



wwPDB X-ray Structure Validation Summary Report ⓘ

May 13, 2020 – 05:27 am BST

PDB ID : 5DM7
Title : Crystal structure of the 50S ribosomal subunit from *Deinococcus radiodurans* in complex with hygromycin A
Authors : Kaminishi, T.; Schedlbauer, A.; Ochoa-Lizarralde, B.; Connell, S.R.; Fucini, P.
Deposited on : 2015-09-08
Resolution : 3.00 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
buster-report : 1.1.7 (2018)
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

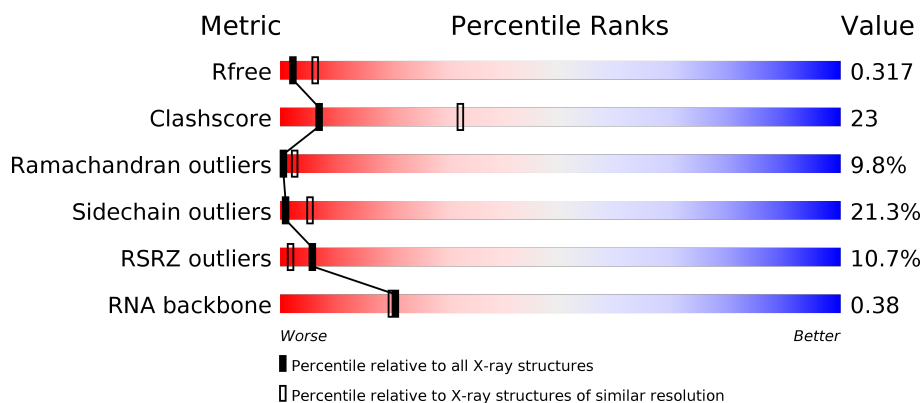
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)
RNA backbone	3102	1173 (3.30-2.70)

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	0	224	<div> <div>80%</div> <div> <div>54%</div> <div>39%</div> <div>6%</div> </div> </div>
2	A	274	<div> <div>14%</div> <div> <div>43%</div> <div>47%</div> <div>9%</div> </div> </div>
3	B	205	<div> <div>2%</div> <div> <div>33%</div> <div>50%</div> <div>17%</div> </div> </div>
4	C	197	<div> <div>5%</div> <div> <div>30%</div> <div>50%</div> <div>17%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
5	D	177	
6	E	171	
7	F	144	
8	G	142	
9	H	134	
10	I	141	
11	J	136	
12	K	113	
13	L	104	
14	M	109	
15	N	117	
16	O	94	
17	P	127	
18	Q	93	
19	R	110	
20	S	175	
21	T	84	
22	U	72	
23	V	66	
24	W	55	
25	Z	57	
26	1	54	
27	2	47	
28	3	65	
29	X	2881	

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Mol	Chain	Length	Quality of chain
30	Y	122	

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
31	MG	X	6006	-	-	-	X
31	MG	X	6035	-	-	-	X
31	MG	X	6051	-	-	-	X
31	MG	X	6076	-	-	-	X
31	MG	X	6099	-	-	-	X
31	MG	X	6101	-	-	-	X
31	MG	X	6111	-	-	-	X
31	MG	X	6114	-	-	-	X
31	MG	X	6116	-	-	-	X
31	MG	X	6118	-	-	-	X
31	MG	X	6124	-	-	-	X
31	MG	X	6125	-	-	-	X
31	MG	X	6127	-	-	-	X
31	MG	X	6135	-	-	-	X
31	MG	X	6139	-	-	-	X
31	MG	X	6140	-	-	-	X
31	MG	X	6149	-	-	-	X
31	MG	X	6150	-	-	-	X
31	MG	X	6159	-	-	-	X
31	MG	X	6160	-	-	-	X
31	MG	X	6162	-	-	-	X
31	MG	X	6168	-	-	-	X
31	MG	X	6169	-	-	-	X
31	MG	X	6176	-	-	-	X
31	MG	Y	205	-	-	-	X

2 Entry composition

There are 32 unique types of molecules in this entry. The entry contains 89361 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 L1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	0	224	Total	C	N	O	S	0	0	0
			1651	1031	302	313	5			

- Molecule 2 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	274	Total	C	N	O	S	0	0	0
			2107	1313	423	368	3			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	7	LYS	ARG	conflict	UNP Q9RXJ9
A	25	ALA	THR	conflict	UNP Q9RXJ9
A	270	LEU	ILE	conflict	UNP Q9RXJ9

- Molecule 3 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	B	205	Total	C	N	O	S	0	0	0
			1540	965	295	272	8			

- Molecule 4 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	C	197	Total	C	N	O	S	0	0	0
			1507	935	287	283	2			

- Molecule 5 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	D	177	Total	C	N	O	S	0	0	0
			1401	892	247	255	7			

- Molecule 6 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	E	171	Total	C	N	O	S	0	0	0
			1287	812	237	237	1			

- Molecule 7 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	F	144	Total	C	N	O	S	0	0	0
			1048	663	183	197	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	2	ARG	LYS	conflict	UNP Q9RSS7
F	3	ARG	LYS	conflict	UNP Q9RSS7

- Molecule 8 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	G	142	Total	C	N	O	S	0	0	0
			1115	704	209	199	3			

- Molecule 9 is a protein called 50S ribosomal protein L14.

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

- Molecule 10 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	I	141	Total	C	N	O		0	0	0
			1068	655	216	197				

- Molecule 11 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	J	136	Total	C	N	O	S	0	0	0
			1091	696	202	186	7			

- Molecule 12 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	K	113	Total	C	N	O	S	0	0	0
			879	541	178	158	2			

- Molecule 13 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	L	104	Total	C	N	O	0	0	0
			778	476	159	143			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	26	LYS	ARG	conflict	UNP Q9RSL2

- Molecule 14 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	M	109	Total	C	N	O	0	0	0
			867	540	171	156			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	?	-	LEU	deletion	UNP Q9RWB4
M	?	-	ARG	deletion	UNP Q9RWB4
M	?	-	GLU	deletion	UNP Q9RWB4
M	?	-	LEU	deletion	UNP Q9RWB4

- Molecule 15 is a protein called 50S ribosomal protein L20.

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

- Molecule 16 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
16	O	94	Total	C	N	O	0	0	0
			742	465	139	138			

- Molecule 17 is a protein called 50S ribosomal protein L22.

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

- Molecule 18 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	Q	93	Total	C	N	O	S	0	0	0
			727	458	136	131	2			

- Molecule 19 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	R	110	Total	C	N	O	S	0	0	0
			826	513	160	152	1			

- Molecule 20 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	S	175	Total	C	N	O	S	0	0	0
			1346	849	236	255	6			

- Molecule 21 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	T	84	Total	C	N	O	S	0	0	0
			626	393	122	110	1			

- Molecule 22 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
22	U	72	Total	C	N	O	0	0	0
			553	341	116	96			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
U	67	ILE	LEU	conflict	UNP Q9RRG8

- Molecule 23 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	V	66	Total	C	N	O	S	0	0	0
			534	327	107	97	3			

- Molecule 24 is a protein called 50S ribosomal protein L30.

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

- Molecule 25 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	Z	57	Total	C	N	O	S	0	0	0
			453	278	93	77	5			

- Molecule 26 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	1	54	Total	C	N	O	S	0	0	0
			404	256	73	74	1			

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	0	ALA	-	insertion	UNP Q9RSS4
1	1	ALA	-	insertion	UNP Q9RSS4
1	3	GLY	LYS	conflict	UNP Q9RSS4
1	4	ALA	ASP	conflict	UNP Q9RSS4
1	5	ALA	GLY	conflict	UNP Q9RSS4
1	45	ALA	LYS	conflict	UNP Q9RSS4
1	46	HIS	LYS	conflict	UNP Q9RSS4
1	47	VAL	HIS	conflict	UNP Q9RSS4
1	49	PHE	VAL	conflict	UNP Q9RSS4
1	50	ALA	PHE	conflict	UNP Q9RSS4
1	51	ALA	-	insertion	UNP Q9RSS4
1	52	ALA	-	insertion	UNP Q9RSS4
1	53	ALA	-	insertion	UNP Q9RSS4

- Molecule 27 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	2	47	Total	C	N	O	S	0	0	0
			393	235	92	64	2			

- Molecule 28 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	3	65	Total	C	N	O	S	0	0	0
			509	320	104	80	5			

- Molecule 29 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	X	2780	Total	C	N	O	P	0	0	0
			59673	26617	11011	19265	2780			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	1526	U	UNK	conflict	GB 11612676

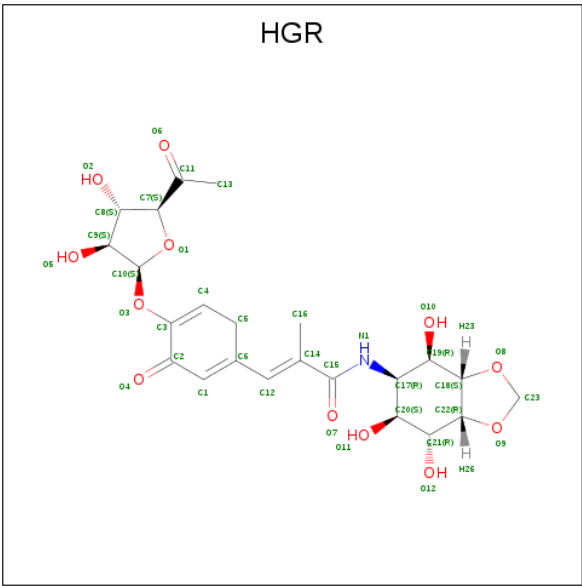
- Molecule 30 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	Y	122	Total	C	N	O	P	0	0	0
			2601	1161	476	842	122			

- Molecule 31 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
31	H	1	Total	Mg	0	0
			1	1		
31	A	1	Total	Mg	0	0
			1	1		
31	N	1	Total	Mg	0	0
			1	1		
31	X	177	Total	Mg	0	0
			177	177		
31	Y	5	Total	Mg	0	0
			5	5		
31	M	1	Total	Mg	0	0
			1	1		

- Molecule 32 is Hygromycin A (three-letter code: HGR) (formula: C₂₃H₂₉NO₁₂).

