156	137	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	124	Total	C	N	O	S	0	0	0
			970	611	195	163	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	M	118	Total	C	N	O	S	0	0	0
			937	579	193	163	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	83	Total	C	N	O	S	0	0	0
			700	443	139	117	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	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
Q	96	GLN	ALA	CONFLICT	UNP Q5SHP7

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

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

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

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

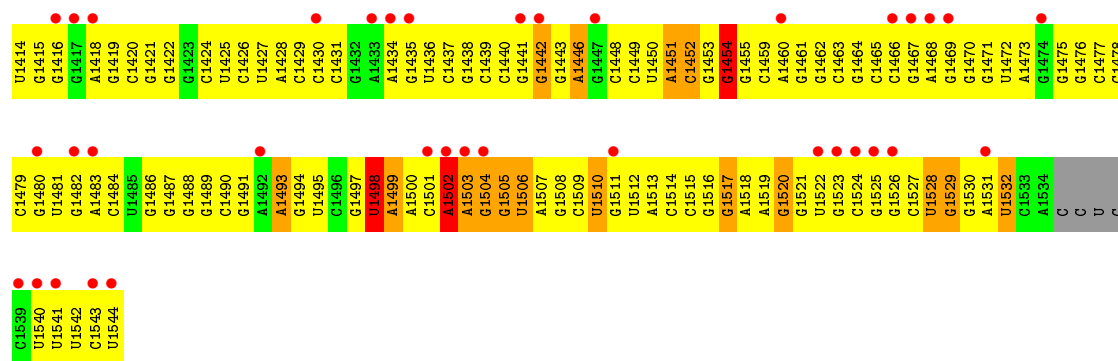
- Molecule 22 is a protein called 30S RIBOSOMAL PROTEIN THX.

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

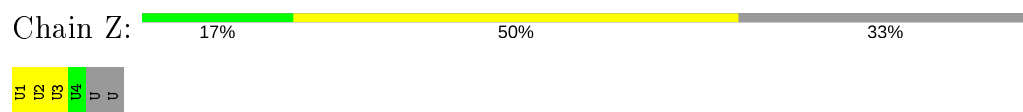
- Molecule 23 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

