



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 7, 2020 – 12:09 am BST

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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

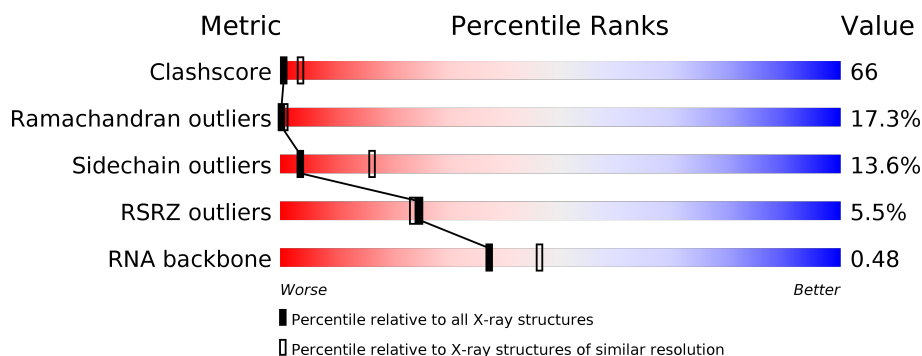
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)
RNA backbone	3102	1117 (3.70-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	1	55	<div> <div>71%</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>
6	A	274	<div> <div>2%</div> <div>17%</div> <div>54%</div> <div>15%</div> <div>12%</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
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	
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
5	BB9	5	13	-	X	-	-
5	BB9	5	15	-	-	-	X
5	DHA	5	16	-	-	-	X
5	DHA	5	3	-	-	-	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			

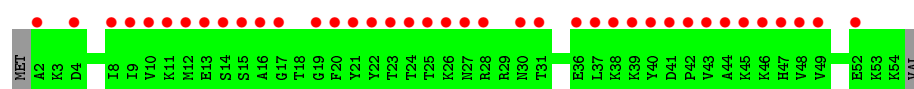
- Molecule 32 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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		

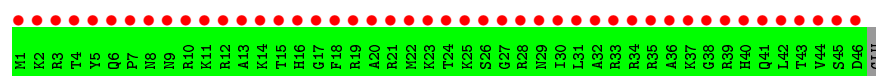
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

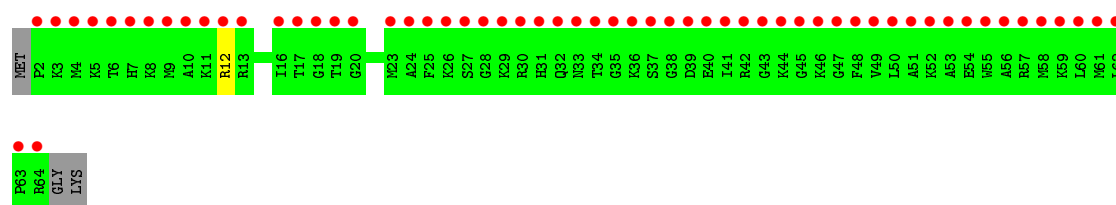
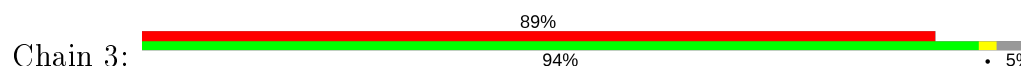
• Molecule 1: 50S RIBOSOMAL PROTEIN L33



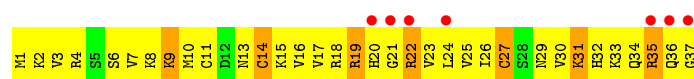
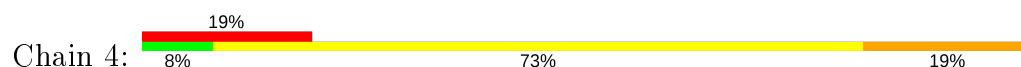
• Molecule 2: 50S RIBOSOMAL PROTEIN L34



