



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 24, 2018 – 09:06 AM EST

PDB ID : 1Q7Y  
Title : Crystal Structure of CCdAP-Puromycin bound at the Peptidyl transferase center of the 50S ribosomal subunit  
Authors : Hansen, J.L.; Schmeing, T.M.; Moore, P.B.; Steitz, T.A.  
Deposited on : 2003-08-20  
Resolution : 3.20 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](mailto: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.

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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 : rb-20030736  
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) : rb-20030736

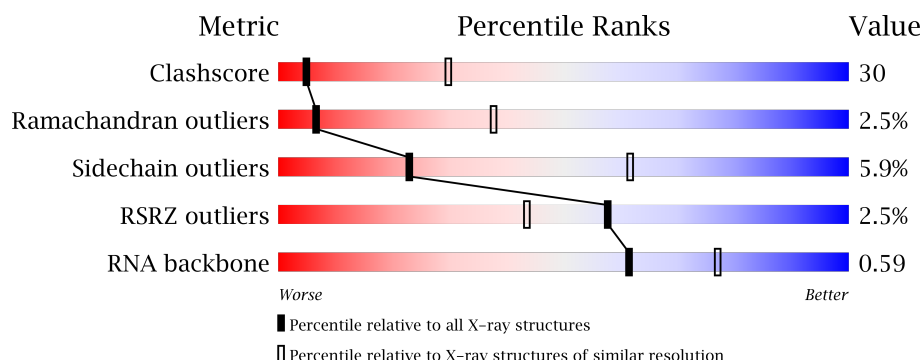
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	112137	1009 (3.20-3.20)
Ramachandran outliers	110173	1118 (3.22-3.18)
Sidechain outliers	110143	1117 (3.22-3.18)
RSRZ outliers	101464	1020 (3.22-3.18)
RNA backbone	2435	1045 (3.60-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	A	2922	<div> <div>0.1%</div> <div>32%</div> <div>45%</div> <div>15%</div> <div>6%</div> </div>
2	B	122	<div> <div>3%</div> <div>30%</div> <div>48%</div> <div>17%</div> <div>4%</div> </div>
3	5	3	<div> <div>33%</div> <div>67%</div> </div>
4	C	239	<div> <div>4%</div> <div>46%</div> <div>46%</div> <div>6%</div> </div>
5	D	337	<div> <div>42%</div> <div>52%</div> <div>6%</div> </div>


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Mol	Chain	Length	Quality of chain
6	E	246	
7	F	176	
8	G	177	
9	H	119	
10	I	348	
11	J	167	
12	K	145	
13	L	132	
14	M	164	
15	N	194	
16	O	186	
17	P	115	
18	Q	148	
19	R	95	
20	S	154	
21	T	84	
22	U	119	
23	V	66	
24	W	70	
25	X	154	
26	Y	91	
27	Z	240	
28	1	73	
29	2	56	
30	3	48	

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Mol	Chain	Length	Quality of chain
31	4	92	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
32	MG	1	8105	-	-	-	X
32	MG	A	8044	-	-	-	X
32	MG	A	8049	-	-	-	X
32	MG	A	8060	-	-	-	X
32	MG	A	8110	-	-	-	X
33	K	A	8201	-	-	-	X
34	NA	A	8303	-	-	-	X
34	NA	A	8321	-	-	-	X
34	NA	A	8323	-	-	-	X
34	NA	A	8331	-	-	-	X
34	NA	A	8332	-	-	-	X
34	NA	A	8335	-	-	-	X
34	NA	A	8340	-	-	-	X
34	NA	A	8350	-	-	-	X
34	NA	A	8356	-	-	-	X
34	NA	A	8361	-	-	-	X
34	NA	A	8362	-	-	-	X
34	NA	A	8369	-	-	-	X
34	NA	A	8371	-	-	-	X
34	NA	A	8374	-	-	-	X
34	NA	A	8377	-	-	-	X
34	NA	B	8383	-	-	-	X
34	NA	M	8380	-	-	-	X
34	NA	S	8386	-	-	-	X
35	CL	A	8505	-	-	-	X
35	CL	A	8510	-	-	-	X
35	CL	A	8511	-	-	-	X
35	CL	A	8513	-	-	-	X
35	CL	A	8515	-	-	-	X
35	CL	D	8519	-	-	-	X
35	CL	P	8508	-	-	-	X
37	PUY	5	78	-	-	-	X
38	CD	4	8404	-	-	X	-

## 2 Entry composition [i](#)

There are 39 unique types of molecules in this entry. The entry contains 98616 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 23S ribosomal rna.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	2754	Total	C	N	O	P	0	0	0
			59017	26346	10878	19048	2745			

- Molecule 2 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	122	Total	C	N	O	P	0	0	0
			2600	1160	472	847	121			

- Molecule 3 is DNA/RNA hybrid called CCdA-P-Puromycin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	5	3	Total	C	N	O	P	0	0	0
			58	28	11	17	2			