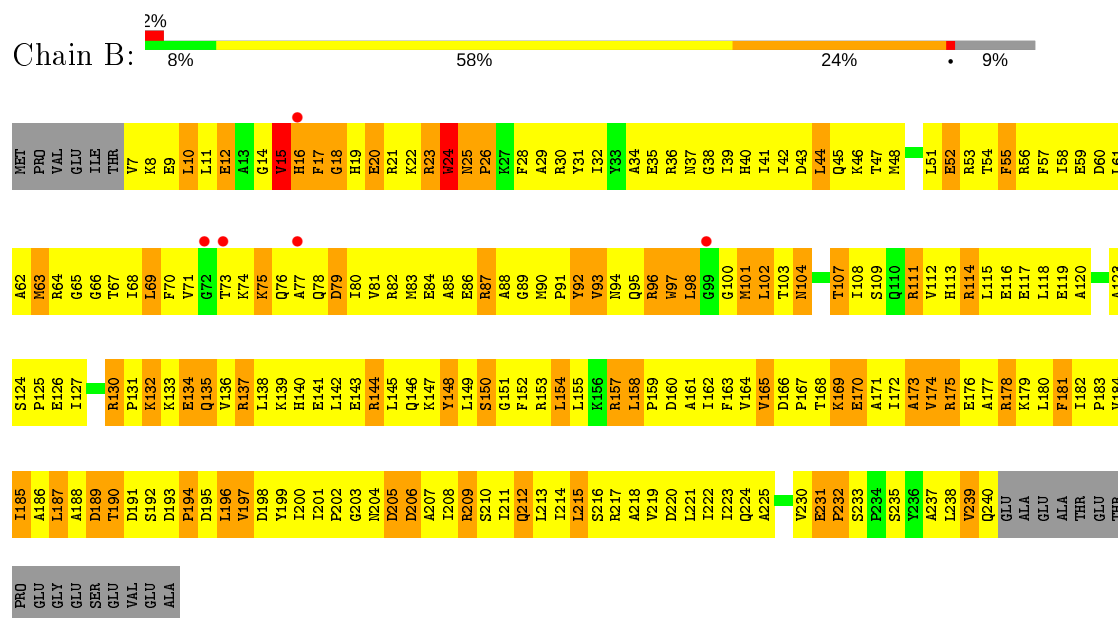
G1353	U1292	U1232	G1172	A1111	G1053	A996	C936	A873	C506	A746	U686	U626
G1354	G1293	G1233	G1173	C1112	U1052	U997	A937	G874	A807	C747	A687	G627
G1355	G1294	G1234	G1174	C1113	G1053	G998	A938	G875	C308	C748	G688	G628
G1356	G1295	U1235	G1175	C1114	C1054	C999	G939	G876	G809	C749	G689	G629
A1357	C1296	A1236	A1176	C1115	U1055	U1001	C940	C877	C810	U751	G690	G630
G1358	G1237	G1237	G1177	C1116	U1056	A1001	G941	G878	C911	U752	G691	G631
G1359	A1238	A1238	G1178	C1117	G1057	G1002	G942	C879	C912	G753	U692	A632
A1360	G1300	A1239	A1179	C1118	G1058	U943	U943	C880	U913	A754	G693	A633
G1361	U1301	U1240	A1180	C1119	C1059	G1003	G944	G881	A314	C755	A694	G634
C1361A	U1302	G1241	G1181	C1120	U1060	G1003A	G945	G882	A815	G755	A695	G635
C1362	C1303	C1242	G1182	U1121	A1005	A1004	A946	C883	A816	C756	A696	U636
G1363	G1304	C1243	A1183	U1122	U1062	A1005	G947	U884	C817	U757	U697	G637
U1364	G1305	C1244	G1184	A1123	G1063	C1007	C948	G885	G818	U758	G698	G638
G1365	A1306	A1245	G1185	G1124	C1064	C1008	A949	G886	A819	A759	C699	G639
G1366	U1307	C1246	G1186	U1125	U1065	G1009	U950	G887	U820	G760	G700	A640
C1367	U1308	U1247	G1187	U1126	C1066	G1010	G951	G888	U821	G761	C701	U641
G1368	G1309	A1248	A1188	G1127	A1067	U952	U952	A889	C922	G762	A702	A642
C1369	G1310	C1249	C1189	U1128	G1068	U1012	G953	G890	G823	G763	G703	G643
G1370	G1311	A1250	G1190	C1129	C1069	G1013	G954	U891	C924	C764	A704	G644
G1371	G1312	A1251	A1191	A1130	U1070	A1014	U955	A892	G825	G765	U705	G645
U1372	C1313	A1252	C1192	G1131	C1071	A1015	U956	A893	G826	A766	A706	U646
C1314	C1314	G1253	G1193	C1132	G1072	A1016	U957	G894	U827	A767	C707	C647
A1373	C1315	C1254	U1194	G1133	U1073	G1017	A958	G895	A828	A768	C708	A648
U1375	G1316	C1255	C1195	G1134	G1074	C1018	A959	C896	G829	G769	G709	G649
G1376	C1317	U1256	U1196	U1135	C1075	U960	U960	C897	G830	C770	G710	G650
A1378	A1318	U1257	G1197	U1136	C1076	U961	U961	G898	U831	G771	G711	C651
C1379	A1319	G1258	G1198	C1137	U1077	U1020	C962	C899	C932	U772	A712	U652
G1379	G1320	C1259	U1199	G1138	U1078	G1021	A968	G906	U833	G773	G713	A653
U1380	C1321	C1260	C1200	G1139	G1079	G1022	A969	A907	U834	A900	G714	G654
U1381	C1322	A1261	A1201	C1140	A1080	G1023	A964	A909	U841	G775	A715	A655
C1382	G1323	C1262	G1202	C1141	G1081	U1025	A965	G902	U835	G776	A716	C656
C1383	A1324	C1263	C1203	G1142	G1082	G1026	G966	G903	G836	G777	A717	G657
C1384	C1325	G1264	A1204	G1143	U1083	C1027	C967	G906	G837	A778	C717	G658
G1385	C1326	G1265	U1205	G1144	C1084	G1028	A968	A907	U838	G778	G718	U659
G1386	C1327	G1266	G1206	C1145	U1085	C1029	A969	A908	U839	C779	C719	G660
G1387	C1328	C1267	G1207	A1146	G1086	G1030	C970	A909	U840	A781	A721	G661
C1388	A1268	A1268	C1208	C1147	G1087	U1030A	C971	C910	C848	A782	G722	G662
C1389	U1330	A1269	C1209	U1148	G1088	G1300B	G973	U911	C849	C783	U723	A663
U1390	G1331	C1270	C1210	C1149	G1089	A974	A974	C912	U850	C784	G724	A664
U1391	A1332	G1271	U1211	U1150	U1090	G1300C	A975	A913	G851	G785	G725	A665
G1392	G1333	G1272	U1212	A1151	U1091	G1031	G976	A914	G852	G786	G726	G666
U1393	C1334	G1273	A1213	A1152	A1092	G1032	A977	A915	G853	A787	G727	G667
A1394	C1335	G1274	G1214	C1153	A1093	G1033	A978	G916	G854	U788	G728	G668
G1395	C1336	A1275	G1215	G1154	G1094	G1034	C979	G917	G855	U789	A729	U669
A1396	G1337	G1276	G1216	G1155	U1095	A1035	C980	A918	U856	A790	G730	G670
C1397	G1338	C1277	C1217	G1156	C1096	U981	U981	A919	G858	G791	G731	G671
A1398	A1339	U1278	C1218	A1157	C1097	G1037	U982	U920	A859	A792	C732	U672
C1399	A1340	A1279	U1219	C1158	C1098	C1038	A983	U921	A860	U793	A733	G673
C1400	U1341	A1280	U1220	U1159	G1099	C1039	G984	G922	G861	A794	G734	G674
G1401	C1342	U1281	G1221	G1160	C1100	U1040	C985	A923	C862	C795	C735	A675
C1402	G1343	C1282	G1222	C1161	A1101	A1041	A986	C924	U863	C796	C736	A676
C1403	C1344	G1283	C1223	C1162	A1102	G1042	G987	G925	A864	C797	A737	U677
C1404	U1345	C1284	G1224	C1163	C1103	C1043	G988	G926	A865	G798	C738	U678
G1405	A1346	A1285	A1225	G1164	G1104	A1044	C989	G927	C866	G799	G739	C679
U1406	G1347	A1286	C1226	C1165	A1105	C1045	C990	G928	G867	G800	U740	G680
C1407	U1348	A1287	A1227	G1166	G1106	A1046	U991	U981	C868	U801	G741	C681
A1408	A1349	A1288	C1228	A1167	C1107	G1047	U992	C932	G869	A802	G742	G682
	U1350	A1289	A1229	A1168	G1108	G1048	G993	G933	U870	G803	G743	G683
	U1351	C1290	C1230	A1169	C1109	U1049	A994	G934	U871	U804	C744	A684
A1412				G1171	A1110	G1050	C995	A935	A872	C805	C745	G685