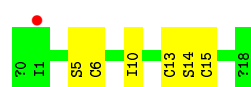
• Molecule 3: 50S RIBOSOMAL PROTEIN L35



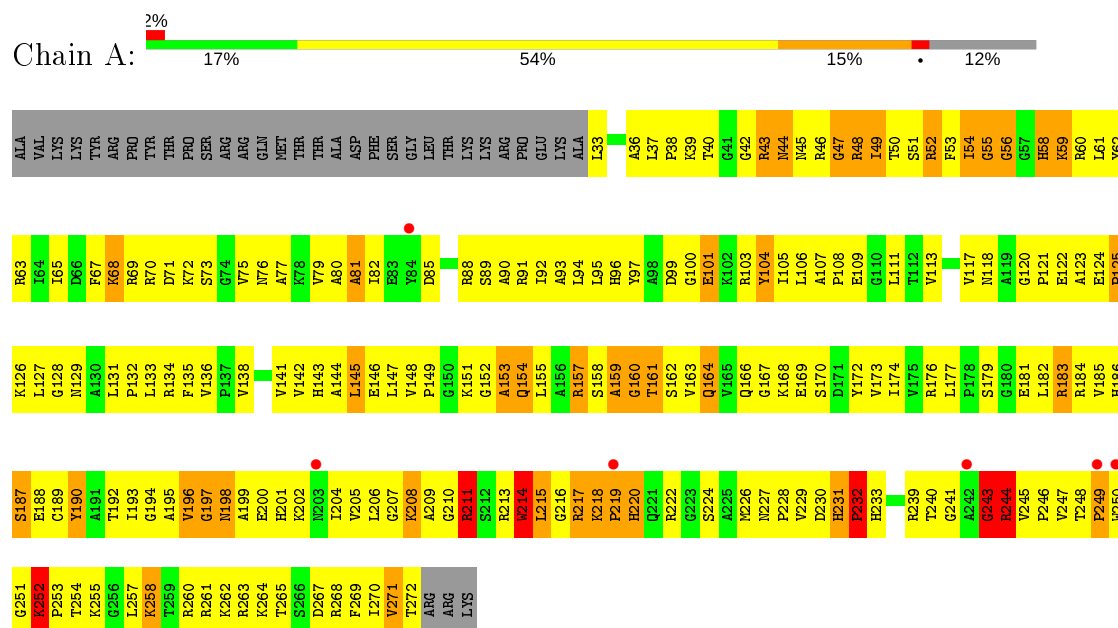
• Molecule 4: 50S RIBOSOMAL PROTEIN L36



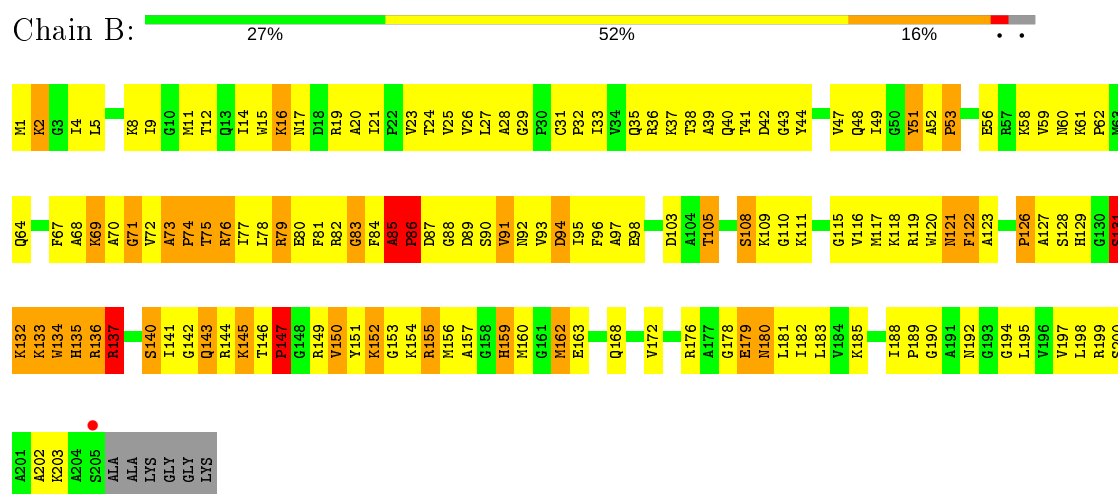
• Molecule 5: THIOSTREPTON



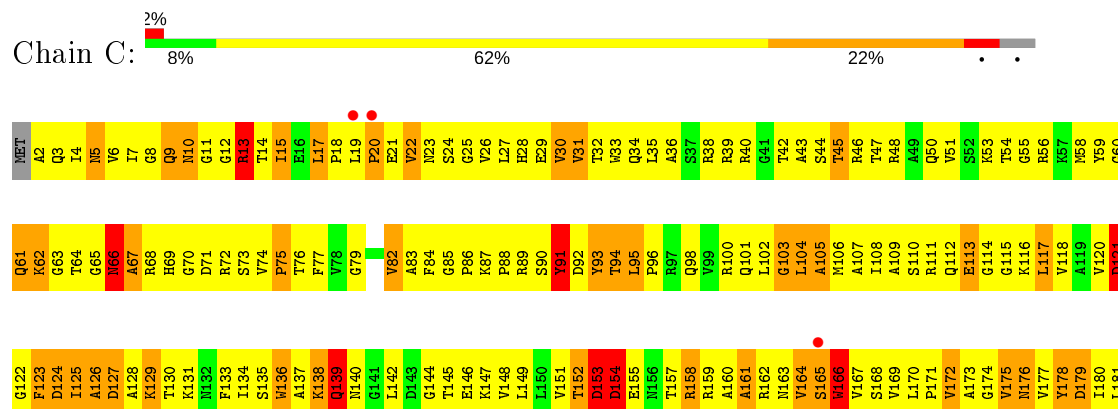
• Molecule 6: 50S RIBOSOMAL PROTEIN L2



• Molecule 7: 50S RIBOSOMAL PROTEIN L3

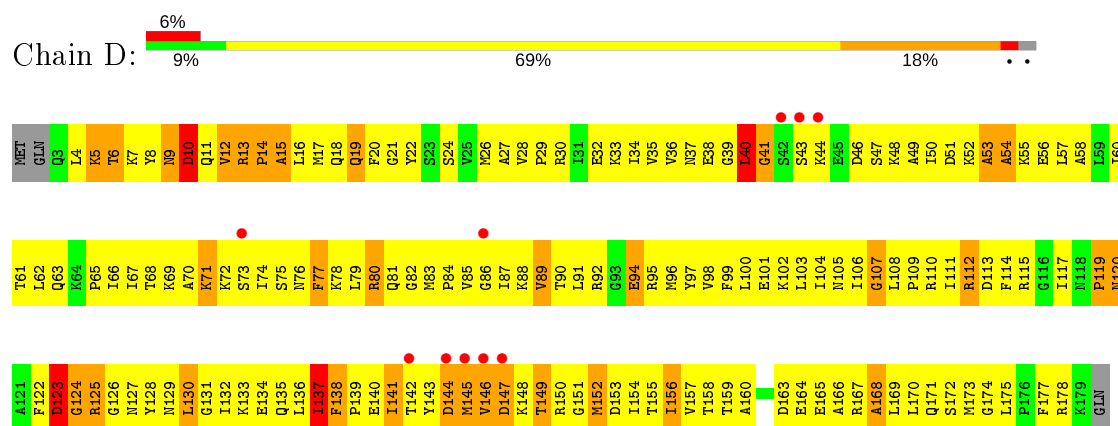


• Molecule 8: 50S RIBOSOMAL PROTEIN L4

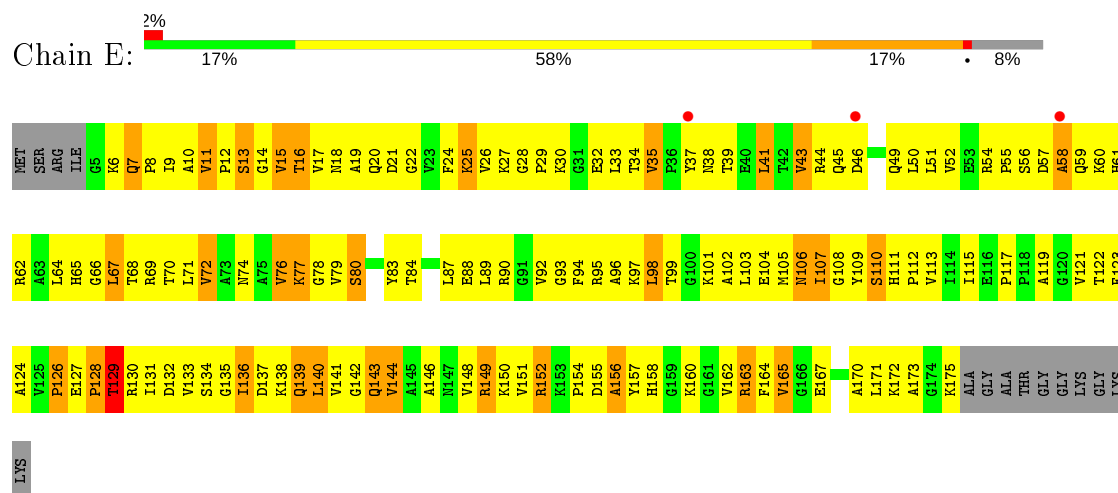




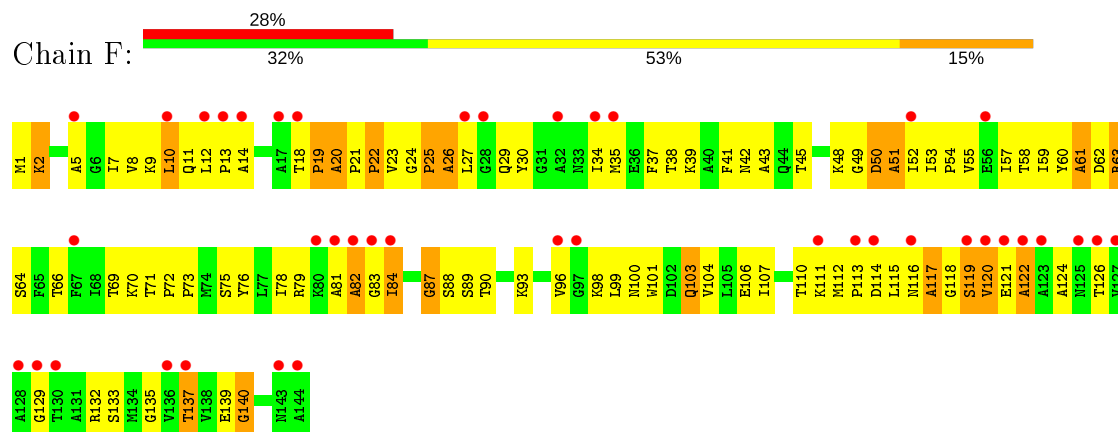
• Molecule 9: 50S RIBOSOMAL PROTEIN L5



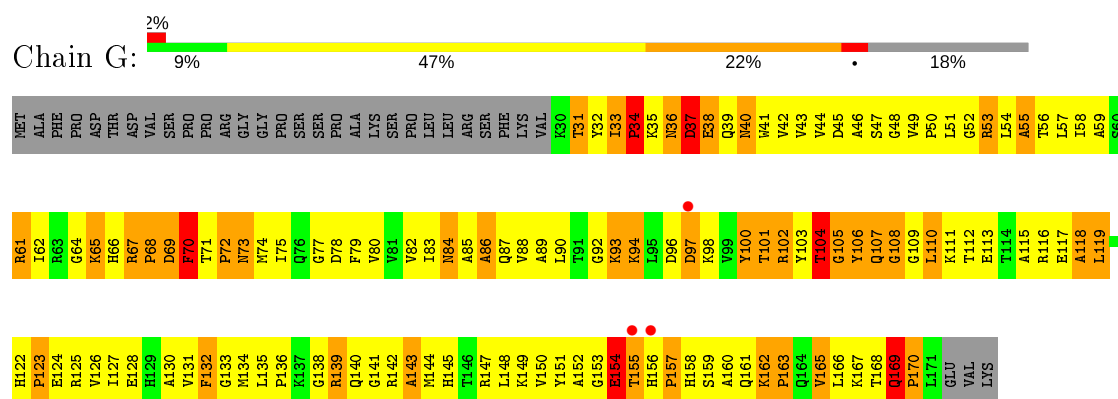
