



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 07:56 AM GMT

PDB ID : 3CF5
Title : Thiopeptide antibiotic Thiostrepton bound to the large ribosomal subunit of *Deinococcus radiodurans*
Authors : Harms, J.M.; Wilson, D.N.; Schlutzen, F.; Connell, S.R.; Stachelhaus, T.; Zaborowska, Z.; Spahn, C.M.T.; Fucini, P.
Deposited on : 2008-03-02
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
<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

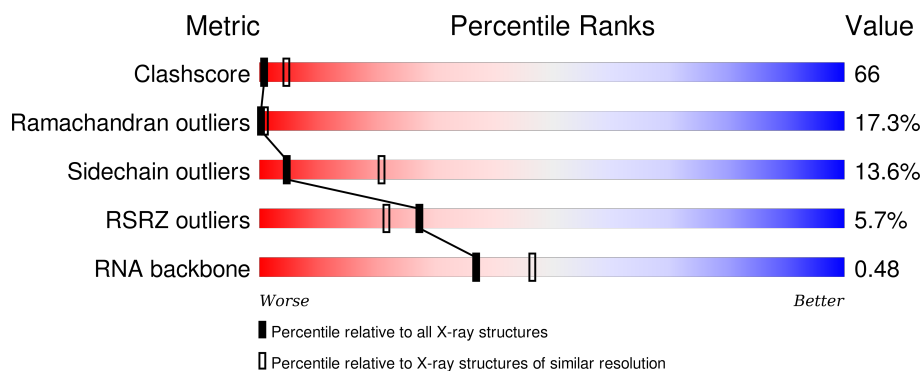
1 Overall quality at a glance

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))
Clashscore	102246	1058 (3.38-3.22)
Ramachandran outliers	100387	1038 (3.38-3.22)
Sidechain outliers	100360	1037 (3.38-3.22)
RSRZ outliers	91569	2070 (3.40-3.20)
RNA backbone	2183	1005 (3.82-2.78)

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	1	55	<div> <div>73%</div> <div>96%</div> <div>.</div> </div>
2	2	47	<div> <div>98%</div> <div>98%</div> <div>.</div> </div>
3	3	66	<div> <div>89%</div> <div>94%</div> <div>5%</div> </div>
4	4	37	<div> <div>19%</div> <div>8%</div> <div>73%</div> <div>19%</div> </div>
5	5	19	<div> <div>5%</div> <div>68%</div> <div>32%</div> </div>

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Mol	Chain	Length	Quality of chain
6	A	274	
7	B	211	
8	C	205	
9	D	180	
10	E	185	
11	F	144	
12	G	174	
13	H	134	
14	I	156	
15	J	142	
16	K	116	
17	L	114	
18	M	166	
19	N	118	
20	O	100	
21	P	134	
22	Q	95	
23	R	115	
24	S	237	
25	T	91	
26	U	81	
27	V	67	
28	W	55	
29	X	2880	
30	Y	60	

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Mol	Chain	Length	Quality of chain
31	Z	123	

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
32	MG	X	2888	-	-	-	X
32	MG	X	2903	-	-	-	X
32	MG	X	2905	-	-	-	X
32	MG	X	2907	-	-	-	X
32	MG	X	2909	-	-	-	X
32	MG	Z	124	-	-	-	X

2 Entry composition

There are 32 unique types of molecules in this entry. The entry contains 84475 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 protein called 50S RIBOSOMAL PROTEIN L33.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
1	1	53	Total C 53 53	0	0	53

- Molecule 2 is a protein called 50S RIBOSOMAL PROTEIN L34.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	2	46	Total C 46 46	0	0	46

- Molecule 3 is a protein called 50S RIBOSOMAL PROTEIN L35.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
3	3	63	Total C 63 63	0	0	63

- Molecule 4 is a protein called 50S RIBOSOMAL PROTEIN L36.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
4	4	37	Total C N O S 297 179 66 47 5	0	0	0

- Molecule 5 is a protein called THIOSTREPTON.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
5	5	19	Total C N O S 114 72 19 18 5	0	0	1

- Molecule 6 is a protein called 50S RIBOSOMAL PROTEIN L2.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
6	A	240	Total C N O S 1826 1137 366 321 2	0	0	0

- Molecule 7 is a protein called 50S RIBOSOMAL PROTEIN L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	B	205	Total	C	N	O	S	0	0	0
			1539	965	295	271	8			

- Molecule 8 is a protein called 50S RIBOSOMAL PROTEIN L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	C	197	Total	C	N	O	S	0	0	0
			1506	935	287	282	2			

- Molecule 9 is a protein called 50S RIBOSOMAL PROTEIN L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	D	177	Total	C	N	O	S	0	0	0
			1400	892	247	254	7			

- Molecule 10 is a protein called 50S RIBOSOMAL PROTEIN L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	E	171	Total	C	N	O	S	0	0	0
			1286	812	237	236	1			

- Molecule 11 is a protein called 50S RIBOSOMAL PROTEIN L11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	F	144	Total	C	N	O	S	0	0	0
			1044	663	179	197	5			

- Molecule 12 is a protein called 50S RIBOSOMAL PROTEIN L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	G	142	Total	C	N	O	S	0	0	0
			1114	704	209	198	3			

- Molecule 13 is a protein called 50S RIBOSOMAL PROTEIN L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	H	134	Total	C	N	O	S	0	0	0
			997	614	198	180	5			

- Molecule 14 is a protein called 50S RIBOSOMAL PROTEIN L15.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	I	141	Total	C	N	O	0	0	0
			1067	655	216	196			

- Molecule 15 is a protein called 50S RIBOSOMAL PROTEIN L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	J	136	Total	C	N	O	S	0	0	0
			1090	696	202	185	7			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	1	MET	-	INITIATING METHIONINE	UNP Q9RXJ5

- Molecule 16 is a protein called 50S RIBOSOMAL PROTEIN L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	K	113	Total	C	N	O	S	0	0	0
			878	541	178	157	2			

- Molecule 17 is a protein called 50S RIBOSOMAL PROTEIN L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
17	L	104	Total	C	N	O	0	0	0
			779	476	161	142			

- Molecule 18 is a protein called 50S RIBOSOMAL PROTEIN L19.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	M	108	Total	C	N	O	0	0	0
			871	543	172	156			

- Molecule 19 is a protein called 50S RIBOSOMAL PROTEIN L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	N	117	Total	C	N	O	S	0	0	0
			978	608	210	159	1			

- Molecule 20 is a protein called 50S RIBOSOMAL PROTEIN L21.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
20	O	94	Total	C	N	O	0	0	0
			741	465	139	137			

- Molecule 21 is a protein called 50S RIBOSOMAL PROTEIN L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	P	127	Total	C	N	O	S	0	0	0
			1014	639	199	174	2			

- Molecule 22 is a protein called 50S RIBOSOMAL PROTEIN L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	Q	93	Total	C	N	O	S	0	0	0
			726	458	136	130	2			

- Molecule 23 is a protein called 50S RIBOSOMAL PROTEIN L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	R	110	Total	C	N	O	S	0	0	0
			825	513	160	151	1			

- Molecule 24 is a protein called 50S RIBOSOMAL PROTEIN L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	S	175	Total	C	N	O	S	0	0	0
			1345	849	236	254	6			

- Molecule 25 is a protein called 50S RIBOSOMAL PROTEIN L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	T	84	Total	C	N	O	S	0	0	0
			625	393	122	109	1			

- Molecule 26 is a protein called 50S RIBOSOMAL PROTEIN L28.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
26	U	72	Total	C	N	O	0	0	0
			552	341	116	95			

- Molecule 27 is a protein called 50S RIBOSOMAL PROTEIN L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	V	66	Total	C	N	O	S	0	0	0
			533	327	107	96	3			

- Molecule 28 is a protein called 50S RIBOSOMAL PROTEIN L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	W	55	Total	C	N	O	S	0	0	0
			424	264	82	76	2			

- Molecule 29 is a RNA chain called RRNA-23S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	X	2686	Total	C	N	O	P	0	0	0
			57651	25718	10642	18606	2685			

- Molecule 30 is a protein called 50S RIBOSOMAL PROTEIN L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	Y	58	Total	C	N	O	S	0	0	0
			457	281	94	77	5			

- Molecule 31 is a RNA chain called RRNA-5S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	Z	122	Total	C	N	O	P	0	0	0
			2598	1161	476	840	121			

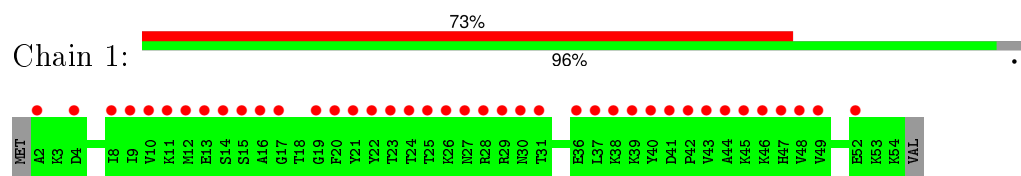
- Molecule 32 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
32	X	30	Total	Mg	0	0
			30	30		
32	Z	5	Total	Mg	0	0
			5	5		
32	M	1	Total	Mg	0	0
			1	1		

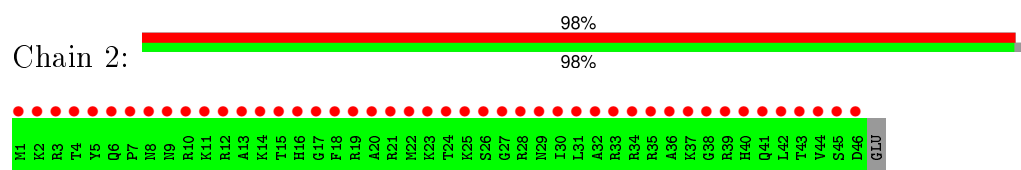
3 Residue-property plots [i](#)

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.

