



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 12:47 PM UTC

PDB ID : 2ZM6 / pdb_00002zm6
Title : Crystal structure of the Thermus thermophilus 30S ribosomal subunit
Authors : Kaminishi, T.; Wang, H.; Kawazoe, M.; Ishii, R.; Schlutzen, F.; Hanawa-Suetsugu, K.; Wilson, D.N.; Nomura, M.; Takemoto, C.; Shirouzu, M.; Fucini, P.; Yokoyama, S.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on : 2008-04-11
Resolution : 3.30 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

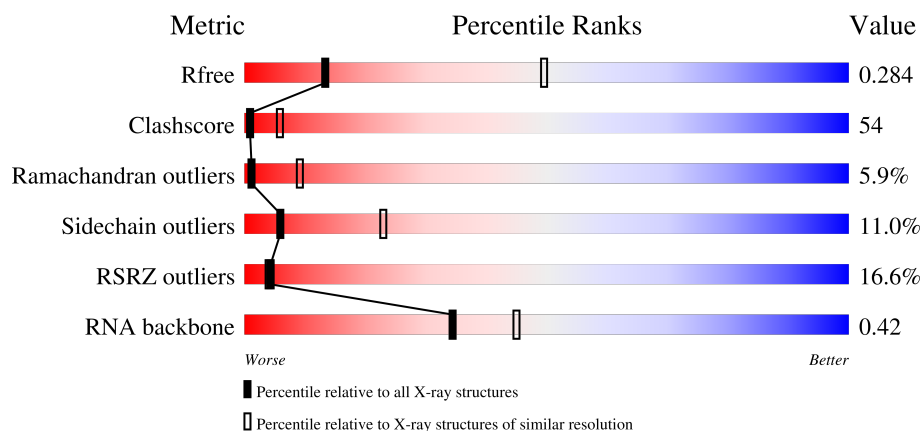
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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}	180053	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)
RNA backbone	3983	1048 (3.60-3.00)

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 of 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	1509	
2	B	255	
3	C	238	
4	D	208	

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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	128	
12	L	131	
13	M	125	
14	N	60	
15	O	88	
16	P	88	
17	Q	104	
18	R	87	
19	S	92	
20	T	105	
21	V	26	

2 Entry composition

There are 22 unique types of molecules in this entry. The entry contains 51308 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	1506	Total	C	N	O	P	0	0	0
			32372	14408	5996	10462	1506			

- Molecule 2 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	222	Total	C	N	O	S	0	0	0
			1810	1154	328	323	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	153	Total	C	N	O	S	0	0	0
			1231	764	246	215	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			

- Molecule 9 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	125	Total	C	N	O	S	0	0	0
			993	629	195	169				

- 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
			794	499	156	138	1			

- Molecule 11 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	115	Total	C	N	O	S	0	0	0
			853	531	160	159	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	120	Total	C	N	O	S	0	0	0
			955	591	197	165	2			

- Molecule 14 is a protein called 30S ribosomal protein S14 type Z.

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	100	Total	C	N	O	S	0	0	0
			834	534	156	142	2			

- Molecule 18 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	R	68	Total	C	N	O	0	0	0
			559	357	109	93			

- 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	94	Total	C	N	O	S	0	0	0
			734	453	157	122	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			

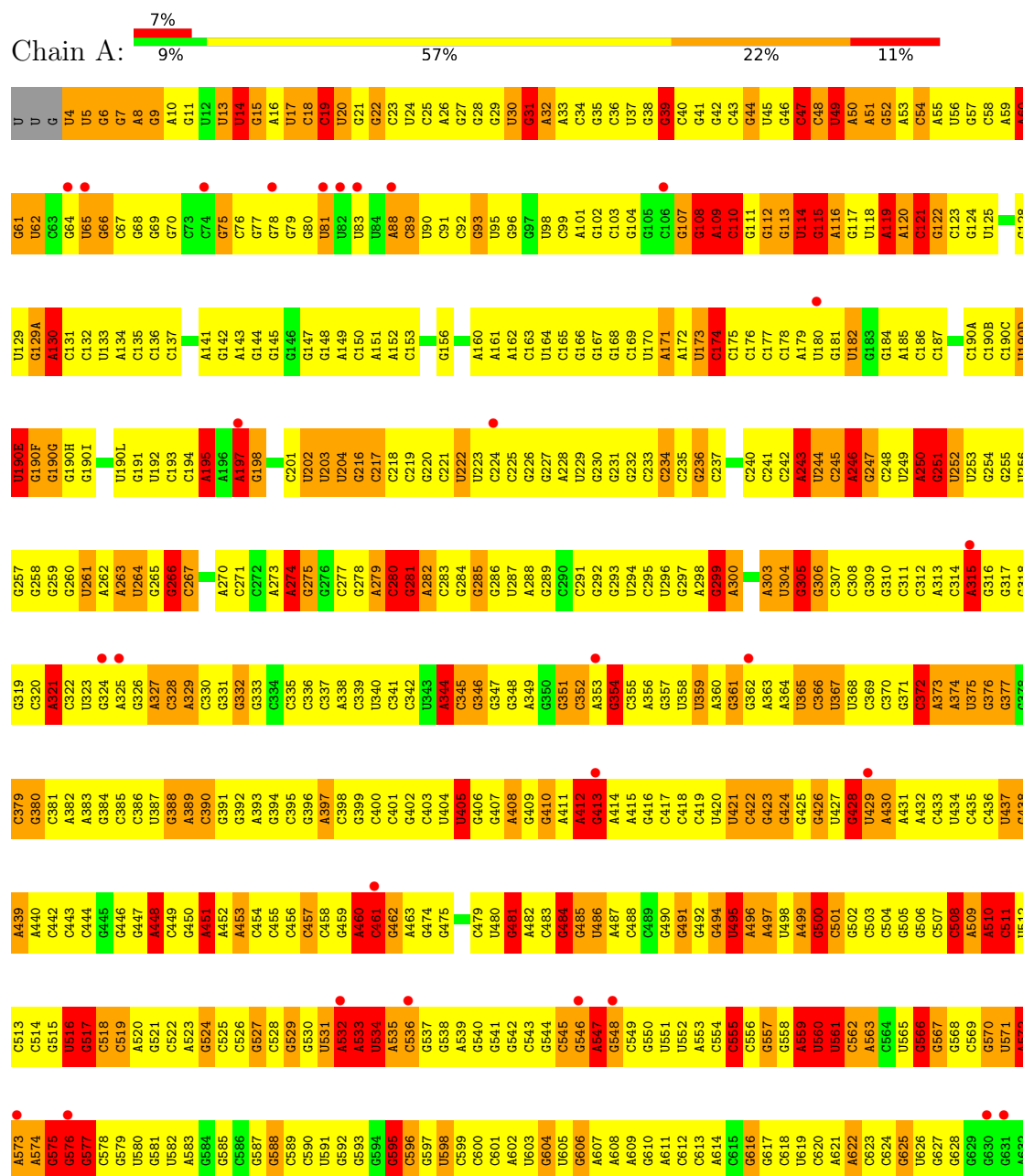
- Molecule 22 is ZINC ION (CCD ID: ZN) (formula: Zn).

