



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 09:53 PM GMT

PDB ID : 1QZW
Title : Crystal structure of the complete core of archaeal SRP and implications for inter-domain communication
Authors : Rosendal, K.R.; Wild, K.; Montoya, G.; Sinning, I.
Deposited on : 2003-09-18
Resolution : 4.10 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
<http://wwpdb.org/validation/2016/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
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

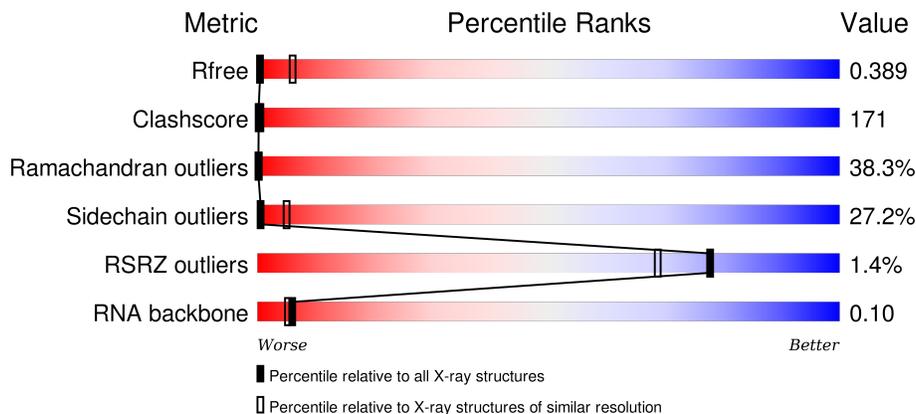
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1018 (4.60-3.60)
Clashscore	102246	1117 (4.60-3.60)
Ramachandran outliers	100387	1063 (4.60-3.60)
Sidechain outliers	100360	1049 (4.60-3.60)
RSRZ outliers	91569	1022 (4.60-3.60)
RNA backbone	2183	1079 (5.04-2.80)

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. 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	B	47	
1	D	47	
1	F	47	
1	H	47	

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Mol	Chain	Length	Quality of chain
2	A	440	 45% 41% 9%
2	C	440	 45% 41% 9%
2	E	440	 45% 41% 9%
2	G	440	 45% 40% 9%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	GTP	B	179	X	-	-	-
1	GTP	D	179	X	-	-	-
1	GTP	F	179	X	-	-	-
1	GTP	H	179	X	-	-	-

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 17720 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 7S RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	B	47	Total	C	N	O	P	0	0	0
			1031	452	197	332	50			
1	D	47	Total	C	N	O	P	0	0	0
			1031	452	197	332	50			
1	F	47	Total	C	N	O	P	0	0	0
			1031	452	197	332	50			
1	H	47	Total	C	N	O	P	0	0	0
			1031	452	197	332	50			

- Molecule 2 is a protein called Signal recognition 54 kDa protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	A	432	Total	C	N	O	S	0	0	0
			3399	2173	574	637	15			
2	C	432	Total	C	N	O	S	0	0	0
			3399	2173	574	637	15			
2	E	432	Total	C	N	O	S	0	0	0
			3399	2173	574	637	15			
2	G	432	Total	C	N	O	S	0	0	0
			3399	2173	574	637	15			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	MET	-	EXPRESSION TAG	UNP Q97ZE7
A	-6	GLY	-	EXPRESSION TAG	UNP Q97ZE7
A	-5	HIS	-	EXPRESSION TAG	UNP Q97ZE7
A	-4	HIS	-	EXPRESSION TAG	UNP Q97ZE7
A	-3	HIS	-	EXPRESSION TAG	UNP Q97ZE7
A	-2	HIS	-	EXPRESSION TAG	UNP Q97ZE7
A	-1	HIS	-	EXPRESSION TAG	UNP Q97ZE7
A	0	HIS	-	EXPRESSION TAG	UNP Q97ZE7
C	-7	MET	-	EXPRESSION TAG	UNP Q97ZE7