- Molecule 4 is a protein called 50S ribosomal protein L2P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	C	237	Total	C	N	O	S	0	0	0
			1754	1072	352	325	5			

- Molecule 5 is a protein called 50S ribosomal protein L3P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	D	337	Total	C	N	O	S	0	0	0
			2624	1616	493	510	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	?	-	PRO	DELETION	UNP P20279
D	310	ARG	PHE	CONFLICT	UNP P20279

- Molecule 6 is a protein called 50S ribosomal protein L4E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	E	246	Total	C	N	O	S	0	0	0
			1858	1131	344	382	1			

- Molecule 7 is a protein called 50S ribosomal protein L5P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	F	140	Total	C	N	O	S	0	0	0
			1094	685	195	210	4			

- Molecule 8 is a protein called 50S ribosomal protein L6P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	G	172	Total	C	N	O	S	0	0	0
			1357	840	224	289	4			

- Molecule 9 is a protein called 50S ribosomal protein L7Ae.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	H	119	Total	C	N	O	S	0	0	0
			885	552	141	191	1			

- Molecule 10 is a protein called Acidic ribosomal protein P0 homolog.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	I	29	Total	C	N	O	S	0	0	0
			240	149	39	51	1			

- Molecule 11 is a protein called L10 Ribosomal Protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	J	156	Total	C	N	O	S	0	0	0
			1215	766	233	212	4			

- Molecule 12 is a protein called 50S ribosomal protein L13P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	K	142	Total	C	N	O	S	0	0	0
			1119	696	199	221	3			

- Molecule 13 is a protein called 50S ribosomal protein L14P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	L	132	Total	C	N	O	S	0	0	0
			993	609	189	191	4			

- Molecule 14 is a protein called 50S ribosomal protein L15P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	M	145	Total	C	N	O	S	0	0	0
			1114	668	222	224				

- Molecule 15 is a protein called L15 Ribosomal Protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	N	194	Total	C	N	O	S	0	0	0
			1605	988	346	266	5			

- Molecule 16 is a protein called 50S ribosomal protein L18P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	O	186	Total	C	N	O	S	0	0	0
			1444	895	262	285	2			

- Molecule 17 is a protein called 50S ribosomal protein L18e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	P	115	Total	C	N	O	S	0	0	0
			864	529	161	174				

- Molecule 18 is a protein called 50S ribosomal protein L19E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	Q	143	Total	C	N	O	S	0	0	0
			1133	680	230	223				

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	71	LYS	TYR	CONFLICT	UNP P14119

- Molecule 19 is a protein called 50S ribosomal protein L21e.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
19	R	95	Total	C	N	O			
			734	450	141	143	0	0	0

- Molecule 20 is a protein called 50S ribosomal protein L22P.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
20	S	150	Total	C	N	O	S		
			1149	713	209	223	4	0	0

- Molecule 21 is a protein called 50S ribosomal protein L23P.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	T	81	Total	C	N	O	S		
			641	389	111	138	3	0	0

- Molecule 22 is a protein called 50S ribosomal protein L24P.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
22	U	119	Total	C	N	O			
			949	568	180	201		0	0

- Molecule 23 is a protein called 50S ribosomal protein L24E.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
23	V	53	Total	C	N	O	S		
			410	244	75	86	5	0	0

- Molecule 24 is a protein called 50S ribosomal protein L29P.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
24	W	65	Total	C	N	O	S		
			499	304	94	100	1	0	0

- Molecule 25 is a protein called 50S ribosomal protein L30P.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
25	X	154	Total	C	N	O	S		
			1195	737	209	243	6	0	0

- Molecule 26 is a protein called 50S ribosomal protein L31e.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	Y	82	Total	C	N	O	S	0	0	0
			654	402	129	122	1			

- Molecule 27 is a protein called 50S ribosomal protein L32E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	Z	142	Total	C	N	O	S	0	0	0
			1130	686	228	216				

- Molecule 28 is a protein called L37Ae 50S ribosomal protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	1	73	Total	C	N	O	S	0	0	0
			563	359	111	86	7			

- Molecule 29 is a protein called 50S ribosomal protein L37e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	2	56	Total	C	N	O	S	0	0	0
			430	258	86	82	4			

- Molecule 30 is a protein called 50S ribosomal protein L39e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	3	46	Total	C	N	O	S	0	0	0
			393	238	86	68	1			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
3	?	-	ARG	DELETION	UNP P22452

- Molecule 31 is a protein called 50S ribosomal protein L44E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	4	92	Total	C	N	O	S	0	0	0
			755	458	153	137	7			

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	1	1	Total Mg 1 1	0	0
32	B	1	Total Mg 1 1	0	0
32	5	1	Total Mg 1 1	0	0
32	C	1	Total Mg 1 1	0	0
32	Z	1	Total Mg 1 1	0	0
32	A	109	Total Mg 109 109	0	0
32	4	1	Total Mg 1 1	0	0
32	U	1	Total Mg 1 1	0	0
32	L	1	Total Mg 1 1	0	0