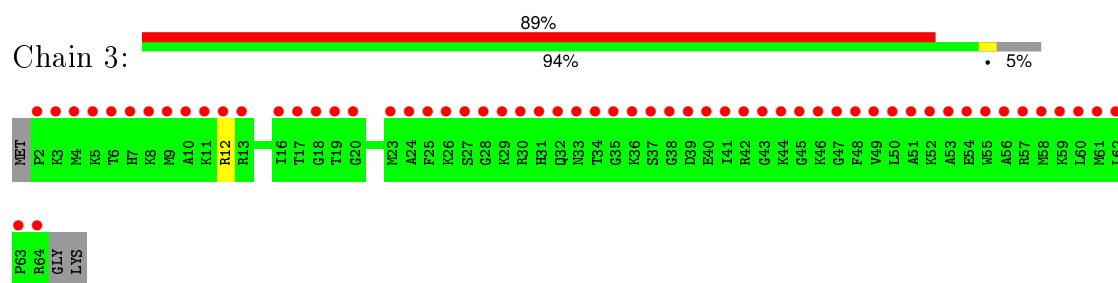
- Molecule 1: 50S RIBOSOMAL PROTEIN L33



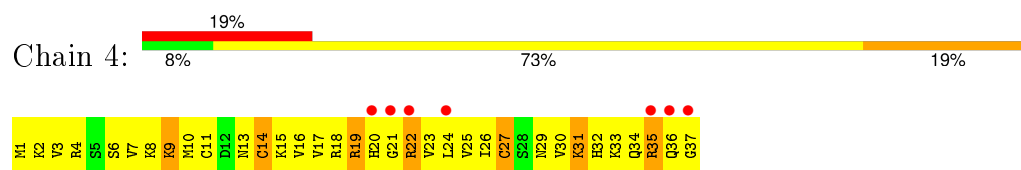
- Molecule 2: 50S RIBOSOMAL PROTEIN L34



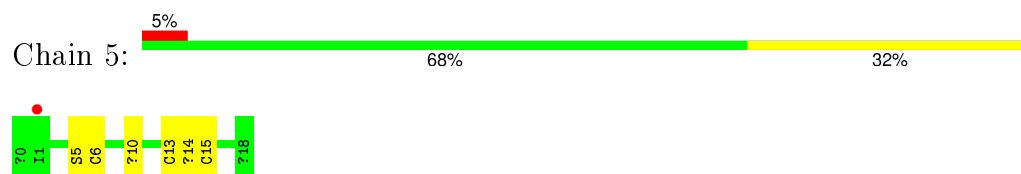
- Molecule 3: 50S RIBOSOMAL PROTEIN L35



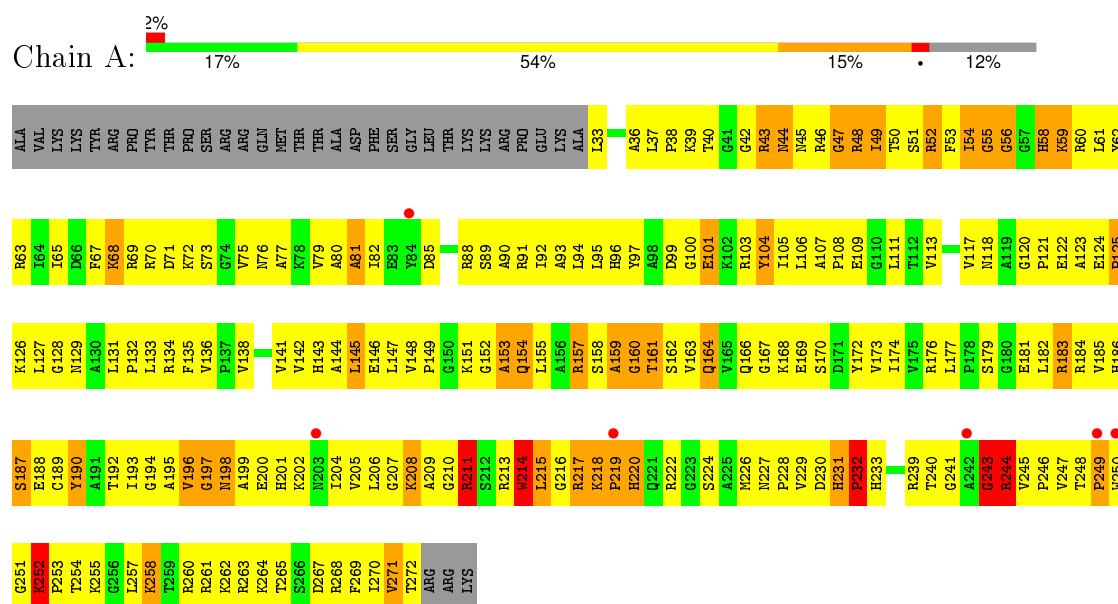
- Molecule 4: 50S RIBOSOMAL PROTEIN L36



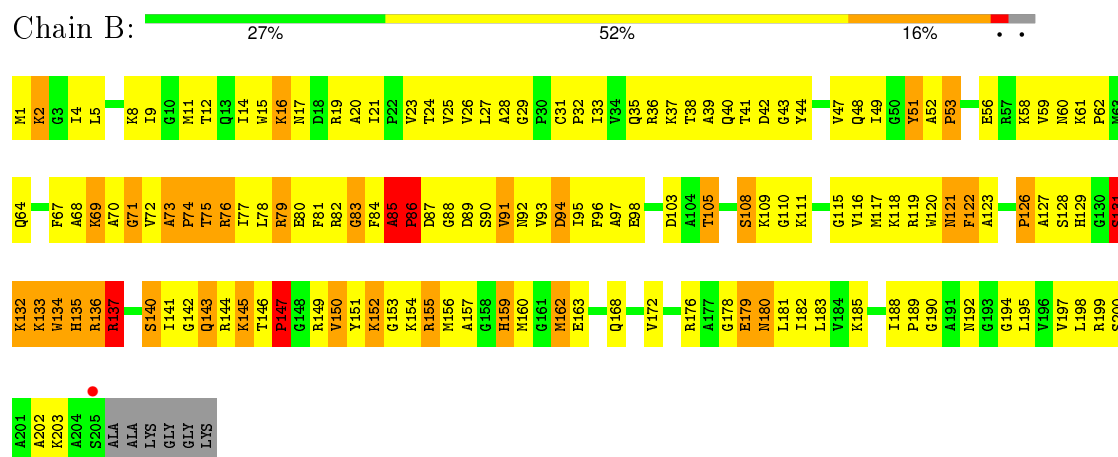
- Molecule 5: THIOSTREPTON



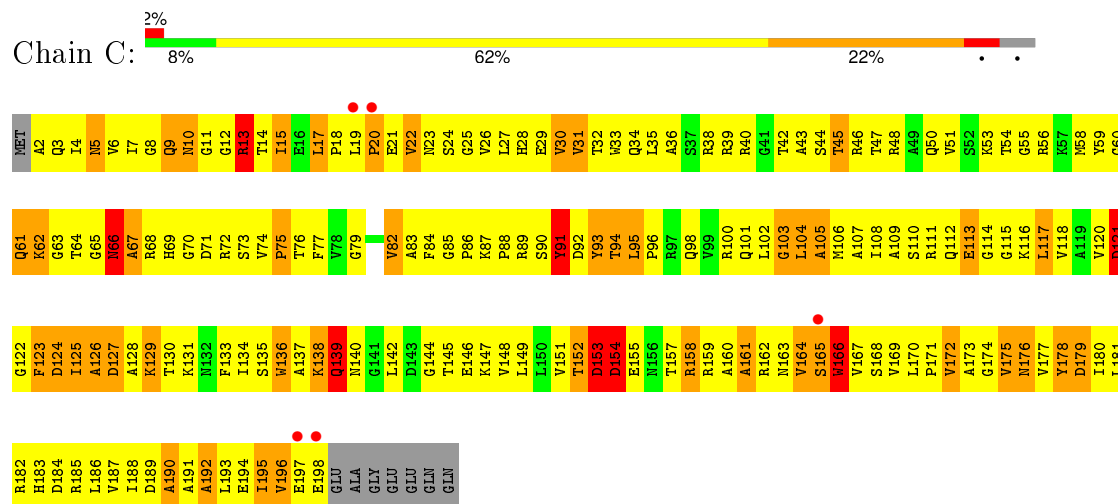
- Molecule 6: 50S RIBOSOMAL PROTEIN L2



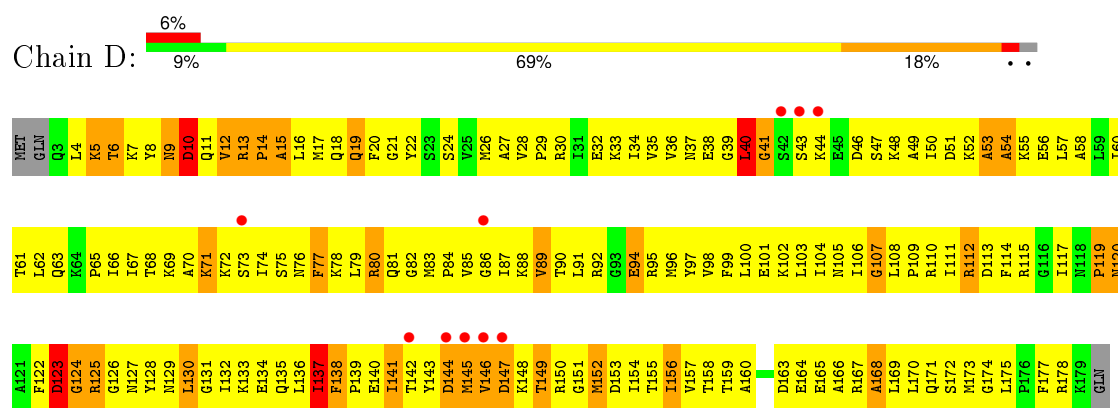
• Molecule 7: 50S RIBOSOMAL PROTEIN L3