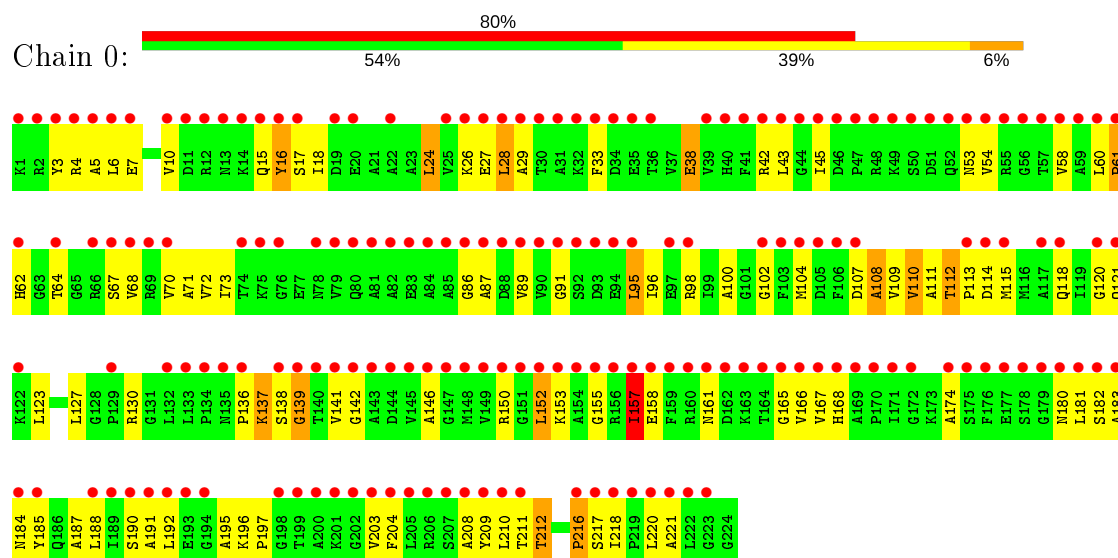


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
32	X	1	Total	C	N	O	0	0
			36	23	1	12		

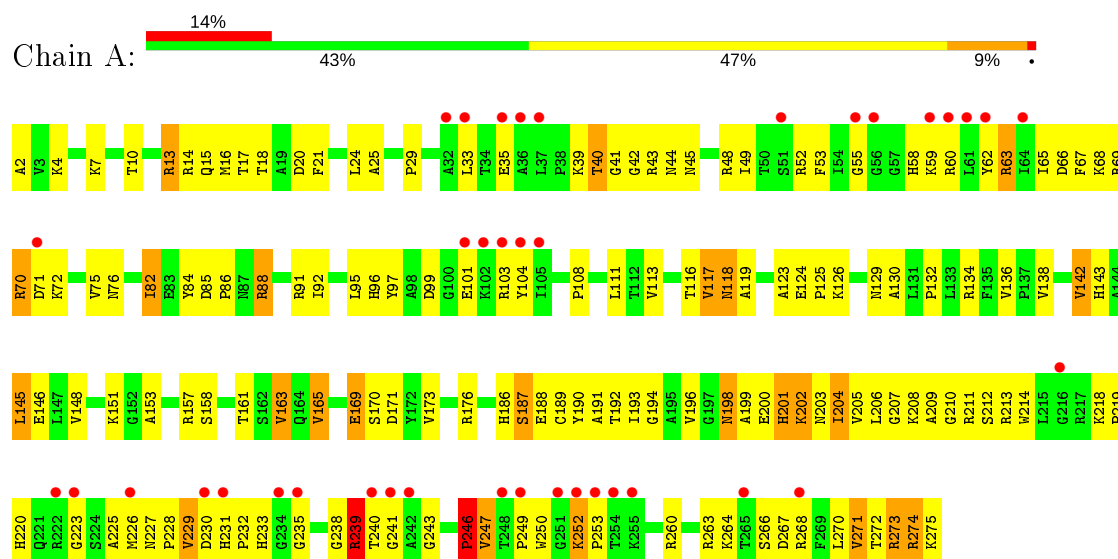
3 Residue-property plots [i](#)

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.

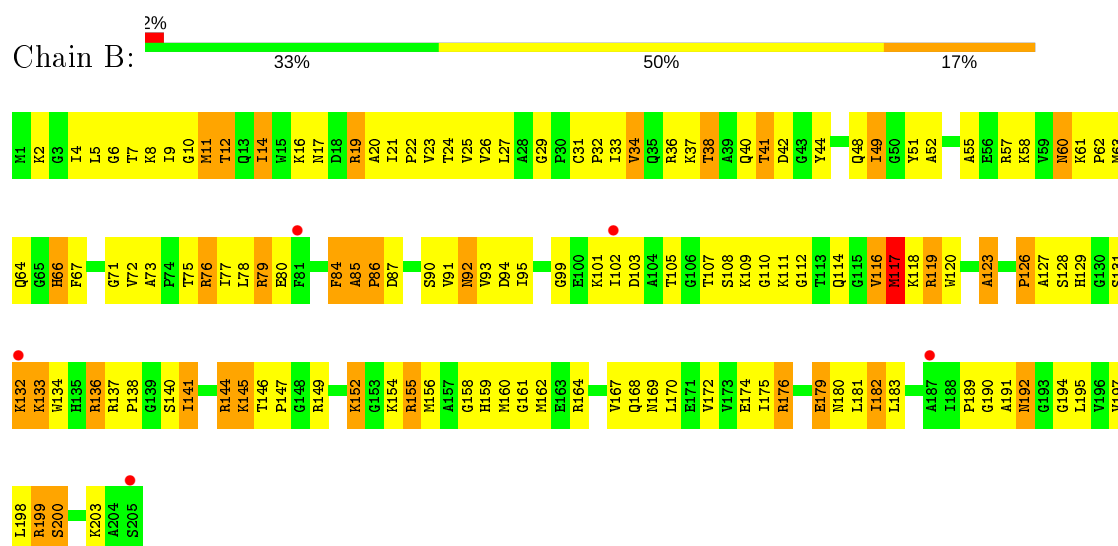
- Molecule 1: 50S ribosomal protein L1



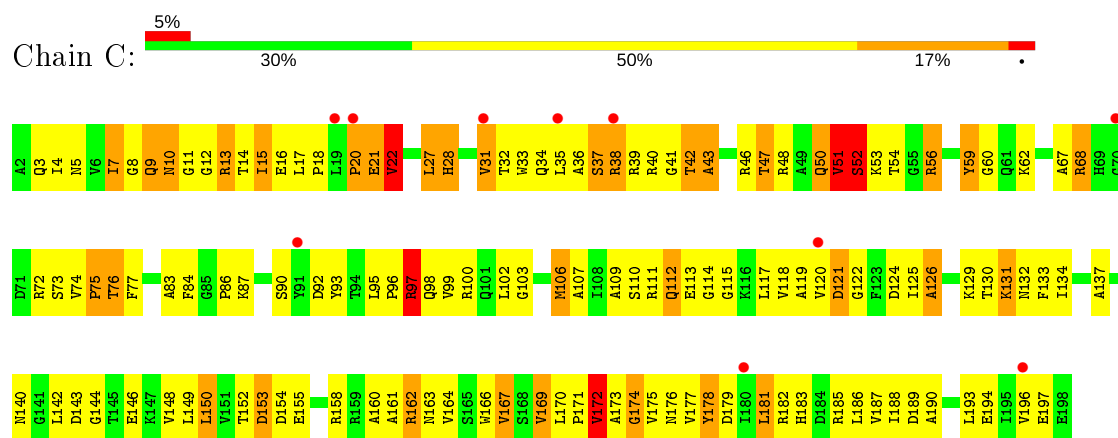
- Molecule 2: 50S ribosomal protein L2

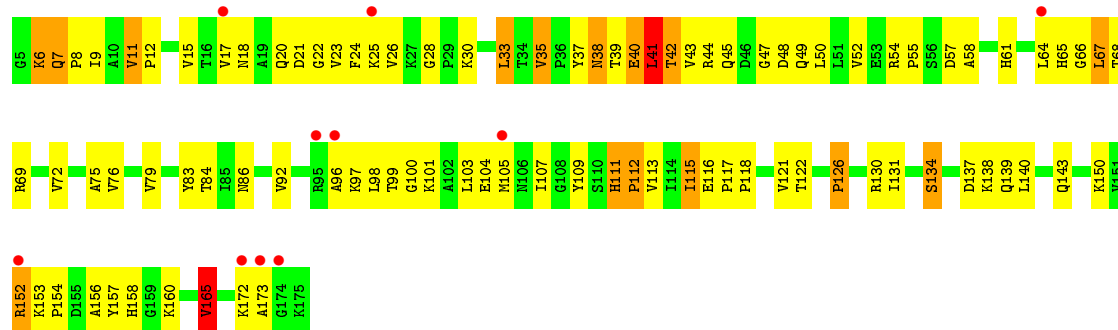


- Molecule 3: 50S ribosomal protein L3

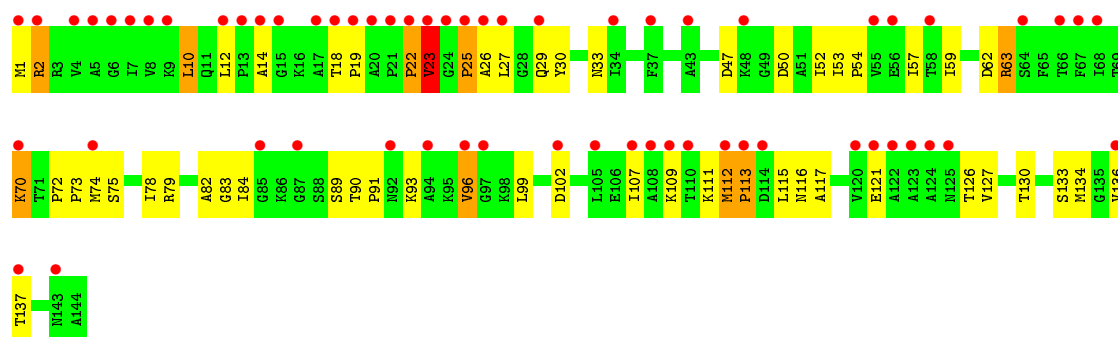
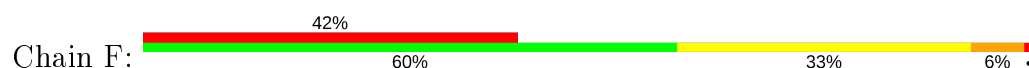