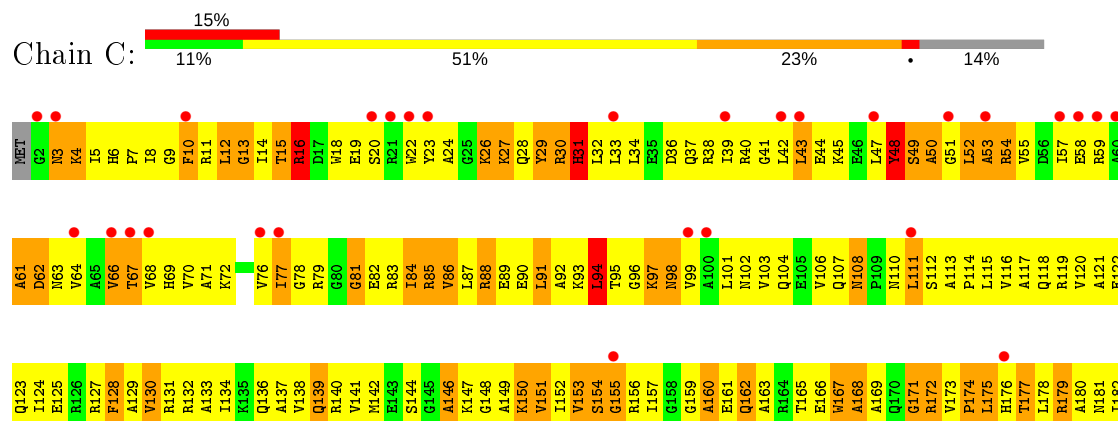
• Molecule 2: A-SITE MESSENGER RNA FRAGMENT