• Molecule 10: 50S RIBOSOMAL PROTEIN L6



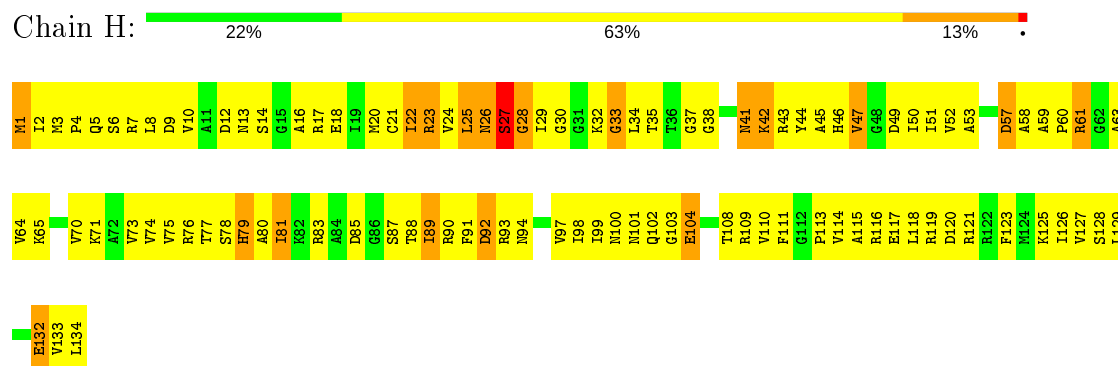
• Molecule 11: 50S RIBOSOMAL PROTEIN L11



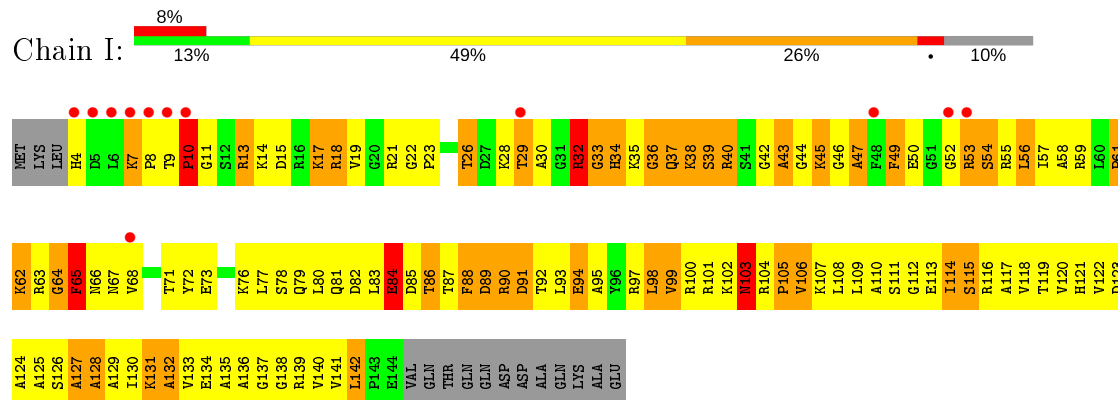
• Molecule 12: 50S RIBOSOMAL PROTEIN L13



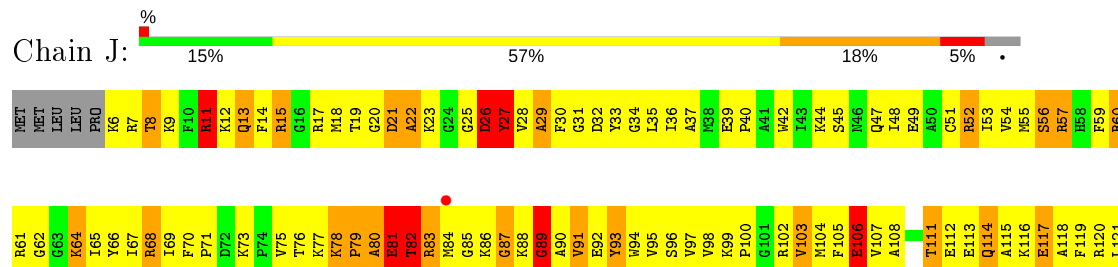
• Molecule 13: 50S RIBOSOMAL PROTEIN L14



• Molecule 14: 50S RIBOSOMAL PROTEIN L15

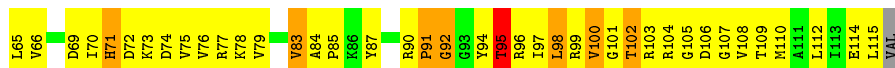


• Molecule 15: 50S RIBOSOMAL PROTEIN L16

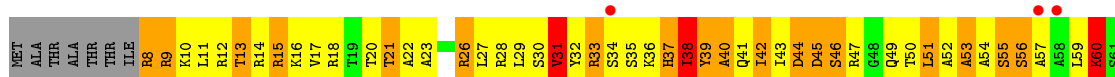




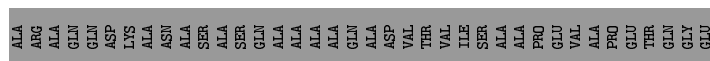
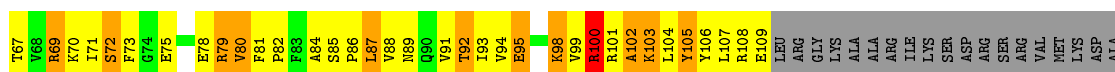
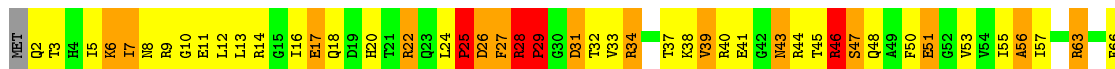
• Molecule 16: 50S RIBOSOMAL PROTEIN L17