• Molecule 4: 50S ribosomal protein L4

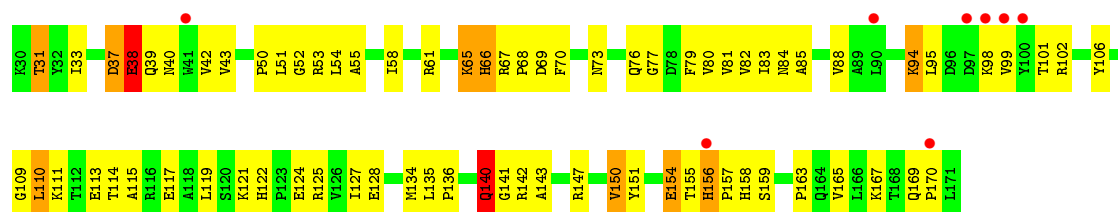




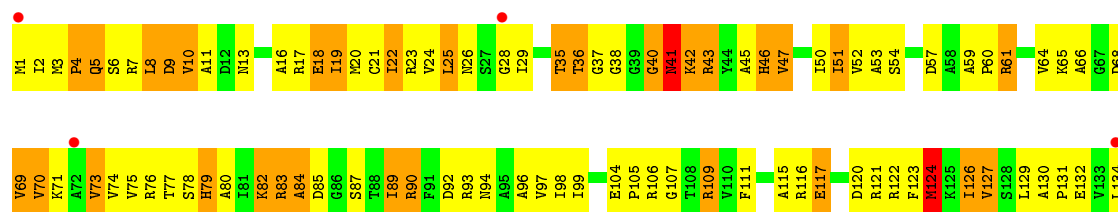
• Molecule 7: 50S ribosomal protein L11



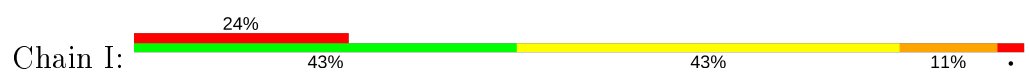
• Molecule 8: 50S ribosomal protein L13

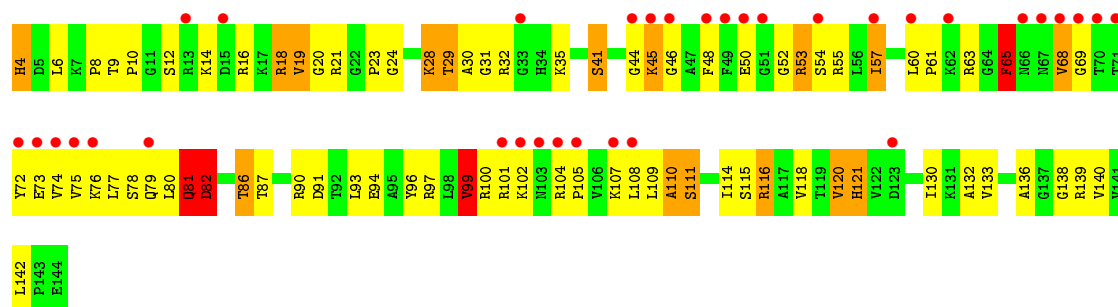


• Molecule 9: 50S ribosomal protein L14

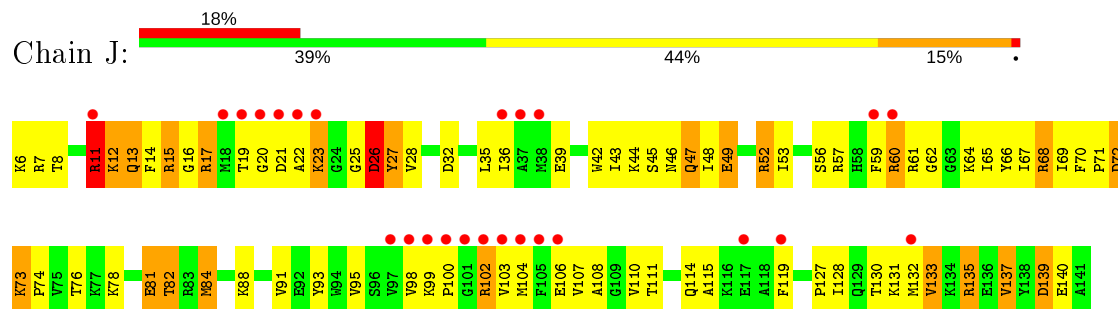


• Molecule 10: 50S ribosomal protein L15

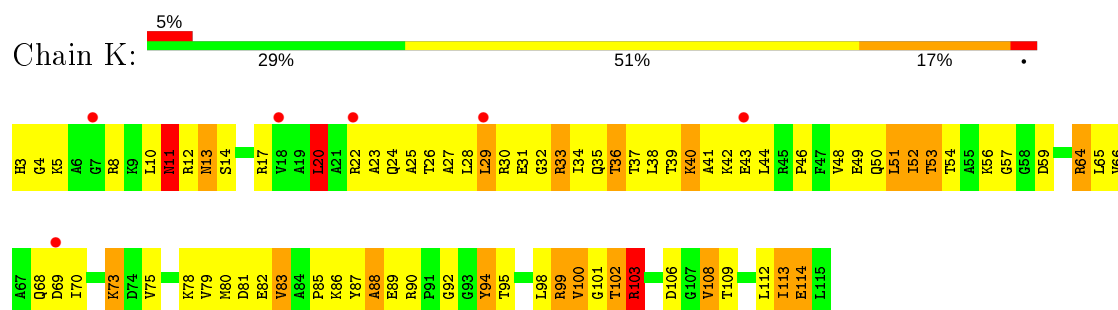




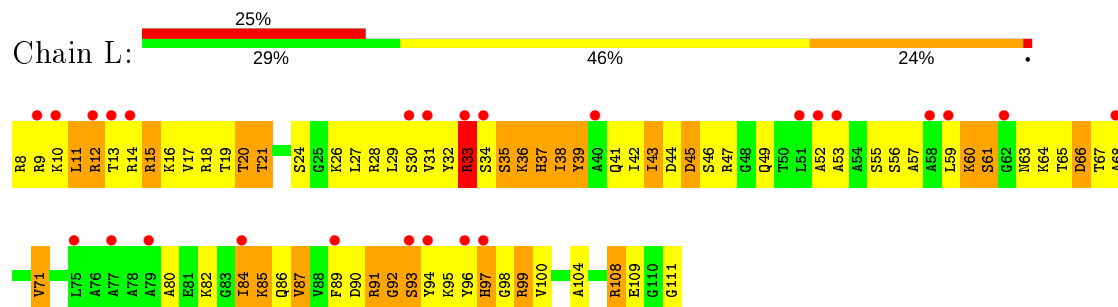
- Molecule 11: 50S ribosomal protein L16



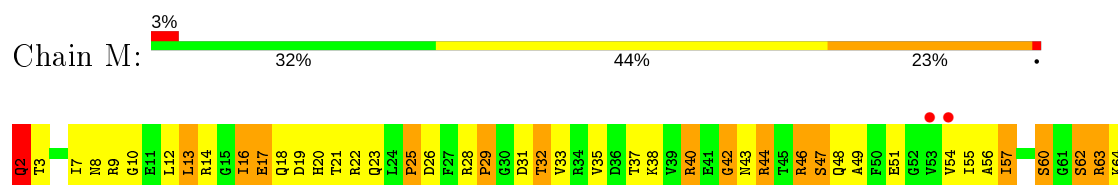
- Molecule 12: 50S ribosomal protein L17

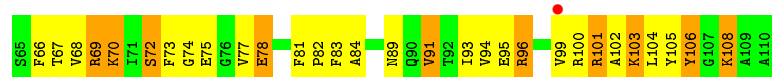


- Molecule 13: 50S ribosomal protein L18

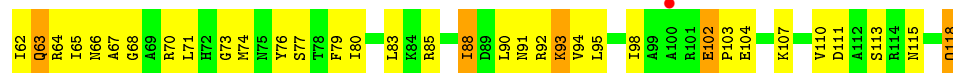


- Molecule 14: 50S ribosomal protein L19

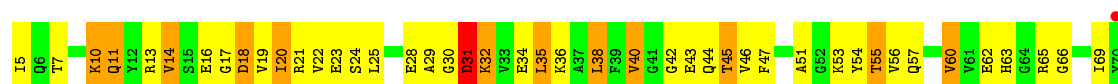




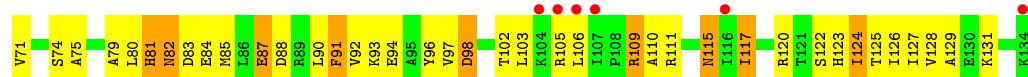
- Molecule 15: 50S ribosomal protein L20



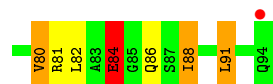
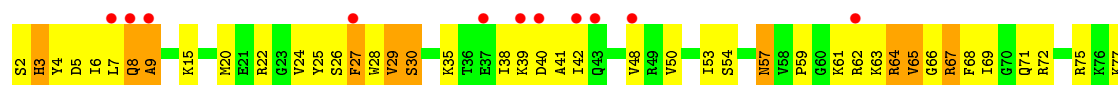
- Molecule 16: 50S ribosomal protein L21



- Molecule 17: 50S ribosomal protein L22

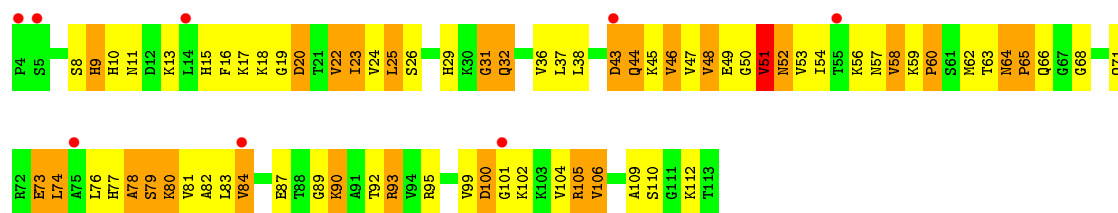


- Molecule 18: 50S ribosomal protein L23

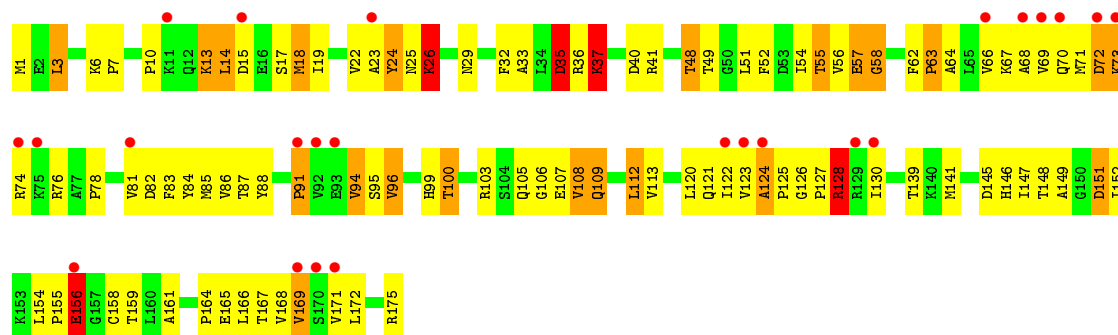


- Molecule 19: 50S ribosomal protein L24

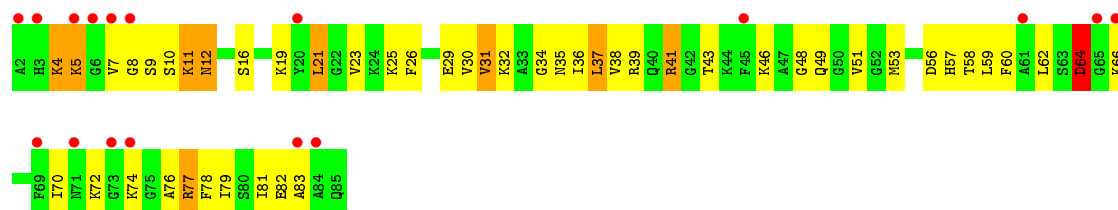




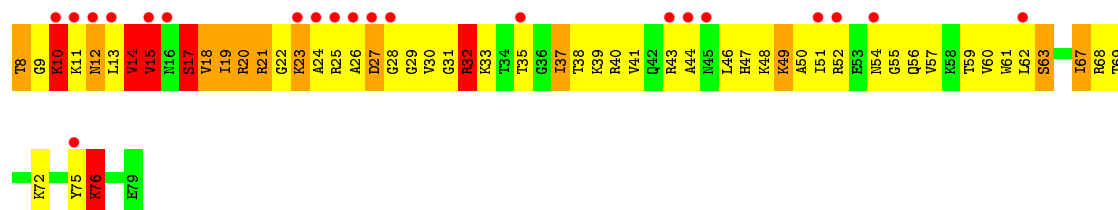
• Molecule 20: 50S ribosomal protein L25