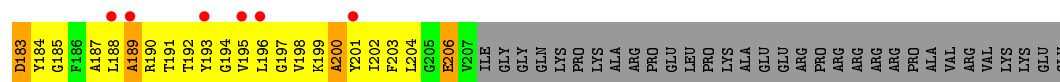


• Molecule 3: 30S RIBOSOMAL PROTEIN S2

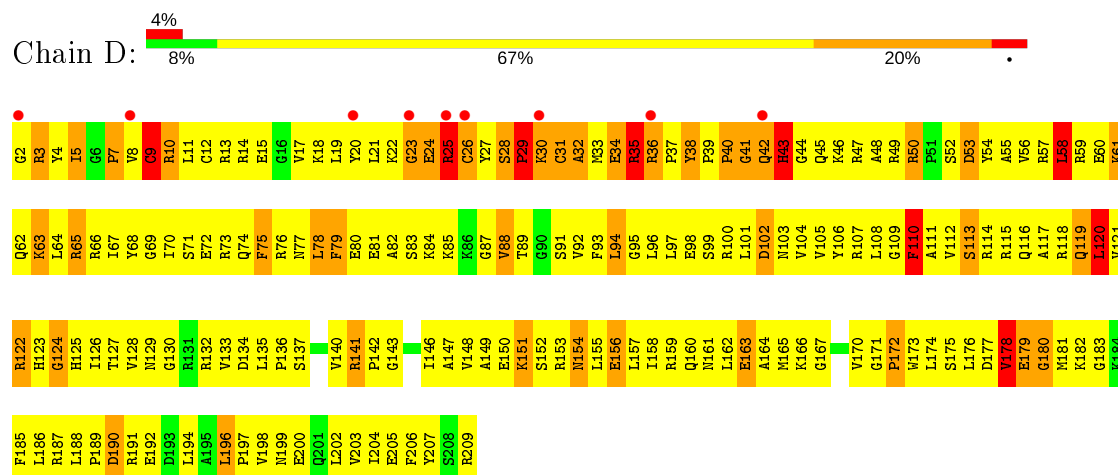


• Molecule 4: 30S RIBOSOMAL PROTEIN S3

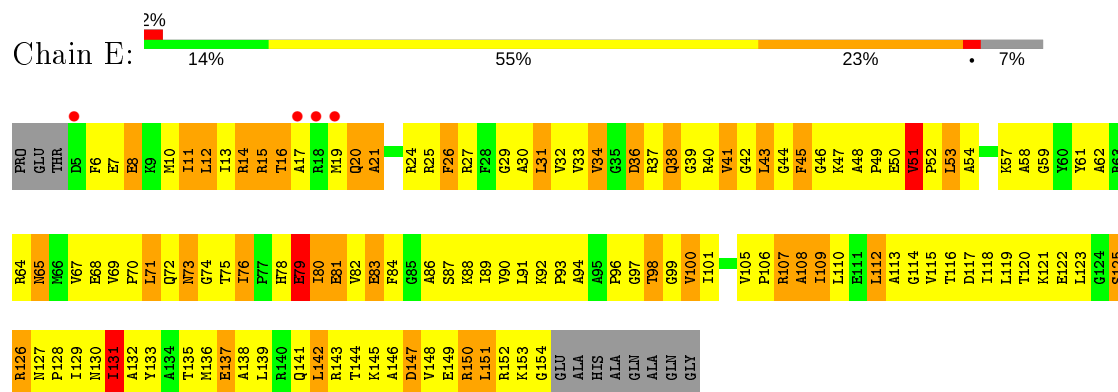




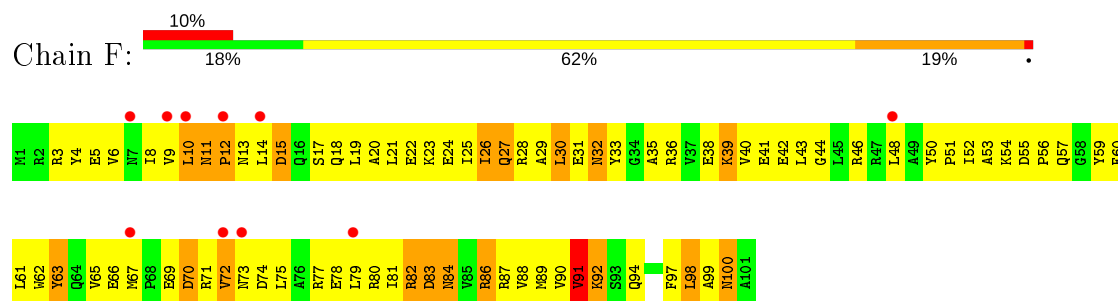
• Molecule 5: 30S RIBOSOMAL PROTEIN S4



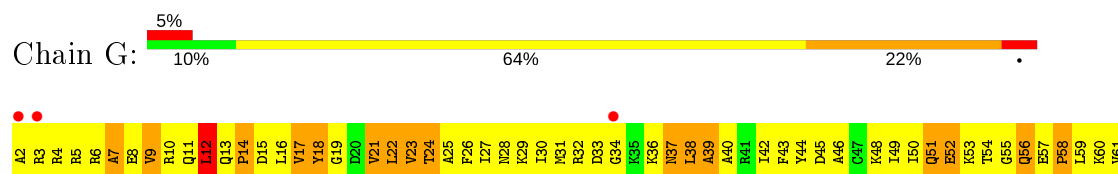
• Molecule 6: 30S RIBOSOMAL PROTEIN S5

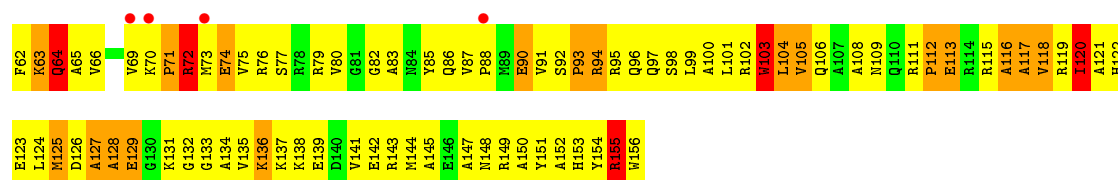


• Molecule 7: 30S RIBOSOMAL PROTEIN S6

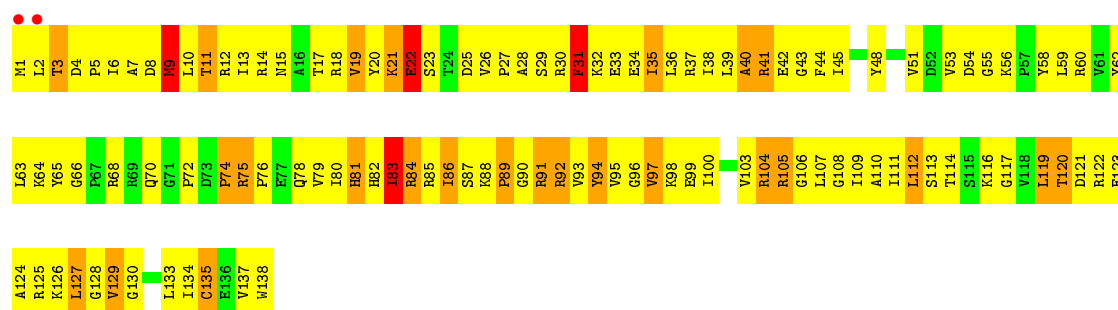


• Molecule 8: 30S RIBOSOMAL PROTEIN S7

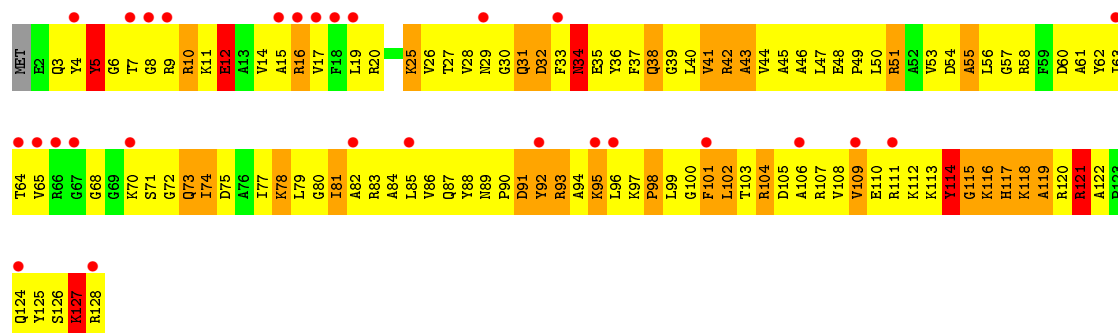
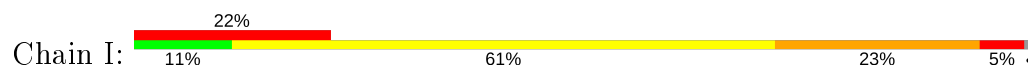