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, DNA and oligosaccharide 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.

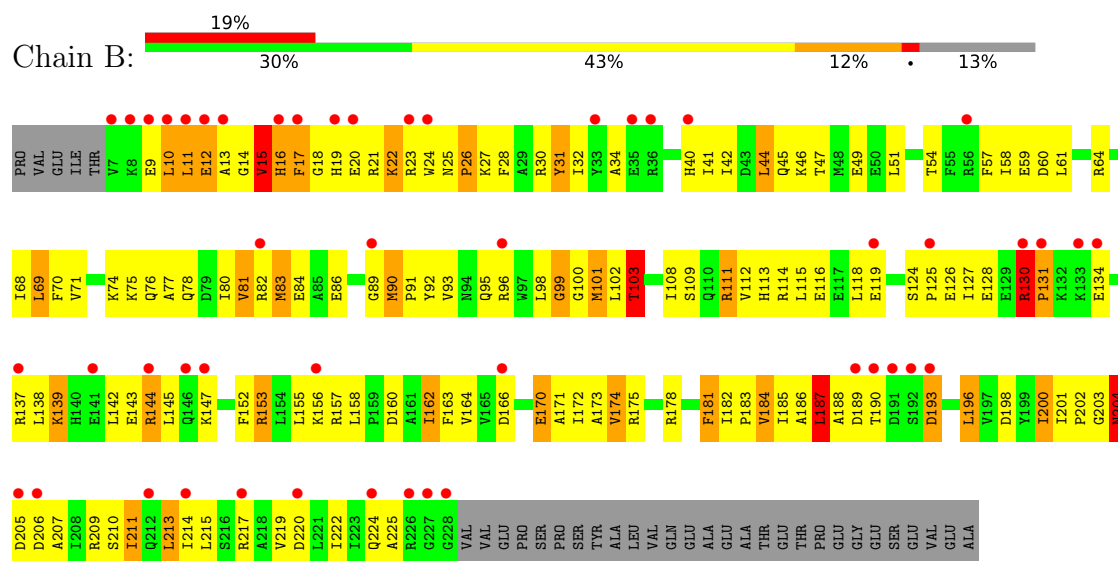
• Molecule 1: 16S ribosomal RNA



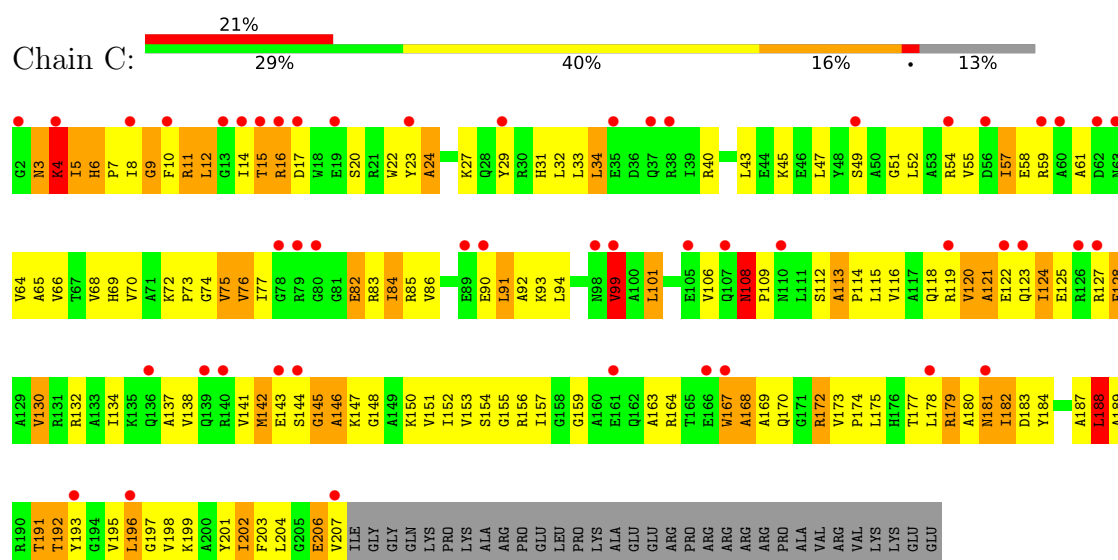
C1430	C1367	U1308	U1247	G1187	A1123	C1063	C1006	A946	G886	A816	C754	G693	G633
C1431	G1368	G1309	A1248	A1188	G1124	G1064	C1007	G947	G887	C817	G755	A694	C634
G1432	C1369	G1310	C1249	C1189	U1126	U1085	C1008	C948	G888	C818	G756	A695	C635
A1433	G1370	G1311	A1250	G1190	U1126	C1066	G1009	A949	A889	A819	U757	A696	U636
A1434	A1371	G1312	A1251	A1191	G1127	A1067	G1010	U950	G890	U820	G758	U697	G637
G1435	U1372	U1313	A1252	C1192	G1128	G1068	G1011	G951	U891	G821	A759	G698	G638
U1436	G1373	G1314	G1253	G1193	G1129	C1069	U1012	U952	A892	C822	G760	C699	G639
A1437	C1254	U1315	C1254	U1194	A1130	U1070	G1013	G853	C893	G823	G761	G700	A640
G1438	G1375	G1316	G1255	C1195	G1131	C1071	A1014	G954	C894	G824	G762	C701	U641
C1439	A1376	C1317	A1256	U1196	G1132	G1072	A1015	U955	C895	G825	A702	A702	A642
C1440	A1377	G1318	U1257	G1197	G1133	U1073	A1016	U956	C896	C826	C764	G703	C643
G1441	C1378	A1319	G1258	U1198	G1134	G1074	G1017	U957	C897	U827	A765	A704	G644
G1442	G1379	C1320	C1259	U1199	U1135	C1075	G1018	A958	G898	A828	A766	U705	C645
G1443	U1380	C1321	G1260	C1200	U1136	G1076	C1019	A959	G899	G829	A767	A706	U646
A1446	C1381	C1322	A1261	A1201	C1137	U1077	U1020	U960	A900	G829	A768	C707	C647
C1447	C1382	G1323	C1262	G1202	G1138	U1078	G1021	A901	A901	U831	G708	G708	A648
C1448	A1383	C1324	C1263	C1203	G1139	G1079	G1022	G962	G902	U831	G709	G649	G650
C1449	G1385	A1325	C1264	A1204	C1140	A1080	G1023	G963	G903	U835	G710	G710	C651
U1450	G1386	C1326	U1265	U1205	C1141	G1081	G1024	A964	C904	G836	G711	G711	C652