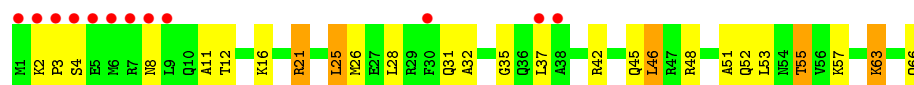
• Molecule 21: 50S ribosomal protein L27



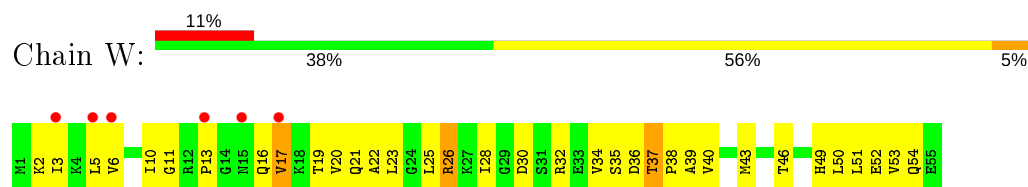
• Molecule 22: 50S ribosomal protein L28



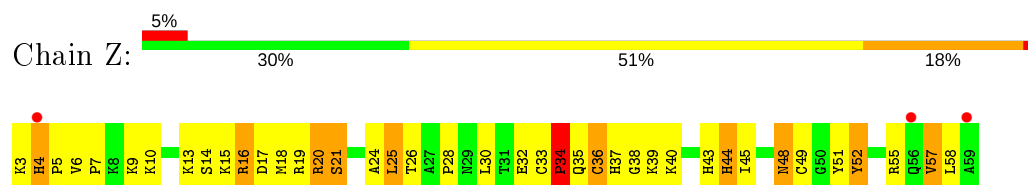
• Molecule 23: 50S ribosomal protein L29



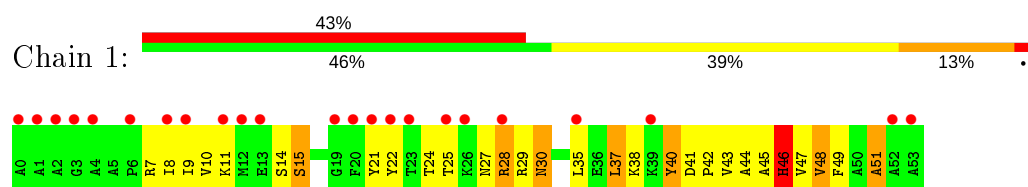
- Molecule 24: 50S ribosomal protein L30



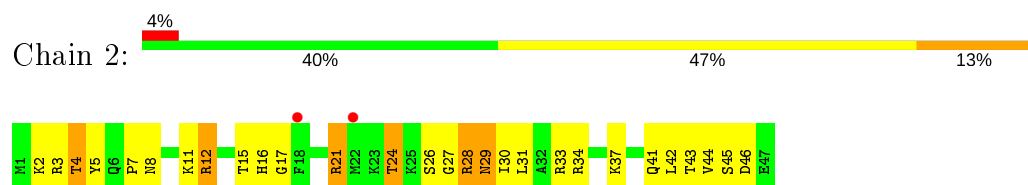
- Molecule 25: 50S ribosomal protein L32



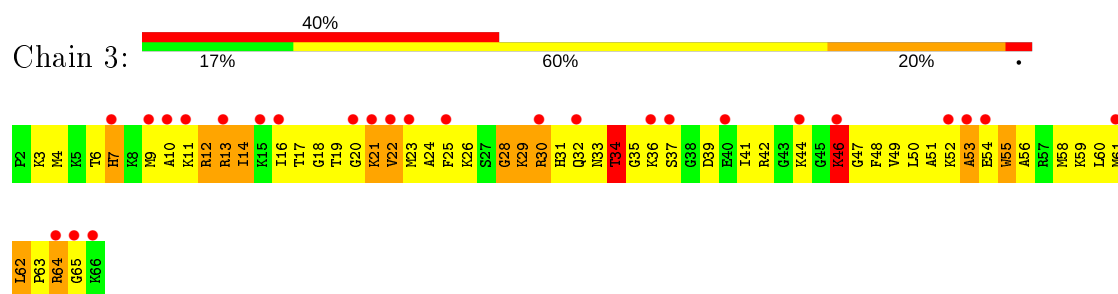
- Molecule 26: 50S ribosomal protein L33



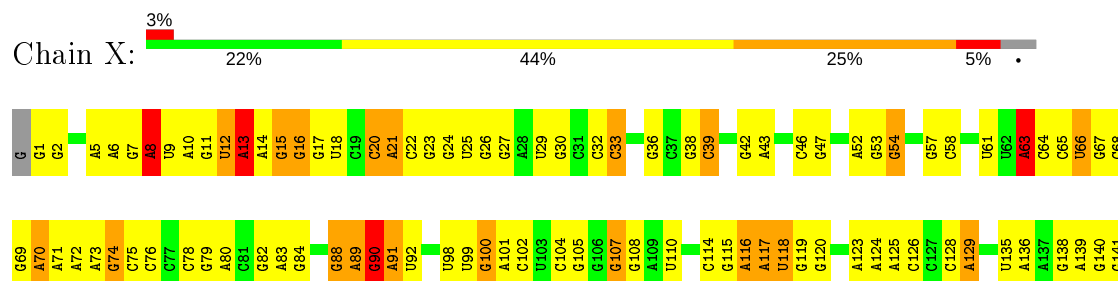
- Molecule 27: 50S ribosomal protein L34



