



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 07:59 am GMT

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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

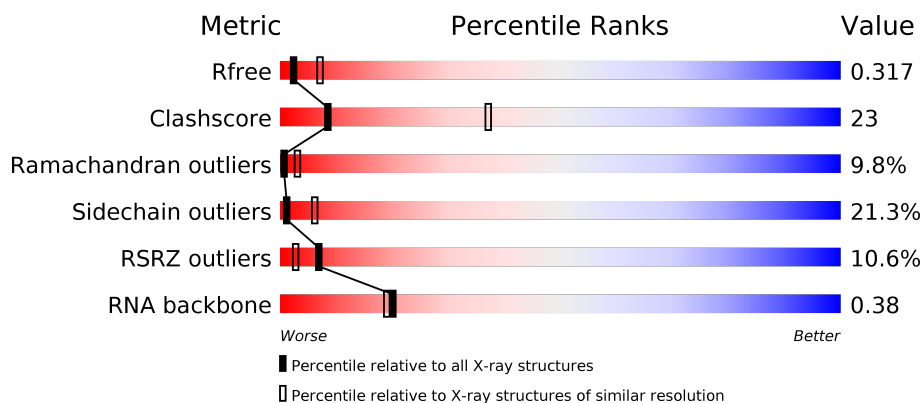
1 Overall quality at a glance

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}	100719	1692 (3.00-3.00)
Clashscore	112137	2037 (3.00-3.00)
Ramachandran outliers	110173	1973 (3.00-3.00)
Sidechain outliers	110143	1976 (3.00-3.00)
RSRZ outliers	101464	1716 (3.00-3.00)
RNA backbone	2435	1007 (3.34-2.66)

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

Mol	Chain	Length	Quality of chain
1	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	M	201	-	-	-	X
31	MG	N	201	-	-	-	X
31	MG	X	6001	-	-	-	X
31	MG	X	6002	-	-	-	X
31	MG	X	6006	-	-	-	X
31	MG	X	6007	-	-	-	X
31	MG	X	6008	-	-	-	X
31	MG	X	6011	-	-	-	X
31	MG	X	6014	-	-	-	X
31	MG	X	6016	-	-	-	X
31	MG	X	6017	-	-	-	X
31	MG	X	6018	-	-	-	X
31	MG	X	6019	-	-	-	X
31	MG	X	6021	-	-	-	X
31	MG	X	6022	-	-	-	X
31	MG	X	6032	-	-	-	X
31	MG	X	6033	-	-	-	X
31	MG	X	6037	-	-	-	X
31	MG	X	6051	-	-	-	X
31	MG	X	6053	-	-	-	X
31	MG	X	6054	-	-	-	X
31	MG	X	6055	-	-	-	X
31	MG	X	6056	-	-	-	X
31	MG	X	6059	-	-	-	X
31	MG	X	6060	-	-	-	X
31	MG	X	6062	-	-	-	X
31	MG	X	6066	-	-	-	X
31	MG	X	6068	-	-	-	X
31	MG	X	6071	-	-	-	X
31	MG	X	6078	-	-	-	X
31	MG	X	6085	-	-	-	X
31	MG	X	6087	-	-	-	X
31	MG	X	6093	-	-	-	X
31	MG	X	6105	-	-	-	X
31	MG	X	6108	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
31	MG	X	6110	-	-	-	X
31	MG	X	6115	-	-	-	X
31	MG	X	6129	-	-	-	X
31	MG	X	6131	-	-	-	X
31	MG	X	6132	-	-	-	X
31	MG	X	6142	-	-	-	X
31	MG	X	6144	-	-	-	X
31	MG	X	6147	-	-	-	X
31	MG	X	6162	-	-	-	X
31	MG	X	6167	-	-	-	X
31	MG	X	6171	-	-	-	X
31	MG	Y	201	-	-	-	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

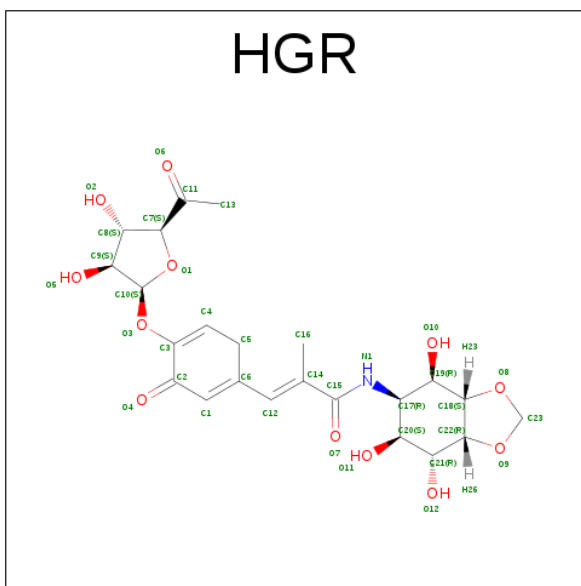
- Molecule 30 is a RNA chain called 5S ribosomal RNA.

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: $C_{23}H_{29}NO_{12}$).

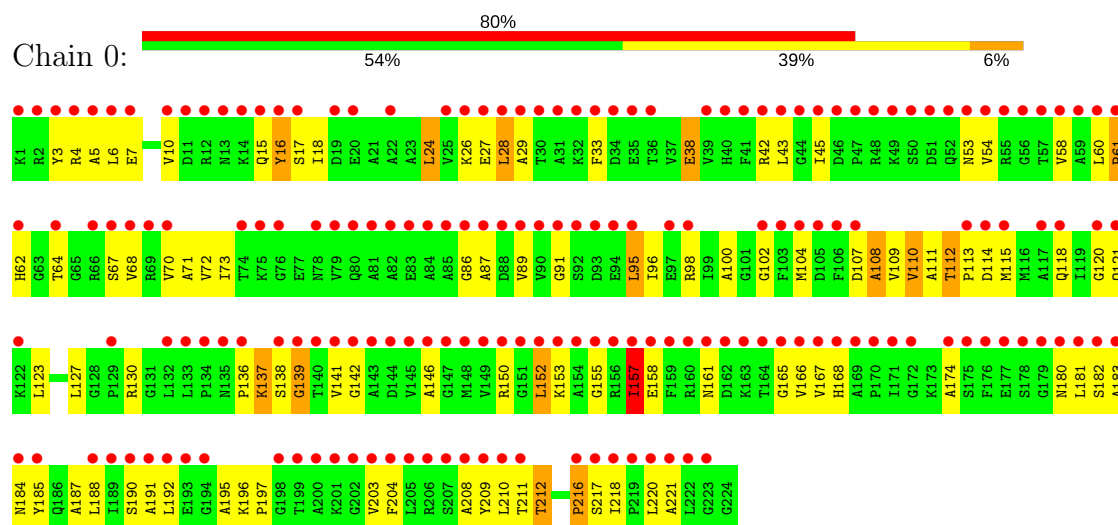


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
32	X	1	Total	C	N	O	0	0
			36	23	1	12		