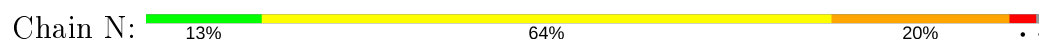
• Molecule 17: 50S RIBOSOMAL PROTEIN L18



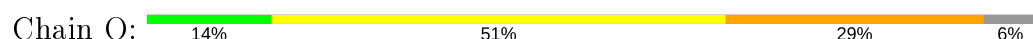
• Molecule 18: 50S RIBOSOMAL PROTEIN L19

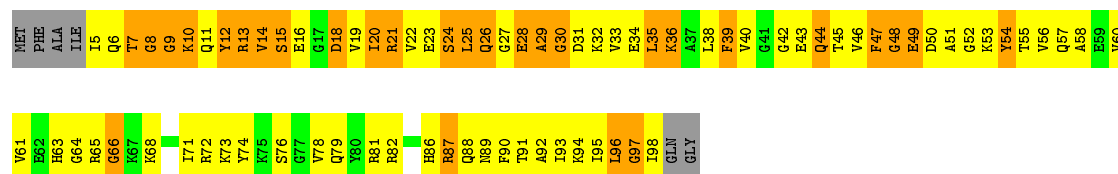


• Molecule 19: 50S RIBOSOMAL PROTEIN L20



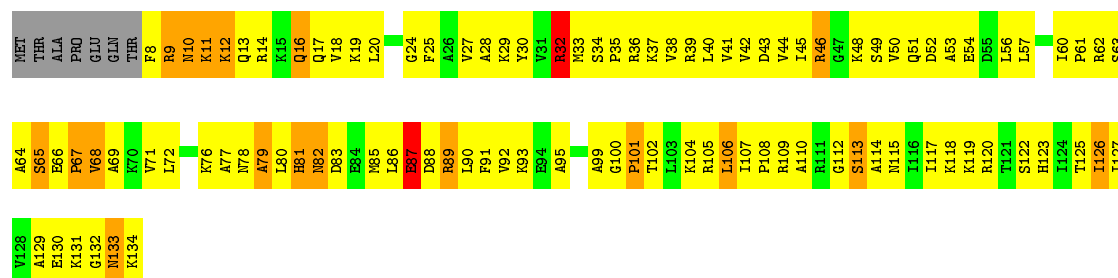
• Molecule 20: 50S RIBOSOMAL PROTEIN L21





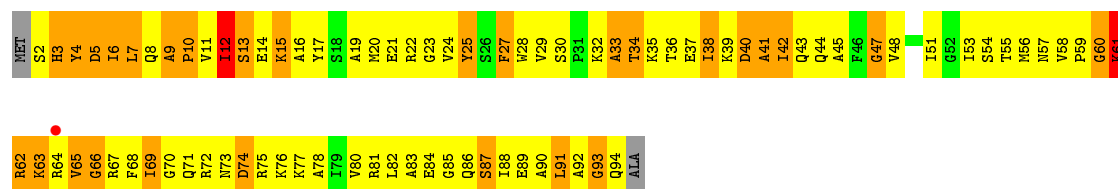
• Molecule 21: 50S RIBOSOMAL PROTEIN L22

Chain P: 19% 61% 13% 5%



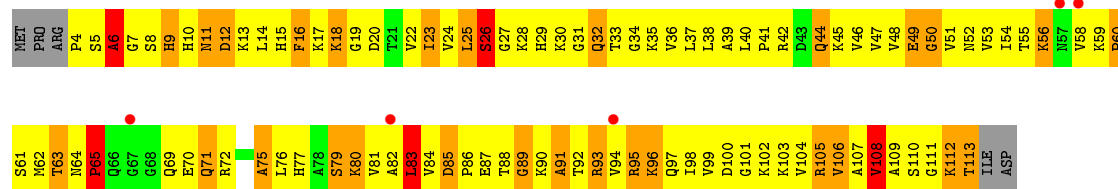
• Molecule 22: 50S RIBOSOMAL PROTEIN L23

Chain Q: 8% 58% 29% . .



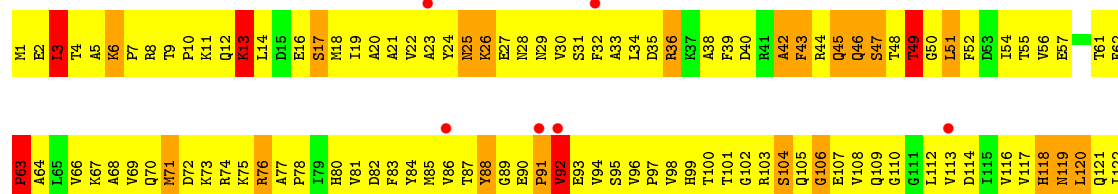
• Molecule 23: 50S RIBOSOMAL PROTEIN L24

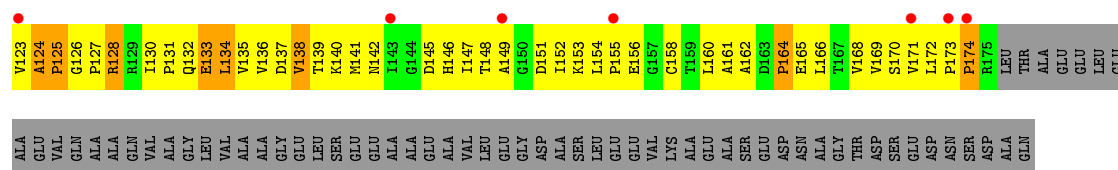
Chain R: 4% 8% 59% 24% . .