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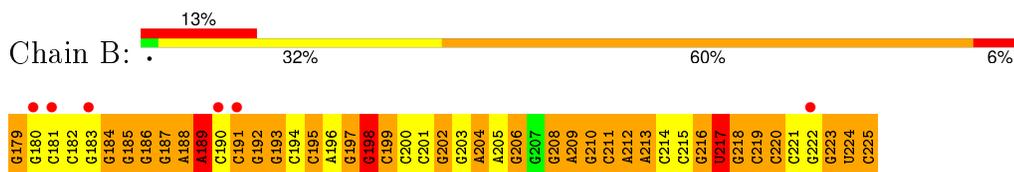
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Chain	Residue	Modelled	Actual	Comment	Reference
C	-6	GLY	-	EXPRESSION TAG	UNP Q97ZE7
C	-5	HIS	-	EXPRESSION TAG	UNP Q97ZE7
C	-4	HIS	-	EXPRESSION TAG	UNP Q97ZE7
C	-3	HIS	-	EXPRESSION TAG	UNP Q97ZE7
C	-2	HIS	-	EXPRESSION TAG	UNP Q97ZE7
C	-1	HIS	-	EXPRESSION TAG	UNP Q97ZE7
C	0	HIS	-	EXPRESSION TAG	UNP Q97ZE7
E	-7	MET	-	EXPRESSION TAG	UNP Q97ZE7
E	-6	GLY	-	EXPRESSION TAG	UNP Q97ZE7
E	-5	HIS	-	EXPRESSION TAG	UNP Q97ZE7
E	-4	HIS	-	EXPRESSION TAG	UNP Q97ZE7
E	-3	HIS	-	EXPRESSION TAG	UNP Q97ZE7
E	-2	HIS	-	EXPRESSION TAG	UNP Q97ZE7
E	-1	HIS	-	EXPRESSION TAG	UNP Q97ZE7
E	0	HIS	-	EXPRESSION TAG	UNP Q97ZE7
G	-7	MET	-	EXPRESSION TAG	UNP Q97ZE7
G	-6	GLY	-	EXPRESSION TAG	UNP Q97ZE7
G	-5	HIS	-	EXPRESSION TAG	UNP Q97ZE7
G	-4	HIS	-	EXPRESSION TAG	UNP Q97ZE7
G	-3	HIS	-	EXPRESSION TAG	UNP Q97ZE7
G	-2	HIS	-	EXPRESSION TAG	UNP Q97ZE7
G	-1	HIS	-	EXPRESSION TAG	UNP Q97ZE7
G	0	HIS	-	EXPRESSION TAG	UNP Q97ZE7

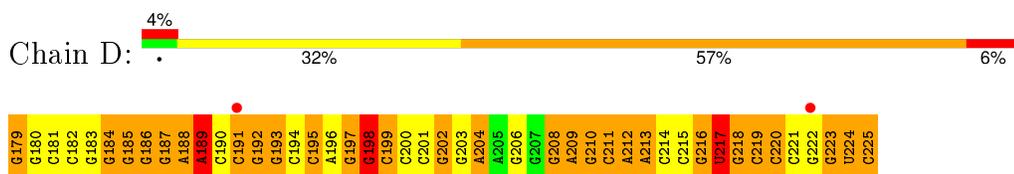
3 Residue-property plots [i](#)