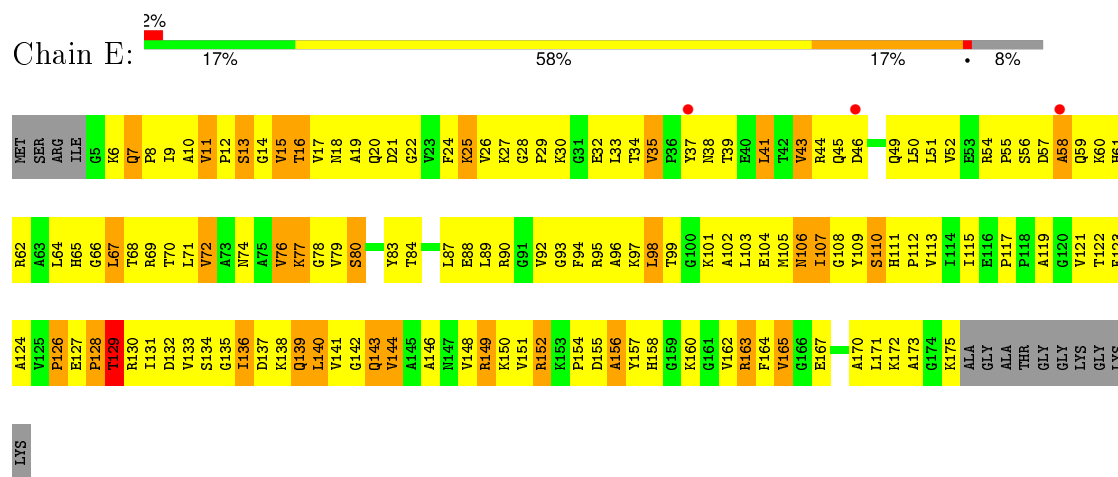
• Molecule 8: 50S RIBOSOMAL PROTEIN L4



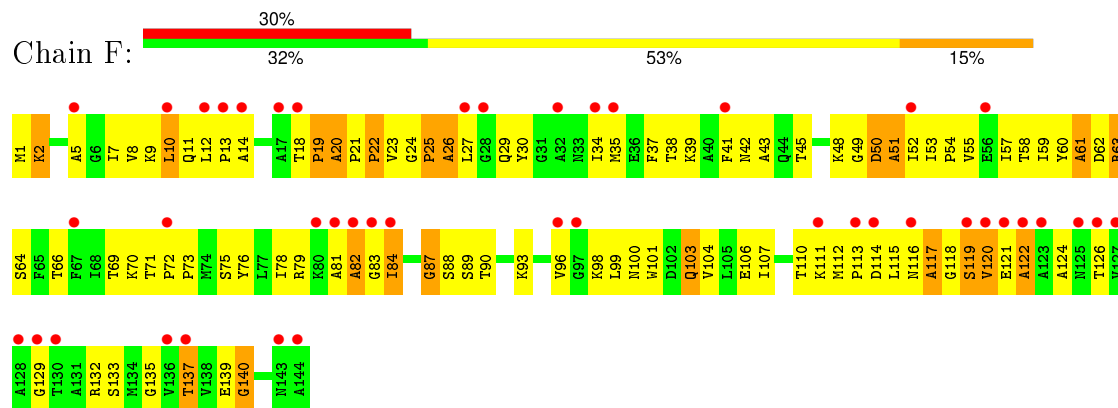
• Molecule 9: 50S RIBOSOMAL PROTEIN L5



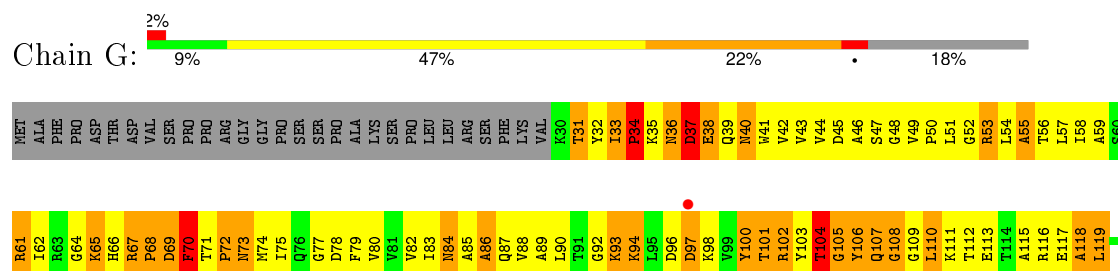
• Molecule 10: 50S RIBOSOMAL PROTEIN L6

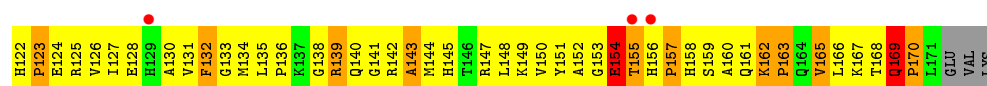


• Molecule 11: 50S RIBOSOMAL PROTEIN L11



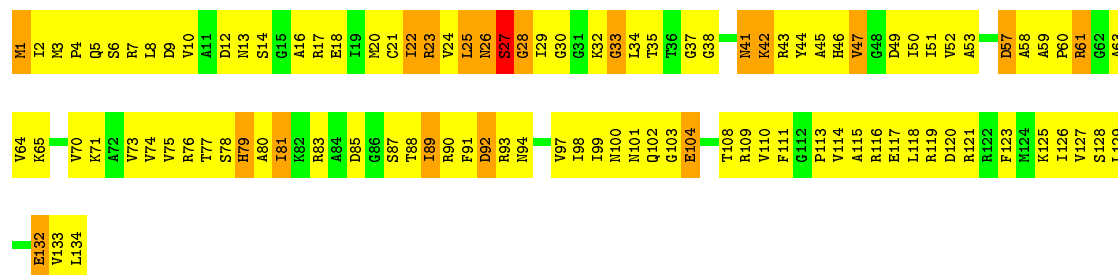
• Molecule 12: 50S RIBOSOMAL PROTEIN L13





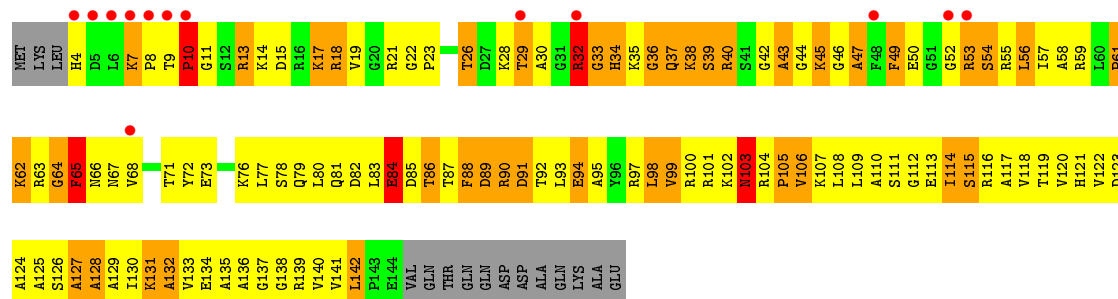
• Molecule 13: 50S RIBOSOMAL PROTEIN L14

Chain H: 22% 63% 13%



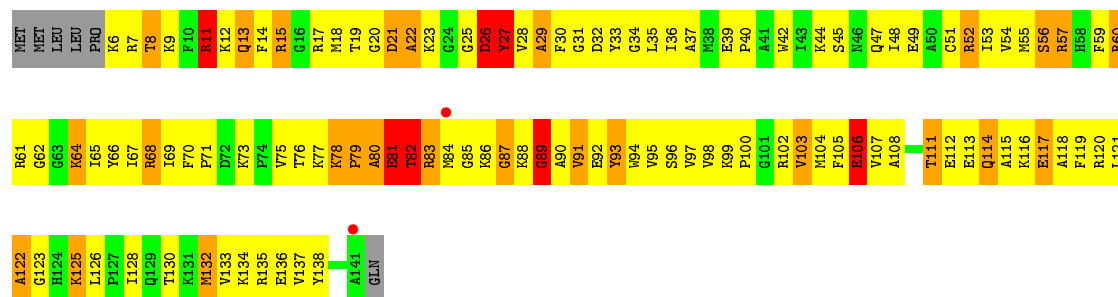
• Molecule 14: 50S RIBOSOMAL PROTEIN L15