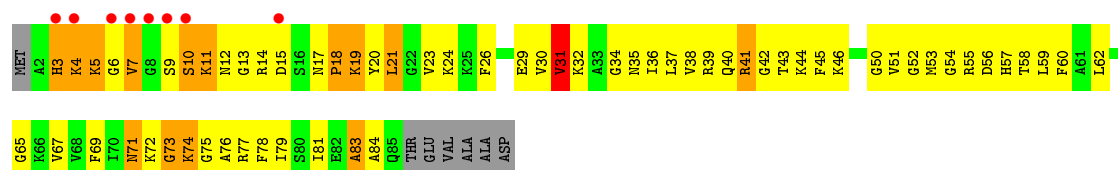
• Molecule 24: 50S RIBOSOMAL PROTEIN L25

Chain S: 5% 8% 51% 12% 26%

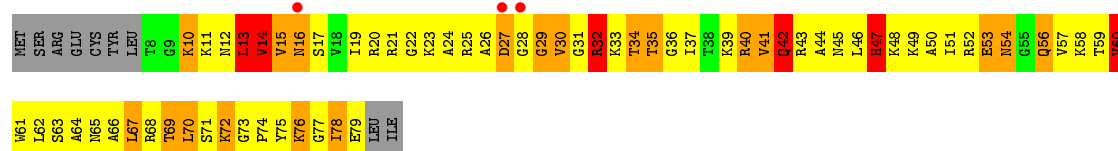




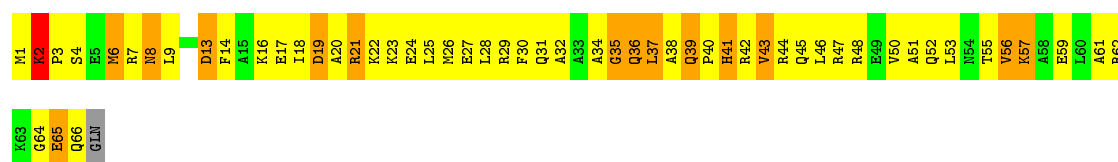
• Molecule 25: 50S RIBOSOMAL PROTEIN L27



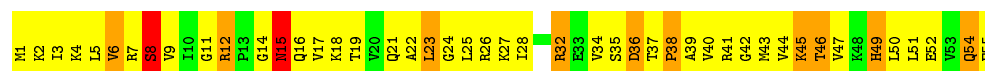
• Molecule 26: 50S RIBOSOMAL PROTEIN L28



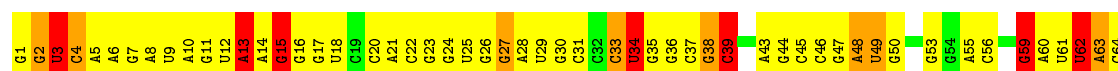
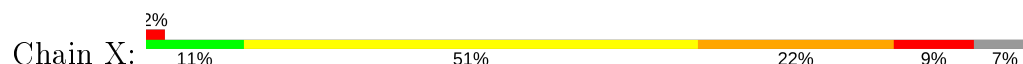
• Molecule 27: 50S RIBOSOMAL PROTEIN L29



• Molecule 28: 50S RIBOSOMAL PROTEIN L30



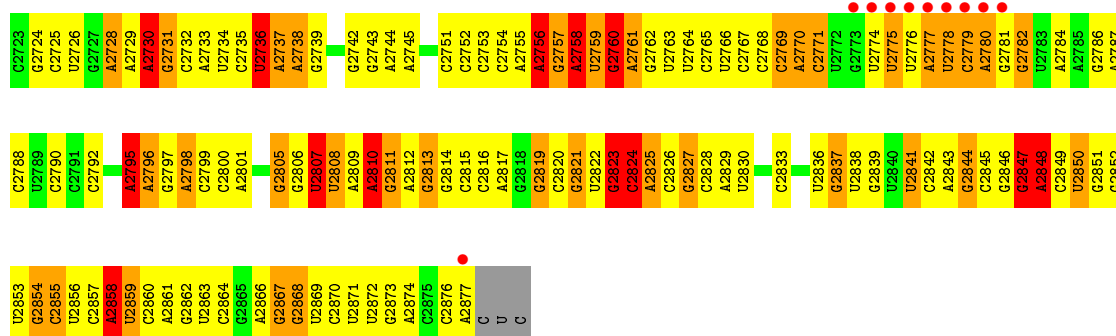
• Molecule 29: RRNA-23S RIBOSOMAL RNA



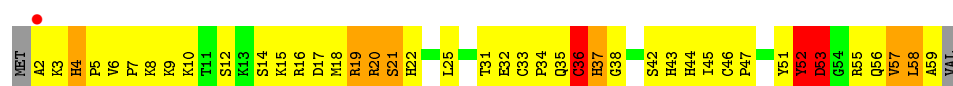
G928	A865	U800	A740	C679	A619	A556	A493	C432	U	A311	C	A189	C127	G65
A929	A866	A801	G741	U680	U694	U557	A494	G433	A	G312	G	A190	C128	U66
A930	G867	A802	G742	A681	G621	G558	A495	C434	C	U313	A	A191	A129	G
G931	U868	C803	A743	G682	U622	C559	C496	A435	U	G314	A	G192	C130	G69
C932	C869	G804	C744	A683	G623	G560	C497	A436	G	G315	A	A193	C131	A70
G933	C870	G805	C745	C684	A624	U561	C498	G437	G	C316	C	G194	U132	A71
G934	U871	A806	G746	U685	A625	U562	G499	G438	C	U317	G	A195		A72
C935	G872	A807	A747	C686	A626	U563	A500	C439	A	G318	C	A196	U135	A73
A936	U873	C808	A748	A687	U564	G501	A501	G440	C	G319	U	G197	A136	G74
C937	A874	C809	C749	A688	A628	A565	A502	A441	C	A320	U	A198	A137	C75
G938	G875	U810	C750	A689	C629	U566	G503		G	A321	G	A199	G138	C76
C939	A876	G811	G751	A690	G630	G567	G504	A443	U	A322	C	A200	A139	C77
G940	G877	G812	G752	C691	G631	G568	G505	U444	A	G323	G	G201	G140	C78
U941	C878	A813	U753	C692	A632	C569	A445	U444	G	U325	U	G202	U141	G79
U942	A879	G814	G754	A693	G633	G570		C446	U	C324	U	G203	U142	A80
U943		A815	C755	G694	G634	U571	G510	U447		A326	U	A204	A143	C81
A944	C884	U816	C756	G695	C635	G572	A511	C448		C327	C	A205	U144	G82
G945	A885	A817	U757	U696	G636	C573	A512	C449		A328	G	U206	C145	A83
U946	A886	G818	G758	G697	G637	C574	A513	C450		C329	G	U207	C146	
C947	G887	C819	C759	A698	A638	U575	G514	A451		C330	G	C208	G391	G84
C948	G888	U820	U760	G699	G639	A576	A515	G452		U331	G	G209	G392	
	C889	A821	G761	C700	C640	U577	G516	U453		C332	U	A210	A149	G87
G951	U890	G822	A762	U701	G641	U578	A517	G454		A333	U	U211	A150	A88
A952	C891	U823	A763		A642	G579	A518	A455		G334	G	U212	A151	A89
G953	G	U824	A764	G704	A643	A880	C519	C456		A335	U	C213	G152	A90
C954	G	C825	C765	A705	A644	G581	C520	C457		U397	A	G214	A153	A91
U955	G	U826	A766	C706	G645	G582	U521	G458		C337	G	U215	U154	A92
A956	G	C827	G767	U707	C646	A883	G522	A459		G338	G	C216	G155	A93
G957	G	C828	U768	G708	G647	C584	A523	U460		U339	A	G217	G156	A94
C958	C	C829	C769	A709	A648	U585	A524	A461		G340	C	A218	G157	A95
G959	U	C830	U770	C710	G649	G586	A525	G462		A401	U	G219	C158	C96
U960	U	G831	C771	C711	U650	A887	C526	C463		A402	C	U220	A158	U97
	C	A832	G772	A712	C651	G588	C527	G464		A341	A	A221	U161	U98
G965	A	C833	G773	G713	C652	C589	G528	C465		A404	G	G222	C162	U99
A966	C	A834	A774	G714	G653	C590	U529	A466		G344	U	C223	A163	G100
G967	A	U835	U775	U715	A654	G591	G530	U467		U345	U	G224	A164	A101
C968	G	C836	G776	U716	A655	G592	G531	A468		C346	U	G225	G164	C102
U969	U	C837	A777	C717	U656	C593	A532	G469		C347	U	C226	G165	U103
A970	C	U838	G778	A718	A657	G594	C533	U470		U348	U	A227	C104	C104
G971	U	U839	U779	A719	G658	A595	U534	A471		G349	A	A228	A167	G105
C972	A	U840	U780	A720	G659	C596		C472		U350	A	G229	C168	G106
U973	C	G841	G781	C721	C660	U597	C537	G473		A411	G	C230	G107	G107
G974	C	A842	U782	C722	C661	U598	A538	G474		G413	A	G231	U170	G108
C975	A911	G843	G783	C723	G662	A599	A539	U475		A414	U	A232	G171	A109
G976	A912	G844	U784	C724	G663	G600	G540	G476		G353	U	A233	A172	U110
G977	A913	U845	U785	C725	C664	A601	C541	A477		U416	C	C234	A173	G111
	C914	A846	U786	G726	A665	C602	A542			A357	A	C235	A174	U112
G980	C915	C947	A787	U727	U666	C603	G543	G480		C418	C	C236	C175	C113
C981	U916	A848	G788	U728	U667		U544	A481		G419	C	G237	A176	C114
G982	U917	C949	G789	A729	U668	U608	C545	A482		C420	C	G238	U177	G115
G983	A918	C950	A790	C730	G669	G809	A546	A483		G421	C	A239	C178	A116
	U919		G791	A731	U670	G610	U547	G484		G422	C	U240	U179	A117
G984	G920	U857	U792	G732	A671	C611	G548	G485		A423	G	C241	C180	U118
A921	C921	G588	G793	G733	C672	G612	G549	U486		G424	C	A242	A181	G119
U922	A922	U889	A794	G734	G673	A613	C550	G487		A425	U	G243	G182	G120
C923	G988	U860	A795	G735	U674	G614	A551	A488		C426	U	C244	U183	G121
G924	U924	G561	A796	G736	C675	C615	C552	A489		G427	G	G245	G184	C122
U925	C925	A862	A797	G737	G676	U616	C553	A490		A	C	C307	C185	A123
A991		C926	G798	U738	C677	U617	G738	A491		C429	C	A248	C186	A124
C992	U992	C964	C799	G739	G678	A818	U554	C492		C430	U	A	U187	C125
A993							U555			C431	C		C189	A126