- Molecule 28: 50S ribosomal protein L35

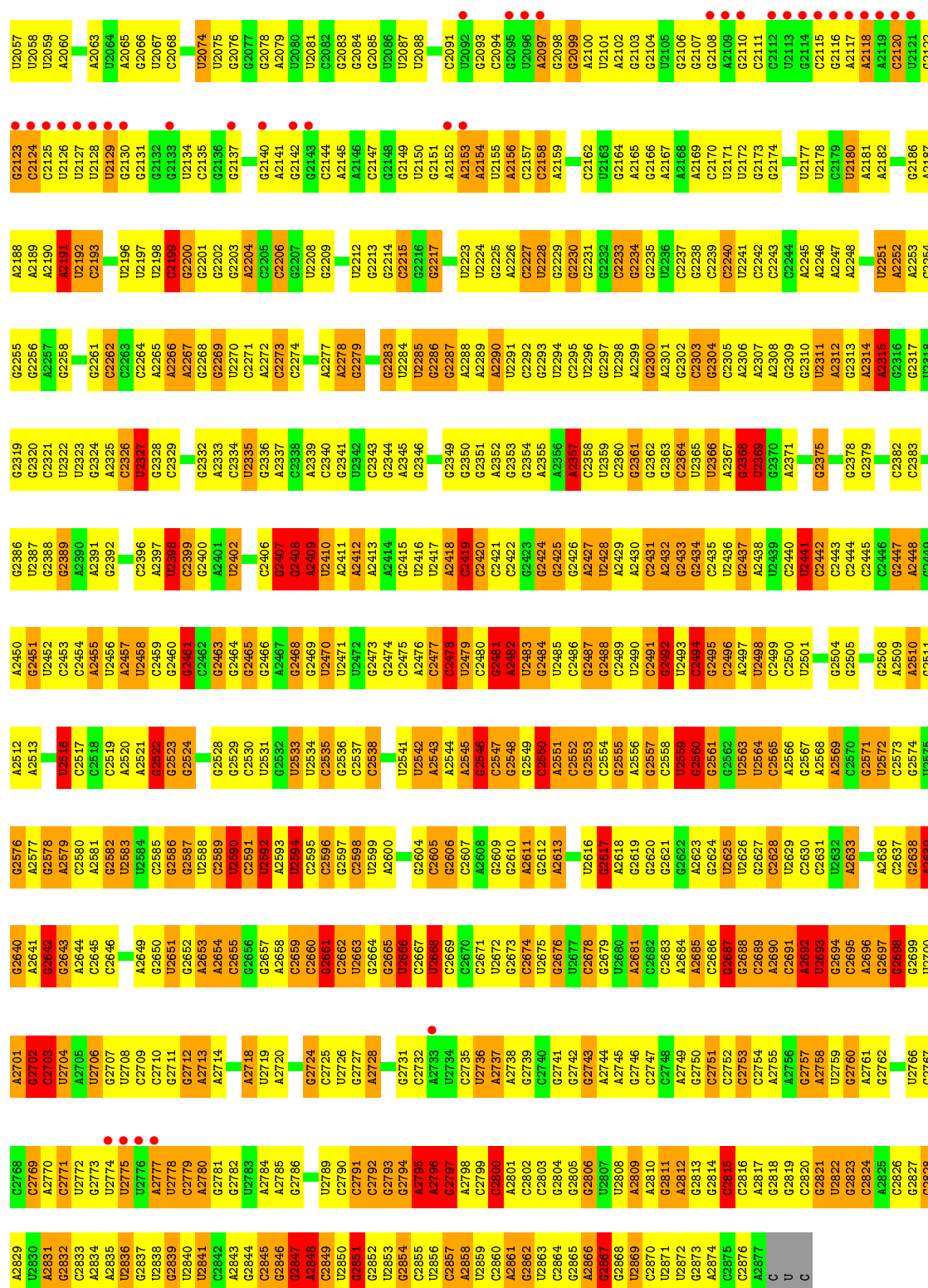


- Molecule 29: 23S ribosomal RNA

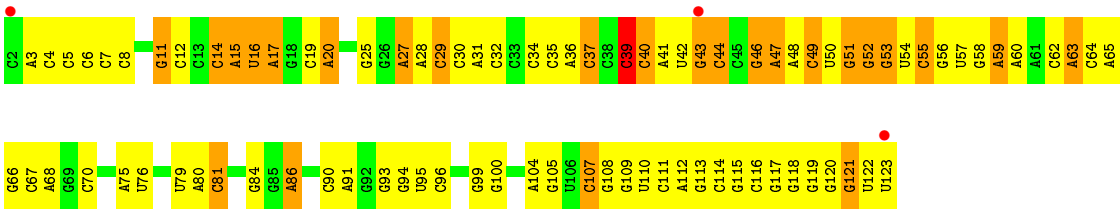


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C926	C927	A928	A929	A930	G931	G932	G933	G934	C935	A936	G937	G938	C939	G940	U941	U942	U943	A944	G945	U946	C947	C948	G949	G950	G951	A952	G953	U954	G955	A956	C957	G958	G959	U960	G961	C962	G963	A964	G965	A966	G967	C968	U969	A970	C971	C972	U973	U974	C975	C976	G980	C981	C982	C983	U984	A985	A986	G987																																																																																																																																																																																																																																																																																																																																								
U860	G861	A862	C863	C864	A865	U866	G867	U868	C869	C870	U871	G872	U873	A874	G875	G876	G877	U878	A879	C880	A881	U882	A883	A884	G885	G886	G887	G888	A889	G890	C891	A892	C893	A894	C895	A896	C897	A898	C899	A900	C901	C902	C903	C904	C905	C906	C907	C908	C909	C910	C911	C912	C913	C914	C915	U916	C917	C918	C919	C920	C921	C922	C923	C924	C925	C926	C927	C928	C929	C930	C931	C932	C933	C934	C935	C936	C937	C938	C939	C940	C941	C942	C943	C944	C945	C946	C947	C948	C949	C950	C951	C952	C953	C954	C955	C956	C957	C958	C959	C960	C961	C962	C963	C964	C965	C966	C967	C968	C969	C970	C971	C972	C973	C974	C975	C976	C977	C978	C979	C980	C981	C982	C983	C984	C985	C986	C987	C988	C989	C990	C991	C992	C993	C994	C995	C996	C997	C998	C999	C1000	C1001	C1002	C1003	C1004	C1005	C1006	C1007	C1008	C1009	C1010	C1011	C1012	C1013	C1014	C1015	C1016	C1017	C1018	C1019	C1020	C1021	C1022	C1023	C1024	C1025	C1026	C1027	C1028	C1029	C1030	C1031	C1032	C1033	C1034	C1035	C1036	C1037	C1038	C1039	C1040	C1041	C1042	C1043	C1044	C1045	C1046	C1047	C1048	C1049	C1050	C1051	C1052	C1053	C1054	C1055	C1056	C1057	C1058	C1059	C1060	C1061	C1062	C1063	C1064	C1065	C1066	C1067	C1068	C1069	C1070	C1071	C1072	C1073	C1074	C1075	C1076	C1077	C1078	C1079	C1080	C1081	C1082	C1083	C1084	C1085	C1086	C1087	C1088	C1089	C1090	C1091	C1092	C1093	C1094	C1095	C1096	C1097	C1098	C1099	C1100	C1101	C1102	C1103	C1104	C1105	C1106	C1107	C1108	C1109	C1110	C1111	C1112	C1113	C1114	C1115	C1116	C1117																																																																																																																																	
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U1999	A1802	A1869	A1803	G1736	U1530	G1460	A1386	G1317	U1257	G1190	G1120
U2000	G1803	G1737	C1606	G1738	G1533	G1461	A1391	A1318	A1258	A1192	G1121
G2001	U1804	U1738	A1607	G1534	G1533	G1462	A1392	C1319	A1259	G1193	A1122
A2002	G1805	G1739	A1608	A1535	A1534	A1463	A1393	A1320	A1260	U1194	G1123
A2003	U1806	U1741	G1609	C1535	C1535	A1464	G1393	A1321	G1261	U1195	U1124
U2004	A1807	G1742	A1610	G1539	G1539	G1465	G1394	G1322	U1262	G1196	G1125
U2005	C1808	G1743	U1611	U1540	U1540	U1466	A1395	G1323	G1263	U1197	
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G2007	U1810	G1745	U1613	G1541	G1541	U1468	G1397	G1325	C1265	U1199	A1129
C2008	A1811	A1746	G1616	G1542	G1542	U1469	G1398	U1326	G1266	G1200	U1130
U2009	U1812	G1747	G1617	G1543	G1543	U1470	G1401	U1327	G1267	U1201	U1131
G2010	A1813	U1748	U1618	A1544	A1544	G1471	G1402	U1328	U1268	U1202	C1132
U2011	G1814	G1749	A1619	G1545	G1545	A1474	U1403	U1329	G1269	A1203	G1133
A2012	G1815	A1750	C1620	U1548	U1548	U1475	C1404	G1330	C1270	G1204	C1134
A2013	A1816	A1751	G1621	C1549	C1549	U1476	A1405	G1332	C1271	G1205	C1135
A2014	U1817	U1752	G1622	C1550	C1550	U1477	A1406	G1333	C1272	G1206	G1136
G2015	G1818	A1753	C1623	U1551	U1551	U1478	G1407	A1334	G1273	G1207	A1137
A2016	U1819	G1754	A1624	U1552	U1552	U1479	A1408	A1335	C1274	A1208	A1138
U2017	G1820	G1755	A1625	G1553	G1553	U1480	U1409	G1336	C1275	G1209	A1139
G2018	A1821	C1756	C1627	G1554	G1554	U1481	U1410	G1337	U1276	G1210	U1141
C2019	U1822	C1757	A1628	A1555	A1555	U1482	C1411	G1338	G1277	G1211	
G2020	G1825	G1760	G1629	U1556	U1556	U1483	U1412	U1339	A1278	U1212	G1142
A2021	U1826	G1761	A1630	G1557	G1557	U1484	U1413	C1340	C1279	U1213	A1143
C2022	G1827	G1762	C1631	A1560	A1560	U1485	G1414	G1341	U1280		U1144
G2023	C1828	G1763	A1632	A1561	A1561	U1490	G1419	U1342	A1281	C1218	C1145
U2024	A1829	A1764	C1633	G1562	G1562	U1491	A1420	G1343	A1282	C1219	G1146
A2025	G1830	G1765	A1634	U1563	U1563	U1492	A1421	G1344	C1283	G1220	G1147
C2026	G1831	C1766	G1635	U1564	U1564	G1493	U1422	G1345	G1284	G1221	G1148
G2027	C1832	U1767	G1636	U1565	U1565	U1494	U1423	C1346	A1285	G1222	G1149
G2028	C1833	G1768	G1637	U1566	U1566	U1495	A1424	C1347	U1286	G1223	G1150
G2029	A1836	U1769	A1642	A1567	A1567	U1496	A1425	C1348	A1287	U1224	U1151
U2030	G1837	G1770	G1643	A1568	A1568	U1497	G1427	G1349	A1288	G1225	A1152
A2031	C1838	U1771	A1644	A1569	A1569	U1498	G1428	G1350	A1289	A1226	A1153
G2032	A1839	G1772	U1645	G1570	G1570	A1499	A1429	G1351	A1290		A1154
C2033	U1840	C1773	G1646	G1571	G1571	U1500	G1430	G1352	G1291	G1229	G1155
A2034	G1841	U1774	U1647	G1572	G1572	U1503	A1433	A1353	A1292	C1230	U1156
G2035	A1845	A1775	U1651	C1573	C1573	U1504	U1434	U1354	A1293	C1231	G1157
G2036	U1846	A1776	G1652	A1574	A1574	U1505	G1435	G1355	G1294	U1232	A1158
A2037	G1847	A1777	C1653	C1575	C1575	U1506	G1436	G1360	U1295	A1233	
C2038	U1848	U1778	A1654	U1578	U1578	A1507	A1437	U1365	A1297	C1234	A1162
A2040	G1850	C1779	C1655	G1579	G1579	U1508	G1438	A1366	G1298	G1235	G1163
A2041	A1851	A1782	U1656	G1580	G1580	U1509	G1439	A1367	A1299	G1236	G1164
A2042	C1852	G1783	A1657	C1581	C1581	A1510	G1440	A1368	A1300	A1237	G1165
G2043	G1853	G1784	A1658	A1582	A1582	A1511	A1441	G1369	U1301	A1238	A1166
A2044	U1854	U1785	A1659	A1583	A1583	U1512	C1442	G1370	G1302	G1240	A1167
G2045	G1855	U1786	G1660	A1585	A1585	U1513	A1445	U1371	U1303	G1241	G1168
C2046	U1856	G1788	C1661	A1586	A1586	U1514		G1372	U1304	G1242	C1169
G2047	G1857	U1789	G1662	U1591	U1591	C1517	C1449	G1374	C1305	G1243	G1174
C2048	C1858	G1790	C1663	U1592	U1592	C1518	G1450	C1375	U1306	G1244	A1175
C2049	A1859	C1791	G1664	C1593	C1593	A1523	C1451	A1378	U1307	G1245	U1176
G2050	U1860	C1792	G1665	U1594	U1594	C1524	A1452	A1379	C1308	G1246	U1177
U2051	G1861	A1793	G1666	U1595	U1595	C1525	A1453	C1380	G1309	U1247	C1178
G2052	C1862	A1794	G1667	U1600	U1600	U1526	U1454	G1381	C1310	A1250	A1179
G2053	U1863	C1795	A1667	U1601	U1601	A1527	C1455	G1382	C1311	G1253	G1185
A2054	G1864	A1796	G1668	U1602	U1602	U1528	C1456	G1383	U1312	G1254	G1186
G2055	C1865	U1797	G1669	U1733	U1733		A1457		A1314		A1187
A2056	G1866	U1799	G1670								



● Molecule 30: 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	169.82Å 411.54Å 695.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	57.02 – 3.00 59.03 – 3.00	Depositor EDS
% Data completeness (in resolution range)	91.9 (57.02-3.00) 76.2 (59.03-3.00)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.27 (at 3.01Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.284 , 0.326 0.272 , 0.317	Depositor DCC
R_{free} test set	22814 reflections (4.77%)	wwPDB-VP
Wilson B-factor (Å ²)	67.3	Xtriage
Anisotropy	0.451	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.16 , 40.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	89361	wwPDB-VP
Average B, all atoms (Å ²)	142.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.33% 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, HGR

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	0	0.25	0/1674	0.46	0/2257
2	A	0.40	0/2149	0.62	0/2890
3	B	0.66	0/1568	0.92	2/2105 (0.1%)
4	C	0.50	0/1530	0.75	0/2070
5	D	0.36	0/1420	0.59	0/1903
6	E	0.39	0/1309	0.61	0/1771
7	F	0.30	0/1067	0.55	0/1446
8	G	0.47	0/1139	0.74	0/1539
9	H	0.72	0/1007	1.02	1/1352 (0.1%)
10	I	0.49	0/1082	0.78	0/1448
11	J	0.60	0/1114	0.83	1/1486 (0.1%)
12	K	0.81	0/887	1.11	4/1188 (0.3%)
13	L	0.54	0/784	0.79	1/1045 (0.1%)
14	M	0.76	0/880	1.02	3/1179 (0.3%)
15	N	0.65	0/994	0.77	0/1323
16	O	0.54	0/751	0.75	0/1000
17	P	0.75	0/1027	0.93	0/1373
18	Q	0.46	0/738	0.63	0/988
19	R	0.58	0/836	0.87	0/1121
20	S	0.40	0/1371	0.68	0/1862
21	T	0.52	0/634	0.70	0/838
22	U	0.52	0/557	0.88	1/741 (0.1%)
23	V	0.40	0/538	0.58	0/714
24	W	0.51	0/426	0.74	0/568
25	Z	0.67	0/465	0.99	1/622 (0.2%)
26	1	0.47	0/411	0.68	0/554
27	2	0.47	0/397	0.70	0/521
28	3	0.56	0/516	0.75	0/673
29	X	0.79	28/66826 (0.0%)	1.38	1078/104247 (1.0%)
30	Y	0.61	0/2907	1.12	10/4529 (0.2%)
All	All	0.73	28/97004 (0.0%)	1.25	1102/145353 (0.8%)