A1451	G1387	C1327	G1267	G1206	G1142	U1082	U1025	A965	U905	G837	G712	A712	A653
C1452	A1268	C1328	A1268	G1207	G1143	U1083	G1026	G966	G906	G838	G713	G713	A654
G1453	A1269	A1329	A1269	C1208	G1144	G1084	C1027	C967	A907	U839	G714	G714	A655
G1454	U1390	U1330	C1270	C1209	G1145	U1085	A1028	A968	A908	C840	A777	A715	A656
G1455	G1391	G1331	G1271	C1210	A1146	U1086	U1029	A969	A909	U841	C778	A716	C656
C1459	G1392	A1332	G1272	U1211	C1147	G1087	C1030	C970	C910	C849	C779	G717	G657
U1460	U1393	A1333	G1273	U1212	U1148	G1088	G1030A	G971	U911	C849	A780	G718	G658
G1461	A1394	G1334	G1274	A1213	C1149	U1089	C1030B	C972	C912	U850	A781	C719	U659
C1462	C1395	C1335	A1275	G1214	U1150	G1090	G1030C	A973	A913	C851	A782	C720	G660
C1463	A1396	G1336	U1276	G1215	A1151	U1091	A1030D	A974	A914	C852	C783	G661	G661
C1397	G1377	G1337	G1277	G1216	A1152	A1092	G1031	A975	A915	C853	C784	A722	G662
A1398	U1278	G1338	U1278	C1217	U1153	A1093	G1032	G976	G916	C854	G785	U723	A663
C1399	A1279	A1339	A1279	C1218	U1154	G1094	G1033	A977	C917	G854	G786	G724	G664
C1400	A1280	A1340	A1280	U1219	C1158	U1095	G1034	A978	A918	G858	A787	G725	A665
G1401	U1281	U1341	U1281	G1220	U1159	C1096	A1035	C979	A919	A859	U788	G726	G666
C1402	C1282	C1342	G1283	G1221	G1160	C1097	U1036	C980	U920	A860	U789	G727	G667
C1403	G1283	G1343	G1284	G1222	C1161	C1098	C1037	U981	U921	C861	A790	A728	G668
C1404	C1284	C1344	C1284	C1223	C1162	G1099	G1038	U982	G922	C862	G791	G729	U669
G1405	A1285	U1345	A1285	G1224	G1163	C1100	C1039	A983	A923	U863	A792	G670	G670
U1406	A1286	A1346	A1286	C1225	G1164	A1101	U1040	C984	C924	A864	U793	C732	G671
C1407	A1287	G1347	C1287	C1226	C1165	A1102	A1041	A985	G925	A865	A794	A733	U672
A1408	A1288	A1348	A1288	A1227	G1166	C1103	U1042	A986	G926	C866	C795	G734	G673
G1411	A1289	U1349	A1289	C1228	A1167	G1104	A1044	G987	G927	C867	C796	C735	G674