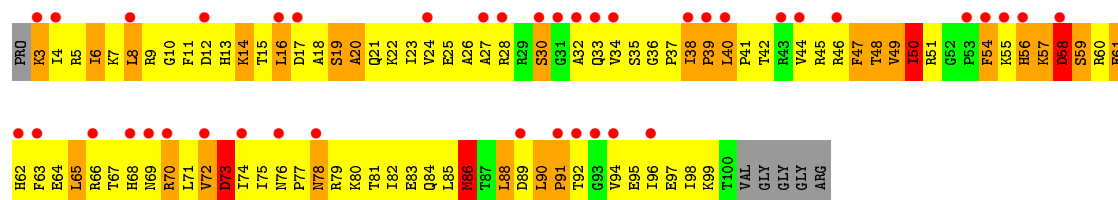
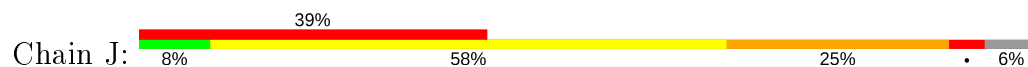
• Molecule 9: 30S RIBOSOMAL PROTEIN S8



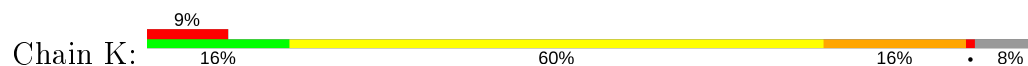
• Molecule 10: 30S RIBOSOMAL PROTEIN S9

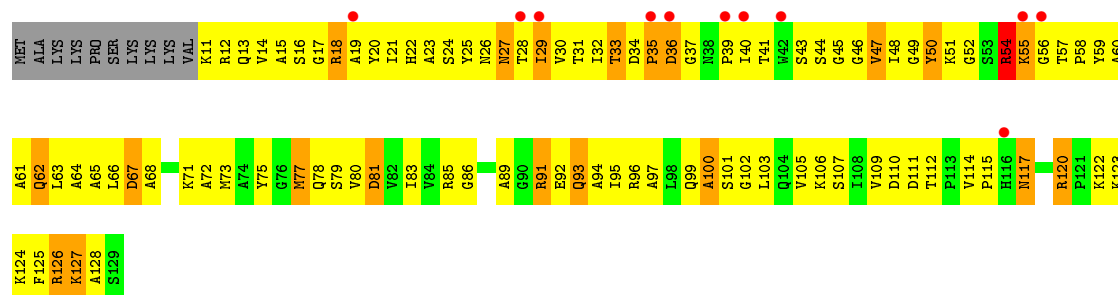


• Molecule 11: 30S RIBOSOMAL PROTEIN S10

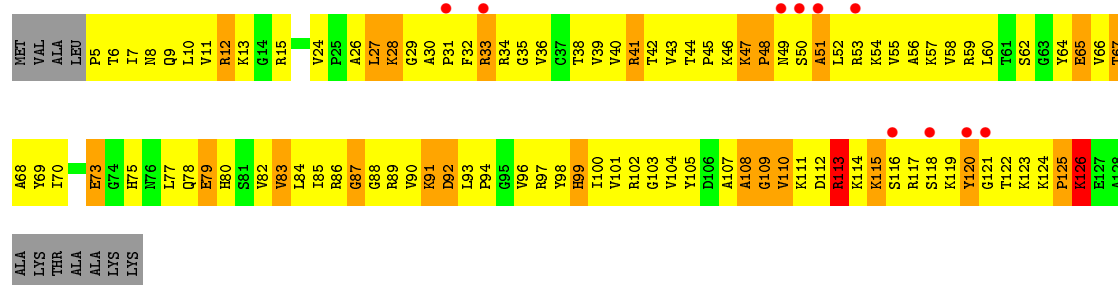
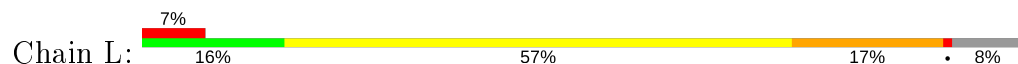


• Molecule 12: 30S RIBOSOMAL PROTEIN S11

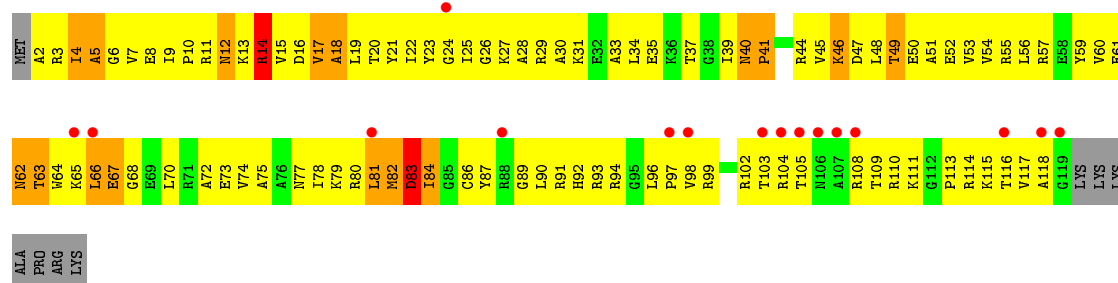
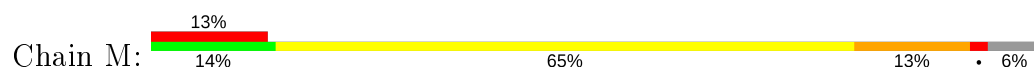