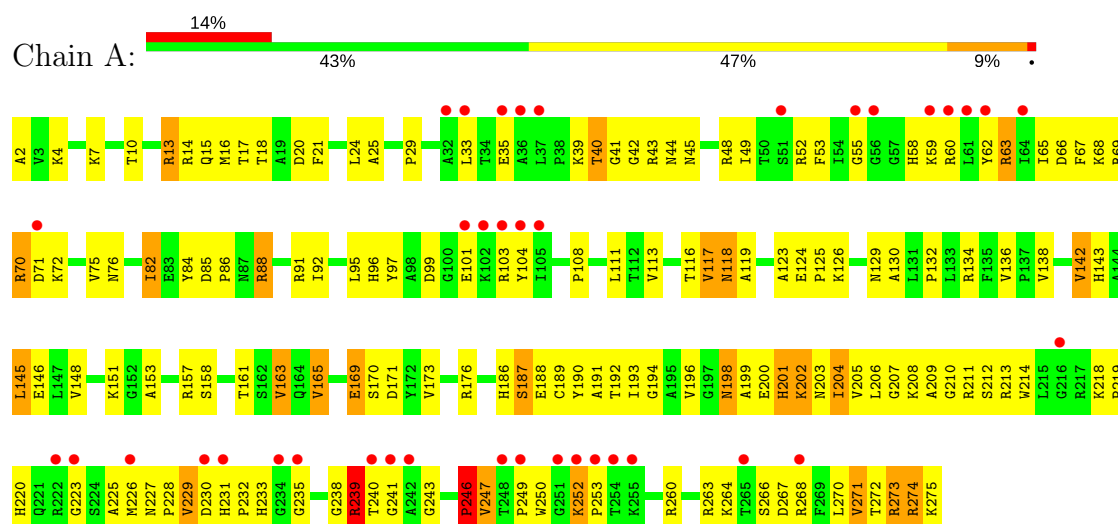
3 Residue-property plots

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

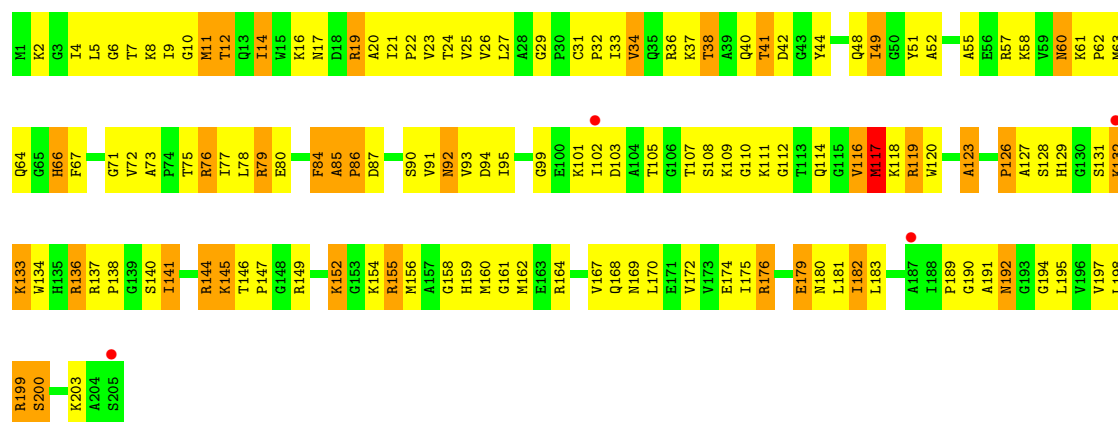


• Molecule 2: 50S ribosomal protein L2

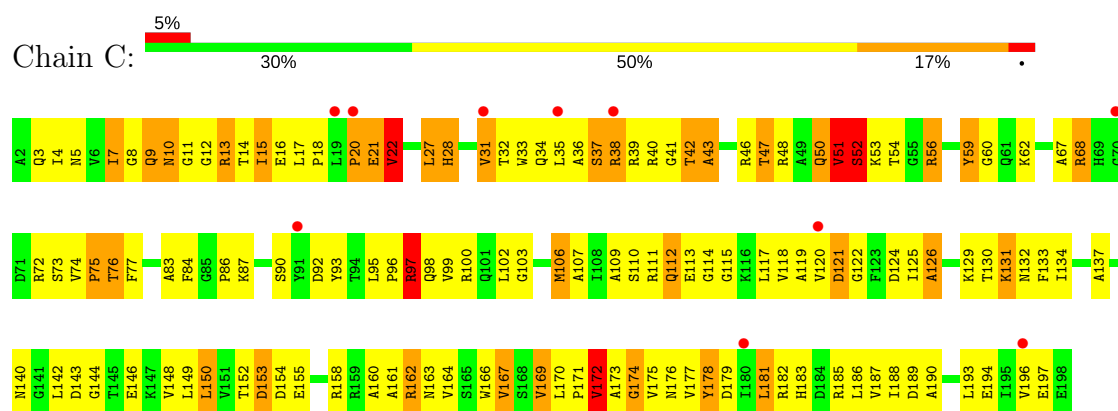


• Molecule 3: 50S ribosomal protein L3

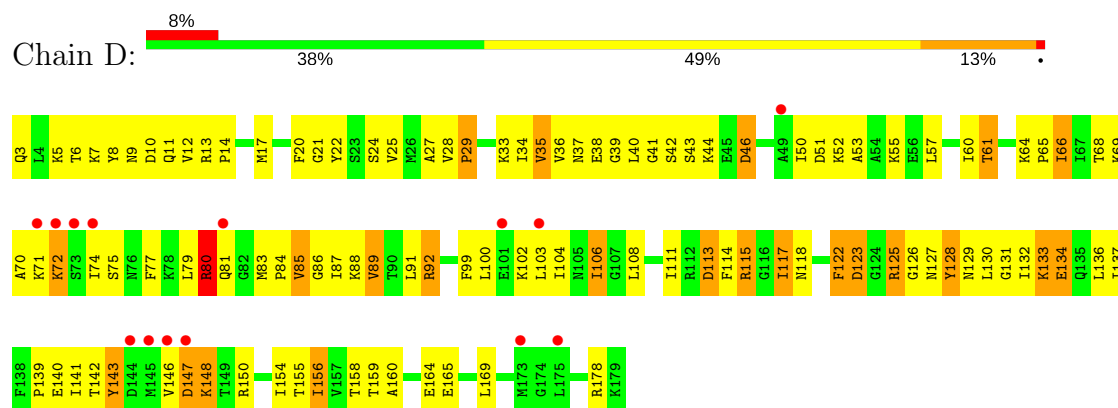




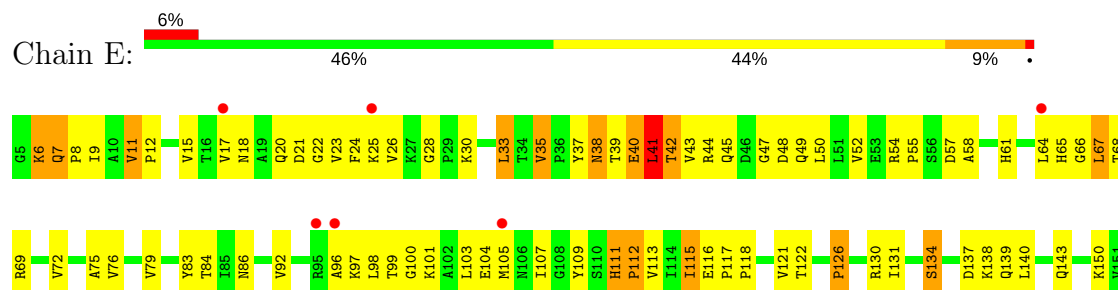
• Molecule 4: 50S ribosomal protein L4



• Molecule 5: 50S ribosomal protein L5

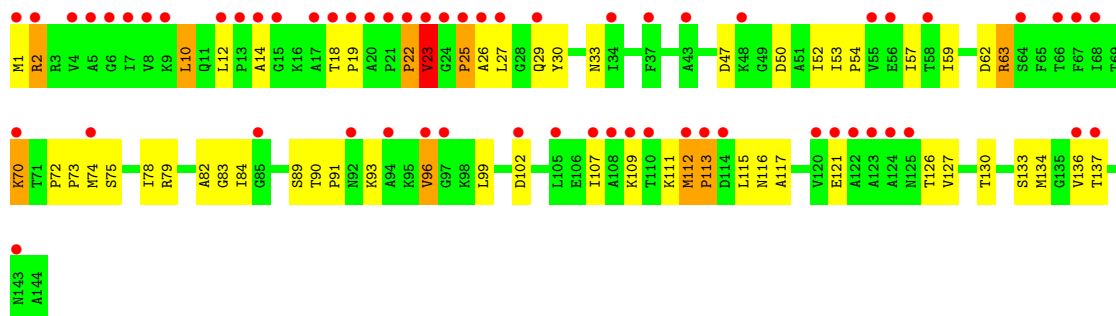
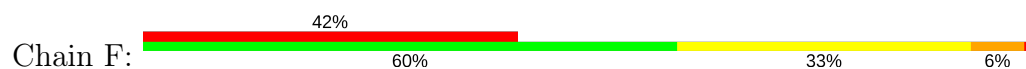


• Molecule 6: 50S ribosomal protein L6

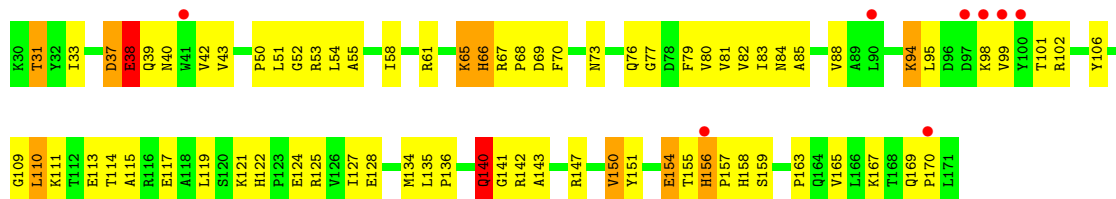




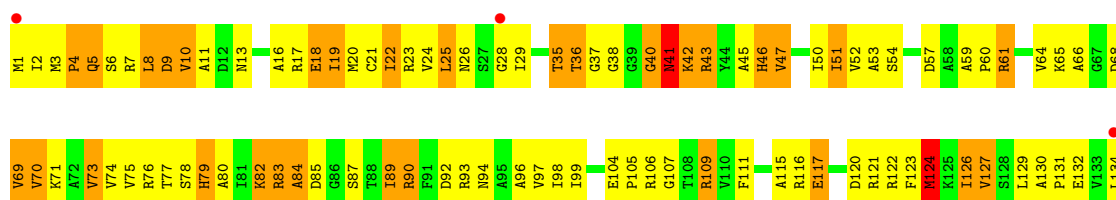
• Molecule 7: 50S ribosomal protein L11



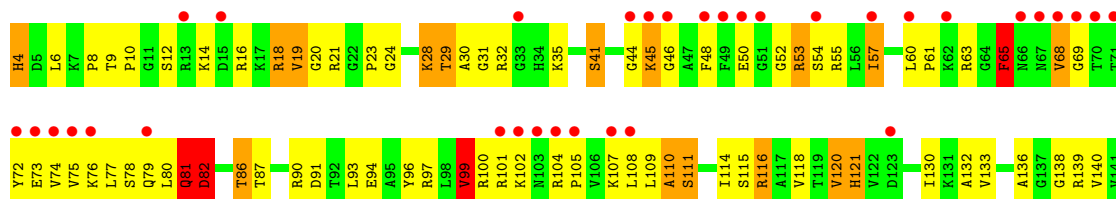
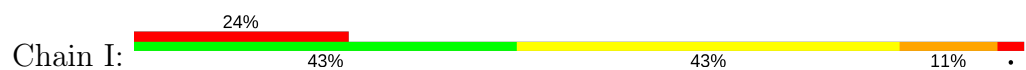
• Molecule 8: 50S ribosomal protein L13