- Molecule 33 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	A	2	Total K 2 2	0	0

- Molecule 34 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	J	2	Total Na 2 2	0	0
34	K	1	Total Na 1 1	0	0
34	E	1	Total Na 1 1	0	0
34	B	2	Total Na 2 2	0	0
34	C	1	Total Na 1 1	0	0
34	A	72	Total Na 72 72	0	0
34	T	1	Total Na 1 1	0	0
34	N	1	Total Na 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	R	1	Total 1	Na 1	0	0
34	S	3	Total 3	Na 3	0	0
34	M	1	Total 1	Na 1	0	0

- Molecule 35 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

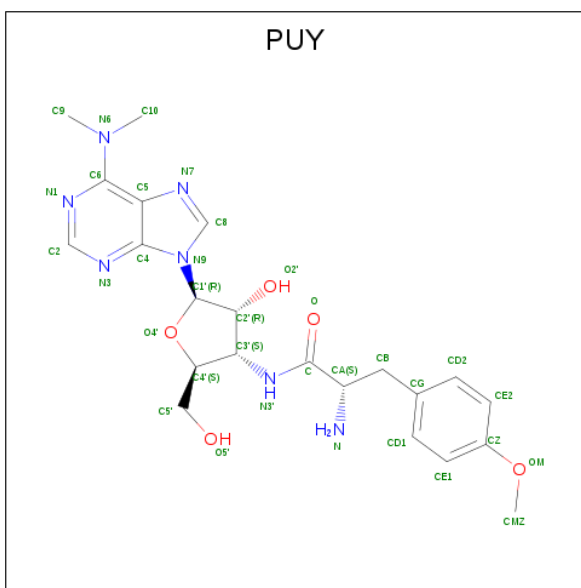
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	P	1	Total 1	Cl 1	0	0
35	D	1	Total 1	Cl 1	0	0
35	K	3	Total 3	Cl 3	0	0
35	C	1	Total 1	Cl 1	0	0
35	Z	1	Total 1	Cl 1	0	0
35	A	11	Total 11	Cl 11	0	0
35	4	1	Total 1	Cl 1	0	0
35	N	1	Total 1	Cl 1	0	0
35	O	1	Total 1	Cl 1	0	0
35	S	1	Total 1	Cl 1	0	0

- Molecule 36 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
36	5	1	Total	O	P	0	0
			3	2	1		

- Molecule 37 is PUROMYCIN (three-letter code: PUY) (formula: C<sub>22</sub>H<sub>29</sub>N<sub>7</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
37	5	1	Total	C	N	O	0	0
			34	22	7	5		

- Molecule 38 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
38	P	1	Total Cd 1 1	0	0
38	2	1	Total Cd 1 1	0	0
38	1	1	Total Cd 1 1	0	0
38	4	1	Total Cd 1 1	0	0
38	V	1	Total Cd 1 1	0	0

- Molecule 39 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
39	A	5861	Total O 5861 5861	0	0
39	B	154	Total O 154 154	0	0
39	5	6	Total O 6 6	0	0
39	C	123	Total O 123 123	0	0
39	D	149	Total O 149 149	0	0
39	E	178	Total O 178 178	0	0
39	F	50	Total O 50 50	0	0
39	G	46	Total O 46 46	0	0
39	H	27	Total O 27 27	0	0
39	I	20	Total O 20 20	0	0
39	J	75	Total O 75 75	0	0
39	K	56	Total O 56 56	0	0
39	L	60	Total O 60 60	0	0
39	M	90	Total O 90 90	0	0
39	N	128	Total O 128 128	0	0