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
3	B	0	1
9	H	0	1
10	I	0	1
13	L	0	1
14	M	0	2
19	R	0	1
All	All	0	7

The worst 5 of 28 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	X	774	A	N3-C4	7.61	1.39	1.34
29	X	774	A	C5-C4	7.18	1.43	1.38
29	X	1682	A	N7-C5	-6.86	1.35	1.39
29	X	1975	G	N7-C5	6.29	1.43	1.39
29	X	2823	G	N9-C8	-6.08	1.33	1.37

The worst 5 of 1102 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	X	1678	G	C8-N9-C4	14.96	112.38	106.40
29	X	1292	A	C8-N9-C4	14.80	111.72	105.80
29	X	774	A	N1-C6-N6	13.97	126.98	118.60
29	X	1679	U	C5-C6-N1	-13.00	116.20	122.70
29	X	1678	G	N7-C8-N9	-12.95	106.62	113.10

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	B	85	ALA	Peptide
9	H	36	THR	Peptide
10	I	52	GLY	Peptide
13	L	87	VAL	Peptide
14	M	2	GLN	Peptide

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	0	1651	0	1693	51	0
2	A	2107	0	2190	133	0
3	B	1540	0	1600	117	0
4	C	1507	0	1525	115	0
5	D	1401	0	1481	81	0
6	E	1287	0	1336	53	0
7	F	1048	0	1088	35	0
8	G	1115	0	1144	50	0
9	H	997	0	1046	81	0
10	I	1068	0	1103	68	0
11	J	1091	0	1125	66	0
12	K	879	0	930	79	0
13	L	778	0	820	57	0
14	M	867	0	890	64	0
15	N	978	0	1020	95	0
16	O	742	0	756	37	0
17	P	1014	0	1096	80	0
18	Q	727	0	753	31	0
19	R	826	0	881	65	0
20	S	1346	0	1372	71	0
21	T	626	0	655	38	0
22	U	553	0	604	50	0
23	V	534	0	558	13	0
24	W	424	0	470	24	0
25	Z	453	0	455	49	0
26	1	404	0	416	25	0
27	2	393	0	420	24	0
28	3	509	0	565	56	0
29	X	59673	0	30060	1967	0
30	Y	2601	0	1327	91	0
31	A	1	0	0	0	0
31	H	1	0	0	0	0
31	M	1	0	0	0	0
31	N	1	0	0	0	0
31	X	177	0	0	1	0
31	Y	5	0	0	0	0
32	X	36	0	29	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	89361	0	59408	3326	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 23.

The worst 5 of 3326 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)
3:B:14:ILE:HB	14:M:20:HIS:HD2	1.16	1.11
12:K:79:VAL:HA	12:K:83:VAL:HG13	1.35	1.06
29:X:1225:G:H1'	29:X:1250:A:H61	1.21	1.03
29:X:517:A:H5''	29:X:518:A:H5'	1.37	1.02
29:X:2690:A:OP1	29:X:2692:A:OP2	1.78	0.99

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	
1	0	222/224 (99%)	139 (63%)	58 (26%)	25 (11%)	0	2
2	A	272/274 (99%)	206 (76%)	50 (18%)	16 (6%)	1	9
3	B	203/205 (99%)	152 (75%)	33 (16%)	18 (9%)	1	3
4	C	195/197 (99%)	123 (63%)	50 (26%)	22 (11%)	0	2
5	D	175/177 (99%)	117 (67%)	42 (24%)	16 (9%)	1	3
6	E	169/171 (99%)	119 (70%)	33 (20%)	17 (10%)	0	2
7	F	142/144 (99%)	100 (70%)	27 (19%)	15 (11%)	0	2
8	G	140/142 (99%)	111 (79%)	19 (14%)	10 (7%)	1	5
9	H	132/134 (98%)	96 (73%)	18 (14%)	18 (14%)	0	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	I	139/141 (99%)	93 (67%)	30 (22%)	16 (12%)	0	2
11	J	134/136 (98%)	97 (72%)	28 (21%)	9 (7%)	1	6
12	K	111/113 (98%)	81 (73%)	18 (16%)	12 (11%)	0	2
13	L	102/104 (98%)	68 (67%)	18 (18%)	16 (16%)	0	1
14	M	107/109 (98%)	83 (78%)	14 (13%)	10 (9%)	0	3
15	N	115/117 (98%)	90 (78%)	19 (16%)	6 (5%)	2	12
16	O	92/94 (98%)	69 (75%)	13 (14%)	10 (11%)	0	2
17	P	125/127 (98%)	102 (82%)	17 (14%)	6 (5%)	2	13
18	Q	91/93 (98%)	67 (74%)	16 (18%)	8 (9%)	1	3
19	R	108/110 (98%)	63 (58%)	28 (26%)	17 (16%)	0	1
20	S	173/175 (99%)	123 (71%)	32 (18%)	18 (10%)	0	2
21	T	82/84 (98%)	68 (83%)	8 (10%)	6 (7%)	1	5
22	U	70/72 (97%)	39 (56%)	15 (21%)	16 (23%)	0	0
23	V	64/66 (97%)	54 (84%)	9 (14%)	1 (2%)	9	40
24	W	53/55 (96%)	36 (68%)	13 (24%)	4 (8%)	1	5
25	Z	55/57 (96%)	36 (66%)	13 (24%)	6 (11%)	0	2
26	1	52/54 (96%)	31 (60%)	13 (25%)	8 (15%)	0	1
27	2	45/47 (96%)	38 (84%)	6 (13%)	1 (2%)	6	31
28	3	63/65 (97%)	38 (60%)	17 (27%)	8 (13%)	0	1
All	All	3431/3487 (98%)	2439 (71%)	657 (19%)	335 (10%)	0	2

5 of 335 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	0	17	SER
1	0	61	PRO
1	0	157	ILE
1	0	216	PRO
2	A	25	ALA

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	
1	0	167/167 (100%)	150 (90%)	17 (10%)	7	28
2	A	214/214 (100%)	177 (83%)	37 (17%)	2	10
3	B	155/155 (100%)	123 (79%)	32 (21%)	1	6
4	C	157/157 (100%)	117 (74%)	40 (26%)	0	3
5	D	153/153 (100%)	126 (82%)	27 (18%)	2	10
6	E	136/136 (100%)	111 (82%)	25 (18%)	1	9
7	F	107/107 (100%)	94 (88%)	13 (12%)	5	21
8	G	118/118 (100%)	97 (82%)	21 (18%)	2	9
9	H	103/103 (100%)	73 (71%)	30 (29%)	0	2
10	I	108/108 (100%)	88 (82%)	20 (18%)	1	8
11	J	110/110 (100%)	82 (74%)	28 (26%)	0	3
12	K	90/90 (100%)	68 (76%)	22 (24%)	0	3
13	L	74/74 (100%)	46 (62%)	28 (38%)	0	0
14	M	92/92 (100%)	58 (63%)	34 (37%)	0	0
15	N	96/96 (100%)	82 (85%)	14 (15%)	3	15
16	O	75/75 (100%)	59 (79%)	16 (21%)	1	5
17	P	109/109 (100%)	85 (78%)	24 (22%)	1	4
18	Q	75/75 (100%)	57 (76%)	18 (24%)	0	3
19	R	91/91 (100%)	71 (78%)	20 (22%)	1	4
20	S	149/149 (100%)	119 (80%)	30 (20%)	1	6
21	T	62/62 (100%)	42 (68%)	20 (32%)	0	1
22	U	57/57 (100%)	38 (67%)	19 (33%)	0	1
23	V	54/54 (100%)	45 (83%)	9 (17%)	2	11
24	W	48/48 (100%)	38 (79%)	10 (21%)	1	5
25	Z	51/51 (100%)	43 (84%)	8 (16%)	2	13
26	1	38/38 (100%)	33 (87%)	5 (13%)	4	18
27	2	40/40 (100%)	32 (80%)	8 (20%)	1	7
28	3	51/51 (100%)	34 (67%)	17 (33%)	0	1
All	All	2780/2780 (100%)	2188 (79%)	592 (21%)	1	5

5 of 592 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	J	27	TYR
13	L	82	LYS
24	W	26	ARG
11	J	64	LYS
12	K	59	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
7	F	11	GLN
13	L	37	HIS
23	V	52	GLN
6	E	139	GLN
26	1	30	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
29	X	2776/2881 (96%)	839 (30%)	30 (1%)
30	Y	121/122 (99%)	35 (28%)	1 (0%)
All	All	2897/3003 (96%)	874 (30%)	31 (1%)

5 of 874 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
29	X	8	A
29	X	13	A
29	X	15	G
29	X	54	G
29	X	63	A

5 of 31 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
29	X	1506	C
29	X	1602	G
29	X	2823	G
29	X	1526	U
29	X	1690	U

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 187 ligands modelled in this entry, 186 are monoatomic - leaving 1 for Mogul analysis.

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	$\# Z > 2$
32	HGR	X	6178	-	39,39,39	1.81	7 (17%)	50,58,58	1.72	9 (18%)

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
32	HGR	X	6178	-	-	4/20/79/79	0/4/4/4

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	X	6178	HGR	C5-C6	-4.19	1.42	1.50
32	X	6178	HGR	C1-C6	4.15	1.41	1.35
32	X	6178	HGR	C12-C14	4.14	1.43	1.33
32	X	6178	HGR	C12-C6	3.87	1.55	1.44
32	X	6178	HGR	C3-C2	-3.78	1.41	1.48

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	X	6178	HGR	C10-O3-C3	4.73	126.09	115.36
32	X	6178	HGR	C4-C5-C6	4.24	121.49	112.36
32	X	6178	HGR	C23-O8-C18	-4.00	100.22	106.31
32	X	6178	HGR	C4-C3-C2	-3.98	118.17	121.83
32	X	6178	HGR	O3-C3-C2	3.09	118.43	112.56

There are no chirality outliers.