Chain I: 8% 13% 49% 26% 10%



• Molecule 15: 50S RIBOSOMAL PROTEIN L16

Chain J: 15% 57% 18% 5%



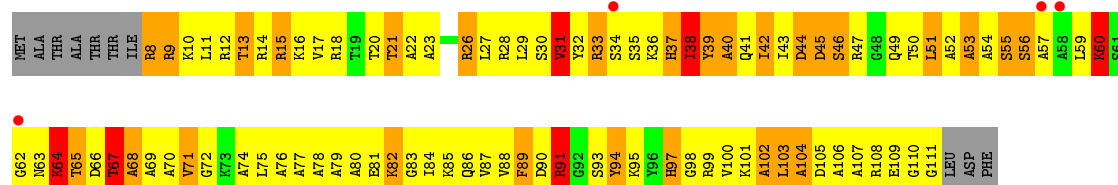
• Molecule 16: 50S RIBOSOMAL PROTEIN L17

Chain K: 24% 53% 19%

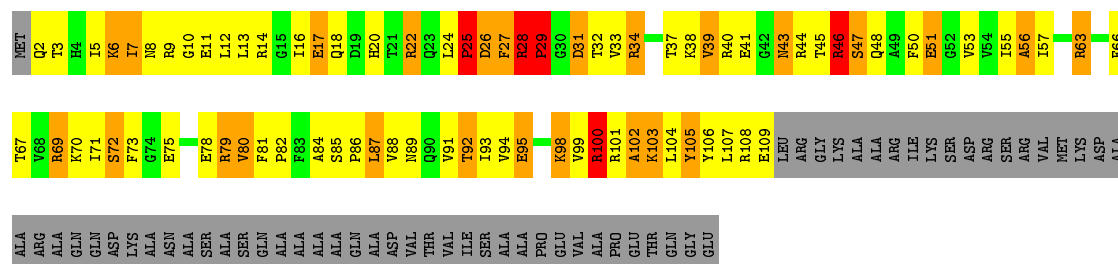
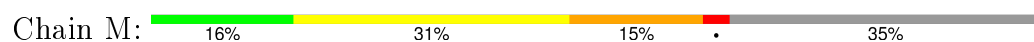




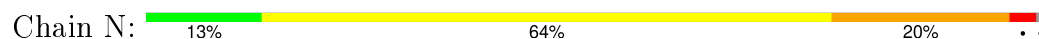
• Molecule 17: 50S RIBOSOMAL PROTEIN L18



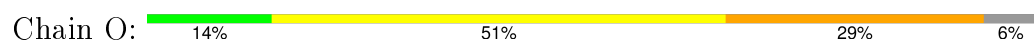
• Molecule 18: 50S RIBOSOMAL PROTEIN L19



• Molecule 19: 50S RIBOSOMAL PROTEIN L20

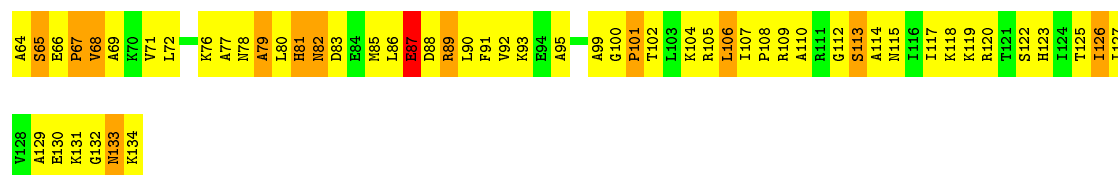


• Molecule 20: 50S RIBOSOMAL PROTEIN L21

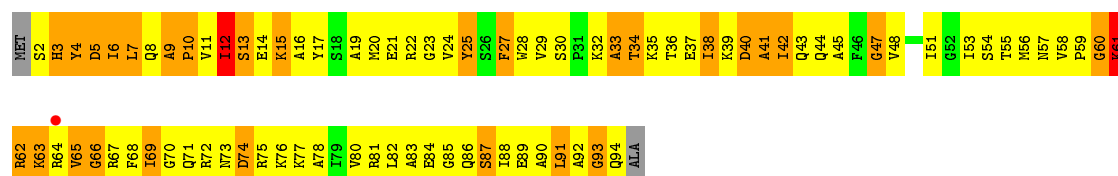
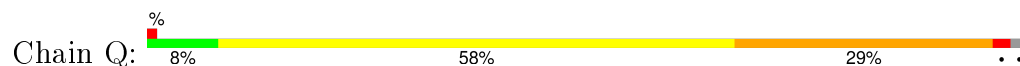


• Molecule 21: 50S RIBOSOMAL PROTEIN L22

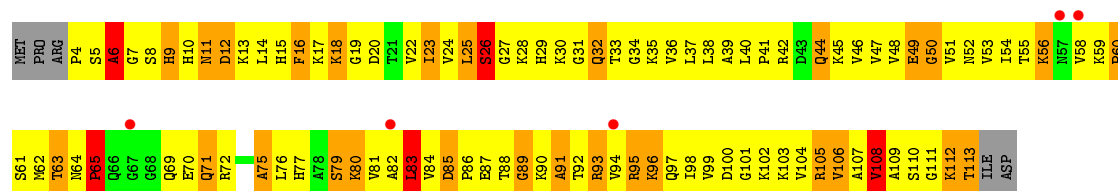
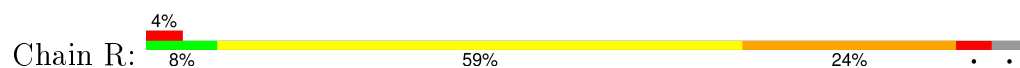




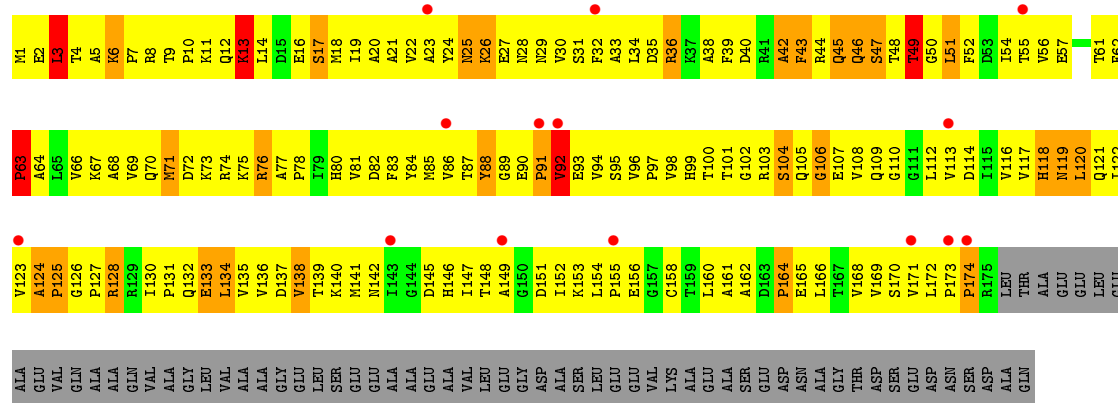
• Molecule 22: 50S RIBOSOMAL PROTEIN L23



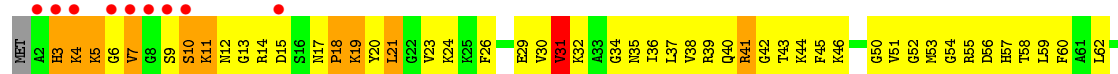
• Molecule 23: 50S RIBOSOMAL PROTEIN L24

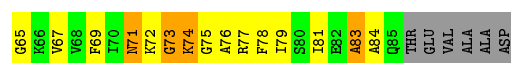


• Molecule 24: 50S RIBOSOMAL PROTEIN L25

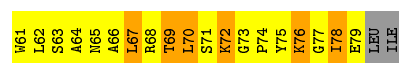


• Molecule 25: 50S RIBOSOMAL PROTEIN L27

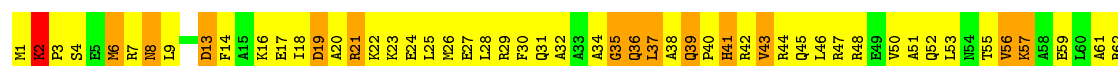




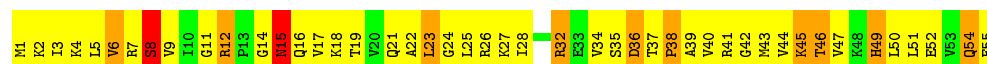
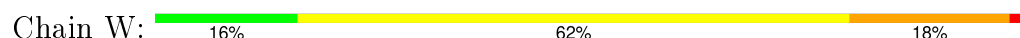
• Molecule 26: 50S RIBOSOMAL PROTEIN L28



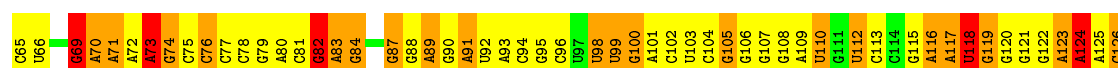
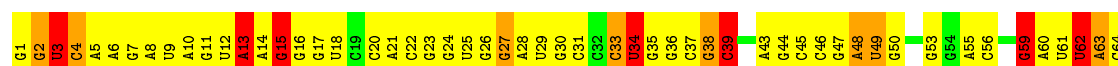
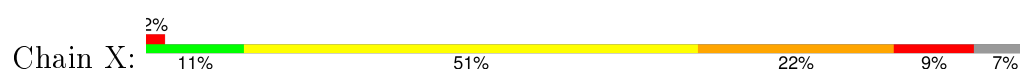
• Molecule 27: 50S RIBOSOMAL PROTEIN L29