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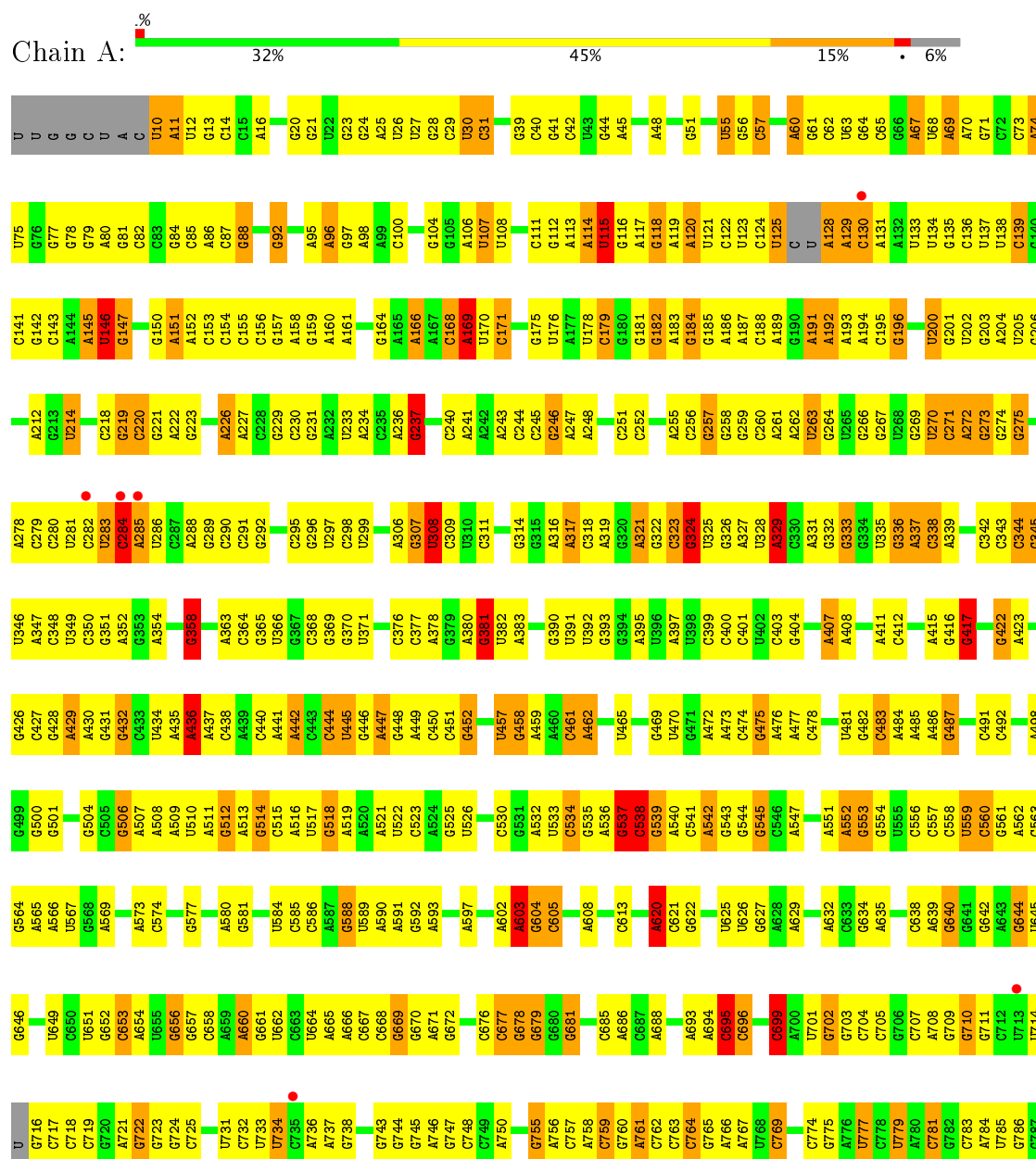
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
39	O	63	Total 63	O 63	0	0
39	P	45	Total 45	O 45	0	0
39	Q	62	Total 62	O 62	0	0
39	R	53	Total 53	O 53	0	0
39	S	86	Total 86	O 86	0	0
39	T	36	Total 36	O 36	0	0
39	U	42	Total 42	O 42	0	0
39	V	30	Total 30	O 30	0	0
39	W	15	Total 15	O 15	0	0
39	X	73	Total 73	O 73	0	0
39	Y	30	Total 30	O 30	0	0
39	Z	99	Total 99	O 99	0	0
39	1	36	Total 36	O 36	0	0
39	2	63	Total 63	O 63	0	0
39	3	42	Total 42	O 42	0	0
39	4	73	Total 73	O 73	0	0