• Molecule 9: 50S ribosomal protein L14

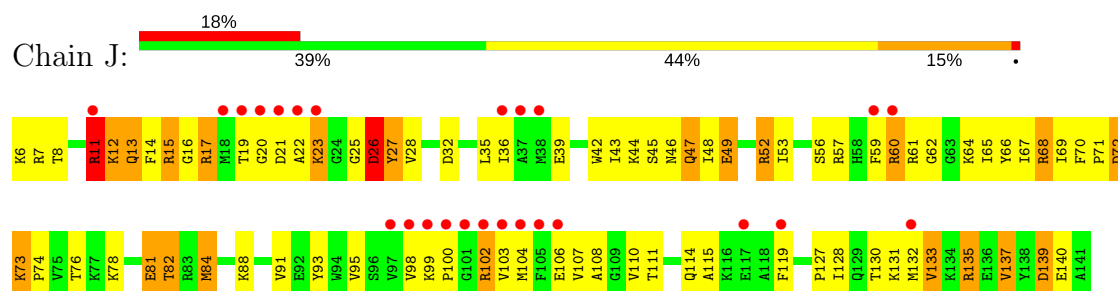


• Molecule 10: 50S ribosomal protein L15

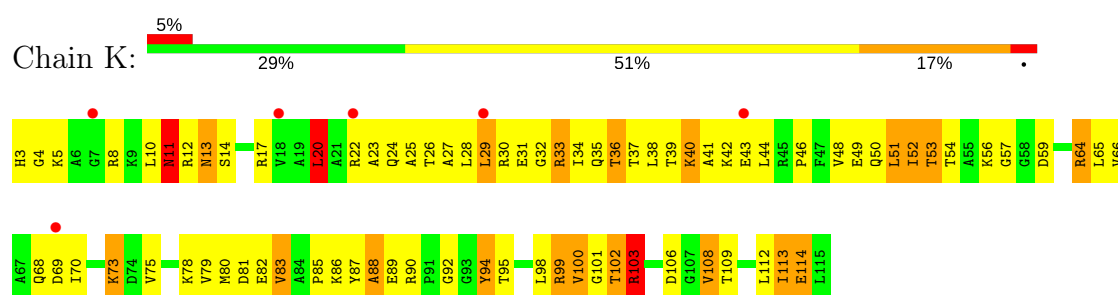




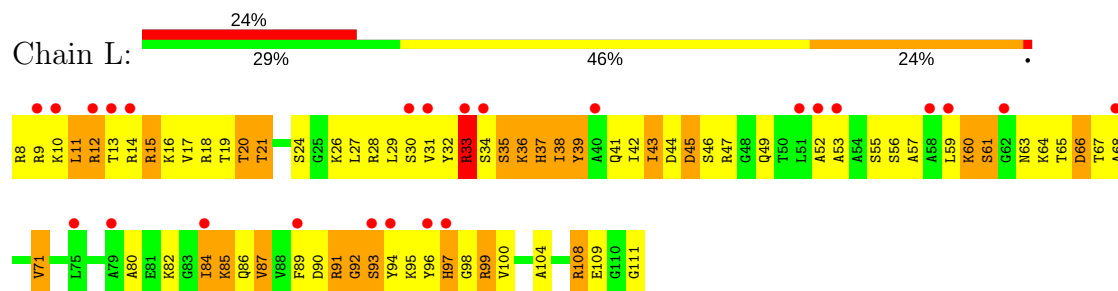
• Molecule 11: 50S ribosomal protein L16



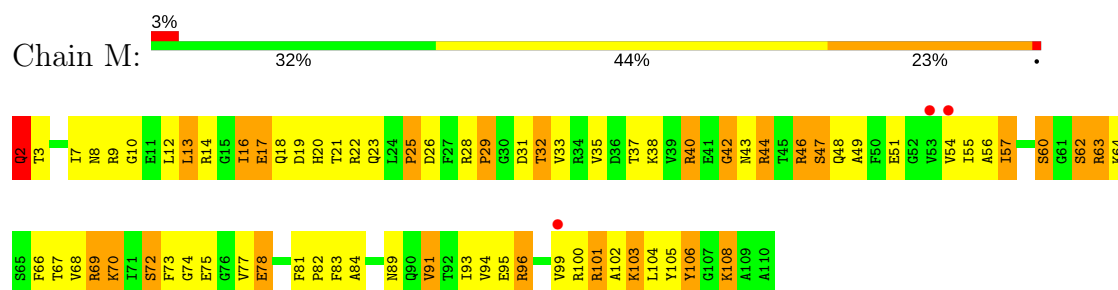
• Molecule 12: 50S ribosomal protein L17



• Molecule 13: 50S ribosomal protein L18



• Molecule 14: 50S ribosomal protein L19

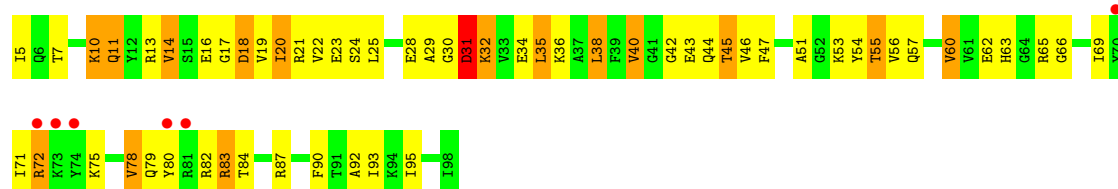


• Molecule 15: 50S ribosomal protein L20

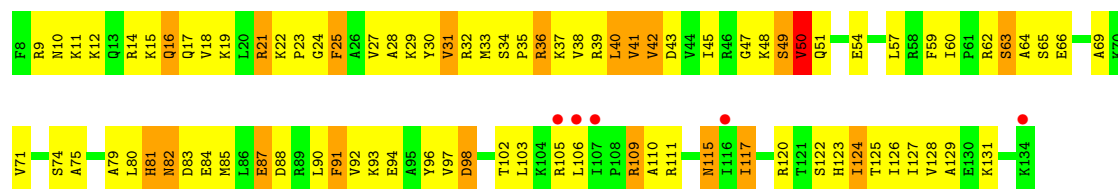




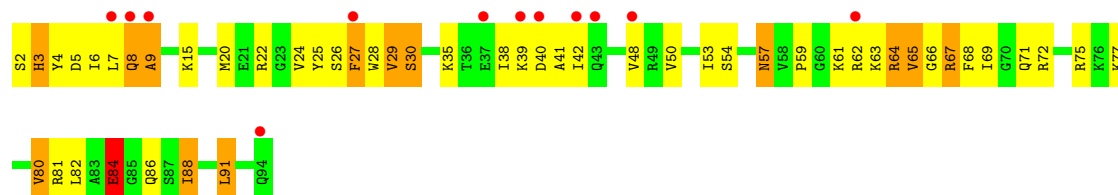
• Molecule 16: 50S ribosomal protein L21



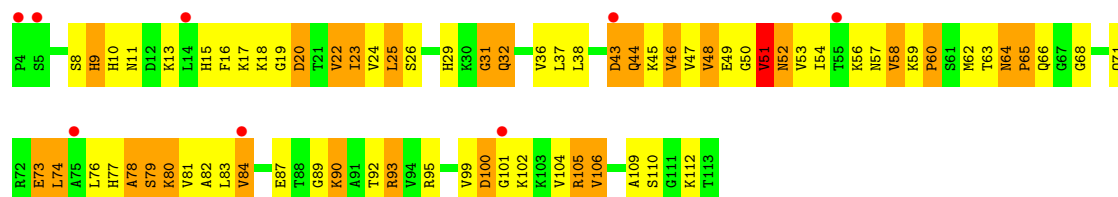
• Molecule 17: 50S ribosomal protein L22