• Molecule 28: 50S RIBOSOMAL PROTEIN L30

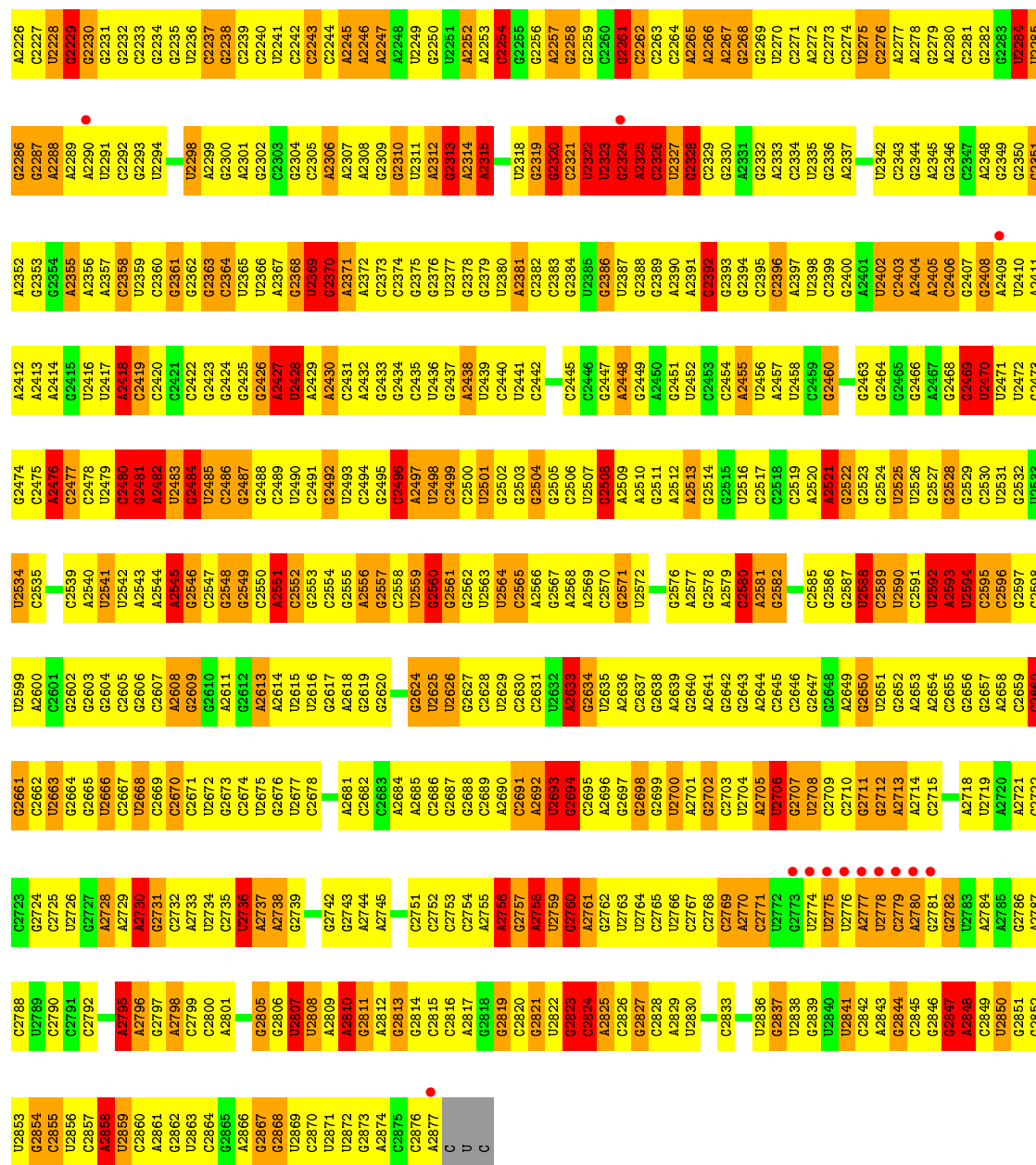


• Molecule 29: RRNA-23S RIBOSOMAL RNA



A1239	C1178	G1117	U1056	A994	G928	A865	U800	A740	C679	A493	C432	U
G1240	A1179	G1118	A1057	A995	A929	U866	A801	G741	U680	A494	G433	A
G1241	A1180	U1119	C1058	C996	A930	G867	A802	G742	G682	C495	G434	C
A1242	C1181	C1120	A1059	C997	G931	U868	C803	A743	G681	C496	A435	U
G1243	U1182	A1121	C1060	C998	G932	C869	C804	G744	A683	C497	A436	G
G1244	C1183	G1122	A1061	A999	G933	C870	G805	G745	C684	C498	G437	G
G1245	G1184	G1123	G1062	G1000	G934	U871	A806	G746	U885	C499	C438	C
G1246	C1185	U1124	C1063	A1001	G935	U872	A807	A747	C686	G500	C439	A
G1247	G1186	G1125	C1064	C1002	A936	G873	C808	A748	U686	G501	U440	C
G1248	A1187	U1126	A1065	A1003	G937	A874	C809	A688	A628	A502	U441	C
G1249	G1188	C1127	G1066	C1004	G938	G875	U810	C750	A689	A503	U442	U
G1250	G1189	A1128	G1067	U1005	G939	A876	G811	A690	G630	G504	A443	G
G1251	C1190	G1129	A1068	C1006	G940	G877	G812	G752	C691	U444	U444	A
C1252	G1191	U1130	G1069	A1007	U941	C878	A813	U753	C692	G505	A445	G
C1253	A1192	G1131	U1070	G1008	U942	A879	G814	G754	A693	G506	C446	U
G1254	G1193	C1132	U1071	C1009	U943	A879	A815	C755	G694	G510	U447	A
A1255	U1194	G1133	U1072	U1010	A944	C884	U816	A685	G695	A511	C448	G
G1256	U1195	C1134	G1073	A1011	G945	A885	A817	U757	U696	A512	C449	G
U1257	G1196	C1135	G1074	A1012	U946	A886	G818	G758	G697	A513	C450	U
G1258	U1197	G1136	U1075	G1013	C947	G887	C819	C759	A698	G514	A451	G
A1259	C1198	A1137	U1076	G1014	C948	G888	U820	U760	G699	A515	A452	U
A1260	U1199	A1138	U1077	U1015	G949	C889	A821	G761	C700	A516	G453	U
G1261	G1200	C1139	A1078	C1016	U890	U890	G822	A762	U701	A517	G454	U
U1262	G1201	A1140	G1079	C1017	A891	G	U823	A763	G704	A518	A455	G
G1263	U1202	U1141	A1080	C1018	G953	G	C824	A764	A643	C519	G456	U
C1264	G1203	G1142	A1081	U1019	U954	G	C825	C765	A644	C520	C457	U
G1265	G1204	A1143	G1082	U1020	G955	G	U826	A766	G645	U521	G458	C
G1266	G1205	U1144	C1083	A1022	A956	G	C827	G767	U707	G522	A459	U
G1267	G1206	A1145	U1023	G1084	G957	G	C828	U768	G708	A523	U460	U
U1268	G1207	G1146	G1085	G1024	G958	C	C829	C769	A709	A461	G401	U
G1269	A1208	G1147	C1086	A1025	C959	C	C830	U770	C710	A524	A402	U
C1270	G1209	G1148	U1087	U1026	U960	U	G831	C771	C711	C525	G462	U
	C1210	G1149	C1088	C1027		A	A832	G772	A712	C526	G463	U
G1273	U1211	C1150	C1089	G773	G965	C	A833	G773	G713	C527	C464	U
C1274	G1212	U1151	C1090	A966	A966	C	U835	A774	G714	G528	C465	U
A1275	C1213	G1152	C1091	G967	G967	A	U836	U775	U715	U529	A466	U
U1276	A1153	A1153	U1092	G1032	G968	G	G836	G776	U716	G530	U467	U
G1277	A1154	A1154	U1093	G1033	U969	C	U837	A777	G717	G531	A468	U
A1278	G1216	G1155	C1094	U1034	A970	U	A838	G778	A718	A532	G469	U
G1279	U1217	U1156	A1095	U1035	A971	U	U839	U779	A719	C533	U471	U
U1280	C1218		C1096	G1036	C972	A	U840	U780	C721	U470	C472	U
A1281	C1219	U1159	A1097	U1037	U973	C	G841	G781	A720	G537	G413	U
C1282	G1220	U1161	G1098	U1038	U974	C	A842	U782	C722	A414	A414	U
C1283		U1162	A1099	A1039	C975	A911	G843	U783	C723	A415	A415	U
G1284	G1223	A1162	G1100	A1040	C976	A912	G844	U784	C724	U416	U416	U
A1285	A1224	C1163	U1101	G1041	G977	A912	U845	U785	G725	U417	U417	U
U1286	G1225	C1164	G1102	G1042	G978	C914	A846	U786	G726	G475	G475	U
A1287	A1226	G1165	C1103	A1043	G979	C915	C847	A787	C602	G476	A477	U
A1288	A1227	A1166	G1104	U1044	G980	U916	A848	G788	U667	G480	G480	U
A1289	G1228	A1167	U1105	U1045	C981	U917	G849	U789	G608	A481	A481	U
A1290	C1229	G1168	A1106	U1046	C982	A918	C850	A790	U609	A482	A482	U
G1291	C1230	C1169	A1107	G1047	A983	U919	U857	G791	G610	A546	C422	U
A1292	A1231	U1170	U1108	G985	G985	G920	U858	U792	A671	U547	G423	U
C1293	U1232	A1171	C1049	A921	G956	A921	G858	G793	G611	G548	G424	U
G1294	A1233	U1172	G1050	A922	G957	A922	U859	A794	G612	U486	A425	U
U1295	C1234	G1173	U1051	G988	G988	A923	U860	G795	A613	C550	C426	U
G1296	C1235	G1174	C1113	C1052	G989	C924	G861	A796	G614	A551	C427	U
A1297	G1236	A1175	C1114	G1053	A991	U925	A862	A797	U616	C552	A428	U
G1298	G1237	U1176	C1115	G798	A992	C926	A863	G798	U617	C553	C429	U
A1299	A1238	U1177	U1116	A1055	C993	C927	C864	G799	G678	U555	G431	U