### 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: 23S ribosomal rna



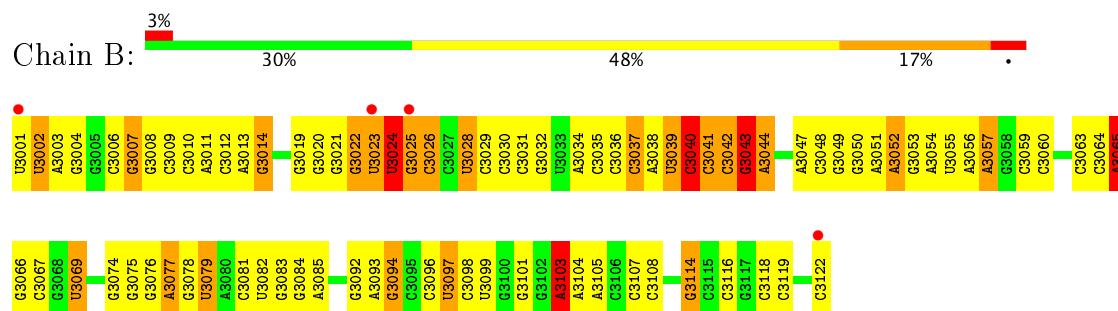
U1758	A1815	G1540	C1469	G1401	U1336	G1273	G1211	A1150	G1074	A	C930	A857	A788
A1687	G1618	G1543	A1470	G1402	A1337	A1274	C1212	G1151	G1075	C	C931	U858	C789
A1688	G1619	U1544	A1471	U1405	G1338	U1275	C1213	A1152	G1076	A	U932	C859	A790
A1689	G1620	U1545	C1472	U1406	G1339	U1276	G1214	C1153	C999	C	U933	U860	A791
A1690	G1621	U1546	C1473	A1407	G1340	A1277	A1215	G1154	C1000	C	U934	A861	C792
A1691	G1622	U1547	C1474	U1408	C1341	A1278	G1216	G1155	C1080	U	U935	U862	A793
A1692	G1623	U1548	C1475	U1409	C1342	U1279	G1217	C1156	A1081	U	U936	U863	U794
A1693	G1624	C1549	A1476	U1410	G1343	A1280	U1218	C1157	A1082	C	C937	A867	C795
A1694	G1625	U1550	A1477	G1410	C1344	U1281	U1219	G1158	C1083	U	U938	C868	A796
A1695	G1626	C1551	U1478	U1411	A1345	U1282	U1220	G1159	C1084	U	U939	C869	C797
A1696	G1627	C1552	U1479	U1412	U1346	G1283	G1221	G1160	C1085	A	U940	C870	A798
A1697	G1628	U1553	G1481	A1413	U1347	U1284	A1222	A1161	C1086	C	U941	C871	C799
A1698	G1629	U1554	C1482	U1414	U1348	U1285	G1223	G1162	U1087	C	U942	G870	C800
A1699	G1630	C1555	C1483	G1415	G1349	A1286	G1224	G1163	A1088	U	U943	U872	U801
A1700	G1631	U1556	G1484	G1416	U1350	A1287	C1225	U1164	A1089	U	U944	A873	C802
A1701	G1632	C1557	A1485	C1417	G1351	U1288	G1226	G1165	C1090	U	U945	A874	C803
A1702	G1633	U1558	U1486	U1418	G1352	C1289	C1227	A1166	U1091	U	U946	A875	C804
A1703	G1634	U1559	U1487	U1419	C1353	U1290	G1228	A1167	A1092	U	U947	A876	C805
A1704	G1635	U1560	C1488	C1420	G1354	G1291	C1229	G1168	A1093	U	U948	A877	C806
A1705	G1636	U1561	G1489	U1421	C1355	U1292	G1230	C1169	A1094	U	U949	A878	C807
A1706	G1637	C1562	G1490	U1422	A1356	U1293	A1231	U1170	A1095	U	U950	C879	C808
A1707	G1638	U1563	G1491	C1423	A1357	U1294	A1232	A1171	C1096	U	U951	C880	C809
A1708	G1639	C1564	A1492	U1424	A1358	G1295	U1233	U1172	A1097	U	U952	C881	C810
A1709	G1640	U1565	A1493	A1425	A1359	A1296	U1234	A1173	C1098	U	U953	C882	C811
A1710	G1641	C1566	A1494	A1426	U1360	U1297	G1235	A1174	A1099	U	U954	A883	C812
A1711	G1642	U1567	G1495	C1430	C1361	G1298	A1236	A1175	C1100	U	U955	C884	C813
A1712	G1643	U1568	G1496	U1431	U1362	U1299	U1237	G1176	A1101	U	U956	A885	C814
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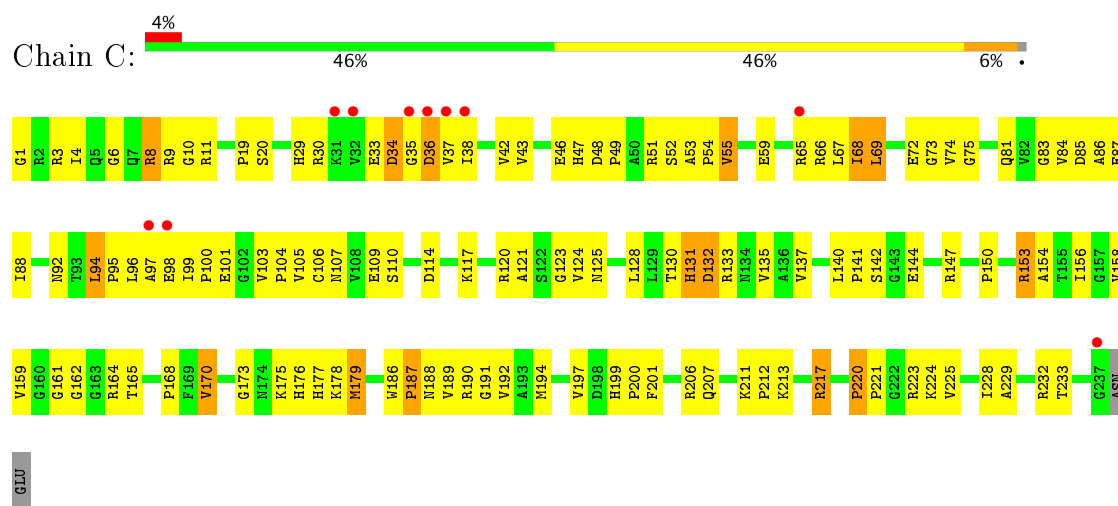
• Molecule 2: 5S ribosomal RNA