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

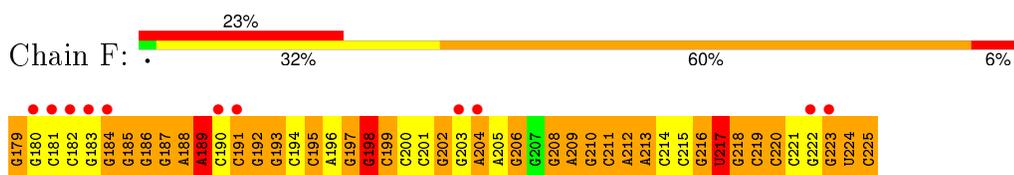
- Molecule 1: 7S RNA



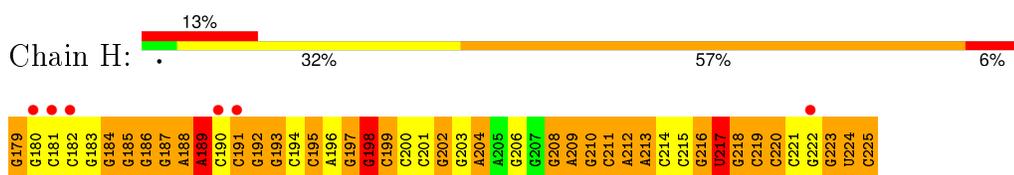
- Molecule 1: 7S RNA



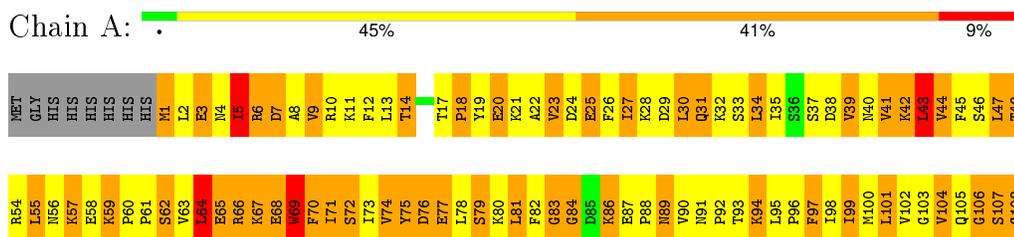
- Molecule 1: 7S RNA



- Molecule 1: 7S RNA



- Molecule 2: Signal recognition 54 kDa protein



G114	K115	L116	M117	N118	O119	P120	Q121	R122	S123	T124	U125	V126	W127	X128	Y129	Z130	A131	B132	C133	D134	E135	F136	G137	H138	I139	J140	K141	L142	M143	N144	O145	P146	Q147	R148	S149	T150	U151	V152	W153	X154	Y155	Z156	A157	B158	C159	D160	E161	F162	G163	H164	I165	J166	K167	L168	M169	N170	O171	P172	Q173	R174																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																															
V175	K176	M177	N178	O179	P180	Q181	R182	S183	T184	U185	V186	W187	X188	Y189	Z190	A191	B192	C193	D194	E195	F196	G197	H198	I199	J200	K201	L202	M203	N204	O205	P206	Q207	R208	S209	T210	U211	V212	W213	X214	Y215	Z216	A217	B218	C219	D220	E221	F222	G223	H224	I225	J226	K227	L228	M229	N230	O231	P232	Q233	R234	S235	T236	U237	V238	W239	X240	Y241	Z242	A243	B244	C245	D246	E247	F248	G249	H250	I251	J252	K253	L254	M255	N256	O257	P258	Q259	R260	S261	T262	U263	V264	W265	X266	Y267	Z268	A269	B270	C271	D272	E273	F274	G275	H276	I277	J278	K279	L280	M281	N282	O283	P284	Q285	R286	S287	T288	U289	V290	W291	X292	Y293	Z294	A295	B296	C297	D298	E299	F300	G301	H302	I303	J304	K305	L306	M307	N308	O309	P310	Q311	R312	S313	T314	U315	V316	W317	X318	Y319	Z320	A321	B322	C323	D324	E325	F326	G327	H328	I329	J330	K331	L332	M333	N334	O335	P336	Q337	R338	S339	T340	U341	V342	W343	X344	Y345	Z346	A347	B348	C349	D350	E351	F352	G353	H354	I355	J356	K357	L358	M359	N360	O361	P362	Q363	R364	S365	T366	U367	V368	W369	X370	Y371	Z372	A373	B374	C375	D376	E377	F378	G379	H380	I381	J382	K383	L384	M385	N386	O387	P388	Q389	R390	S391	T392	U393	V394	W395	X396	Y397	Z398	A399	B400	C401	D402	E403	F404	G405	H406	I407	J408	K409	L410	M411	N412	O413	P414	Q415	R416	S417	T418	U419	V420	W421	X422	Y423	Z424	A425	B426	C427	D428	E429	F430	G431	H432	I433	J434	K435	L436	M437	N438	O439	P440	Q441	R442	S443	T444	U445	V446	W447	X448	Y449	Z450	A451	B452	C453	D454	E455	F456	G457	H458	I459	J460	K461	L462	M463	N464	O465	P466	Q467	R468	S469	T470	U471	V472	W473	X474	Y475	Z476	A477	B478	C479	D480	E481	F482	G483	H484	I485	J486	K487	L488	M489	N490	O491	P492	Q493	R494	S495	T496	U497	V498	W499	X500	Y501	Z502	A503	B504	C505	D506	E507	F508	G509	H510	I511	J512	K513	L514	M515	N516	O517	P518	Q519	R520	S521	T522	U523	V524	W525	X526	Y527	Z528	A529	B530	C531	D532	E533	F534	G535	H536	I537	J538	K539	L540	M541	N542	O543	P544	Q545	R546	S547	T548	U549	V550	W551	X552	Y553	Z554	A555	B556	C557	D558	E559	F560	G561	H562	I563	J564	K565	L566	M567	N568	O569	P570	