C1412	G1290	A1350	G1290	A1229	A1168	G1105	U1045	C988	G928	C868	C797	C736	A675
U1481	G1291	U1351	G1291	C1230	A1169	G1106	A1046	C989	G929	C869	G798	A737	A676
G1482	U1292	C1352	U1292	G1231	G1171	C1107	G1047	C990	C930	U870	G799	C738	U677
C1483	G1293	G1353	G1293	U1232	C1172	G1108	G1048	U991	C931	U871	G800	C739	U678
U1484	G1294	C1354	G1294	G1233	G1173	C1109	U1049	U992	C932	A872	U801	U740	G679
U1485	G1295	G1355	G1295	C1234	G1174	A1110	G1050	G993	G933	A873	A802	G741	C680
G1486	C1296	G1356	C1296	U1235	G1175	A1111	C1051	A994	C934	G874	G803	G742	C681
G1487	U1297	A1357	C1297	U1236	A1176	C1112	U1052	C995	A935	C875	U804	U743	G682
G1488	C1298	U1358	C1298	C1237	G1177	C1113	G1053	A996	G936	G876	C805	C744	G683
G1489	A1299	C1359	A1299	A1238	G1178	C1114	C1054	U997	A937	C877	C806	C745	A684
C1490	U1300	A1360	A1299	A1239	A1179	C1115	U1055	G998	G938	C878	A807	A746	G685
G1491	G1301	U1301	U1301	A1180	G1179	C1116	U1056	C999	G939	C879	C808	A747	G686
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C1424	G1303	C1362	C1242	C1242	G1182	G1118	G1058	G1003	G941	C881	C749	G749	G688
U1425	G1304	A1363	C1243	C1243	A1183	C1119	C1059	G1003	G942	C882	C812	G750	C689
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A1492	G1423	C1361A	G1243	C1243	G1423	C1361A	G1243	C1243	G1423	C1361A	G1243	C1243	G1423
A1493	C1424	C1362	C1303	C1303	G1424	C1362	C1303	C1303	G1424	C1362	C1303	C1303	A1493
G1494	U1425	A1363	G1304	C1243	A1183	C1119	C1059	G1003	G942	C882	C812	G750	C689
U1495	G1426	U1364	G1305	C1244	G1184	C1119	C1060	G1003A	U943	C883	U813	U751	G690
C1496	U1427	G1365	A1306	A1245	G1184	U1121	G1061	A1004	G944	U884	G752	G752	G691
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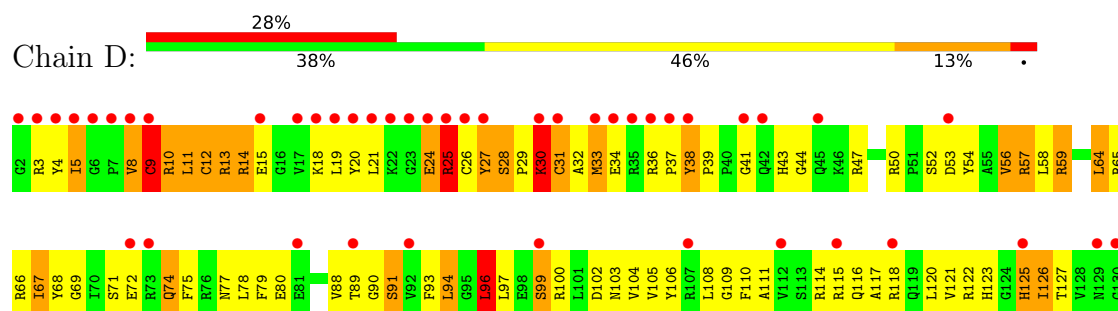
• Molecule 2: 30S ribosomal protein S2