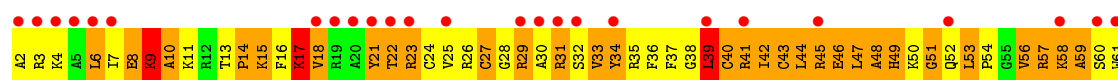
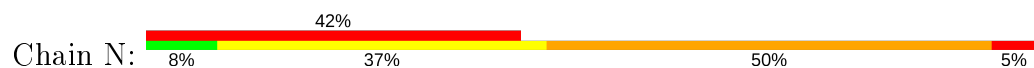
• Molecule 13: 30S RIBOSOMAL PROTEIN S12



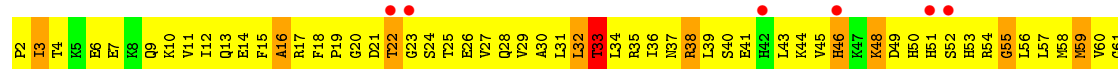
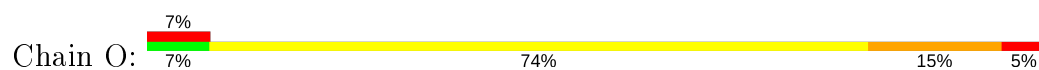
• Molecule 14: 30S RIBOSOMAL PROTEIN S13



• Molecule 15: 30S RIBOSOMAL PROTEIN S14

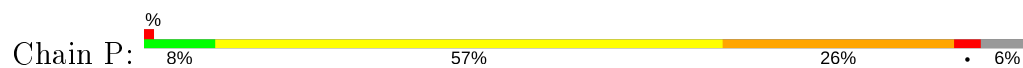


• Molecule 16: 30S RIBOSOMAL PROTEIN S15

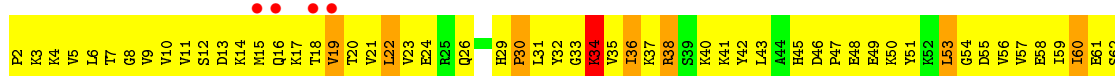
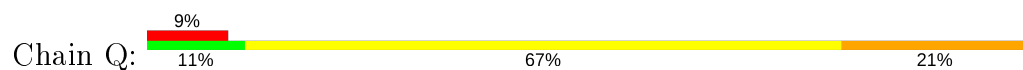




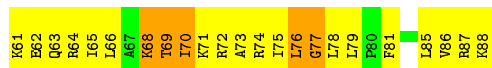
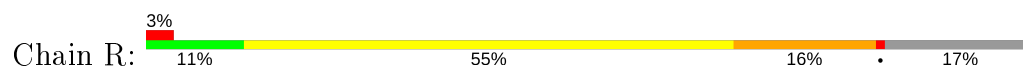
• Molecule 17: 30S RIBOSOMAL PROTEIN S16



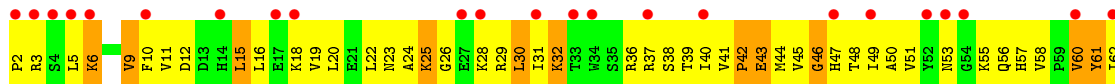
• Molecule 18: 30S RIBOSOMAL PROTEIN S17



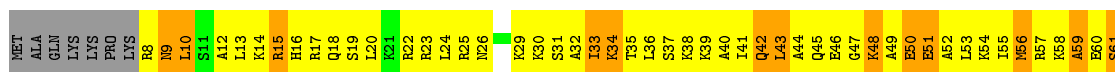
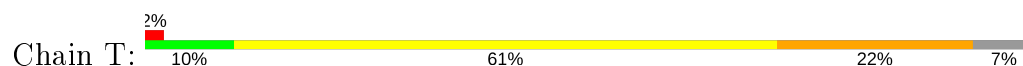
• Molecule 19: 30S RIBOSOMAL PROTEIN S18

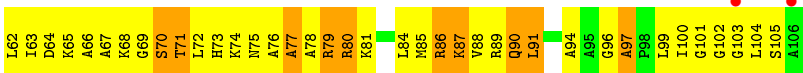


• Molecule 20: 30S RIBOSOMAL PROTEIN S19

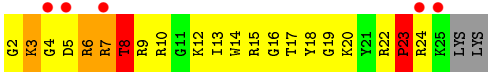
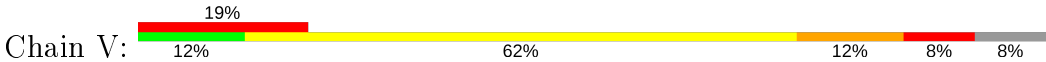