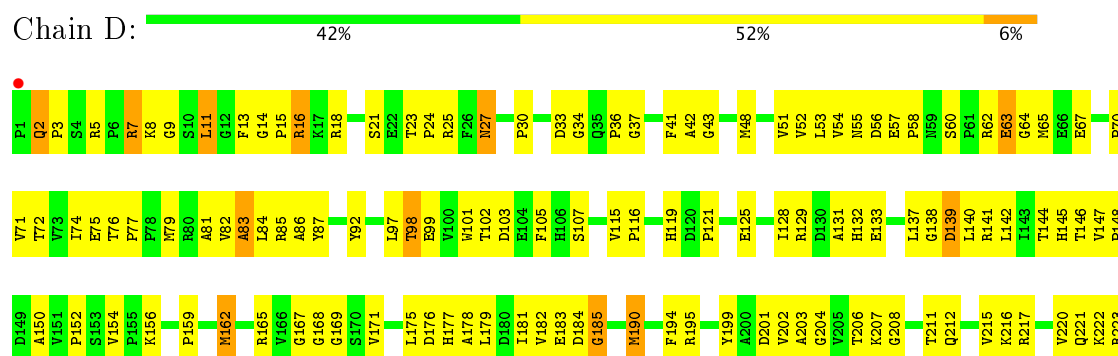
• Molecule 3: CCdA-P-Puromycin

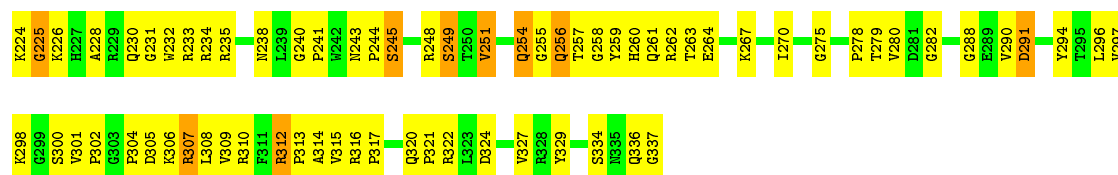


• Molecule 4: 50S ribosomal protein L2P



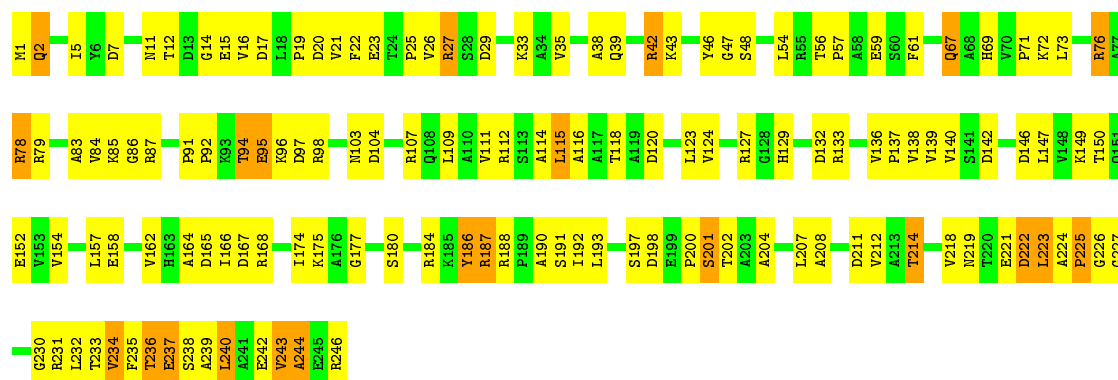
• Molecule 5: 50S ribosomal protein L3P





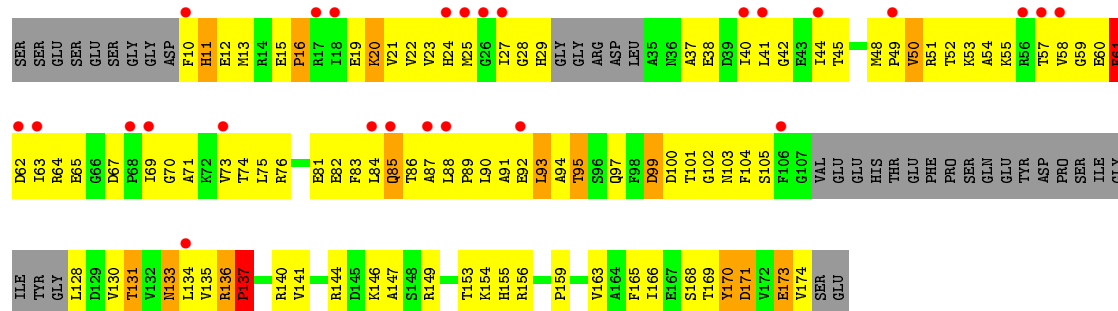
• Molecule 6: 50S ribosomal protein L4E

Chain E: 44% 47% 9%



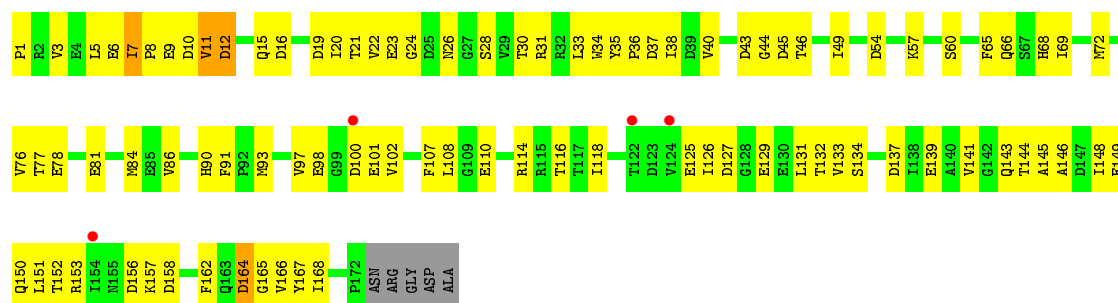
• Molecule 7: 50S ribosomal protein L5P