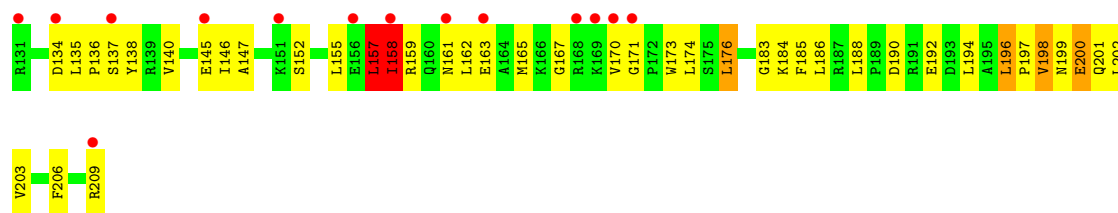


• Molecule 3: 30S ribosomal protein S3

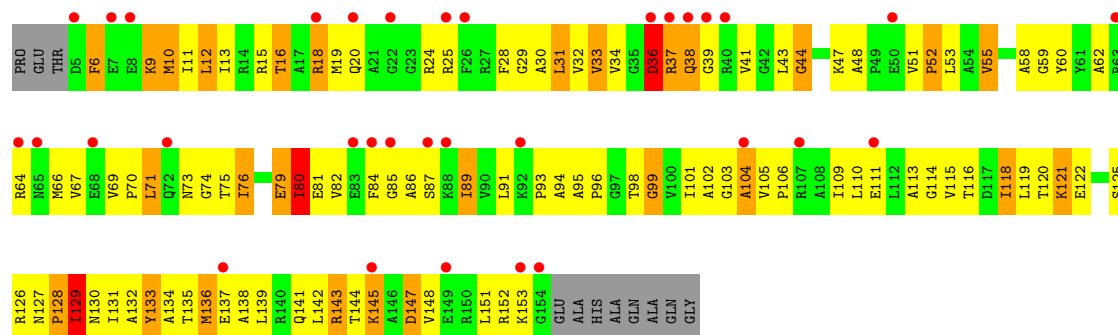


• Molecule 4: 30S ribosomal protein S4

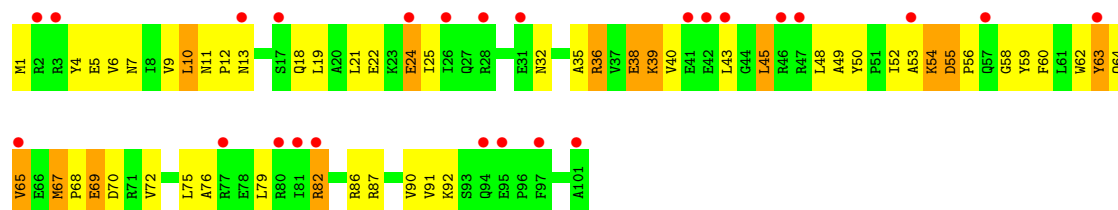




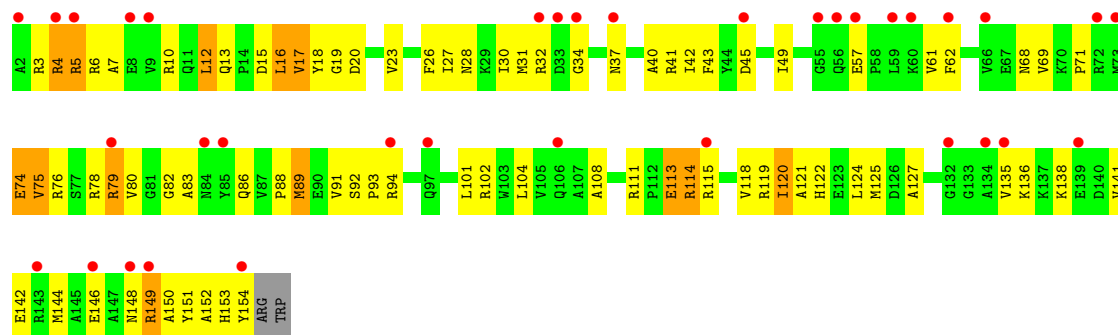
• Molecule 5: 30S ribosomal protein S5



• Molecule 6: 30S ribosomal protein S6

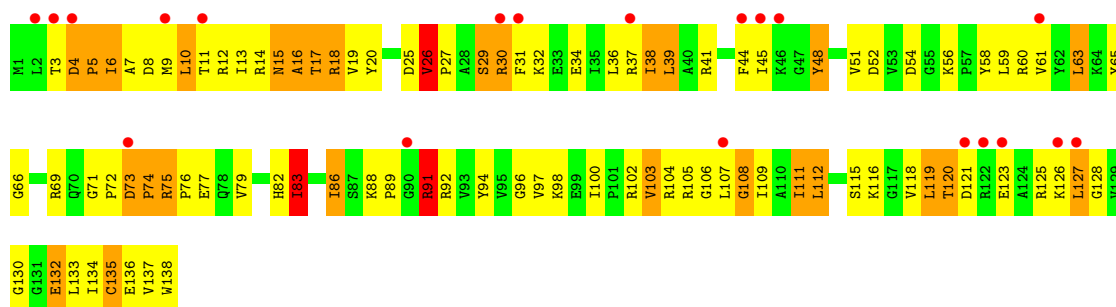


• Molecule 7: 30S ribosomal protein S7

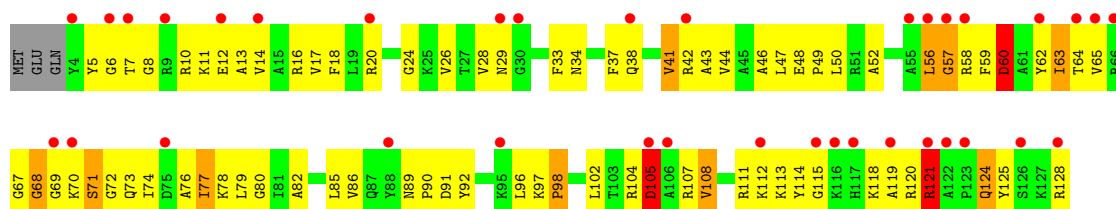


• Molecule 8: 30S ribosomal protein S8

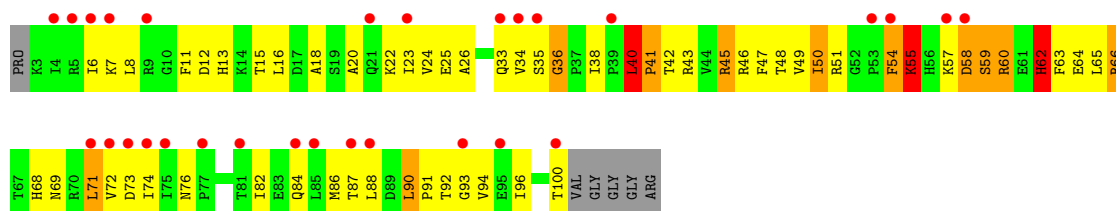




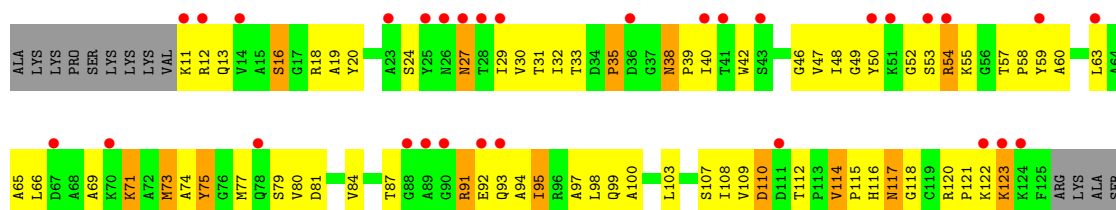
• Molecule 9: 30S ribosomal protein S9



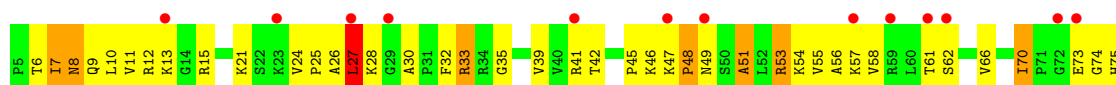
• Molecule 10: 30S ribosomal protein S10

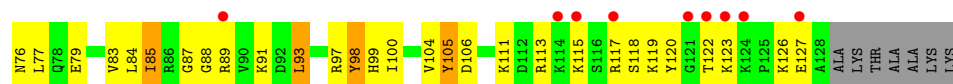


• Molecule 11: 30S ribosomal protein S11

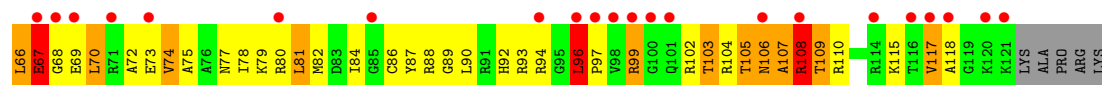