• Molecule 21: 30S RIBOSOMAL PROTEIN S20





● Molecule 22: 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	401.84Å 401.84Å 173.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	141.42 – 3.80 148.30 – 3.78	Depositor EDS
% Data completeness (in resolution range)	92.6 (141.42-3.80) 92.4 (148.30-3.78)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.94 (at 3.78Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.241 , 0.312 0.224 , 0.291	Depositor DCC
R_{free} test set	6465 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	122.1	Xtriage
Anisotropy	0.327	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 194.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.84	EDS
Total number of atoms	51757	wwPDB-VP
Average B, all atoms (Å ²)	101.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.15% 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	0.60	1/36387 (0.0%)	0.76	22/56789 (0.0%)
2	Z	0.62	0/84	0.87	0/128
3	B	0.42	0/1935	0.73	0/2609
4	C	0.37	0/1636	0.70	0/2205
5	D	0.44	0/1733	0.73	0/2318
6	E	0.52	0/1162	0.83	0/1564
7	F	0.37	0/856	0.69	0/1154
8	G	0.35	0/1276	0.66	0/1709
9	H	0.57	0/1136	0.87	0/1527
10	I	0.36	0/1029	0.66	0/1378
11	J	0.36	0/805	0.68	0/1082
12	K	0.42	0/900	0.71	0/1213
13	L	0.41	0/986	0.76	0/1320
14	M	0.36	0/947	0.68	0/1270
15	N	0.38	0/501	0.74	0/664
16	O	0.44	0/745	0.67	0/992
17	P	0.47	0/716	0.71	0/963
18	Q	0.56	0/870	0.83	1/1159 (0.1%)
19	R	0.41	0/603	0.71	0/799
20	S	0.35	0/661	0.67	0/890
21	T	0.37	0/765	0.73	0/1007
22	V	0.40	0/212	0.71	0/277
All	All	0.54	1/55945 (0.0%)	0.75	23/83017 (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	2	42

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Mol	Chain	#Chirality outliers	#Planarity outliers
17	P	0	1
All	All	2	43

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	858	G	C5-C6	-6.02	1.36	1.42

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	51	A	C2'-C3'-O3'	9.80	131.06	109.50
1	A	266	G	C2'-C3'-O3'	9.28	129.91	109.50
1	A	1498	U	C2'-C3'-O3'	9.05	129.41	109.50
1	A	1085	U	C2'-C3'-O3'	7.77	126.60	109.50
1	A	575	G	C2'-C3'-O3'	7.36	125.69	109.50

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	51	A	C3'
1	A	1498	U	C3'

5 of 43 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	127	G	Sidechain
1	A	148	G	Sidechain
1	A	197	A	Sidechain
1	A	28	G	Sidechain
1	A	90	U	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	2480	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	Z	77	0	42	5	0
3	B	1900	0	1951	427	0
4	C	1612	0	1677	396	0
5	D	1703	0	1765	380	0
6	E	1146	0	1207	261	0
7	F	843	0	857	159	0
8	G	1257	0	1296	257	0
9	H	1116	0	1177	235	0
10	I	1011	0	1043	246	0
11	J	792	0	835	245	0
12	K	885	0	904	142	0
13	L	970	0	1057	183	0
14	M	937	0	995	167	0
15	N	492	0	533	140	0
16	O	734	0	771	142	0
17	P	700	0	720	175	0
18	Q	857	0	930	180	0
19	R	597	0	668	143	0
20	S	647	0	673	114	0
21	T	763	0	861	174	0
22	V	208	0	221	53	0
23	D	1	0	0	0	0
23	N	1	0	0	0	0
All	All	51757	0	36597	6246	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 71.

The worst 5 of 6246 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:818:G:O2'	1:A:819:A:H5''	1.44	1.17
1:A:1064:G:H4'	1:A:1065:U:H5'	1.28	1.15
1:A:1443:G:H5''	1:A:1446:A:H5'	1.21	1.14
19:R:53:ARG:HH21	19:R:60:GLY:N	1.46	1.14
6:E:13:ILE:HG22	6:E:30:ALA:HA	1.22	1.13

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	
3	B	232/256 (91%)	134 (58%)	71 (31%)	27 (12%)	0	6
4	C	204/239 (85%)	95 (47%)	64 (31%)	45 (22%)	0	1
5	D	206/208 (99%)	109 (53%)	63 (31%)	34 (16%)	0	3
6	E	148/161 (92%)	98 (66%)	30 (20%)	20 (14%)	0	4
7	F	99/101 (98%)	56 (57%)	30 (30%)	13 (13%)	0	5
8	G	153/155 (99%)	68 (44%)	47 (31%)	38 (25%)	0	1
9	H	136/138 (99%)	91 (67%)	28 (21%)	17 (12%)	0	6
10	I	125/128 (98%)	70 (56%)	27 (22%)	28 (22%)	0	1
11	J	96/104 (92%)	51 (53%)	26 (27%)	19 (20%)	0	2
12	K	117/129 (91%)	72 (62%)	31 (26%)	14 (12%)	0	6
13	L	122/135 (90%)	81 (66%)	22 (18%)	19 (16%)	0	4
14	M	116/126 (92%)	66 (57%)	33 (28%)	17 (15%)	0	4
15	N	58/60 (97%)	25 (43%)	8 (14%)	25 (43%)	0	0
16	O	86/88 (98%)	42 (49%)	30 (35%)	14 (16%)	0	3
17	P	81/88 (92%)	44 (54%)	20 (25%)	17 (21%)	0	1
18	Q	102/104 (98%)	60 (59%)	27 (26%)	15 (15%)	0	4
19	R	71/88 (81%)	36 (51%)	24 (34%)	11 (16%)	0	4
20	S	78/92 (85%)	45 (58%)	24 (31%)	9 (12%)	0	7
21	T	97/106 (92%)	34 (35%)	42 (43%)	21 (22%)	0	1
22	V	22/26 (85%)	10 (46%)	7 (32%)	5 (23%)	0	1
All	All	2349/2532 (93%)	1287 (55%)	654 (28%)	408 (17%)	0	3