Q571	R572	S573	T574	U575	V576	W577	X578	Y579	Z580	A581	B582	C583	D584	E585	F586	G587	H588	I589	J590	K591	L592	M593	N594	O595	P596	Q597	R598	S599	T600	U601	V602	W603	X604	Y605	Z606	A607	B608	C609	D610	E611	F612	G613	H614	I615	J616	K617	L618	M619	N620	O621	P622	Q623	R624	S625	T626	U627	V628	W629	X630	Y631	Z632	A633	B634	C635	D636	E637	F638	G639	H640	I641	J642	K643	L644	M645	N646	O647	P648	Q649	R650	S651	T652	U653	V654	W655	X656	Y657	Z658	A659	B660	C661	D662	E663	F664	G665	H666	I667	J668	K669	L670	M671	N672	O673	P674	Q675	R676	S677	T678	U679	V680	W681	X682	Y683	Z684	A685	B686	C687	D688	E689	F690	G691	H692	I693	J694	K695	L696	M697	N698	O699	P700	Q701	R702	S703	T704	U705	V706	W707	X708	Y709	Z710	A711	B712	C713	D714	E715	F716	G717	H718	I719	J720	K721	L722	M723	N724	O725	P726	Q727	R728	S729	T730	U731	V732	W733	X734	Y735	Z736	A737	B738	C739	D740	E741	F742	G743	H744	I745	J746	K747	L748	M749	N750	O751	P752	Q753	R754	S755	T756	U757	V758	W759	X760	Y761	Z762	A763	B764	C765	D766	E767	F768	G769	H770	I771	J772	K773	L774	M775	N776	O777	P778	Q779	R780	S781	T782	U783	V784	W785	X786	Y787	Z788	A789	B790	C791	D792	E793	F794	G795	H796	I797	J798	K799	L800	M801	N802	O803	P804	Q805	R806	S807	T808	U809	V810	W811	X812	Y813	Z814	A815	B816	C817	D818	E819	F820	G821	H822	I823	J824	K825	L826	M827	N828	O829	P830	Q831	R832	S833	T834	U835	V836	W837	X838	Y839	Z840	A841	B842	C843	D844	E845	F846	G847	H848	I849	J850	K851	L852	M853	N854	O855	P856	Q857	R858	S859	T860	U861	V862	W863	X864	Y865	Z866	A867	B868	C869	D870	E871	F872	G873	H874	I875	J876	K877	L878	M879	N880	O881	P882	Q883	R884	S885	T886	U887	V888	W889	X890	Y891	Z892	A893	B894	C895	D896	E897	F898	G899	H900	I901	J902	K903	L904	M905	N906	O907	P908	Q909	R910	S911	T912	U913	V914	W915	X916	Y917	Z918	A919	B920	C921	D922	E923	F924	G925	H926	I927	J928	K929	L930	M931	N932	O933	P934	Q935	R936	S937	T938	U939	V940	W941	X942	Y943	Z944	A945	B946	C947	D948	E949	F950	G951	H952	I953	J954	K955	L956	M957	N958	O959	P960	Q961	R962	S963	T964	U965	V966	W967	X968	Y969	Z970	A971	B972	C973	D974	E975	F976	G977	H978	I979	J980	K981	L982	M983	N984	O985	P986	Q987	R988	S989	T990	U991	V992	W993	X994	Y995	Z996	A997	B998	C999	D1000	E1001	F1002	G1003	H1004	I1005	J1006	K1007	L1008	M1009	N1010	O1011	P1012	Q1013	R1014	S1015	T1016	U1017	V1018	W1019	X1020	Y1021	Z1022	A1023	B1024	C1025	D1026	E1027	F1028	G1029	H1030	I1031	J1032	K1033	L1034	M1035	N1036	O1037	P1038	Q1039	R1040	S1041	T1042	U1043	V1044	W1045	X1046	Y1047	Z1048	A1049	B1050	C1051	D1052	E1053	F1054	G1055	H1056	I1057	J1058	K1059	L1060	M1061	N1062	O1063	P1064	Q1065	R1066	S1067	T1068	U1069	V1070	W1071	X1072	Y1073	Z1074	A1075	B1076	C1077	D1078	E1079	F1080	G1081	H1082	I1083	J1084	K1085	L1086	M1087	N1088	O1089	P1090	Q1091	R1092	S1093	T1094	