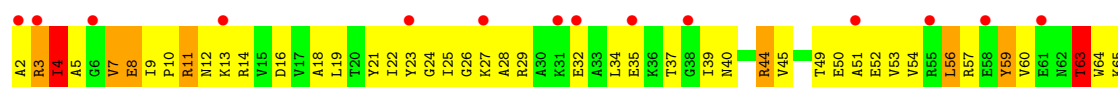


• Molecule 12: 30S ribosomal protein S12





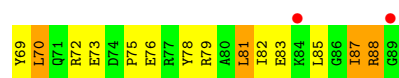
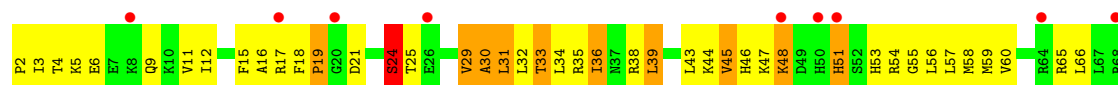
• Molecule 13: 30S ribosomal protein S13



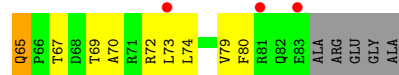
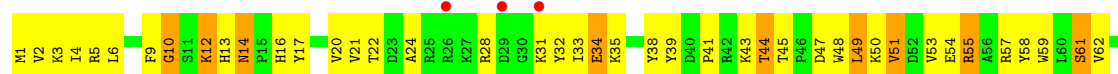
• Molecule 14: 30S ribosomal protein S14 type Z



• Molecule 15: 30S ribosomal protein S15

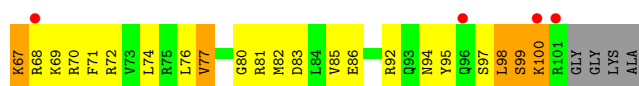


• Molecule 16: 30S ribosomal protein S16

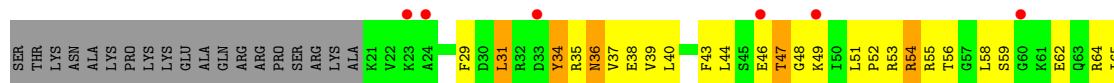


• Molecule 17: 30S ribosomal protein S17

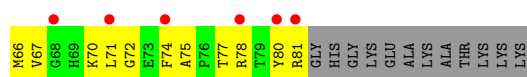
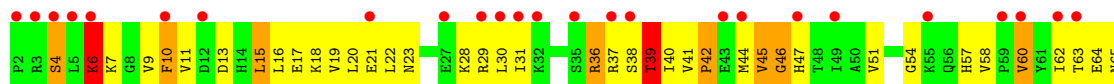




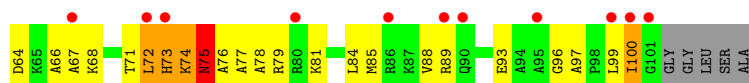
• Molecule 18: 30S ribosomal protein S18



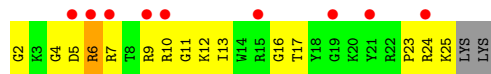
• Molecule 19: 30S ribosomal protein S19