G2166	G2044	A1921	A1860	A1799	C1736	C1674	A1607	G1483	A1300
A2167	A2045	U1922	G1861	A1800	G1737	C1675	U1608	G1484	A1301
A2168	C2046	U1923	C1862	C1801	U1738	U1676	C1609	A1362	A1302
A2169	C2047	U1924	U1863	A1802	U1739	C1677	A1610	U1485	C1363
C2170	C2048	C1925	G1864	G1803	G1740	G1678	U1611	A1486	U1303
C2171	C2049	U1926	C1865	U1804	G1741	U1679	U1612	U1487	A1304
C2172	C2050	U1927	G1866	G1805	G1742	U1680	C1613	A1365	C1305
G2173	U2051	G1928	A1867	G1806	C1743	A1681	C1614	U1366	U1306
G2174	G2052	U1929	A1868	A1807	G1744	A1682	C1615	U1367	U1307
A2175	G2053	C1930	A1869	C1808	C1745	G1683	U1616	G1368	C1308
U2176	G2054	U1931	U1870	G1809	A1746	G1684	U1618	U1370	C1310
U2177	A2055	G1933	G1871	U1810	G1747	A1685	C1621	A1372	C1311
U2178	A2056	U1934	A1872	U1811	U1748	A1686	G1622	G1373	C1312
C2179	U2057	A1935	A1873	U1812	G1749	C1687	G1623	G1374	U1313
U2180	U2058	A1936	U1874	A1813	U1750	U1688	C1624	A1375	A1314
A2181	U2059	G1937	C1875	G1814	A1751	U1689	A1625	C1376	A1315
A2182	A2060	U1938	C1877	U1815	U1752	U1690	A1626	A1377	G1316
C2183	C2061	U1939	G1878	G1816	A1753	G1691	A1627	G1378	G1317
C2184	U2062	C1940	G1879	U1817	G1754	G1692	C1627	A1379	A1318
C2185	A2063	C1941	G1880	G1818	G1755	A1693	G1628	C1380	C1319
G2186	U2064	U1942	U1881	U1819	C1756	U1694	G1629	G1381	A1320
A2187	U2065	U1943	A1882	G1820	C1757	U1695	C1630	G1382	A1321
A2188	G2066	A1945	A1883	A1821	C1758	C1696	C1631	G1383	G1322
A2189	U2067	U1946	A1884	C1822	A1759	U1697	A1569	A1384	G1323
A2190	C2068	G1947	C1885	G1823	U1760	G1698	C1570	A1385	G1324
A2191	U2069	C1948	G1886	C1824	C1762	A1699	G1571	U1487	U1325
U2192	G2070	A1949	G1887	C1825	U1763	C1700	A1574	G1387	U1326
C2193	U2011	C1950	C1888	U1826	G1764	C1701	G1575	A1388	
A2194	A2012	U1951	G	G1827	C1765	C1702	C1576	G1389	
C2195	A2013	G1952	G	C1830	U1766	C1703	G1577	G1390	U1329
U2196	A2014	A1953	C	G1831	U1769	G1704	A1543	G1391	G1330
U2197	G2015	A1954	C	G1832	U1770	U1705	U1645	U1392	G1331
U2198	A2016	G1956	G	G1833	C1771	A1706	U1646	G1393	G1332
C2199	U2017	C1957	U	U1834	C1772	A1707	C1647	G1394	G1333
G2200	G2018	G1958	A	G1835	C1773	C1708	U1647	A1395	A1334
G2201	C2019	U1959	C	C1836	A1774	U1709	C1648	A1396	A1335
G2202	G2020	U1960	U	G1837	C1775	U1710	A1583	G1397	G1336
G2203	C2021	A1961	C	C1837	A1776	C1711	G1584	G1398	G1337
A2204	C2022	C1962	U	G1838	A1777	G1712	G1585	G1399	G1338
C2205	C2023	G1963	U	A1839	C1778	G1713	A1586	A1400	U1339
U2086	U2024	A1964	A	A1840	U1779	A1714	A1587	G1401	G1340
G2207	A2025	U1965	C	G1941	C1779	A1715	A1588	A1464	G1341
U2088	C2026	C1966	C	G1942	A1780	G1716	G1589	G1402	U1342
G2209	C2027	C1967	G	U1943	C1781	A1717	G1590	G1403	C1343
C2210	U2028	U1968	U	C1944	A1782	A1718	A1591	G1404	C1344
U2211	C	G1969	U	A1845	U1783	G1722	U1592	A1405	G1345
U2212	U2030	G1970	C	A1846	A1785	G1723	C1593	A1406	G1346
G2213	A2031	C1971	C	G1947	C1786	U1724	U1594	G1407	C1347
A2214	C2032	C1972	U	U1848	U1787	G1725	C1661	A1408	C1348
C2215	C2033	G1973	A1910	G1849	C1788	C1726	C1662	G1471	A1349
G2216	A2034	C1974	A1911	G1850	U1789	C1727	C1663	U1410	G1350
G2217	C2035	G1975	G1912	A1851	C1790	C1728	C1664	U1473	G1351
G2218	G2036	U1976	G1913	G1852	C1791	A1728	G1665	A1474	G1352
U2219	A2037	C1977	U1914	C1853	C1792	C1729	G1666	U1475	A1353
A2220	C2038	U1978	A1915	G1854	A1793	G1730	G1667	G1476	G1414
G2221	G2039	U1979	G1916	G1855	A1794	C1731	A1668	A1538	A1355
U2222	A2040	C1979	C1917	U1856	C1795	U1732	G1670	U1478	A1415
U2223	U2041	A1980	G1918	G1857	A1796	U1733	A1671	G1479	U1357
U2224	A2042	A1981	G1919	C1858	C1797	C1734	A1672	U1480	G1358
G2225	U2043	C1982	A1920	A1859	G1798	G1735	C1673	U1481	G1359
								U1482	G1360



C62	A63	C64	A65	G66	C67	A68	G69	C70	G71	C72	A73	C74	A75	G76	C77	A78	C79	A80	C81	G82	C83	G84	G85	G88	G94	C95	C96	C97	G100	A101	A102	A103	U106	C107	G108	G109	U110	C111	A112	G113	C114	G115	C116	G117	G118	G119	G120	G121	U122	U123
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4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	169.90Å 408.90Å 694.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.30 29.76 – 3.31	Depositor EDS
% Data completeness (in resolution range)	94.1 (30.00-3.30) 93.2 (29.76-3.31)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.14 (at 3.31Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.276 , 0.318 0.241 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	67.5	Xtriage
Anisotropy	0.110	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.18 , 60.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Outliers	1 of 332876 reflections (0.000%)	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	84475	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.08% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² Theoretical 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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, DCY, DHA, QUA, BB9, NH2, MH6, DBU, TS9

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$
4	4	0.46	0/298	0.67	0/390
5	5	1.46	0/31	1.18	0/38
6	A	0.55	0/1862	0.85	2/2510 (0.1%)
7	B	0.77	0/1567	1.04	4/2105 (0.2%)
8	C	0.63	0/1529	0.91	0/2070
9	D	0.48	0/1419	0.71	0/1903
10	E	0.48	0/1308	0.80	1/1771 (0.1%)
11	F	0.50	0/1063	0.71	0/1440
12	G	0.69	0/1138	1.00	3/1539 (0.2%)
13	H	0.79	0/1007	0.96	1/1352 (0.1%)
14	I	0.65	0/1081	0.94	3/1448 (0.2%)
15	J	0.67	0/1113	0.91	2/1486 (0.1%)
16	K	0.87	0/886	1.06	2/1188 (0.2%)
17	L	0.52	0/785	0.86	0/1048
18	M	0.73	0/884	1.20	6/1186 (0.5%)
19	N	0.63	0/994	0.89	0/1323
20	O	0.61	0/750	0.90	0/1000
21	P	0.77	0/1027	0.93	1/1373 (0.1%)
22	Q	0.67	0/737	0.98	4/988 (0.4%)
23	R	0.55	0/835	0.95	2/1121 (0.2%)
24	S	0.50	0/1370	0.75	0/1862
25	T	0.56	0/633	0.83	1/838 (0.1%)
26	U	0.58	0/556	0.95	1/741 (0.1%)
27	V	0.44	0/537	0.67	0/714
28	W	0.56	0/426	0.84	0/568
29	X	0.88	59/64561 (0.1%)	1.05	497/100708 (0.5%)
30	Y	0.70	0/469	1.11	2/629 (0.3%)
31	Z	0.55	0/2904	0.76	0/4525
All	All	0.81	59/91770 (0.1%)	1.01	532/137864 (0.4%)