All (4) torsion outliers are listed below:

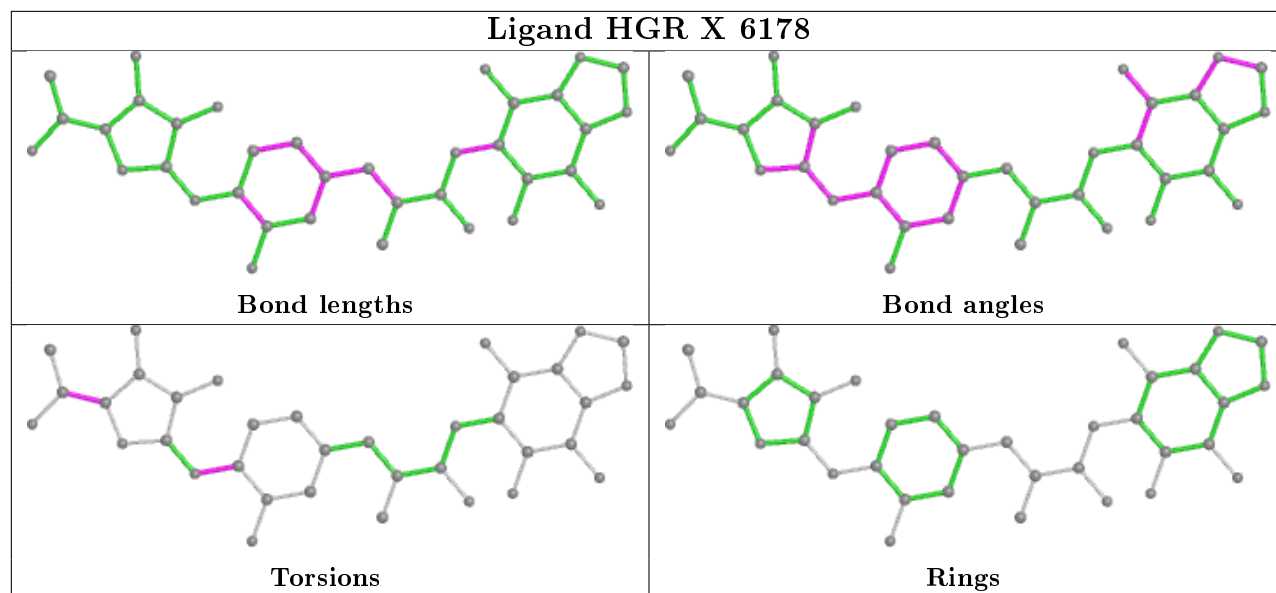
Mol	Chain	Res	Type	Atoms
32	X	6178	HGR	C2-C3-O3-C10
32	X	6178	HGR	C13-C11-C7-O1
32	X	6178	HGR	C13-C11-C7-C8
32	X	6178	HGR	O6-C11-C7-C8

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	X	6178	HGR	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	0	224/224 (100%)	4.90	179 (79%) 0 0	291, 311, 319, 322	0
2	A	274/274 (100%)	0.62	39 (14%) 2 1	108, 151, 172, 185	0
3	B	205/205 (100%)	0.04	5 (2%) 59 30	67, 102, 129, 146	0
4	C	197/197 (100%)	0.12	10 (5%) 28 10	93, 133, 158, 177	0
5	D	177/177 (100%)	0.30	14 (7%) 12 4	165, 183, 200, 214	0
6	E	171/171 (100%)	0.09	10 (5%) 23 7	116, 167, 191, 198	0
7	F	144/144 (100%)	2.34	61 (42%) 0 0	233, 259, 275, 281	0
8	G	142/142 (100%)	0.28	8 (5%) 24 8	87, 125, 139, 169	0
9	H	134/134 (100%)	-0.10	4 (2%) 50 22	70, 92, 108, 118	0
10	I	141/141 (100%)	1.05	34 (24%) 0 0	98, 150, 173, 182	0
11	J	136/136 (100%)	0.94	25 (18%) 1 0	107, 126, 156, 159	0
12	K	113/113 (100%)	0.22	6 (5%) 26 10	63, 82, 95, 99	0
13	L	104/104 (100%)	1.12	26 (25%) 0 0	126, 147, 162, 173	0
14	M	109/109 (100%)	-0.06	3 (2%) 53 25	72, 89, 117, 147	0
15	N	117/117 (100%)	0.36	10 (8%) 10 3	90, 118, 144, 153	0
16	O	94/94 (100%)	-0.28	6 (6%) 19 6	103, 129, 156, 173	0
17	P	127/127 (100%)	0.16	6 (4%) 31 11	81, 96, 120, 180	0
18	Q	93/93 (100%)	0.59	12 (12%) 3 1	108, 137, 160, 176	0
19	R	110/110 (100%)	0.37	8 (7%) 15 4	111, 131, 166, 180	0
20	S	175/175 (100%)	0.48	24 (13%) 3 1	134, 167, 185, 193	0
21	T	84/84 (100%)	1.16	17 (20%) 1 0	111, 130, 148, 171	0
22	U	72/72 (100%)	1.51	21 (29%) 0 0	134, 163, 177, 182	0
23	V	66/66 (100%)	0.82	12 (18%) 1 0	147, 163, 190, 201	0
24	W	55/55 (100%)	0.66	6 (10%) 5 2	112, 124, 142, 157	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	Z	57/57 (100%)	0.05	3 (5%) 26 10	82, 97, 120, 130	0
26	1	54/54 (100%)	1.72	23 (42%) 0 0	140, 153, 179, 189	0
27	2	47/47 (100%)	0.17	2 (4%) 35 13	108, 121, 132, 134	0
28	3	65/65 (100%)	1.63	26 (40%) 0 0	115, 132, 143, 153	0
29	X	2780/2881 (96%)	-0.16	79 (2%) 53 25	59, 127, 241, 397	0
30	Y	122/122 (100%)	-0.36	3 (2%) 57 29	110, 157, 182, 203	0
All	All	6389/6490 (98%)	0.37	682 (10%) 6 2	59, 134, 276, 397	0

The worst 5 of 682 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	0	204	PHE	18.3
1	0	200	ALA	18.1
1	0	205	LEU	17.5
1	0	85	ALA	15.5
1	0	47	PRO	15.3