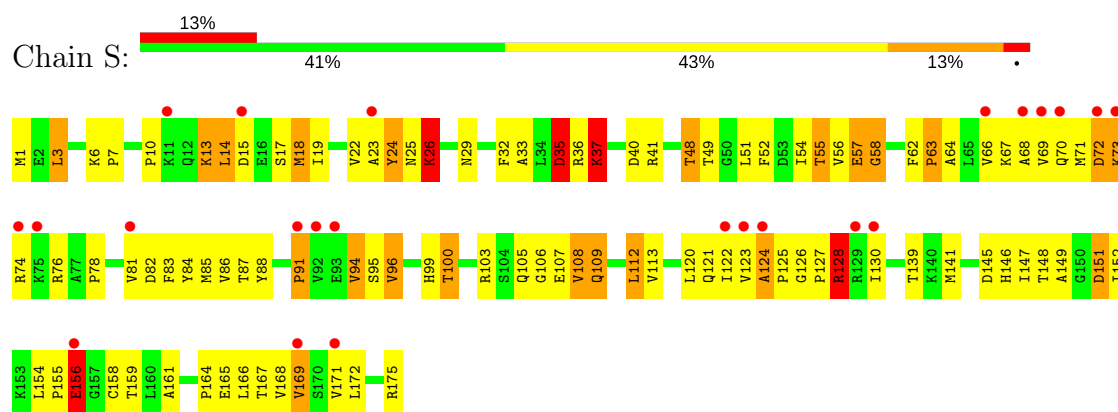
• Molecule 18: 50S ribosomal protein L23



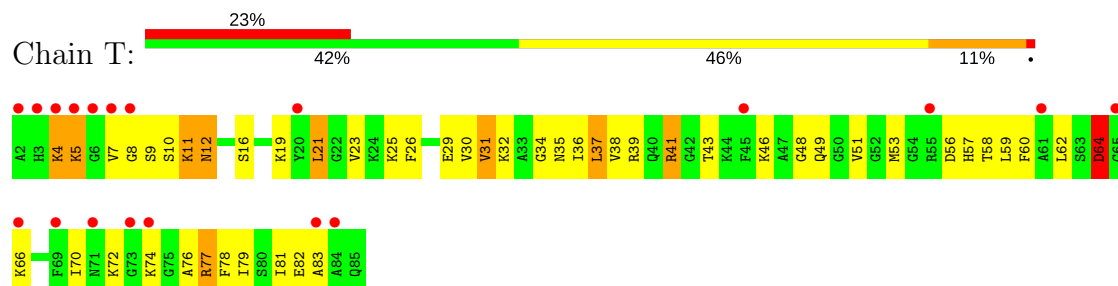
• Molecule 19: 50S ribosomal protein L24



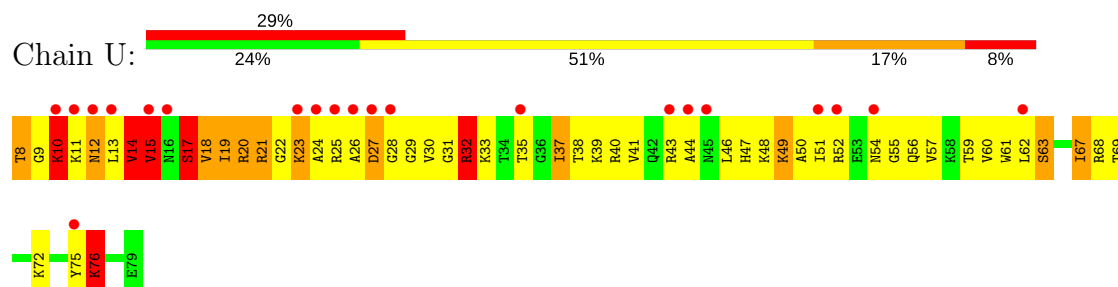
• Molecule 20: 50S ribosomal protein L25



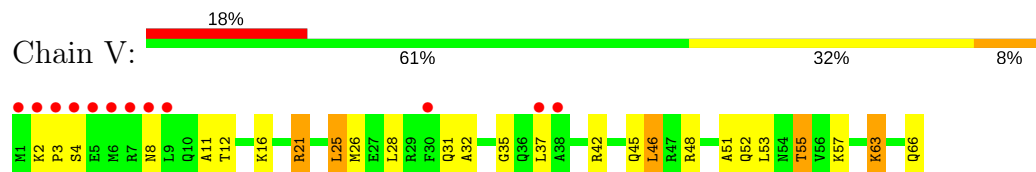
• Molecule 21: 50S ribosomal protein L27



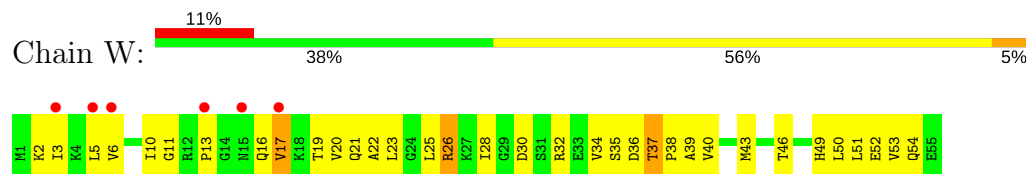
• Molecule 22: 50S ribosomal protein L28



• Molecule 23: 50S ribosomal protein L29



• Molecule 24: 50S ribosomal protein L30

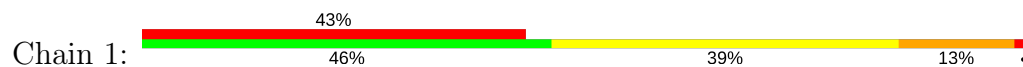


• Molecule 25: 50S ribosomal protein L32

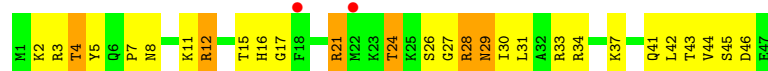




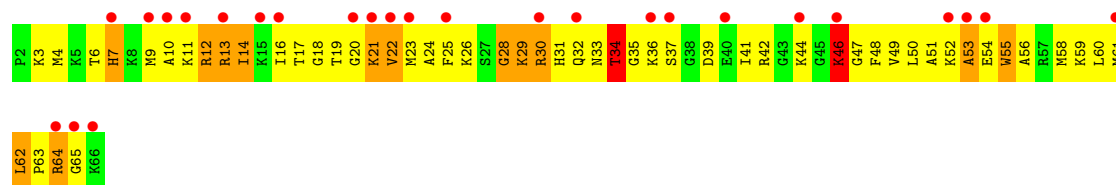
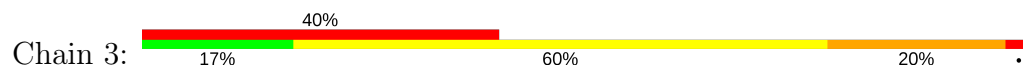
• Molecule 26: 50S ribosomal protein L33



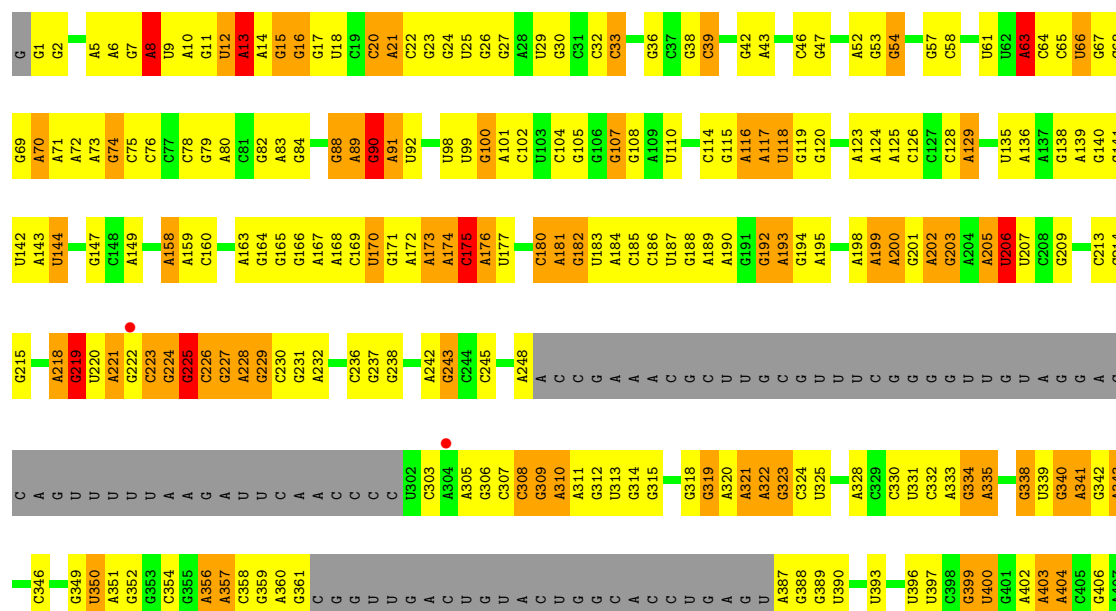
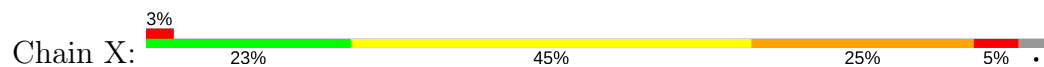
• Molecule 27: 50S ribosomal protein L34