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
6	A	0	1
19	N	0	2
22	Q	0	1
29	X	2	257
30	Y	0	1
31	Z	0	4
All	All	2	266

The worst 5 of 59 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	X	1856	U	C4'-C3'	-9.30	1.43	1.53
29	X	1856	U	O3'-P	-8.64	1.50	1.61
29	X	1056	U	P-O5'	8.52	1.68	1.59
29	X	1855	G	O3'-P	-8.11	1.51	1.61
29	X	551	A	O3'-P	-8.05	1.51	1.61

The worst 5 of 532 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	X	1055	A	N9-C1'-C2'	-29.46	75.70	114.00
29	X	2324	G	N9-C1'-C2'	22.22	142.88	114.00
29	X	557	U	N1-C1'-C2'	19.61	139.50	114.00
29	X	417	C	N1-C1'-C2'	18.73	138.35	114.00
18	M	28	ARG	C-N-CD	-18.52	79.85	120.60

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
29	X	1278	A	C1'
29	X	2592	U	C1'

5 of 266 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	A	104	TYR	Sidechain
19	N	32	TYR	Sidechain
19	N	76	TYR	Sidechain
22	Q	25	TYR	Sidechain

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Mol	Chain	Res	Type	Group
29	X	12	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	1	53	0	0	0	0
2	2	46	0	0	0	0
3	3	63	0	0	1	0
4	4	297	0	330	62	0
5	5	114	0	79	5	0
6	A	1826	0	1885	451	0
7	B	1539	0	1600	303	0
8	C	1506	0	1525	371	0
9	D	1400	0	1481	373	0
10	E	1286	0	1336	264	0
11	F	1044	0	1088	176	0
12	G	1114	0	1144	310	0
13	H	997	0	1046	194	0
14	I	1067	0	1103	301	0
15	J	1090	0	1125	273	0
16	K	878	0	930	135	0
17	L	779	0	820	231	0
18	M	871	0	894	208	0
19	N	978	0	1020	239	0
20	O	741	0	756	186	0
21	P	1014	0	1096	181	0
22	Q	726	0	753	150	0
23	R	825	0	881	266	0
24	S	1345	0	1372	303	0
25	T	625	0	655	111	0
26	U	552	0	604	207	0
27	V	533	0	558	109	0
28	W	424	0	470	83	0
29	X	57651	0	29049	4301	0
30	Y	457	0	462	86	0
31	Z	2598	0	1328	185	0
32	M	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	X	30	0	0	0	0
32	Z	5	0	0	0	0
All	All	84475	0	55390	9214	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 66.

The worst 5 of 9214 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)
7:B:116:VAL:N	7:B:136:ARG:HE	1.23	1.30
29:X:1053:G:H2'	29:X:1054:C:C6	1.70	1.26
29:X:2196:U:H2'	29:X:2197:U:O4'	1.31	1.23
29:X:2736:U:O2'	29:X:2737:A:H5''	1.36	1.21
29:X:2496:C:O2'	29:X:2497:A:H3'	1.40	1.19

There are no symmetry-related clashes.

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	
4	4	35/37 (95%)	20 (57%)	10 (29%)	5 (14%)	0	1
5	5	5/19 (26%)	4 (80%)	1 (20%)	0	100	100
6	A	238/274 (87%)	154 (65%)	50 (21%)	34 (14%)	0	1
7	B	203/211 (96%)	148 (73%)	32 (16%)	23 (11%)	0	3
8	C	195/205 (95%)	97 (50%)	54 (28%)	44 (23%)	0	0
9	D	175/180 (97%)	95 (54%)	48 (27%)	32 (18%)	0	1
10	E	169/185 (91%)	100 (59%)	38 (22%)	31 (18%)	0	1
11	F	142/144 (99%)	94 (66%)	29 (20%)	19 (13%)	0	2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	G	140/174 (80%)	76 (54%)	34 (24%)	30 (21%)	0	0
13	H	132/134 (98%)	105 (80%)	18 (14%)	9 (7%)	1	12
14	I	139/156 (89%)	59 (42%)	45 (32%)	35 (25%)	0	0
15	J	134/142 (94%)	82 (61%)	31 (23%)	21 (16%)	0	1
16	K	111/116 (96%)	74 (67%)	25 (22%)	12 (11%)	0	4
17	L	102/114 (90%)	59 (58%)	19 (19%)	24 (24%)	0	0
18	M	106/166 (64%)	70 (66%)	23 (22%)	13 (12%)	0	2
19	N	115/118 (98%)	57 (50%)	40 (35%)	18 (16%)	0	1
20	O	92/100 (92%)	57 (62%)	10 (11%)	25 (27%)	0	0
21	P	125/134 (93%)	89 (71%)	21 (17%)	15 (12%)	0	3
22	Q	91/95 (96%)	39 (43%)	28 (31%)	24 (26%)	0	0
23	R	108/115 (94%)	62 (57%)	27 (25%)	19 (18%)	0	1
24	S	173/237 (73%)	93 (54%)	46 (27%)	34 (20%)	0	1
25	T	82/91 (90%)	47 (57%)	19 (23%)	16 (20%)	0	1
26	U	70/81 (86%)	35 (50%)	16 (23%)	19 (27%)	0	0
27	V	64/67 (96%)	35 (55%)	16 (25%)	13 (20%)	0	1
28	W	53/55 (96%)	38 (72%)	9 (17%)	6 (11%)	0	3
30	Y	56/60 (93%)	40 (71%)	9 (16%)	7 (12%)	0	2
All	All	3055/3410 (90%)	1829 (60%)	698 (23%)	528 (17%)	0	1

5 of 528 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	A	59	LYS
6	A	145	LEU
6	A	168	LYS
6	A	217	ARG
6	A	220	HIS

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	
4	4	35/35 (100%)	32 (91%)	3 (9%)	13	45
5	5	3/4 (75%)	3 (100%)	0	100	100
6	A	185/215 (86%)	161 (87%)	24 (13%)	5	22
7	B	155/157 (99%)	132 (85%)	23 (15%)	4	17
8	C	157/163 (96%)	131 (83%)	26 (17%)	3	13
9	D	153/156 (98%)	138 (90%)	15 (10%)	10	37
10	E	136/144 (94%)	128 (94%)	8 (6%)	24	63
11	F	107/107 (100%)	100 (94%)	7 (6%)	21	59
12	G	118/146 (81%)	96 (81%)	22 (19%)	2	9
13	H	103/103 (100%)	88 (85%)	15 (15%)	4	18
14	I	108/121 (89%)	91 (84%)	17 (16%)	3	15
15	J	110/116 (95%)	89 (81%)	21 (19%)	2	8
16	K	90/93 (97%)	76 (84%)	14 (16%)	3	16
17	L	74/82 (90%)	54 (73%)	20 (27%)	0	2
18	M	94/134 (70%)	72 (77%)	22 (23%)	1	4
19	N	96/97 (99%)	83 (86%)	13 (14%)	5	21
20	O	75/79 (95%)	70 (93%)	5 (7%)	20	58
21	P	109/115 (95%)	100 (92%)	9 (8%)	14	47
22	Q	75/76 (99%)	67 (89%)	8 (11%)	8	32
23	R	91/96 (95%)	72 (79%)	19 (21%)	1	6
24	S	149/192 (78%)	137 (92%)	12 (8%)	15	48
25	T	62/67 (92%)	57 (92%)	5 (8%)	15	48
26	U	57/66 (86%)	44 (77%)	13 (23%)	1	4
27	V	54/55 (98%)	48 (89%)	6 (11%)	8	31
28	W	48/48 (100%)	38 (79%)	10 (21%)	1	6
30	Y	51/53 (96%)	48 (94%)	3 (6%)	24	63
All	All	2495/2720 (92%)	2155 (86%)	340 (14%)	5	21

5 of 340 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
14	I	65	PHE

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Mol	Chain	Res	Type
16	K	83	VAL
26	U	47	HIS
14	I	103	ASN
15	J	82	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 78 such sidechains are listed below:

Mol	Chain	Res	Type
13	H	41	ASN
16	K	13	ASN
27	V	45	GLN
13	H	79	HIS
14	I	66	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
29	X	2680/2880 (93%)	688 (25%)	313 (11%)
31	Z	121/123 (98%)	24 (19%)	1 (0%)
All	All	2801/3003 (93%)	712 (25%)	314 (11%)

5 of 712 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
29	X	2	G
29	X	4	C
29	X	13	A
29	X	14	A
29	X	27	G

5 of 314 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
29	X	1261	G
29	X	1552	C
29	X	2660	C
29	X	1278	A
29	X	1345	G

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

11 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	$\# Z > 2$
5	TS9	5	10	5	6,8,10	0.89	0	6,12,15	1.16	0
5	BB9	5	11	5	3,5,6	1.35	0	1,5,7	2.19	1 (100%)
5	BB9	5	13	5	0,4,6	0.00	-	0,4,7	0.00	-
5	MH6	5	14	5	3,3,6	1.61	1 (33%)	1,3,7	0.51	0
5	BB9	5	15	5	3,5,6	3.63	1 (33%)	1,5,7	3.43	1 (100%)
5	DHA	5	16	5	4,4,5	4.09	2 (50%)	3,4,6	4.29	1 (33%)
5	DHA	5	17	5	4,4,5	1.86	1 (25%)	3,4,6	2.19	2 (66%)
5	DHA	5	3	5	4,4,5	2.07	2 (50%)	3,4,6	1.71	1 (33%)
5	BB9	5	6	5	3,5,6	1.81	1 (33%)	1,5,7	2.21	1 (100%)
5	DBU	5	8	5	2,4,6	0.78	0	0,4,7	0.00	-
5	DCY	5	9	5	4,5,6	0.33	0	3,5,7	3.07	2 (66%)