U1095	V1096	W1097	X1098	Y1099	Z1100	A1101	B1102	C1103	D1104	E1105	F1106	G1107	H1108	I1109	J1110	K1111	L1112	M1113	N1114	O1115	P1116	Q1117	R1118	S1119	T1120	U1121	V1122	W1123	X1124	Y1125	Z1126	A1127	B1128	C1129	D1130	E1131	F1132	G1133	H1134	I1135	J1136	K1137	L1138	M1139	N1140	O1141	P1142	Q1143	R1144	S1145	T1146	U1147	V1148	W1149	X1150	Y1151	Z1152	A1153	B1154	C1155	D1156	E1157	F1158	G1159	H1160	I1161	J1162	K1163	L1164	M1165	N1166	O1167	P1168	Q1169	R1170	S1171	T1172	U1173	V1174	W1175	X1176	Y1177	Z1178	A1179	B1180	C1181	D1182	E1183	F1184	G1185	H1186	I1187	J1188	K1189	L1190	M1191	N1192	O1193	P1194	Q1195	R1196	S1197	T1198	U1199	V1200	W1201	X1202	Y1203	Z1204	A1205	B1206	C1207	D1208	E1209	F1210	G1211	H1212	I1213	J1214	K1215	L1216	M1217	N1218	O1219	P1220	Q1221	R1222	S1223	T1224	U1225	V1226	W1227	X1228	Y1229	Z1230	A1231	B1232	C1233	D1234	E1235	F1236	G1237	H1238	I1239	J1240	K1241	L1242	M1243	N1244	O1245	P1246	Q1247	R1248	S1249	T1250	U1251	V1252	W1253	X1254	Y1255	Z1256	A1257	B1258	C1259	D1260	E1261	F1262	G1263	H1264	I1265	J1266	K1267	L1268	M1269	N1270	O1271	P1272	Q1273	R1274	S1275	T1276	U1277	V1278	W1279	X1280	Y1281	Z1282	A1283	B1284	C1285	D1286	E1287	F1288	G1289	H1290	I1291	J1292	K1293	L1294	M1295	N1296	O1297	P1298	Q1299	R1300	S1301	T1302	U1303	V1304	W1305	X1306	Y1307	Z1308	A1309	B1310	C1311	D1312	E1313	F1314	G1315	H1316	I1317	J1318	K1319	L1320	M1321	N1322	O1323	P1324	Q1325	R1326	S1327	T1328	U1329	V1330	W1331	X1332	Y1333	Z1334	A1335	B1336	C1337	D1338	E1339	F1340	G1341	H1342	I1343	J1344	K1345	L1346	M1347	N1348	O1349	P1350	Q1351	R1352	S1353	T1354	U1355	V1356	W1357	X1358	Y1359	Z1360	A1361	B1362	C1363	D1364	E1365	F1366	G1367	H1368	I1369	J1370	K1371	L1372	M1373	N1374	O1375	P1376	Q1377	R1378	S1379	T1380	U1381	V1382	W1383	X1384	Y1385	Z1386	A1387	B1388	C1389	D1390	E1391	F1392	G1393	H1394	I1395	J1396	K1397	L1398	M1399	N1400	O1401	P1402	Q1403	R1404	S1405	T1406	U1407	V1408	W1409	X1410	Y1411	Z1412	A1413	B1414	C1415	D1416	E1417	F1418	G1419	H1420	I1421	J1422	K1423	L1424	M1425	N1426	O1427	P1428	Q1429	R1430	S1431	T1432	U1433	V1434	W1435	X1436	Y1437	Z1438	A1439	B1440	C1441	D1442	E1443	F1444	G1445	H1446	I1447	J1448	K1449	L1450	M1451	N1452	O1453	P1454	Q1455	R1456	S1457	T1458	U1459	V1460	W1461	X1462	Y1463	Z1464	A1465	B1466	C1467	D1468	E1469	F1470	G1471	H1472	I1473	J1474	K1475	L1476	M1477	N1478	O1479	P1480	Q1481	R1482	S1483	T1484	U1485	V1486	W1487	X1488	Y1489	Z1490	A1491	B1492	C1493	D1494	E1495	F1496	G1497	H1498	I1499	J1500	K1501	L1502	M1503	N1504	O1505	P1506	Q1507	R1508	S1509	T1510	U1511	V1512	W1513	X1514	Y1515	Z1516	A1517	B1518	C1519	D1520	E1521	F1522	G1523	H1524	I1525	J1526	K1527	L1528	M1529	N1530	O1531	P1532	Q1533	R1534	S1535	T1536	U1537	V1538	W1539	X1540	Y1541	Z1542	A1543	B1544	C1545	D1