• Molecule 28: 50S ribosomal protein L35

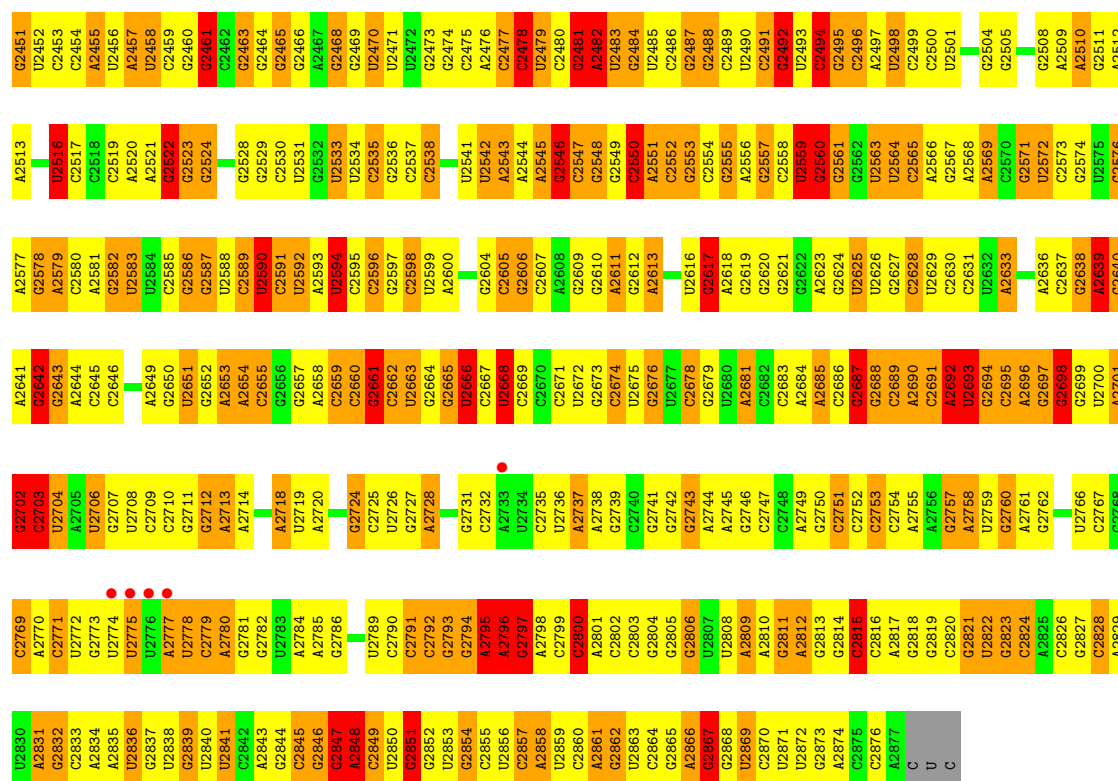


• Molecule 29: 23S ribosomal RNA



C1385	C1386	G1316	G1317	C1256	G1189	U1119	C1054	G988	C926	U860	A795	G562	U597	A536	U475	U408
A1391	A1392	A1318	A1319	U1257	A1192	C1120	A1055	G989	C927	G861	A796	G563	U598	C537	G476	G409
A1393	A1394	A1259	A1260	G1258	A1056	C1121	U1057	A990	A928	A862	A797	C564	A601	A538	A477	A410
G1393	G1394	U1195	U1196	U1194	G1058	A1122	A1057	A991	A929	C863	G798	A865	A602	A539	G478	C411
A1395	A1396	U1124	U1125	U1123	A1059	G1123	A1058	A992	A930	C864	A801	U866	G603	C541	G479	U412
G1397	G1398	U1197	A1061	G1125	C1060	G1126	C1060	A994	C932	A866	A805	U867	U604	A542	C480	G413
A1401	A1402	U1198	A1065	G1128	A1065	G1128	A1065	A995	G933	U867	G805	A868	A544	A481	A414	A415
U1403	U1404	U1199	A1066	A1129	A1066	A1129	A1066	C996	G934	U868	A806	U869	U609	A483	A418	C418
A1405	A1406	U1200	A1067	U1130	A1067	U1130	A1067	C997	G935	U869	A807	C545	G610	A484	G419	G419
G1407	G1408	U1201	A1068	G1131	A1068	G1131	A1068	C998	G936	U870	C808	C572	G611	G485	G485	C420
A1409	A1410	U1202	A1069	G1132	A1069	G1132	A1069	A1001	C937	U871	C809	U874	G612	U486	G486	C421
U1410	U1411	U1203	G1068	G1133	G1068	G1133	G1068	A1002	C938	U872	U810	U874	G613	C487	G487	C422
C1412	C1413	G1204	G1070	C1134	G1070	C1134	G1070	C1003	G940	A874	G812	G876	C615	A488	A488	G423
G1414	G1415	U1205	A1071	G1135	A1071	G1135	A1071	A1004	U941	G875	G813	G877	U616	A489	A489	G424
A1419	A1420	U1206	U1072	G1136	U1072	G1136	U1072	A1005	U942	A876	G814	G878	G617	A491	A491	A425
U1426	U1427	G1207	G1073	G1137	G1073	G1137	G1073	C1006	U943	G877	G815	C749	U617	A493	A493	C426
G1428	G1429	U1208	A1074	C1138	A1074	C1138	A1074	C1007	U944	G878	U816	U880	G618	A494	A494	C427
A1433	A1434	U1209	G1074	G1139	G1074	G1139	G1074	A1007	U945	C879	A817	U881	G620	A495	A495	C428
U1435	U1436	U1210	C1075	A1140	C1075	A1140	C1075	G1008	U946	C880	G818	G882	U621	C496	C496	C430
G1438	G1439	U1211	U1077	G1141	U1077	G1141	U1077	A1009	U947	A886	U820	G884	G622	C497	C497	C431
A1440	A1441	U1212	A1078	G1142	A1078	G1142	A1078	C1010	C948	G887	U821	U885	G623	C498	C498	C432
C1442	C1443	U1213	U1079	G1143	U1079	G1143	U1079	C1011	U949	G888	G822	C886	A624	G500	G500	A435
A1445	A1446	U1214	A1080	U1144	A1080	U1144	A1080	G1013	G950	G889	G823	C887	A625	A501	A501	A436
G1449	G1450	C1218	A1081	G1145	A1081	G1145	A1081	G1014	C951	A891	U824	G888	A626	G502	G502	A437
U1451	U1452	U1219	C1082	G1146	C1082	G1146	C1082	U1015	A952	G	C825	U864	A627	A503	A503	C439
A1453	A1454	U1220	U1083	G1147	U1083	G1147	U1083	C1016	G953	G	U826	A890	G628	G504	G504	A443
G1455	G1456	C1221	A1084	G1148	A1084	G1148	A1084	C1017	U954	G	G827	C891	G630	A507	A507	U444
U1457	U1458	U1222	G1085	C1150	G1085	C1150	G1085	C1018	U955	G	C828	C892	G631	G505	G505	A445
A1459	A1460	U1223	U1086	G1151	U1086	G1151	U1086	U1019	A956	G	C829	C893	A632	G506	G506	U446
G1461	G1462	U1224	C1087	G1152	C1087	G1152	C1087	A1020	C957	C	C830	C894	A633	A509	A509	U447
C1463	C1464	U1225	A1088	G1153	A1088	G1153	A1088	A1021	G958	U	G831	G895	G634	G510	G510	A451
A1465	A1466	U1226	C1089	G1154	C1089	G1154	C1089	U1022	U960	C	A832	U896	G635	A512	A512	G452
U1467	U1468	U1227	C1091	G1155	C1091	G1155	C1091	A1023	C961	A	A833	G897	G636	A513	A513	G453
G1469	G1470	C1229	U1092	G1156	U1092	G1156	U1092	G1024	C962	C	A834	C769	G637	A514	A514	G454
A1471	A1472	U1230	A1096	G1157	A1096	G1157	A1096	A1025	G963	C	U835	C770	G638	A515	A515	G455
U1473	U1474	U1231	A1097	G1158	A1097	G1158	A1097	G1026	A964	A	U836	C771	A644	A517	A517	G456
C1475	C1476	U1232	A1098	G1159	A1098	G1159	A1098	C1027	A965	G	U837	C772	G645	A518	A518	G457
A1477	A1478	U1233	U1099	G1160	U1099	G1160	U1099	C1028	G966	C	A838	G773	G646	C519	C519	G458
G1479	G1480	C1234	A1099	G1161	A1099	G1161	A1099	C1029	A966	C	U839	A774	G647	C520	C520	A459
U1481	U1482	U1235	U1100	G1162	U1100	G1162	U1100	C1030	A967	C	U840	A775	A648	A521	A521	G460
A1483	A1484	U1236	C1163	G1163	C1163	G1163	C1163	C1031	C967	U	G841	A776	G649	G522	G522	G461
G1485	G1486	U1237	U1101	G1164	U1101	G1164	U1101	A1032	U968	A	A842	C705	U650	A525	A525	G462
U1487	U1488	A1238	U1102	G1165	U1102	G1165	U1102	G1033	U969	C	A843	G706	G651	G526	G526	G463
A1489	A1490	U1239	C1103	G1166	C1103	G1166	C1103	U1034	A970	C	A844	A707	G652	C527	C527	A466
C1491	C1492	G1104	G1104	G1167	G1104	G1167	G1104	G1035	A971	A911	G845	G708	G653	G528	G528	U467
G1493	G1494	U1240	A1107	G1168	A1107	G1168	A1107	C972	U973	A912	U846	C711	G654	G529	G529	A468
U1495	U1496	U1241	U1108	G1169	U1108	G1169	U1108	C975	C976	A913	U847	A712	G655	G530	G530	G469
A1497	A1498	C1242	U1109	G1170	U1109	G1170	U1109	C977	G980	A914	A848	G713	C651	G531	G531	U470
G1499	G1500	U1243	G1110	G1171	G1110	G1171	G1110	C978	U981	C915	U849	G714	G652	A532	A532	A471
U1501	U1502	U1244	C1111	G1172	C1111	G1172	C1111	U1040	C982	U916	G851	G715	G653	G533	G533	A472
A1503	A1504	U1245	U1112	G1173	U1112	G1173	U1112	A1041	C983	U917	A852	A716	G654	G534	G534	C473
G1505	G1506	C1246	U1113	G1174	U1113	G1174	U1113	G1042	U984	A918	U853	A717	A654	U535	U535	G474
U1507	U1508	U1247	C1114	G1175	C1114	G1175	C1114	U1043	C985	U919	U854	A718	G655	G536	G536	
A1509	A1510	A1179	A1114	G1176	A1114	G1176	A1114	U1044	G986	A920	G854	A719	U656	G537	G537	
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U1513	U1514	G1185	C1116	G1178	C1116	G1178	C1116	U1046	A985	A922	U856	G790	G658	G539	G539	
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G2389	C2322	U2322	G2258	A2191	U2126	A2060	U2000	U1938	A1890	A1803	G1737	C1674	C1533	C1461
A2390	U2323	U2323		U2192	U2127		G2001	U1939	A1872	U1804	U1738	C1675	G1533	C1462
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G2392	A2325	C2326	G2262	C2193	U2129	U2064	U2004	G1942	C1882	A1807	G1742	G1678	C1535	A1464
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A2397	G2328	U2328	C2264	U2197	G2131	G2066	U2006	A1943	G1882	G1809	G1744	U1680	U1611	C1466
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C2399	U2330	U2330	A2266	C2199	U2133	C2068	C2008	G1947	A1884	U1811	C1746	A1682	G1541	U1468