Chain F: 15% 23% 47% 8% 20%

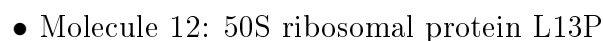


• Molecule 8: 50S ribosomal protein L6P

Chain G: 2% 45% 50%



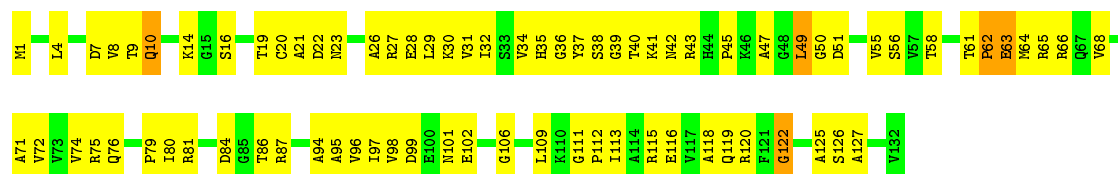
• Molecule 9: 50S ribosomal protein L7Ae





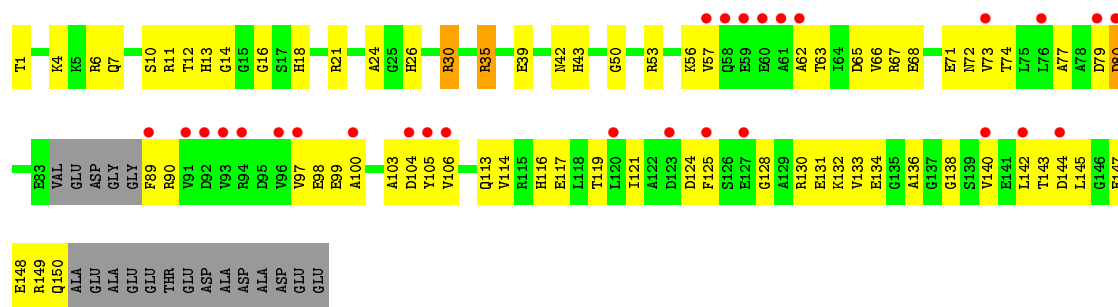
• Molecule 13: 50S ribosomal protein L14P

Chain L: 41% 55%



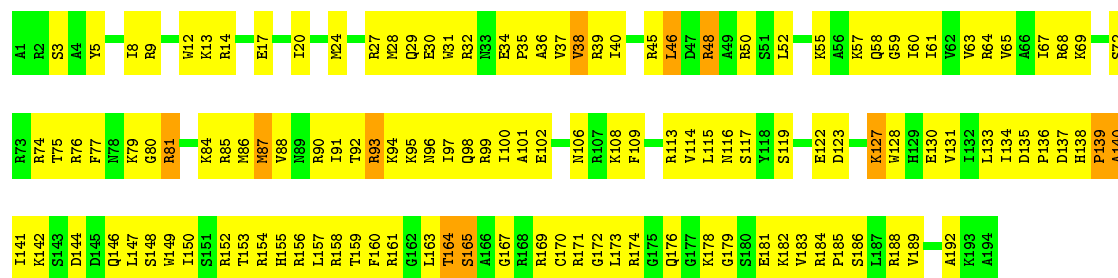
• Molecule 14: 50S ribosomal protein L15P