5 of 408 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	B	20	GLU

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Mol	Chain	Res	Type
3	B	158	LEU
3	B	232	PRO
3	B	239	VAL
4	C	4	LYS

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	
3	B	202/220 (92%)	156 (77%)	46 (23%)	1	6
4	C	160/188 (85%)	140 (88%)	20 (12%)	4	24
5	D	180/180 (100%)	150 (83%)	30 (17%)	2	15
6	E	115/122 (94%)	90 (78%)	25 (22%)	1	7
7	F	90/90 (100%)	81 (90%)	9 (10%)	7	32
8	G	126/126 (100%)	111 (88%)	15 (12%)	5	26
9	H	119/119 (100%)	102 (86%)	17 (14%)	3	20
10	I	98/99 (99%)	79 (81%)	19 (19%)	1	9
11	J	87/91 (96%)	70 (80%)	17 (20%)	1	9
12	K	90/99 (91%)	76 (84%)	14 (16%)	2	17
13	L	104/111 (94%)	94 (90%)	10 (10%)	8	34
14	M	94/101 (93%)	85 (90%)	9 (10%)	8	34
15	N	49/49 (100%)	35 (71%)	14 (29%)	0	2
16	O	79/79 (100%)	68 (86%)	11 (14%)	3	21
17	P	72/74 (97%)	59 (82%)	13 (18%)	1	12
18	Q	96/96 (100%)	83 (86%)	13 (14%)	4	22
19	R	64/77 (83%)	59 (92%)	5 (8%)	12	42
20	S	71/79 (90%)	63 (89%)	8 (11%)	6	28
21	T	76/82 (93%)	71 (93%)	5 (7%)	16	48
22	V	19/21 (90%)	17 (90%)	2 (10%)	7	30

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1991/2103 (95%)	1689 (85%)	302 (15%)	3 18

5 of 302 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	G	56	GLN
10	I	91	ASP
18	Q	93	GLN
8	G	94	ARG
9	H	84	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
7	F	94	GLN
8	G	122	HIS
19	R	36	ASN
8	G	37	ASN
8	G	86	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1511/1522 (99%)	234 (15%)	51 (3%)
2	Z	3/6 (50%)	0	0
All	All	1514/1528 (99%)	234 (15%)	51 (3%)

5 of 234 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 51 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	575	G

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Mol	Chain	Res	Type
1	A	960	U
1	A	1364	U
1	A	748	C
1	A	976	G

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	1511/1522 (99%)	1.96	572 (37%) 0 0	15, 89, 187, 199	0
2	Z	4/6 (66%)	1.03	0 100 100	168, 184, 185, 199	0
3	B	234/256 (91%)	0.02	5 (2%) 63 55	23, 99, 178, 199	0
4	C	206/239 (86%)	0.91	35 (16%) 1 1	46, 134, 198, 199	0
5	D	208/208 (100%)	0.21	9 (4%) 35 30	14, 86, 165, 189	0
6	E	150/161 (93%)	0.12	4 (2%) 54 45	6, 56, 121, 160	0
7	F	101/101 (100%)	0.53	10 (9%) 7 6	44, 111, 171, 185	0
8	G	155/155 (100%)	0.15	7 (4%) 33 28	43, 141, 195, 199	0
9	H	138/138 (100%)	0.06	2 (1%) 75 68	3, 46, 115, 127	0
10	I	127/128 (99%)	0.92	28 (22%) 0 1	40, 146, 195, 199	0
11	J	98/104 (94%)	1.78	41 (41%) 0 0	63, 154, 199, 199	0
12	K	119/129 (92%)	0.38	11 (9%) 9 7	16, 93, 164, 199	0
13	L	124/135 (91%)	0.35	10 (8%) 12 10	19, 96, 159, 196	0
14	M	118/126 (93%)	0.59	16 (13%) 3 3	61, 125, 173, 199	0
15	N	60/60 (100%)	2.04	25 (41%) 0 0	42, 134, 185, 199	0
16	O	88/88 (100%)	0.17	6 (6%) 17 13	25, 70, 145, 189	0
17	P	83/88 (94%)	0.20	1 (1%) 79 72	12, 69, 141, 188	0
18	Q	104/104 (100%)	0.28	9 (8%) 10 8	2, 69, 140, 199	0
19	R	73/88 (82%)	0.33	3 (4%) 37 31	27, 87, 168, 194	0
20	S	80/92 (86%)	1.82	26 (32%) 0 0	55, 152, 198, 199	0
21	T	99/106 (93%)	-0.02	2 (2%) 65 58	24, 82, 169, 199	0
22	V	24/26 (92%)	1.16	5 (20%) 1 1	39, 125, 181, 195	0
All	All	3904/4060 (96%)	1.06	827 (21%) 0 1	2, 98, 186, 199	0

The worst 5 of 827 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1221	G	10.4
4	C	2	GLY	10.3
1	A	1053	G	9.4
20	S	2	PRO	9.0
5	D	42	GLN	8.5

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 monosaccharides 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
23	ZN	D	306	1/1	0.88	0.39	78,78,78,78	0
23	ZN	N	307	1/1	0.99	0.11	78,78,78,78	0

6.5 Other polymers [i](#)

There are no such residues in this entry.