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	U2335	U2335	G2271	A2204	G2137	G2077	A2012	G1951	G1889	A1815	G1750	U1686		
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G2408	A2337	U2337	C2273	C2206	A2141	U2079	A2014	A1953	C1891	A1817	U1752	U1688	C1549	G1476
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A2412	A2341	U2341	A2145	G2212	A2145	G2083	C2019	C1957	A1896	C1825		C1693	U1553	G1480
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G2414	C2343	U2343	G2147	G2214	C2147	G2085	G2021	A1961	U1898	G1827	G1761	C1696	C1555	U1482
A2415	A2344	U2344	G2148	G2215	G2148	U2086	C2022	C1962	A1899	C1828	C1762	U1697	A1556	G1483
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A2417	U2346	U2346	G2151	G2217	A2151	C2091	U2024	A1964	A1901	G1831	U1764	U1705	G1561	U1485
A2418	G2349	U2349	A2152	U2223	A2152	U2092	U2025	U1965	A1902	C1831	G1765	C1700	A1562	U1490
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G2420	G2351	U2351	G2155	U2225	U2155	C2094	C2027	U1967	G1904	U1836	G1767	C1703	U1564	G1494
A2421	A2352	U2352	A2156	G2226	A2156	G2095	G2028	G1968	G1905	C1836	U1768	C1704	G1495	G1496
C2422	G2353	U2353	C2157	A2227	C2157	U2096	U2030	G1970	U1906	G1837	U1769	U1705	A1567	C1497
G2423	A2354	U2354	A2158	G2228	C2158	G2098	A2031	G1971	U1909	A1839	U1770	A1706	G1569	G1498
U2424	C2355	U2355	C2159	U2229	A2159	C2099	G2032	C1972	A1910	A1840	C1772	C1707	C1570	A1499
A2425	A2356	U2356	G2160	G2230	C2160	U2100	C2033	U1974	A1911	G1841	C1773	U1709	G1571	U1500
G2426	G2357	U2357	U2161	G2231	C2161	U2101	G2035	G1975	G1912	A1845	A1774	U1709	G1572	
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U2428	A2359	U2359	G2164	G2233	G2164	G2103	U2037	C1977	U1914		A1776	C1711	A1574	G1504
A2429	C2360	U2360	A2165	U2234	A2165	G2104	C2038	U1978	G1849	G1851	U1777	G1712	C1575	U1505
C2430	G2361	U2361	G2166	U2235	G2166	U2105	G2039	C1979	G1850	G1852	U1778	G1713	C1575	C1506
A2431	C2362	U2362	A2167	U2236	A2167	G2106	C2040	U1980	A1918	G1853	C1779	A1714	U1578	C1507
G2432	G2363	U2363	G2168	U2237	A2168	G2107	A2041	A1981	A1919	U1854	U1780	A1715	G1579	A1508
C2433	C2364	U2364	A2169	G2238	A2169	G2108	A2042	A1982	A1920	G1855	U1781	G1716	C1580	A1509
G2434	U2365	U2365	C2170	U2239	C2170	A2109	A2043	G1983	A1921	C1853	G1782	U1717	C1581	A1510
C2435	G2366	U2366	U2171	G2240	U2171	G2110	G2044	U1984	U1922	G1854	G1783	A1718	A1582	A1511
U2436	C2367	U2367	U2172	U2241	U2172	G2111	C2045	G1985	C1923	G1855	U1784	G1719	G1585	U1512
A2437	G2368	U2368	G2173	U2242	G2173	C2111	C2046	G1986	C1924	U1856	U1785	G1720	A1585	U1513
U2438	C2369	U2369	G2174	C2243	G2174	C2112	C2047	G1987	C1925	G1857	U1786	G1721	A1586	C1517
G2439	G2370	U2370	U2177	U2244	U2177	U2113	C2048	A1988	U1926	C1858	U1789	G1722	C1586	C1518
C2440	A2371	U2371	U2178	A2245	U2178	G2114	C2049	C1989	U1927	A1859	G1790	G1723	U1591	
U2441	G2372	U2372	U2179	A2246	U2179	C2115	C2050	U1990	G1928	C1791	C1792	U1724	U1592	C1522
C2442	C2373	U2373	U2180	U2247	U2180	A2116	U2051	U1991	G1929	G1861	C1793	C1725	C1593	A1523
A2443	G2374	U2374	A2181	A2248	U2181	G2117	G2052	G1992	G1930	C1862	U1794	C1726	U1594	C1524
U2444	C2375	U2375	A2182	U2251	A2182	A2119	G2053	G1993	G1931	G1864	C1795	C1727	A1667	A1525
C2445	G2376	U2376	U2183	U2252	A2183	C2120	A2054	U1994	G1932	C1865	U1796	A1728	U1800	A1526
U2446	A2377	U2377	G2186	A2253	U2186	U2121	G2055	G1995	U1933	C1866	A1799	U1733	U1601	G1527
G2447	C2378	U2378	A2187	C2254	A2187	G2122	C2056	U1996	U1934	C1867		C1734	A1800	C1528
A2448	G2379	U2379	A2188	U2255	A2188	G2123	U2057	A1997	A1935	A1867				



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	1.32 (at 3.01Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.284 , 0.326 0.271 , 0.317	Depositor DCC
R_{free} test set	21382 reflections (4.83%)	DCC
Wilson B-factor (Å ²)	66.7	Xtriage
Anisotropy	0.402	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.16 , 40.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	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	O	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%)	2	11
3	B	203/205 (99%)	152 (75%)	33 (16%)	18 (9%)	1	4
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	4
6	E	169/171 (99%)	119 (70%)	33 (20%)	17 (10%)	1	3
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	6
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	7
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%)	1	4
15	N	115/117 (98%)	90 (78%)	19 (16%)	6 (5%)	2	14
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	16
18	Q	91/93 (98%)	67 (74%)	16 (18%)	8 (9%)	1	4
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	3
21	T	82/84 (98%)	68 (83%)	8 (10%)	6 (7%)	1	6
22	U	70/72 (97%)	39 (56%)	15 (21%)	16 (23%)	0	0
23	V	64/66 (97%)	54 (84%)	9 (14%)	1 (2%)	11	46
24	W	53/55 (96%)	36 (68%)	13 (24%)	4 (8%)	1	6
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%)	8	36
28	3	63/65 (97%)	38 (60%)	17 (27%)	8 (13%)	0	1
All	All	3431/3487 (98%)	2439 (71%)	657 (19%)	335 (10%)	1	3

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

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%)	0
30	Y	121/122 (99%)	35 (28%)	0
All	All	2897/3003 (96%)	874 (30%)	0

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

There are no RNA pucker outliers to report.

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

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	1.80	7 (17%)	48,58,58	1.70	8 (16%)

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	-	-	0/20/79/79	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	-4.43	1.42	1.50
32	X	6178	HGR	C3-C2	-3.85	1.41	1.48
32	X	6178	HGR	C5-C4	-3.36	1.43	1.49
32	X	6178	HGR	C17-N1	2.06	1.49	1.45
32	X	6178	HGR	C12-C14	3.84	1.43	1.33

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	X	6178	HGR	C23-O8-C18	-3.83	100.22	106.22
32	X	6178	HGR	C4-C3-C2	-3.79	118.17	121.88
32	X	6178	HGR	O1-C10-C9	-2.67	101.47	104.97
32	X	6178	HGR	C1-C2-C3	2.48	120.84	115.87
32	X	6178	HGR	O10-C19-C17	2.60	114.88	109.61

There are no chirality outliers.