A1799	C1736	A1607	A1544	G1483	G1361	A1300	C1178	G1117	U1056	A894
A1800	G1737	U1608	G1545	G1484	A1362	U1301	A1179	G1118	A1057	A995
A1801	U1738	G1609	G1546	U1485	C1363	C1302	C1180	U1119	G1058	C996
A1802	G1677	A1610	U1547	A1486	C1364	U1303	C1181	C1120	A1059	C997
G1803	G1678	U1611	U1548	G1487	U1365	U1304	U1182	G1121	C1060	C998
U1804	G1679	G1612	U1549	G1488	G1366	C1305	G1427	A1122	A1061	A999
G1805	U1680	G1613	C1550	G1489	A1367	U1306	G1245	G1123	G1062	G1000
G1806	G1742	G1614	U1551	U1490	G1368	U1307	G1246	G1124	C1063	A1001
A1807	C1743	C1615	G1552	U1491	G1369	C1308	C1185	U1125	G1064	A1002
C1808	G1744	G1616	G1553	A1492	U1370	G1309	U1247	G1126	A1065	C1003
G1809	G1684	U1617	G1554	A1493	G1371	C1310	A1187	A1127	G1066	A1004
U1810	U1618	U1618	A1555	G1494	G1372	C1311	A1188	G1128	G1067	U1005
A1811	A1685	G1621	A1556	G1495	A1373	G1312	C1199	A1129	A1068	U1006
G1812	G1747	G1622	G1557	G1496	G1374	U1313	G1191	U1130	G1069	A1007
U1813	G1749	G1623	C1558	A1497	C1375	A1314	A1192	G1131	G1070	G1008
A1814	A1750	A1624	G1559	G1498	C1376	A1315	G1254	U1071	U1071	C1009
G1815	U1752	A1625	A1560	A1499	G1377	G1316	U1194	G1072	U1072	U1010
G1816	A1753	A1626	A1561	U1500	A1378	G1317	U1195	G1073	G1073	A1011
U1817	G1754	C1627	G1562	C1501	A1379	A1318	G1196	G1074	G1074	A1012
G1818	G1755	C1628	U1563	G1502	C1380	C1319	U1197	G1075	G1075	G1013
A1819	A1694	G1629	U1564	G1503	G1381	A1320	C1198	U1076	U1076	G1014
G1820	C1757	A1630	G1565	U1504	G1382	A1321	U1199	U1077	U1077	U1015
A1821	C1758	C1631	G1566	U1505	G1383	G1322	G1200	A1078	A1078	C1016
U1822	A1759	U1697	G1567	A1506	A1384	G1323	G1201	G1079	G1079	G1017
G1823	G1762	A1632	G1570	C1507	G1385	G1324	U1202	A1080	A1080	C1018
C1824	G1763	C1633	G1571	A1507	U1486	U1325	A1283	A1081	A1081	U1019
G1825	A1764	A1634	C1572	G1508	U1447	U1326	G1204	G1082	G1082	A1022
U1826	G1765	G1635	A1573	A1509	G1387	U1327	G1205	C1083	C1083	U1023
G1827	U1766	G1636	G1574	A1510	C1388	G1328	G1206	G1085	G1085	G1024
C1830	G1769	G1637	C1575	A1511	G1389	U1329	G1207	G1086	G1086	A1025
G1831	U1770	A1638	G1576	A1512	C1481	G1330	G1208	C1087	C1087	U1026
A1832	A1705	G1644	U1577	U1513	A1391	G1331	G1209	A1088	A1088	C1027
U1833	U1771	U1645	G1578	C1514	U1392	G1332	C1210	C1089	C1089	U1030
G1834	C1772	C1647	C1580	U1515	G1393	U1333	G1211	C1090	C1090	C1031
C1835	G1773	U1648	G1581	A1516	G1394	A1334	U1212	C1091	C1091	A1032
G1836	A1774	G1649	A1582	C1517	A1395	G1335	C1214	U1092	U1092	G1033
G1837	A1775	U1651	A1583	G1518	C1396	U1336	A1215	U1093	U1093	G1034
G1838	A1776	U1652	G1584	U1520	A1397	G1337	G1277	A1154	A1154	G1036
A1839	C1777	G1653	A1585	C1521	C1461	U1338	A1278	C1094	C1094	U1037
A1840	U1778	A1654	A1586	C1522	A1462	U1339	G1279	A1095	A1095	U1038
G1841	A1779	C1655	A1587	A1523	G1401	G1340	C1217	U1159	U1159	A1039
G1842	C1780	U1656	A1588	C1524	A1463	G1341	C1218	C1162	C1162	A1040
U1843	G1781	A1657	A1589	A1525	G1402	U1342	C1219	C1163	C1163	G1041
C1844	C1782	A1658	G1590	U1526	U1403	C1343	G1220	C1164	C1164	G1042
A1845	A1785	G1659	U1591	G1527	C1466	C1344	G1223	G1165	G1165	A1043
G1846	A1786	G1660	U1592	C1528	A1467	G1345	A1224	A1166	A1166	U1044
U1847	U1723	C1661	C1593	C1529	U1468	C1346	G1225	A1167	A1167	G1045
G1848	G1787	C1662	U1594	U1530	G1470	C1347	A1226	C1168	C1168	U1046
C1849	C1788	C1663	A1595	C1531	A1408	C1348	C1227	C1169	C1169	G1047
G1850	U1789	G1664	A1596	G1532	U1410	G1349	G1228	U1170	U1170	U1048
A1851	G1790	C1665	A1597	A1534	C1411	G1350	C1229	A1171	A1171	C1049
G1852	C1791	G1666	U1598	C1535	C1412	G1351	C1290	G1172	G1172	G1050
C1853	C1792	A1667	G1599	G1536	U1413	A1352	G1291	C1173	C1173	U1051
G1854	A1793	G1668	U1600	U1537	G1414	A1353	U1231	C1174	C1174	C1052
G1855	G1794	A1669	U1601	U1538	C1415	A1354	A1232	A1175	A1175	G1053
U1856	C1795	G1670	G1602	U1539	U1416	A1355	C1233	U1176	U1176	C1054
G1857	A1796	A1671	A1603	C1540	C1417	U1357	C1235	U1112	U1112	U1055
G1858	C1797	C1672	A1604	G1541	G1418	C1358	G1236	C1113	C1113	
A1859	G1798	C1673	U1605	G1542	U1419	G1359	G1237	C1114	C1114	
			C1606	G1543	A1420	G1360	A1238	U1177	U1177	