• 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	411.50Å 411.50Å 172.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	184.03 – 3.30 184.03 – 3.30	Depositor EDS
% Data completeness (in resolution range)	97.7 (184.03-3.30) 97.7 (184.03-3.30)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.86 (at 3.33Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.292 , 0.323 0.251 , 0.284	Depositor DCC
R_{free} test set	10942 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	95.8	Xtriage
Anisotropy	0.188	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 999.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.35$, $\langle L^2 \rangle = 0.18$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	51308	wwPDB-VP
Average B, all atoms (Å ²)	109.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.66% 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	1/36237 (0.0%)	1.05	237/56558 (0.4%)
2	B	0.88	3/1842 (0.2%)	1.36	30/2479 (1.2%)
3	C	0.81	2/1636 (0.1%)	1.23	21/2205 (1.0%)
4	D	0.93	1/1733 (0.1%)	1.44	30/2318 (1.3%)
5	E	1.14	3/1162 (0.3%)	1.51	21/1564 (1.3%)
6	F	0.73	0/856	1.31	11/1154 (1.0%)
7	G	0.65	0/1248	1.14	8/1672 (0.5%)
8	H	1.02	1/1136 (0.1%)	1.55	24/1527 (1.6%)
9	I	0.69	0/1011	1.20	9/1354 (0.7%)
10	J	0.68	0/807	1.24	14/1085 (1.3%)
11	K	0.67	0/868	1.35	16/1173 (1.4%)
12	L	0.77	1/986 (0.1%)	1.33	12/1320 (0.9%)
13	M	0.67	0/965	1.35	15/1292 (1.2%)
14	N	0.77	0/501	1.43	9/664 (1.4%)
15	O	0.90	1/745 (0.1%)	1.30	8/992 (0.8%)
16	P	0.88	1/716 (0.1%)	1.17	4/963 (0.4%)
17	Q	0.93	2/847 (0.2%)	1.30	9/1131 (0.8%)
18	R	0.73	0/564	1.26	7/748 (0.9%)
19	S	0.70	0/661	1.36	11/890 (1.2%)
20	T	0.68	0/736	1.24	9/970 (0.9%)
21	V	0.76	0/212	0.98	0/277
All	All	0.71	16/55469 (0.0%)	1.15	505/82336 (0.6%)

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	0	160
4	D	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
5	E	0	1
8	H	0	1
17	Q	0	1
All	All	0	164

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	12	CYS	CA-CB	8.39	1.66	1.53
5	E	55	VAL	CA-CB	-6.63	1.47	1.54
1	A	1077	G	C5-C6	-6.22	1.29	1.42
8	H	16	ALA	CA-CB	-6.10	1.43	1.53
2	B	182	ILE	CA-CB	-5.67	1.47	1.54

The worst 5 of 505 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	31	CYS	N-CA-C	-15.37	95.54	113.21
8	H	75	ARG	CA-C-N	13.32	133.49	119.90
8	H	75	ARG	C-N-CA	13.32	133.49	119.90
13	M	3	ARG	N-CA-C	12.70	127.97	109.69
6	F	55	ASP	CA-C-N	12.03	134.88	119.84

There are no chirality outliers.

5 of 164 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	14	U	Sidechain
1	A	15	G	Sidechain
1	A	17	U	Sidechain
1	A	19	C	Sidechain
1	A	30	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	32372	0	16335	3393	0
2	B	1810	0	1861	129	0
3	C	1612	0	1677	177	0
4	D	1703	0	1763	143	0
5	E	1146	0	1207	120	0
6	F	843	0	857	45	0
7	G	1231	0	1273	84	0
8	H	1116	0	1177	118	0
9	I	993	0	1029	109	0
10	J	794	0	840	67	0
11	K	853	0	868	54	0
12	L	970	0	1057	81	0
13	M	955	0	1021	98	0
14	N	492	0	529	65	0
15	O	734	0	771	47	0
16	P	700	0	720	67	0
17	Q	834	0	906	73	0
18	R	559	0	624	51	0
19	S	647	0	673	59	0
20	T	734	0	832	60	0
21	V	208	0	221	15	0
22	D	1	0	0	0	0
22	N	1	0	0	0	0
All	All	51308	0	36241	4658	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 54.

The worst 5 of 4658 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:1027:C:C2'	1:A:1028:C:H5''	1.52	1.36
1:A:1250:A:H2'	1:A:1251:A:C8	1.72	1.25
14:N:24:CYS:SG	14:N:39:LEU:HA	1.79	1.21
1:A:1027:C:H2'	1:A:1028:C:C5'	1.72	1.19
1:A:109:A:H2'	1:A:326:G:N2	1.58	1.18

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	220/255 (86%)	165 (75%)	41 (19%)	14 (6%)	1	8
3	C	204/238 (86%)	140 (69%)	47 (23%)	17 (8%)	0	5
4	D	206/208 (99%)	153 (74%)	42 (20%)	11 (5%)	1	10
5	E	148/161 (92%)	113 (76%)	24 (16%)	11 (7%)	1	6
6	F	99/101 (98%)	86 (87%)	9 (9%)	4 (4%)	2	15
7	G	151/155 (97%)	126 (83%)	21 (14%)	4 (3%)	4	23
8	H	136/138 (99%)	117 (86%)	13 (10%)	6 (4%)	2	13
9	I	123/128 (96%)	98 (80%)	21 (17%)	4 (3%)	3	19
10	J	96/104 (92%)	74 (77%)	14 (15%)	8 (8%)	0	5
11	K	113/128 (88%)	88 (78%)	17 (15%)	8 (7%)	1	6
12	L	122/131 (93%)	87 (71%)	26 (21%)	9 (7%)	1	6
13	M	118/125 (94%)	75 (64%)	31 (26%)	12 (10%)	0	2
14	N	58/60 (97%)	46 (79%)	12 (21%)	0	100	100
15	O	86/88 (98%)	62 (72%)	17 (20%)	7 (8%)	1	5
16	P	81/88 (92%)	58 (72%)	19 (24%)	4 (5%)	1	12
17	Q	98/104 (94%)	77 (79%)	16 (16%)	5 (5%)	1	11
18	R	66/87 (76%)	45 (68%)	17 (26%)	4 (6%)	1	9
19	S	78/92 (85%)	62 (80%)	15 (19%)	1 (1%)	9	35
20	T	92/105 (88%)	70 (76%)	16 (17%)	6 (6%)	1	8
21	V	22/26 (85%)	17 (77%)	3 (14%)	2 (9%)	0	3
All	All	2317/2522 (92%)	1759 (76%)	421 (18%)	137 (6%)	1	9