4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	137.76Å 137.76Å 307.89Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 4.10 29.81 – 4.10	Depositor EDS
% Data completeness (in resolution range)	97.2 (30.00-4.10) 98.3 (29.81-4.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.90 (at 4.11Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.340 , 0.387 0.354 , 0.389	Depositor DCC
R_{free} test set	4666 reflections (10.23%)	DCC
Wilson B-factor (Å ²)	167.7	Xtriage
Anisotropy	0.020	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.19 , 76.8	EDS
Estimated twinning fraction	0.337 for -h,-k,l 0.339 for h,-h-k,-l 0.377 for -k,-h,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	0 of 50404 reflections	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	17720	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.22% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: GTP, CCC

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	B	0.88	0/1093	1.14	7/1706 (0.4%)
1	D	0.88	0/1093	1.14	7/1706 (0.4%)
1	F	0.88	0/1093	1.14	7/1706 (0.4%)
1	H	0.88	0/1093	1.14	7/1706 (0.4%)
2	A	0.63	0/3450	0.95	7/4636 (0.2%)
2	C	0.62	0/3450	0.96	7/4636 (0.2%)
2	E	0.62	0/3450	0.95	7/4636 (0.2%)
2	G	0.63	0/3450	0.95	7/4636 (0.2%)
All	All	0.69	0/18172	1.01	56/25368 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	1	0
1	D	1	0
1	F	1	0
1	H	1	0
All	All	4	0

There are no bond length outliers.