There are no torsion outliers.

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

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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	0	224/224 (100%)	4.90	179 (79%) 0 0	291, 311, 319, 322	0
2	A	274/274 (100%)	0.62	39 (14%) 3 1	108, 151, 172, 185	0
3	B	205/205 (100%)	0.04	4 (1%) 65 36	67, 102, 129, 146	0
4	C	197/197 (100%)	0.12	10 (5%) 29 12	93, 133, 158, 177	0
5	D	177/177 (100%)	0.29	14 (7%) 13 5	165, 183, 200, 214	0
6	E	171/171 (100%)	0.09	10 (5%) 24 9	116, 167, 191, 198	0
7	F	144/144 (100%)	2.33	60 (41%) 0 0	233, 259, 275, 281	0
8	G	142/142 (100%)	0.28	8 (5%) 25 10	87, 125, 139, 169	0
9	H	134/134 (100%)	-0.10	3 (2%) 62 33	70, 92, 108, 118	0
10	I	141/141 (100%)	1.05	34 (24%) 1 0	98, 150, 173, 182	0
11	J	136/136 (100%)	0.94	25 (18%) 1 1	107, 126, 156, 159	0
12	K	113/113 (100%)	0.22	6 (5%) 27 11	63, 82, 95, 99	0
13	L	104/104 (100%)	1.12	25 (24%) 1 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%) 11 4	90, 118, 144, 153	0
16	O	94/94 (100%)	-0.28	6 (6%) 20 7	103, 129, 156, 173	0
17	P	127/127 (100%)	0.16	5 (3%) 40 16	81, 96, 120, 180	0
18	Q	93/93 (100%)	0.59	12 (12%) 4 1	108, 137, 160, 176	0
19	R	110/110 (100%)	0.37	8 (7%) 16 6	111, 131, 166, 180	0
20	S	175/175 (100%)	0.47	23 (13%) 4 1	134, 167, 185, 193	0
21	T	84/84 (100%)	1.16	19 (22%) 1 0	111, 130, 148, 171	0
22	U	72/72 (100%)	1.51	21 (29%) 1 0	134, 163, 177, 182	0
23	V	66/66 (100%)	0.82	12 (18%) 1 1	147, 163, 190, 201	0
24	W	55/55 (100%)	0.66	6 (10%) 6 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%) 27 11	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%) 36 15	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%) 58 29	110, 157, 182, 203	0
All	All	6389/6490 (98%)	0.37	678 (10%) 7 3	59, 134, 276, 397	0

The worst 5 of 678 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	17.4
1	0	85	ALA	15.6
29	X	2127	U	15.3