5 of 137 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	10	LEU

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Mol	Chain	Res	Type
2	B	12	GLU
2	B	21	ARG
2	B	24	TRP
2	B	95	GLN

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	191/219 (87%)	162 (85%)	29 (15%)	3	13
3	C	160/187 (86%)	136 (85%)	24 (15%)	3	13
4	D	180/180 (100%)	161 (89%)	19 (11%)	6	24
5	E	115/122 (94%)	99 (86%)	16 (14%)	3	15
6	F	90/90 (100%)	81 (90%)	9 (10%)	7	27
7	G	124/126 (98%)	118 (95%)	6 (5%)	23	52
8	H	119/119 (100%)	102 (86%)	17 (14%)	3	14
9	I	96/99 (97%)	89 (93%)	7 (7%)	13	39
10	J	88/91 (97%)	78 (89%)	10 (11%)	5	21
11	K	87/98 (89%)	81 (93%)	6 (7%)	14	41
12	L	104/108 (96%)	98 (94%)	6 (6%)	18	47
13	M	96/100 (96%)	82 (85%)	14 (15%)	3	14
14	N	49/49 (100%)	40 (82%)	9 (18%)	1	7
15	O	79/79 (100%)	66 (84%)	13 (16%)	2	11
16	P	72/74 (97%)	66 (92%)	6 (8%)	10	34
17	Q	95/96 (99%)	86 (90%)	9 (10%)	8	29
18	R	60/76 (79%)	56 (93%)	4 (7%)	15	42
19	S	71/79 (90%)	64 (90%)	7 (10%)	7	27
20	T	74/81 (91%)	68 (92%)	6 (8%)	11	36
21	V	19/21 (90%)	19 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1969/2094 (94%)	1752 (89%)	217 (11%)	6 23

5 of 217 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	H	111	ILE
12	L	7	ILE
17	Q	100	LYS
8	H	132	GLU
10	J	45	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 37 such sidechains are listed below:

Mol	Chain	Res	Type
12	L	75	HIS
19	S	23	ASN
13	M	77	ASN
15	O	46	HIS
5	E	130	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1506/1509 (99%)	336 (22%)	181 (12%)

5 of 336 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	5	U
1	A	6	G
1	A	7	G
1	A	8	A
1	A	9	G

5 of 181 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	993	G
1	A	1240	U
1	A	1065	U

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Mol	Chain	Res	Type
1	A	1157	A
1	A	1297	C

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 oligosaccharides 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	1506/1509 (99%)	0.43	104 (6%) 23 16	29, 94, 180, 218	0
2	B	222/255 (87%)	1.25	49 (22%) 2 2	43, 111, 195, 218	0
3	C	206/238 (86%)	1.39	50 (24%) 2 1	49, 123, 192, 215	0
4	D	208/208 (100%)	1.39	59 (28%) 1 1	25, 101, 171, 218	0
5	E	150/161 (93%)	1.12	33 (22%) 2 2	42, 85, 151, 185	0
6	F	101/101 (100%)	1.22	25 (24%) 2 1	53, 122, 186, 211	0
7	G	153/155 (98%)	1.38	35 (22%) 2 2	74, 136, 196, 218	0
8	H	138/138 (100%)	0.79	20 (14%) 6 5	30, 83, 156, 193	0
9	I	125/128 (97%)	1.50	36 (28%) 1 1	69, 144, 201, 218	0
10	J	98/104 (94%)	1.63	29 (29%) 1 1	61, 150, 210, 218	0
11	K	115/128 (89%)	1.37	31 (26%) 1 1	60, 118, 181, 209	0
12	L	124/131 (94%)	1.02	22 (17%) 4 3	41, 108, 169, 204	0
13	M	120/125 (96%)	1.51	36 (30%) 1 1	66, 133, 198, 218	0
14	N	60/60 (100%)	1.15	11 (18%) 3 3	56, 110, 174, 203	0
15	O	88/88 (100%)	0.68	11 (12%) 8 6	50, 103, 167, 203	0
16	P	83/88 (94%)	0.72	6 (7%) 21 15	36, 91, 152, 216	0
17	Q	100/104 (96%)	0.67	13 (13%) 7 6	43, 95, 166, 211	0
18	R	68/87 (78%)	0.84	9 (13%) 7 6	49, 102, 184, 196	0
19	S	80/92 (86%)	1.60	31 (38%) 1 1	66, 143, 208, 218	0
20	T	94/105 (89%)	1.46	21 (22%) 2 2	64, 126, 190, 218	0
21	V	24/26 (92%)	1.63	9 (37%) 1 1	93, 129, 158, 188	0
All	All	3863/4031 (95%)	0.92	640 (16%) 4 4	25, 104, 188, 218	0

The worst 5 of 640 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	107	GLN	12.5
1	A	1129	C	11.5
20	T	101	GLY	10.5
3	C	56	ASP	9.1
3	C	14	ILE	8.4

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 oligosaccharides 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($\text{\AA}^2$)	Q<0.9
22	ZN	D	210	1/1	0.94	0.21	90,90,90,90	0
22	ZN	N	62	1/1	1.00	0.02	101,101,101,101	0

6.5 Other polymers [i](#)

There are no such residues in this entry.