The worst 5 of 56 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	217	U	C5'-C4'-C3'	-14.93	92.11	116.00
1	F	217	U	C5'-C4'-C3'	-14.90	92.15	116.00
1	B	217	U	C5'-C4'-C3'	-14.90	92.16	116.00
1	D	217	U	C5'-C4'-C3'	-14.89	92.18	116.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	217	U	N1-C1'-C2'	13.30	131.29	114.00

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	179	GTP	C3'
1	D	179	GTP	C3'
1	F	179	GTP	C3'
1	H	179	GTP	C3'

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	B	1031	0	514	96	1
1	D	1031	0	514	94	0
1	F	1031	0	514	93	1
1	H	1031	0	514	92	1
2	A	3399	0	3543	1366	5
2	C	3399	0	3543	1401	15
2	E	3399	0	3543	1413	17
2	G	3399	0	3543	1356	4
All	All	17720	0	16228	5797	22

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 171.

The worst 5 of 5797 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)
2:A:59:LYS:HD3	2:A:59:LYS:O	1.18	1.34
2:A:151:GLY:HA2	2:G:151:GLY:CA	1.68	1.23
2:A:151:GLY:CA	2:G:151:GLY:HA2	1.73	1.18
2:E:48:THR:HA	2:E:51:ILE:HD12	1.29	1.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:153:GLN:HG3	2:E:153:GLN:CG	1.76	1.14

The worst 5 of 22 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:59:LYS:O	2:E:361:THR:O[2_655]	1.08	1.12
2:C:315:LYS:CG	2:E:312:LYS:NZ[2_655]	1.56	0.64
2:C:61:PRO:CB	2:E:359:LEU:O[2_655]	1.59	0.61
2:C:361:THR:O	2:E:59:LYS:O[2_655]	1.59	0.61
2:A:59:LYS:CD	2:G:361:THR:O[2_665]	1.73	0.47

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	A	430/440 (98%)	142 (33%)	123 (29%)	165 (38%)	0	0
2	C	430/440 (98%)	143 (33%)	123 (29%)	164 (38%)	0	0
2	E	430/440 (98%)	143 (33%)	122 (28%)	165 (38%)	0	0
2	G	430/440 (98%)	142 (33%)	123 (29%)	165 (38%)	0	0
All	All	1720/1760 (98%)	570 (33%)	491 (28%)	659 (38%)	0	0

5 of 659 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	18	PRO
2	A	20	GLU
2	A	23	VAL
2	A	33	SER
2	A	39	VAL

5.3.2 Protein sidechains [i](#)

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	A	370/377 (98%)	270 (73%)	100 (27%)	0	5
2	C	370/377 (98%)	269 (73%)	101 (27%)	0	5
2	E	370/377 (98%)	269 (73%)	101 (27%)	0	5
2	G	370/377 (98%)	270 (73%)	100 (27%)	0	5
All	All	1480/1508 (98%)	1078 (73%)	402 (27%)	0	5

5 of 402 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	362	PRO
2	E	101	LEU
2	G	319	ASP
2	C	393	ASN
2	E	7	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 58 such sidechains are listed below:

Mol	Chain	Res	Type
2	C	350	GLN
2	E	153	GLN
2	G	283	ASN
2	C	351	HIS
2	E	31	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	B	46/47 (97%)	31 (67%)	3 (6%)
1	D	46/47 (97%)	31 (67%)	3 (6%)
1	F	46/47 (97%)	31 (67%)	3 (6%)
1	H	46/47 (97%)	31 (67%)	3 (6%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
All	All	184/188 (97%)	124 (67%)	12 (6%)

5 of 124 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	B	181	C
1	B	182	C
1	B	184	G
1	B	185	G
1	B	186	G

5 of 12 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	D	217	U
1	F	179	GTP
1	H	179	GTP
1	D	210	G
1	F	217	U