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
31	MG	X	6033	1/1	0.83	0.69	50.68	76,76,76,76	0
31	MG	X	6001	1/1	0.89	0.72	46.73	67,67,67,67	0
31	MG	X	6162	1/1	0.76	0.77	41.13	104,104,104,104	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
31	MG	X	6147	1/1	0.93	1.07	30.90	93,93,93,93	0
31	MG	X	6018	1/1	0.95	0.78	25.79	86,86,86,86	0
31	MG	X	6167	1/1	0.90	1.05	25.64	97,97,97,97	0
31	MG	X	6129	1/1	0.90	0.45	19.53	89,89,89,89	0
31	MG	X	6132	1/1	0.92	0.56	19.09	84,84,84,84	0
31	MG	X	6087	1/1	0.82	0.61	18.86	85,85,85,85	0
31	MG	X	6085	1/1	0.82	0.41	17.47	66,66,66,66	0
31	MG	X	6105	1/1	0.90	0.41	14.75	86,86,86,86	0
31	MG	X	6014	1/1	0.80	0.47	13.89	99,99,99,99	0
31	MG	X	6142	1/1	0.92	0.55	12.91	106,106,106,106	0
31	MG	X	6011	1/1	0.91	0.39	11.98	104,104,104,104	0
31	MG	X	6016	1/1	0.96	0.35	10.99	74,74,74,74	0
31	MG	X	6019	1/1	0.93	0.48	10.81	75,75,75,75	0
31	MG	X	6066	1/1	0.93	0.40	10.57	105,105,105,105	0
31	MG	X	6054	1/1	0.96	0.38	10.32	79,79,79,79	0
31	MG	X	6053	1/1	0.94	0.35	9.81	85,85,85,85	0
31	MG	X	6006	1/1	0.78	0.56	9.65	70,70,70,70	0
31	MG	M	201	1/1	0.94	0.67	9.22	71,71,71,71	0
31	MG	Y	201	1/1	0.81	0.41	8.70	96,96,96,96	0
31	MG	X	6022	1/1	0.84	0.58	8.63	92,92,92,92	0
31	MG	X	6017	1/1	0.86	0.45	8.42	54,54,54,54	0
31	MG	X	6068	1/1	0.93	0.38	8.22	111,111,111,111	0
31	MG	X	6007	1/1	0.96	0.39	7.55	78,78,78,78	0
31	MG	X	6062	1/1	0.86	0.72	6.89	87,87,87,87	0
31	MG	X	6055	1/1	0.97	0.45	6.87	85,85,85,85	0
31	MG	X	6037	1/1	0.89	0.41	5.74	65,65,65,65	0
31	MG	X	6093	1/1	0.65	0.34	5.65	96,96,96,96	0
31	MG	X	6171	1/1	0.85	0.32	5.58	118,118,118,118	0
31	MG	N	201	1/1	0.76	0.38	5.42	74,74,74,74	0
31	MG	X	6115	1/1	0.91	0.30	5.21	133,133,133,133	0
31	MG	X	6008	1/1	0.95	0.26	4.65	58,58,58,58	0
31	MG	X	6032	1/1	0.95	0.36	4.21	86,86,86,86	0
31	MG	X	6060	1/1	0.92	0.64	4.21	80,80,80,80	0
31	MG	X	6078	1/1	0.81	0.36	3.55	89,89,89,89	0
31	MG	X	6071	1/1	0.89	0.33	3.17	99,99,99,99	0
31	MG	X	6056	1/1	0.91	0.32	3.16	81,81,81,81	0
31	MG	X	6021	1/1	0.94	0.26	3.15	91,91,91,91	0
31	MG	X	6144	1/1	0.80	0.26	3.11	132,132,132,132	0
31	MG	X	6131	1/1	0.80	0.39	2.97	80,80,80,80	0
31	MG	X	6002	1/1	0.85	0.32	2.78	91,91,91,91	0
31	MG	X	6051	1/1	0.73	0.54	2.64	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
31	MG	X	6110	1/1	0.91	0.22	2.59	84,84,84,84	0
31	MG	X	6059	1/1	0.90	0.24	2.16	88,88,88,88	0
32	HGR	X	6178	36/36	0.90	0.25	1.98	79,99,109,111	0
31	MG	X	6108	1/1	0.92	0.52	1.93	108,108,108,108	0
31	MG	X	6158	1/1	0.87	0.21	1.68	76,76,76,76	0
31	MG	X	6023	1/1	0.97	0.37	1.35	83,83,83,83	0
31	MG	X	6012	1/1	0.86	0.24	1.25	78,78,78,78	0
31	MG	X	6004	1/1	0.96	0.28	1.03	93,93,93,93	0
31	MG	A	301	1/1	0.73	0.34	-0.14	108,108,108,108	0
31	MG	X	6086	1/1	0.96	0.17	-0.21	104,104,104,104	0
31	MG	X	6038	1/1	0.94	0.08	-4.26	82,82,82,82	0
31	MG	X	6119	1/1	0.91	0.40	-	89,89,89,89	0
31	MG	X	6042	1/1	0.86	1.01	-	96,96,96,96	0
31	MG	X	6036	1/1	0.94	0.35	-	70,70,70,70	0
31	MG	X	6174	1/1	0.73	0.30	-	117,117,117,117	0
31	MG	X	6101	1/1	0.08	1.25	-	138,138,138,138	0
31	MG	X	6127	1/1	0.80	0.62	-	81,81,81,81	0
31	MG	X	6172	1/1	0.77	0.34	-	88,88,88,88	0
31	MG	X	6044	1/1	0.94	0.41	-	66,66,66,66	0
31	MG	X	6100	1/1	0.91	0.42	-	111,111,111,111	0
31	MG	X	6140	1/1	0.46	0.42	-	97,97,97,97	0
31	MG	X	6126	1/1	0.87	0.42	-	114,114,114,114	0
31	MG	X	6107	1/1	0.92	0.22	-	76,76,76,76	0
31	MG	X	6079	1/1	0.86	0.33	-	99,99,99,99	0
31	MG	X	6164	1/1	0.86	0.23	-	86,86,86,86	0
31	MG	X	6092	1/1	0.92	0.72	-	97,97,97,97	0
31	MG	X	6169	1/1	0.77	0.48	-	91,91,91,91	0
31	MG	X	6143	1/1	0.97	0.63	-	99,99,99,99	0
31	MG	X	6076	1/1	0.74	0.55	-	73,73,73,73	0
31	MG	X	6120	1/1	0.88	0.27	-	78,78,78,78	0
31	MG	X	6046	1/1	0.85	0.58	-	76,76,76,76	0
31	MG	X	6005	1/1	0.98	0.55	-	58,58,58,58	0
31	MG	X	6039	1/1	0.90	0.39	-	79,79,79,79	0
31	MG	X	6177	1/1	0.90	0.49	-	125,125,125,125	0
31	MG	X	6088	1/1	0.99	0.28	-	88,88,88,88	0
31	MG	X	6149	1/1	0.75	0.41	-	99,99,99,99	0
31	MG	X	6074	1/1	0.84	0.39	-	89,89,89,89	0
31	MG	X	6003	1/1	0.82	0.31	-	72,72,72,72	0
31	MG	X	6045	1/1	0.86	0.72	-	94,94,94,94	0
31	MG	X	6109	1/1	0.94	0.37	-	92,92,92,92	0
31	MG	X	6137	1/1	0.84	0.47	-	136,136,136,136	0
31	MG	X	6083	1/1	0.89	0.29	-	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
31	MG	X	6134	1/1	0.94	0.11	-	100,100,100,100	0
31	MG	X	6072	1/1	0.96	0.51	-	101,101,101,101	0
31	MG	X	6152	1/1	0.56	0.30	-	158,158,158,158	0
31	MG	X	6165	1/1	0.89	0.44	-	88,88,88,88	0
31	MG	X	6025	1/1	0.91	0.65	-	76,76,76,76	0
31	MG	X	6135	1/1	0.44	1.17	-	129,129,129,129	0
31	MG	X	6031	1/1	0.94	0.61	-	85,85,85,85	0
31	MG	X	6026	1/1	0.97	0.34	-	79,79,79,79	0
31	MG	X	6013	1/1	0.92	0.49	-	76,76,76,76	0
31	MG	X	6148	1/1	0.84	0.31	-	104,104,104,104	0
31	MG	X	6099	1/1	0.60	0.86	-	120,120,120,120	0
31	MG	Y	202	1/1	0.91	0.18	-	130,130,130,130	0
31	MG	X	6090	1/1	0.80	0.46	-	72,72,72,72	0
31	MG	X	6160	1/1	0.74	0.71	-	108,108,108,108	0
31	MG	X	6024	1/1	0.95	0.37	-	100,100,100,100	0
31	MG	X	6104	1/1	0.93	0.54	-	89,89,89,89	0
31	MG	X	6156	1/1	0.82	0.25	-	91,91,91,91	0
31	MG	X	6064	1/1	0.85	0.48	-	77,77,77,77	0
31	MG	X	6041	1/1	0.91	0.41	-	64,64,64,64	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	6063	1/1	0.97	0.31	-	87,87,87,87	0
31	MG	X	6124	1/1	0.68	0.58	-	100,100,100,100	0
31	MG	X	6028	1/1	0.92	0.30	-	75,75,75,75	0
31	MG	X	6081	1/1	0.96	0.33	-	90,90,90,90	0
31	MG	X	6168	1/1	0.56	0.67	-	100,100,100,100	0
31	MG	X	6154	1/1	0.90	0.67	-	96,96,96,96	0
31	MG	X	6111	1/1	0.71	0.41	-	98,98,98,98	0
31	MG	X	6096	1/1	0.93	0.33	-	99,99,99,99	0
31	MG	X	6141	1/1	0.78	0.38	-	87,87,87,87	0
31	MG	X	6009	1/1	0.94	0.30	-	50,50,50,50	0
31	MG	X	6048	1/1	0.95	0.57	-	66,66,66,66	0
31	MG	X	6098	1/1	0.87	0.20	-	71,71,71,71	0
31	MG	X	6035	1/1	0.76	0.46	-	80,80,80,80	0
31	MG	X	6123	1/1	0.93	0.54	-	89,89,89,89	0
31	MG	X	6175	1/1	0.85	0.54	-	121,121,121,121	0
31	MG	X	6052	1/1	0.81	0.43	-	86,86,86,86	0
31	MG	X	6128	1/1	0.96	0.21	-	131,131,131,131	0
31	MG	X	6146	1/1	0.89	0.15	-	125,125,125,125	0
31	MG	X	6112	1/1	0.71	0.34	-	80,80,80,80	0
31	MG	X	6113	1/1	0.93	0.58	-	143,143,143,143	0
31	MG	X	6057	1/1	0.95	0.68	-	92,92,92,92	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
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	6163	1/1	0.76	0.33	-	82,82,82,82	0
31	MG	X	6097	1/1	0.90	0.52	-	122,122,122,122	0
31	MG	X	6106	1/1	0.92	0.50	-	100,100,100,100	0
31	MG	Y	204	1/1	0.88	0.59	-	116,116,116,116	0
31	MG	X	6077	1/1	0.92	0.56	-	80,80,80,80	0
31	MG	X	6116	1/1	0.78	0.67	-	99,99,99,99	0
31	MG	X	6058	1/1	0.86	0.34	-	70,70,70,70	0
31	MG	X	6091	1/1	0.89	0.27	-	72,72,72,72	0
31	MG	Y	203	1/1	0.81	0.76	-	96,96,96,96	0
31	MG	X	6010	1/1	0.91	0.50	-	64,64,64,64	0
31	MG	X	6118	1/1	0.62	0.41	-	82,82,82,82	0
31	MG	X	6153	1/1	0.89	0.30	-	114,114,114,114	0
31	MG	X	6114	1/1	0.60	0.70	-	93,93,93,93	0
31	MG	X	6015	1/1	0.82	0.27	-	74,74,74,74	0
31	MG	X	6047	1/1	0.84	0.25	-	79,79,79,79	0
31	MG	X	6065	1/1	0.87	0.28	-	93,93,93,93	0
31	MG	X	6159	1/1	0.76	1.13	-	109,109,109,109	0
31	MG	X	6138	1/1	0.93	0.15	-	86,86,86,86	0
31	MG	X	6103	1/1	0.50	0.24	-	126,126,126,126	0
31	MG	X	6161	1/1	0.69	0.23	-	113,113,113,113	0
31	MG	Y	205	1/1	0.77	0.64	-	123,123,123,123	0
31	MG	X	6151	1/1	0.94	0.15	-	88,88,88,88	0
31	MG	X	6133	1/1	0.81	0.48	-	91,91,91,91	0
31	MG	X	6030	1/1	0.82	0.33	-	101,101,101,101	0
31	MG	X	6102	1/1	0.95	0.30	-	98,98,98,98	0
31	MG	X	6061	1/1	0.83	0.23	-	100,100,100,100	0
31	MG	X	6027	1/1	0.94	0.72	-	65,65,65,65	0
31	MG	X	6050	1/1	0.98	0.45	-	91,91,91,91	0
31	MG	X	6029	1/1	0.91	0.40	-	82,82,82,82	0
31	MG	X	6157	1/1	0.90	0.56	-	96,96,96,96	0
31	MG	X	6136	1/1	0.95	0.68	-	84,84,84,84	0
31	MG	X	6125	1/1	0.73	0.49	-	109,109,109,109	0
31	MG	X	6034	1/1	0.94	0.27	-	69,69,69,69	0
31	MG	X	6080	1/1	0.94	0.69	-	82,82,82,82	0
31	MG	X	6150	1/1	0.80	0.47	-	97,97,97,97	0
31	MG	X	6075	1/1	0.81	0.27	-	85,85,85,85	0
31	MG	X	6117	1/1	0.90	0.42	-	130,130,130,130	0
31	MG	X	6173	1/1	0.81	0.14	-	87,87,87,87	0
31	MG	X	6095	1/1	0.93	0.58	-	78,78,78,78	0
31	MG	X	6170	1/1	0.81	0.37	-	97,97,97,97	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
31	MG	X	6049	1/1	0.78	0.40	-	91,91,91,91	0
31	MG	H	201	1/1	0.90	0.14	-	104,104,104,104	0
31	MG	X	6130	1/1	0.86	0.41	-	132,132,132,132	0
31	MG	X	6122	1/1	0.90	0.36	-	84,84,84,84	0
31	MG	X	6121	1/1	0.93	0.60	-	85,85,85,85	0
31	MG	X	6176	1/1	0.69	0.55	-	73,73,73,73	0
31	MG	X	6020	1/1	0.83	0.44	-	76,76,76,76	0
31	MG	X	6082	1/1	0.94	0.68	-	105,105,105,105	0
31	MG	X	6069	1/1	0.91	0.34	-	65,65,65,65	0
31	MG	X	6067	1/1	0.97	0.18	-	72,72,72,72	0
31	MG	X	6070	1/1	0.81	0.47	-	69,69,69,69	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	6139	1/1	0.72	0.43	-	113,113,113,113	0
31	MG	X	6155	1/1	0.83	0.79	-	108,108,108,108	0
31	MG	X	6040	1/1	0.94	0.54	-	63,63,63,63	0
31	MG	X	6089	1/1	0.94	0.26	-	89,89,89,89	0

6.5 Other polymers [i](#)

There are no such residues in this entry.