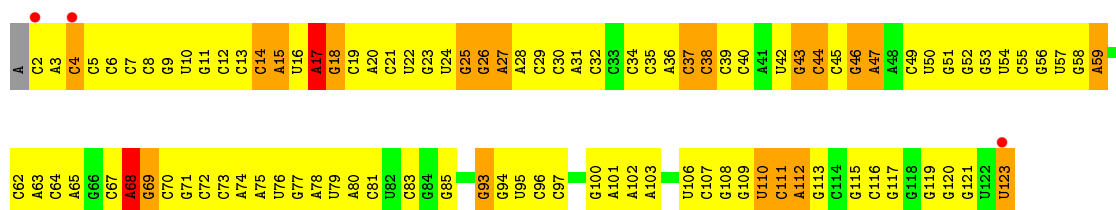




• Molecule 30: 50S RIBOSOMAL PROTEIN L32



• Molecule 31: RRNA-5S RIBOSOMAL RNA



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	Depositor
R, R_{free}	0.276 , 0.318 0.241 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
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 , 60.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	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.*

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: 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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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	2
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	1

Continued on next page...

Continued from previous page...

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	8
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	2
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	1
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	2
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	0
25	T	82/91 (90%)	47 (57%)	19 (23%)	16 (20%)	0	0
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	0
28	W	53/55 (96%)	38 (72%)	9 (17%)	6 (11%)	0	2
30	Y	56/60 (93%)	40 (71%)	9 (16%)	7 (12%)	0	1
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%)	10	35
5	5	3/4 (75%)	3 (100%)	0	100	100
6	A	185/215 (86%)	161 (87%)	24 (13%)	4	17
7	B	155/157 (99%)	132 (85%)	23 (15%)	3	13
8	C	157/163 (96%)	131 (83%)	26 (17%)	2	10
9	D	153/156 (98%)	138 (90%)	15 (10%)	8	29
10	E	136/144 (94%)	128 (94%)	8 (6%)	19	49
11	F	107/107 (100%)	100 (94%)	7 (6%)	17	46
12	G	118/146 (81%)	96 (81%)	22 (19%)	1	7
13	H	103/103 (100%)	88 (85%)	15 (15%)	3	14
14	I	108/121 (89%)	91 (84%)	17 (16%)	2	12
15	J	110/116 (95%)	89 (81%)	21 (19%)	1	6
16	K	90/93 (97%)	76 (84%)	14 (16%)	2	12
17	L	74/82 (90%)	54 (73%)	20 (27%)	0	1
18	M	94/134 (70%)	72 (77%)	22 (23%)	1	3
19	N	96/97 (99%)	83 (86%)	13 (14%)	4	16
20	O	75/79 (95%)	70 (93%)	5 (7%)	16	45
21	P	109/115 (95%)	100 (92%)	9 (8%)	11	36
22	Q	75/76 (99%)	67 (89%)	8 (11%)	6	25
23	R	91/96 (95%)	72 (79%)	19 (21%)	1	4
24	S	149/192 (78%)	137 (92%)	12 (8%)	11	36
25	T	62/67 (92%)	57 (92%)	5 (8%)	11	36
26	U	57/66 (86%)	44 (77%)	13 (23%)	1	3
27	V	54/55 (98%)	48 (89%)	6 (11%)	6	23
28	W	48/48 (100%)	38 (79%)	10 (21%)	1	4
30	Y	51/53 (96%)	48 (94%)	3 (6%)	19	49
All	All	2495/2720 (92%)	2155 (86%)	340 (14%)	3	16

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

Mol	Chain	Res	Type
14	I	65	PHE

Continued on next page...

Continued from previous page...

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	BB9	5	15	5	3,5,6	3.69	1 (33%)	1,5,7	3.99	1 (100%)
5	TS9	5	10	5	6,8,10	0.89	0	5,12,15	1.14	0
5	BB9	5	6	5	3,5,6	1.82	1 (33%)	1,5,7	2.55	1 (100%)
5	BB9	5	11	5	3,5,6	1.31	0	1,5,7	2.53	1 (100%)
5	DHA	5	3	5	4,4,5	2.01	2 (50%)	2,4,6	1.79	1 (50%)
5	DHA	5	16	5	4,4,5	4.20	2 (50%)	2,4,6	5.51	1 (50%)
5	BB9	5	13	5	2,4,6	1.67	1 (50%)	3,4,7	2.70	3 (100%)
5	DHA	5	17	5	4,4,5	1.82	1 (25%)	2,4,6	2.55	1 (50%)
5	MH6	5	14	5	3,3,6	1.53	1 (33%)	1,3,7	0.42	0
5	DBU	5	8	5	4,4,6	3.15	2 (50%)	4,4,7	1.52	1 (25%)

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

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	5	16	DHA	CA-N	7.94	1.55	1.35
5	5	15	BB9	O-C	-6.34	1.07	1.22
5	5	8	DBU	CA-N	5.83	1.47	1.33
5	5	17	DHA	CA-N	3.10	1.43	1.35
5	5	6	BB9	O-C	2.87	1.28	1.22