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

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

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(Å ²)	Q<0.9
31	MG	X	6101	1/1	0.05	1.26	138,138,138,138	0
31	MG	X	6135	1/1	0.44	1.17	129,129,129,129	0
31	MG	X	6140	1/1	0.45	0.42	97,97,97,97	0
31	MG	X	6103	1/1	0.49	0.23	126,126,126,126	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
31	MG	X	6168	1/1	0.55	0.67	100,100,100,100	0
31	MG	X	6152	1/1	0.57	0.30	158,158,158,158	0
31	MG	X	6099	1/1	0.58	0.86	120,120,120,120	0
31	MG	X	6118	1/1	0.62	0.41	82,82,82,82	0
31	MG	X	6114	1/1	0.62	0.70	93,93,93,93	0
31	MG	X	6093	1/1	0.66	0.34	96,96,96,96	0
31	MG	X	6124	1/1	0.68	0.58	100,100,100,100	0
31	MG	X	6161	1/1	0.69	0.23	113,113,113,113	0
31	MG	X	6176	1/1	0.69	0.55	73,73,73,73	0
31	MG	X	6111	1/1	0.71	0.41	98,98,98,98	0
31	MG	X	6139	1/1	0.71	0.42	113,113,113,113	0
31	MG	X	6112	1/1	0.72	0.33	80,80,80,80	0
31	MG	X	6125	1/1	0.72	0.49	109,109,109,109	0
31	MG	X	6051	1/1	0.73	0.54	83,83,83,83	0
31	MG	A	301	1/1	0.73	0.35	108,108,108,108	0
31	MG	X	6174	1/1	0.74	0.30	117,117,117,117	0
31	MG	X	6163	1/1	0.74	0.34	82,82,82,82	0
31	MG	X	6160	1/1	0.74	0.72	108,108,108,108	0
31	MG	X	6076	1/1	0.74	0.55	73,73,73,73	0
31	MG	X	6149	1/1	0.75	0.40	99,99,99,99	0
31	MG	Y	205	1/1	0.75	0.64	123,123,123,123	0
31	MG	X	6035	1/1	0.76	0.46	80,80,80,80	0
31	MG	X	6162	1/1	0.76	0.76	104,104,104,104	0
31	MG	N	201	1/1	0.77	0.38	74,74,74,74	0
31	MG	X	6006	1/1	0.78	0.56	70,70,70,70	0
31	MG	X	6169	1/1	0.78	0.48	91,91,91,91	0
31	MG	X	6049	1/1	0.78	0.40	91,91,91,91	0
31	MG	X	6172	1/1	0.78	0.34	88,88,88,88	0
31	MG	X	6116	1/1	0.78	0.67	99,99,99,99	0
31	MG	X	6159	1/1	0.79	1.13	109,109,109,109	0
31	MG	X	6141	1/1	0.79	0.38	87,87,87,87	0
31	MG	X	6127	1/1	0.80	0.62	81,81,81,81	0
31	MG	X	6150	1/1	0.80	0.46	97,97,97,97	0
31	MG	X	6075	1/1	0.80	0.26	85,85,85,85	0
31	MG	Y	203	1/1	0.80	0.76	96,96,96,96	0
31	MG	X	6131	1/1	0.80	0.39	80,80,80,80	0
31	MG	X	6090	1/1	0.80	0.46	72,72,72,72	0
31	MG	X	6052	1/1	0.81	0.43	86,86,86,86	0
31	MG	X	6014	1/1	0.81	0.47	99,99,99,99	0
31	MG	X	6070	1/1	0.81	0.47	69,69,69,69	0
31	MG	X	6078	1/1	0.81	0.36	89,89,89,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
31	MG	Y	201	1/1	0.81	0.41	96,96,96,96	0
31	MG	X	6144	1/1	0.81	0.26	132,132,132,132	0
31	MG	X	6133	1/1	0.81	0.48	91,91,91,91	0
31	MG	X	6173	1/1	0.82	0.14	87,87,87,87	0
31	MG	X	6030	1/1	0.82	0.33	101,101,101,101	0
31	MG	X	6003	1/1	0.82	0.31	72,72,72,72	0
31	MG	X	6085	1/1	0.82	0.41	66,66,66,66	0
31	MG	X	6156	1/1	0.82	0.25	91,91,91,91	0
31	MG	X	6155	1/1	0.82	0.79	108,108,108,108	0
31	MG	X	6170	1/1	0.83	0.37	97,97,97,97	0
31	MG	X	6061	1/1	0.83	0.23	100,100,100,100	0
31	MG	X	6015	1/1	0.83	0.27	74,74,74,74	0
31	MG	X	6047	1/1	0.83	0.25	79,79,79,79	0
31	MG	X	6020	1/1	0.83	0.44	76,76,76,76	0
31	MG	X	6033	1/1	0.83	0.69	76,76,76,76	0
31	MG	X	6087	1/1	0.83	0.62	85,85,85,85	0
31	MG	X	6022	1/1	0.84	0.58	92,92,92,92	0
31	MG	X	6137	1/1	0.84	0.47	136,136,136,136	0
31	MG	X	6074	1/1	0.84	0.39	89,89,89,89	0
31	MG	X	6002	1/1	0.85	0.32	91,91,91,91	0
31	MG	X	6148	1/1	0.85	0.31	104,104,104,104	0
31	MG	X	6064	1/1	0.85	0.48	77,77,77,77	0
31	MG	X	6171	1/1	0.85	0.32	118,118,118,118	0
31	MG	X	6046	1/1	0.85	0.58	76,76,76,76	0
31	MG	X	6079	1/1	0.86	0.33	99,99,99,99	0
31	MG	X	6058	1/1	0.86	0.34	70,70,70,70	0
31	MG	X	6017	1/1	0.86	0.45	54,54,54,54	0
31	MG	X	6130	1/1	0.86	0.41	132,132,132,132	0
31	MG	X	6042	1/1	0.86	1.02	96,96,96,96	0
31	MG	X	6062	1/1	0.86	0.72	87,87,87,87	0
31	MG	X	6175	1/1	0.86	0.54	121,121,121,121	0
31	MG	X	6012	1/1	0.86	0.24	78,78,78,78	0
31	MG	X	6164	1/1	0.86	0.23	86,86,86,86	0
31	MG	X	6045	1/1	0.87	0.72	94,94,94,94	0
31	MG	X	6158	1/1	0.87	0.20	76,76,76,76	0
31	MG	X	6065	1/1	0.87	0.28	93,93,93,93	0
31	MG	X	6126	1/1	0.88	0.41	114,114,114,114	0
31	MG	X	6098	1/1	0.88	0.20	71,71,71,71	0
31	MG	X	6091	1/1	0.88	0.27	72,72,72,72	0
31	MG	X	6120	1/1	0.88	0.27	78,78,78,78	0
31	MG	X	6083	1/1	0.88	0.28	83,83,83,83	0
31	MG	X	6153	1/1	0.88	0.30	114,114,114,114	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
31	MG	Y	204	1/1	0.88	0.59	116,116,116,116	0
31	MG	X	6165	1/1	0.89	0.44	88,88,88,88	0
31	MG	X	6146	1/1	0.89	0.15	125,125,125,125	0
31	MG	X	6001	1/1	0.89	0.72	67,67,67,67	0
31	MG	X	6037	1/1	0.89	0.40	65,65,65,65	0
31	MG	X	6071	1/1	0.89	0.34	99,99,99,99	0
31	MG	H	201	1/1	0.89	0.14	104,104,104,104	0
31	MG	X	6011	1/1	0.90	0.39	104,104,104,104	0
31	MG	X	6097	1/1	0.90	0.52	122,122,122,122	0
31	MG	X	6117	1/1	0.90	0.42	130,130,130,130	0
31	MG	X	6105	1/1	0.90	0.40	86,86,86,86	0
31	MG	X	6154	1/1	0.90	0.66	96,96,96,96	0
31	MG	X	6039	1/1	0.90	0.39	79,79,79,79	0
32	HGR	X	6178	36/36	0.90	0.24	79,99,109,111	0
31	MG	X	6177	1/1	0.90	0.49	125,125,125,125	0
31	MG	X	6122	1/1	0.90	0.36	84,84,84,84	0
31	MG	X	6100	1/1	0.90	0.42	111,111,111,111	0
31	MG	X	6059	1/1	0.90	0.24	88,88,88,88	0
31	MG	X	6167	1/1	0.90	1.06	97,97,97,97	0
31	MG	X	6157	1/1	0.90	0.56	96,96,96,96	0
31	MG	X	6129	1/1	0.90	0.45	89,89,89,89	0
31	MG	X	6115	1/1	0.91	0.30	133,133,133,133	0
31	MG	X	6025	1/1	0.91	0.65	76,76,76,76	0
31	MG	X	6029	1/1	0.91	0.40	82,82,82,82	0
31	MG	X	6119	1/1	0.91	0.41	89,89,89,89	0
31	MG	X	6069	1/1	0.91	0.34	65,65,65,65	0
31	MG	X	6041	1/1	0.91	0.41	64,64,64,64	0
31	MG	X	6110	1/1	0.91	0.21	84,84,84,84	0
31	MG	X	6142	1/1	0.91	0.56	106,106,106,106	0
31	MG	X	6010	1/1	0.91	0.49	64,64,64,64	0
31	MG	Y	202	1/1	0.92	0.17	130,130,130,130	0
31	MG	X	6108	1/1	0.92	0.52	108,108,108,108	0
31	MG	X	6060	1/1	0.92	0.65	80,80,80,80	0
31	MG	X	6013	1/1	0.92	0.49	76,76,76,76	0
31	MG	X	6092	1/1	0.92	0.72	97,97,97,97	0
31	MG	X	6132	1/1	0.92	0.56	84,84,84,84	0
31	MG	X	6056	1/1	0.92	0.32	81,81,81,81	0
31	MG	X	6077	1/1	0.92	0.56	80,80,80,80	0
31	MG	X	6028	1/1	0.92	0.30	75,75,75,75	0
31	MG	X	6107	1/1	0.92	0.22	76,76,76,76	0
31	MG	X	6096	1/1	0.93	0.33	99,99,99,99	0
31	MG	X	6019	1/1	0.93	0.48	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
31	MG	X	6068	1/1	0.93	0.38	111,111,111,111	0
31	MG	X	6138	1/1	0.93	0.15	86,86,86,86	0
31	MG	X	6104	1/1	0.93	0.54	89,89,89,89	0
31	MG	X	6121	1/1	0.93	0.60	85,85,85,85	0
31	MG	X	6147	1/1	0.93	1.06	93,93,93,93	0
31	MG	X	6106	1/1	0.93	0.50	100,100,100,100	0
31	MG	X	6044	1/1	0.93	0.42	66,66,66,66	0
31	MG	X	6123	1/1	0.93	0.55	89,89,89,89	0
31	MG	X	6043	1/1	0.93	0.39	106,106,106,106	0
31	MG	X	6073	1/1	0.93	0.30	105,105,105,105	0
31	MG	X	6095	1/1	0.93	0.58	78,78,78,78	0
31	MG	X	6066	1/1	0.93	0.39	105,105,105,105	0
31	MG	X	6166	1/1	0.93	0.12	76,76,76,76	0
31	MG	X	6084	1/1	0.94	0.29	124,124,124,124	0
31	MG	X	6080	1/1	0.94	0.69	82,82,82,82	0
31	MG	X	6151	1/1	0.94	0.16	88,88,88,88	0
31	MG	X	6134	1/1	0.94	0.12	100,100,100,100	0
31	MG	X	6036	1/1	0.94	0.35	70,70,70,70	0
31	MG	X	6027	1/1	0.94	0.72	65,65,65,65	0
31	MG	X	6089	1/1	0.94	0.27	89,89,89,89	0
31	MG	X	6021	1/1	0.94	0.26	91,91,91,91	0
31	MG	X	6082	1/1	0.94	0.68	105,105,105,105	0
31	MG	X	6145	1/1	0.94	0.39	84,84,84,84	0
31	MG	X	6094	1/1	0.94	0.37	95,95,95,95	0
31	MG	X	6034	1/1	0.94	0.27	69,69,69,69	0
31	MG	X	6113	1/1	0.94	0.59	143,143,143,143	0
31	MG	X	6031	1/1	0.94	0.61	85,85,85,85	0
31	MG	X	6009	1/1	0.94	0.31	50,50,50,50	0
31	MG	M	201	1/1	0.94	0.67	71,71,71,71	0
31	MG	X	6040	1/1	0.94	0.54	63,63,63,63	0
31	MG	X	6109	1/1	0.94	0.36	92,92,92,92	0
31	MG	X	6048	1/1	0.95	0.57	66,66,66,66	0
31	MG	X	6038	1/1	0.95	0.08	82,82,82,82	0
31	MG	X	6053	1/1	0.95	0.36	85,85,85,85	0
31	MG	X	6136	1/1	0.95	0.68	84,84,84,84	0
31	MG	X	6032	1/1	0.95	0.36	86,86,86,86	0
31	MG	X	6018	1/1	0.95	0.78	86,86,86,86	0
31	MG	X	6008	1/1	0.95	0.26	58,58,58,58	0
31	MG	X	6024	1/1	0.95	0.37	100,100,100,100	0
31	MG	X	6102	1/1	0.95	0.30	98,98,98,98	0
31	MG	X	6057	1/1	0.95	0.68	92,92,92,92	0
31	MG	X	6016	1/1	0.96	0.35	74,74,74,74	0

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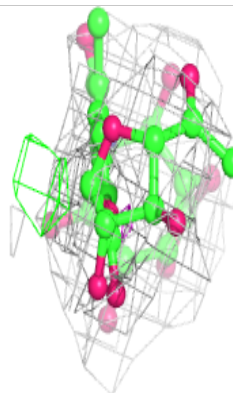
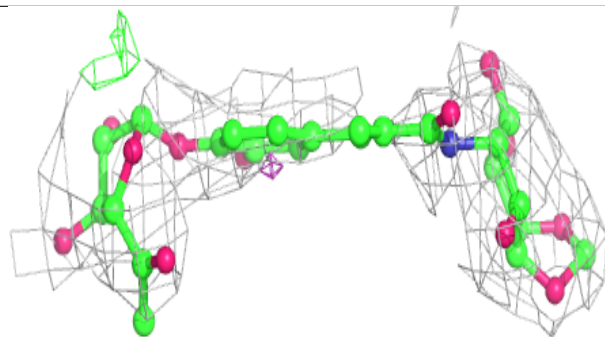
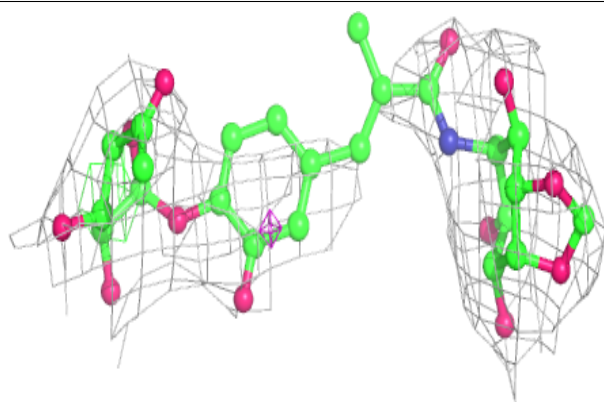
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
31	MG	X	6128	1/1	0.96	0.21	131,131,131,131	0
31	MG	X	6054	1/1	0.96	0.39	79,79,79,79	0
31	MG	X	6007	1/1	0.96	0.39	78,78,78,78	0
31	MG	X	6086	1/1	0.96	0.17	104,104,104,104	0
31	MG	X	6072	1/1	0.96	0.51	101,101,101,101	0
31	MG	X	6004	1/1	0.96	0.28	93,93,93,93	0
31	MG	X	6081	1/1	0.96	0.34	90,90,90,90	0
31	MG	X	6055	1/1	0.97	0.45	85,85,85,85	0
31	MG	X	6143	1/1	0.97	0.63	99,99,99,99	0
31	MG	X	6026	1/1	0.97	0.34	79,79,79,79	0
31	MG	X	6063	1/1	0.97	0.31	87,87,87,87	0
31	MG	X	6023	1/1	0.97	0.37	83,83,83,83	0
31	MG	X	6050	1/1	0.98	0.44	91,91,91,91	0
31	MG	X	6067	1/1	0.98	0.18	72,72,72,72	0
31	MG	X	6005	1/1	0.98	0.55	58,58,58,58	0
31	MG	X	6088	1/1	0.99	0.29	88,88,88,88	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around HGR X 6178:

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.