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
5	TS9	5	10	5	-	0/9/12/16	0/0/0/0
5	BB9	5	11	5	-	0/0/4/6	0/0/0/0
5	BB9	5	13	5	-	0/0/2/6	0/0/0/0
5	MH6	5	14	5	-	0/0/0/6	0/0/0/0
5	BB9	5	15	5	-	0/0/4/6	0/0/0/0
5	DHA	5	16	5	-	0/0/2/4	0/0/0/0
5	DHA	5	17	5	-	0/0/2/4	0/0/0/0
5	DHA	5	3	5	-	0/0/2/4	0/0/0/0
5	BB9	5	6	5	-	0/0/4/6	0/0/0/0
5	DBU	5	8	5	-	0/1/2/6	0/0/0/0
5	DCY	5	9	5	-	0/1/4/6	0/0/0/0

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	5	15	BB9	O-C	-6.26	1.07	1.22
5	5	16	DHA	C-CA	-2.72	1.40	1.45
5	5	14	MH6	C-CA	2.17	1.53	1.49
5	5	3	DHA	C-CA	2.48	1.48	1.45
5	5	3	DHA	CA-N	2.82	1.42	1.34

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	5	16	DHA	O-C-CA	-7.39	111.08	125.35
5	5	9	DCY	CA-CB-SG	-4.49	104.20	114.48
5	5	9	DCY	O-C-CA	-2.86	118.03	125.49
5	5	17	DHA	O-C-CA	-2.81	119.92	125.35
5	5	3	DHA	O-C-CA	-2.35	120.82	125.35

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	5	10	TS9	1	0
5	5	13	BB9	1	0
5	5	14	MH6	1	0
5	5	15	BB9	1	0
5	5	6	BB9	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 36 ligands modelled in this entry, 36 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 [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	1	53/55 (96%)	3.55	40 (75%) 0 0	48, 56, 77, 82	0
2	2	46/47 (97%)	5.68	46 (100%) 0 0	9, 29, 38, 40	0
3	3	63/66 (95%)	5.20	59 (93%) 0 0	23, 41, 51, 57	0
4	4	37/37 (100%)	1.21	7 (18%) 2 1	60, 69, 77, 81	0
5	5	6/19 (31%)	1.14	1 (16%) 2 2	79, 83, 86, 86	0
6	A	240/274 (87%)	-0.09	6 (2%) 61 54	25, 63, 77, 84	0
7	B	205/211 (97%)	-0.68	1 (0%) 91 90	3, 22, 49, 63	0
8	C	197/205 (96%)	-0.29	5 (2%) 61 54	8, 51, 73, 83	0
9	D	177/180 (98%)	0.06	10 (5%) 28 22	60, 75, 85, 91	0
10	E	171/185 (92%)	-0.33	3 (1%) 71 65	44, 66, 79, 88	0
11	F	144/144 (100%)	1.53	43 (29%) 1 1	74, 89, 98, 102	0
12	G	142/174 (81%)	-0.27	4 (2%) 56 50	22, 43, 67, 72	0
13	H	134/134 (100%)	-0.77	0 100 100	3, 16, 37, 45	0
14	I	141/156 (90%)	0.28	13 (9%) 11 9	22, 62, 77, 85	0
15	J	136/142 (95%)	-0.30	2 (1%) 76 71	27, 51, 73, 80	0
16	K	113/116 (97%)	-0.83	0 100 100	3, 9, 24, 34	0
17	L	104/114 (91%)	-0.04	4 (3%) 44 37	43, 62, 72, 75	0
18	M	108/166 (65%)	-0.73	0 100 100	4, 19, 43, 64	0
19	N	117/118 (99%)	-0.56	0 100 100	4, 40, 62, 73	0
20	O	94/100 (94%)	-0.42	0 100 100	18, 53, 71, 81	0
21	P	127/134 (94%)	-0.71	0 100 100	4, 18, 53, 76	0
22	Q	93/95 (97%)	-0.39	1 (1%) 82 78	32, 50, 69, 80	0
23	R	110/115 (95%)	-0.13	5 (4%) 37 30	36, 54, 80, 87	0
24	S	175/237 (73%)	0.26	14 (8%) 15 12	61, 71, 82, 87	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	T	84/91 (92%)	0.04	9 (10%) 8 6	35, 51, 80, 90	0
26	U	72/81 (88%)	0.11	3 (4%) 40 33	45, 61, 72, 78	0
27	V	66/67 (98%)	-0.48	0 100 100	49, 61, 81, 88	0
28	W	55/55 (100%)	-0.41	0 100 100	23, 41, 61, 78	0
29	X	2686/2880 (93%)	-0.36	67 (2%) 61 54	4, 41, 116, 151	0
30	Y	58/60 (96%)	-0.51	1 (1%) 73 67	4, 17, 44, 52	0
31	Z	122/123 (99%)	-0.09	3 (2%) 61 54	30, 75, 102, 129	0
All	All	6076/6581 (92%)	-0.13	347 (5%) 27 22	3, 49, 95, 151	0

The worst 5 of 347 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	3	39	ASP	16.2
2	2	26	SER	9.9
2	2	4	THR	9.8
1	1	2	ALA	9.8
3	3	31	HIS	9.7

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(Å ²)	Q<0.9
5	BB9	5	15	6/7	0.78	0.48	-	88,88,88,88	0
5	TS9	5	10	9/11	0.87	0.38	-	87,88,89,89	0
5	BB9	5	6	6/7	0.89	0.18	-	82,84,85,86	0
5	BB9	5	11	6/7	0.86	0.23	-	85,87,87,88	0
5	DHA	5	3	5/6	0.77	0.47	-	82,83,84,85	0
5	DHA	5	16	5/6	0.52	0.55	-	83,83,85,86	0
5	BB9	5	13	5/7	0.83	0.22	-	85,86,86,87	0
5	DHA	5	17	5/6	0.55	0.39	-	76,77,78,80	2
5	MH6	5	14	4/7	0.85	0.30	-	86,86,87,87	0
5	DCY	5	9	6/7	0.81	0.18	-	87,87,87,87	0
5	DBU	5	8	5/7	0.93	0.16	-	85,86,87,87	0

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
32	MG	X	2907	1/1	0.96	0.73	63.93	17,17,17,17	0
32	MG	X	2905	1/1	0.97	0.50	9.56	13,13,13,13	0
32	MG	X	2888	1/1	0.95	0.30	8.43	3,3,3,3	0
32	MG	X	2903	1/1	0.95	0.30	6.38	3,3,3,3	0
32	MG	Z	124	1/1	0.95	0.31	6.24	26,26,26,26	0
32	MG	X	2909	1/1	0.96	0.21	5.32	3,3,3,3	0
32	MG	X	2895	1/1	0.98	0.25	1.39	3,3,3,3	0
32	MG	X	2910	1/1	0.90	0.38	-	19,19,19,19	0
32	MG	X	2885	1/1	0.93	0.41	-	56,56,56,56	0
32	MG	X	2901	1/1	0.98	0.08	-	60,60,60,60	0
32	MG	X	2887	1/1	0.98	0.18	-	3,3,3,3	0
32	MG	X	2881	1/1	0.95	0.25	-	59,59,59,59	0
32	MG	X	2899	1/1	0.99	0.53	-	3,3,3,3	0
32	MG	X	2882	1/1	0.97	0.36	-	12,12,12,12	0
32	MG	X	2906	1/1	0.98	0.19	-	58,58,58,58	0
32	MG	X	2883	1/1	0.99	0.10	-	49,49,49,49	0
32	MG	X	2897	1/1	0.98	0.47	-	3,3,3,3	0
32	MG	X	2884	1/1	0.83	0.79	-	55,55,55,55	0
32	MG	X	2904	1/1	0.97	0.31	-	6,6,6,6	0
32	MG	X	2900	1/1	0.96	0.26	-	3,3,3,3	0
32	MG	Z	126	1/1	0.95	0.34	-	25,25,25,25	0
32	MG	X	2893	1/1	0.96	0.15	-	13,13,13,13	0
32	MG	M	167	1/1	0.98	0.54	-	3,3,3,3	0
32	MG	X	2894	1/1	0.99	0.40	-	15,15,15,15	0
32	MG	X	2898	1/1	0.90	0.54	-	19,19,19,19	0
32	MG	X	2902	1/1	0.96	0.38	-	24,24,24,24	0
32	MG	Z	128	1/1	0.95	0.09	-	41,41,41,41	0
32	MG	X	2889	1/1	0.95	0.77	-	3,3,3,3	0
32	MG	X	2890	1/1	0.91	0.34	-	49,49,49,49	0
32	MG	X	2886	1/1	0.91	0.26	-	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	Z	127	1/1	0.95	0.17	-	12,12,12,12	0
32	MG	X	2892	1/1	0.95	0.16	-	22,22,22,22	0
32	MG	X	2896	1/1	0.95	0.27	-	3,3,3,3	0
32	MG	X	2908	1/1	0.97	0.11	-	3,3,3,3	0
32	MG	X	2891	1/1	0.99	0.41	-	12,12,12,12	0
32	MG	Z	125	1/1	0.98	0.29	-	9,9,9,9	0

6.5 Other polymers [i](#)

There are no such residues in this entry.