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

8 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	GTP	B	179	1	25,34,34	1.39	3 (12%)	34,54,54	3.15	13 (38%)
1	CCC	B	225	1	14,25,26	0.94	0	20,38,41	1.46	4 (20%)
1	GTP	D	179	1	25,34,34	1.39	3 (12%)	34,54,54	3.15	14 (41%)
1	CCC	D	225	1	14,25,26	0.94	0	20,38,41	1.45	4 (20%)
1	GTP	F	179	1	25,34,34	1.39	3 (12%)	34,54,54	3.15	14 (41%)
1	CCC	F	225	1	14,25,26	0.95	0	20,38,41	1.46	4 (20%)
1	GTP	H	179	1	25,34,34	1.39	3 (12%)	34,54,54	3.15	13 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	CCC	H	225	1	14,25,26	0.94	0	20,38,41	1.45	4 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	GTP	B	179	1	1/1/7/7	0/18/38/38	0/3/3/3
1	CCC	B	225	1	-	0/3/35/36	0/3/3/3
1	GTP	D	179	1	1/1/7/7	0/18/38/38	0/3/3/3
1	CCC	D	225	1	-	0/3/35/36	0/3/3/3
1	GTP	F	179	1	1/1/7/7	0/18/38/38	0/3/3/3
1	CCC	F	225	1	-	0/3/35/36	0/3/3/3
1	GTP	H	179	1	1/1/7/7	0/18/38/38	0/3/3/3
1	CCC	H	225	1	-	0/3/35/36	0/3/3/3

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	179	GTP	C6-C5	2.33	1.45	1.41
1	D	179	GTP	C6-C5	2.33	1.45	1.41
1	B	179	GTP	C6-C5	2.37	1.46	1.41
1	H	179	GTP	C6-C5	2.38	1.46	1.41
1	D	179	GTP	PG-O1G	2.76	1.60	1.51

The worst 5 of 70 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	179	GTP	C5-C6-N1	-8.93	111.38	123.59
1	B	179	GTP	C5-C6-N1	-8.93	111.38	123.59
1	H	179	GTP	C5-C6-N1	-8.92	111.39	123.59
1	F	179	GTP	C5-C6-N1	-8.92	111.39	123.59
1	F	179	GTP	PA-O3A-PB	-7.90	110.54	132.73

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	H	179	GTP	C3'
1	D	179	GTP	C3'
1	F	179	GTP	C3'
1	B	179	GTP	C3'

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	179	GTP	2	0
1	B	225	CCC	1	0
1	D	179	GTP	2	0
1	D	225	CCC	1	0
1	F	179	GTP	2	0
1	F	225	CCC	1	0
1	H	179	GTP	2	0
1	H	225	CCC	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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	B	45/47 (95%)	1.07	6 (13%) 4 5	71, 71, 71, 71	0
1	D	45/47 (95%)	0.83	2 (4%) 38 28	71, 71, 71, 71	0
1	F	45/47 (95%)	1.08	11 (24%) 1 2	71, 71, 71, 71	0
1	H	45/47 (95%)	1.00	6 (13%) 4 5	71, 71, 71, 71	0
2	A	432/440 (98%)	-0.54	0 100 100	71, 71, 71, 71	0
2	C	432/440 (98%)	-0.51	2 (0%) 91 88	71, 71, 71, 71	0
2	E	432/440 (98%)	-0.53	0 100 100	71, 71, 71, 71	0
2	G	432/440 (98%)	-0.57	0 100 100	71, 71, 71, 71	0
All	All	1908/1948 (97%)	-0.39	27 (1%) 78 69	71, 71, 71, 71	0

The worst 5 of 27 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	222	G	4.3
1	F	203	G	3.3
1	F	191	C	3.0
1	H	222	G	3.0
1	F	190	C	2.9

6.2 Non-standard residues in protein, DNA, RNA chains [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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
1	CCC	H	225	23/24	0.82	0.35	-	70,70,70,70	0
1	CCC	F	225	23/24	0.84	0.39	-	70,70,70,70	0
1	CCC	D	225	23/24	0.82	0.34	-	70,70,70,70	0
1	CCC	B	225	23/24	0.89	0.37	-	70,70,70,70	0
1	GTP	H	179	32/32	0.91	0.20	-	70,70,70,70	0
1	GTP	D	179	32/32	0.87	0.22	-	70,70,70,70	0
1	GTP	F	179	32/32	0.86	0.23	-	70,70,70,70	0
1	GTP	B	179	32/32	0.86	0.23	-	70,70,70,70	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.