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	5	16	DHA	O-C-CA	-7.75	111.08	125.54
5	5	15	BB9	O-C-CA	3.99	130.46	125.39
5	5	17	DHA	O-C-CA	-3.01	119.92	125.54
5	5	13	BB9	C-CA-CB	2.89	126.66	121.39
5	5	8	DBU	CB-CA-N	2.75	124.53	122.87

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	15	BB9	1	0
5	5	10	TS9	1	0
5	5	6	BB9	1	0
5	5	13	BB9	1	0
5	5	14	MH6	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%)	3.45	39 (73%) 0 0	48, 56, 77, 82	0
2	2	46/47 (97%)	5.52	46 (100%) 0 0	9, 29, 38, 40	0
3	3	63/66 (95%)	5.06	59 (93%) 0 0	23, 41, 51, 57	0
4	4	37/37 (100%)	1.16	7 (18%) 1 1	60, 69, 77, 81	0
5	5	6/19 (31%)	1.08	1 (16%) 1 1	79, 83, 86, 86	0
6	A	240/274 (87%)	-0.11	6 (2%) 57 54	25, 63, 77, 84	0
7	B	205/211 (97%)	-0.69	1 (0%) 91 91	3, 22, 49, 63	0
8	C	197/205 (96%)	-0.30	4 (2%) 65 64	8, 51, 73, 83	0
9	D	177/180 (98%)	0.03	10 (5%) 24 23	60, 75, 85, 91	0
10	E	171/185 (92%)	-0.34	3 (1%) 68 67	44, 66, 79, 88	0
11	F	144/144 (100%)	1.48	41 (28%) 0 0	74, 89, 98, 102	0
12	G	142/174 (81%)	-0.29	3 (2%) 63 62	22, 43, 67, 72	0
13	H	134/134 (100%)	-0.78	0 100 100	3, 16, 37, 45	0
14	I	141/156 (90%)	0.25	12 (8%) 10 10	22, 62, 77, 85	0
15	J	136/142 (95%)	-0.33	2 (1%) 73 72	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%)	-0.06	4 (3%) 40 37	43, 62, 72, 75	0
18	M	108/166 (65%)	-0.74	0 100 100	4, 19, 43, 64	0
19	N	117/118 (99%)	-0.57	0 100 100	4, 40, 62, 73	0
20	O	94/100 (94%)	-0.43	0 100 100	18, 53, 71, 81	0
21	P	127/134 (94%)	-0.72	0 100 100	4, 18, 53, 76	0
22	Q	93/95 (97%)	-0.41	1 (1%) 80 81	32, 50, 69, 80	0
23	R	110/115 (95%)	-0.15	5 (4%) 33 32	36, 54, 80, 87	0
24	S	175/237 (73%)	0.23	13 (7%) 14 14	61, 71, 82, 87	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	T	84/91 (92%)	0.02	8 (9%) 8 8	35, 51, 80, 90	0
26	U	72/81 (88%)	0.09	3 (4%) 36 34	45, 61, 72, 78	0
27	V	66/67 (98%)	-0.49	0 100 100	49, 61, 81, 88	0
28	W	55/55 (100%)	-0.42	0 100 100	23, 41, 61, 78	0
29	X	2686/2880 (93%)	-0.37	60 (2%) 62 60	4, 41, 116, 151	0
30	Y	58/60 (96%)	-0.52	1 (1%) 70 68	4, 17, 44, 52	0
31	Z	122/123 (99%)	-0.11	3 (2%) 57 54	30, 75, 102, 129	0
All	All	6076/6581 (92%)	-0.15	332 (5%) 25 23	3, 49, 95, 151	0

The worst 5 of 332 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	3	39	ASP	15.9
2	2	26	SER	9.7
1	1	2	ALA	9.6
3	3	31	HIS	9.6
2	2	4	THR	9.5

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. 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(Å ²)	Q<0.9
5	DHA	5	16	5/6	0.52	0.55	83,83,85,86	0
5	DHA	5	17	5/6	0.55	0.39	76,77,78,80	2
5	DHA	5	3	5/6	0.76	0.47	82,83,84,85	0
5	BB9	5	15	6/7	0.78	0.48	88,88,88,88	0
5	DCY	5	9	6/7	0.81	0.18	87,87,87,87	0
5	BB9	5	13	5/7	0.83	0.22	85,86,86,87	0
5	MH6	5	14	4/7	0.85	0.30	86,86,87,87	0
5	BB9	5	11	6/7	0.86	0.23	85,87,87,88	0
5	TS9	5	10	9/11	0.87	0.38	87,88,89,89	0
5	BB9	5	6	6/7	0.88	0.18	82,84,85,86	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. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
32	MG	X	2884	1/1	0.82	0.79	55,55,55,55	0
32	MG	X	2910	1/1	0.90	0.38	19,19,19,19	0
32	MG	X	2898	1/1	0.90	0.54	19,19,19,19	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
32	MG	X	2885	1/1	0.93	0.41	56,56,56,56	0
32	MG	Z	124	1/1	0.95	0.31	26,26,26,26	0
32	MG	Z	126	1/1	0.95	0.34	25,25,25,25	0
32	MG	X	2903	1/1	0.95	0.30	3,3,3,3	0
32	MG	X	2896	1/1	0.95	0.26	3,3,3,3	0
32	MG	X	2889	1/1	0.95	0.77	3,3,3,3	0
32	MG	X	2881	1/1	0.95	0.24	59,59,59,59	0
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	2888	1/1	0.95	0.30	3,3,3,3	0
32	MG	X	2893	1/1	0.96	0.15	13,13,13,13	0
32	MG	X	2905	1/1	0.96	0.50	13,13,13,13	0
32	MG	X	2907	1/1	0.96	0.73	17,17,17,17	0
32	MG	X	2900	1/1	0.96	0.26	3,3,3,3	0
32	MG	X	2902	1/1	0.96	0.39	24,24,24,24	0
32	MG	Z	128	1/1	0.96	0.09	41,41,41,41	0
32	MG	X	2882	1/1	0.97	0.36	12,12,12,12	0
32	MG	X	2909	1/1	0.97	0.21	3,3,3,3	0
32	MG	X	2904	1/1	0.97	0.32	6,6,6,6	0
32	MG	X	2908	1/1	0.97	0.11	3,3,3,3	0
32	MG	X	2897	1/1	0.98	0.47	3,3,3,3	0
32	MG	M	167	1/1	0.98	0.54	3,3,3,3	0
32	MG	X	2895	1/1	0.98	0.25	3,3,3,3	0
32	MG	X	2887	1/1	0.98	0.18	3,3,3,3	0
32	MG	X	2901	1/1	0.98	0.09	60,60,60,60	0
32	MG	X	2906	1/1	0.98	0.19	58,58,58,58	0
32	MG	Z	125	1/1	0.98	0.29	9,9,9,9	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
32	MG	X	2894	1/1	0.99	0.40	15,15,15,15	0
32	MG	X	2883	1/1	0.99	0.10	49,49,49,49	0
32	MG	X	2891	1/1	0.99	0.41	12,12,12,12	0
32	MG	X	2899	1/1	0.99	0.53	3,3,3,3	0

6.5 Other polymers [i](#)

There are no such residues in this entry.