Chain M: 17% 45% 41% 12%



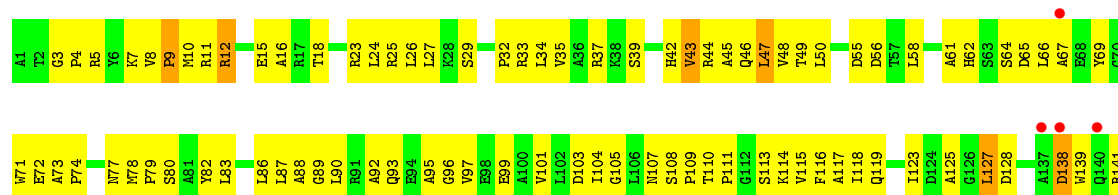
• Molecule 15: L15 Ribosomal Protein

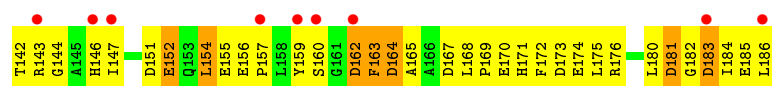
Chain N: 34% 61% 6%



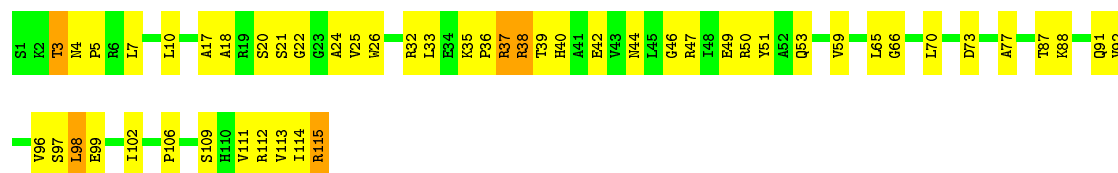
• Molecule 16: 50S ribosomal protein L18P

Chain O: 7% 35% 58% 7%

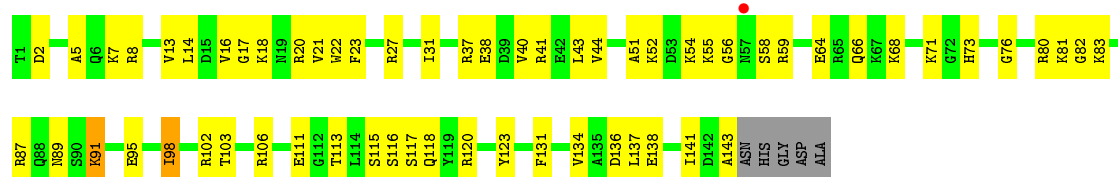




• Molecule 17: 50S ribosomal protein L18e



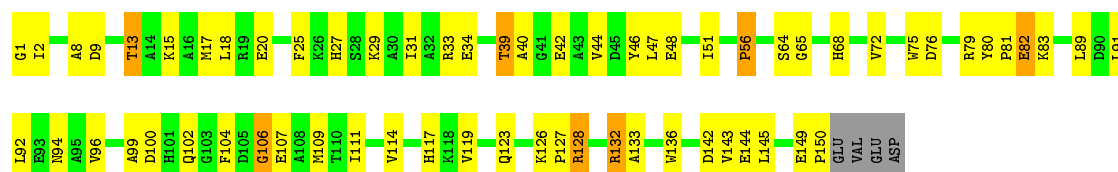
• Molecule 18: 50S ribosomal protein L19E



• Molecule 19: 50S ribosomal protein L21e



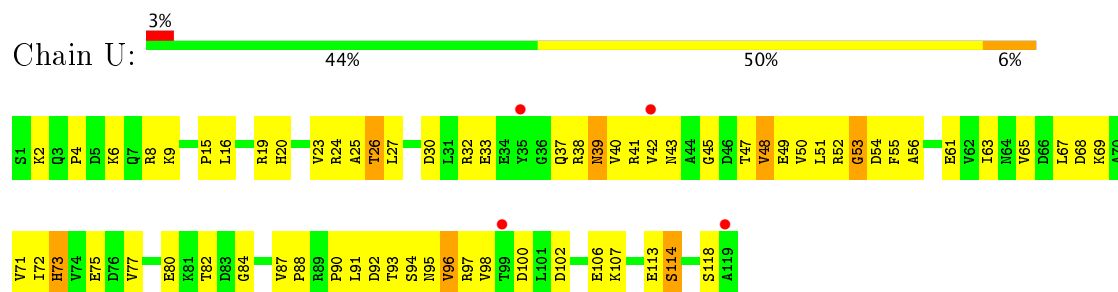
• Molecule 20: 50S ribosomal protein L22P



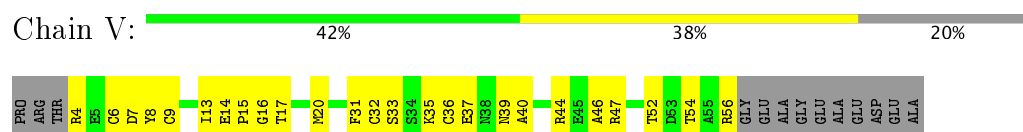
• Molecule 21: 50S ribosomal protein L23P



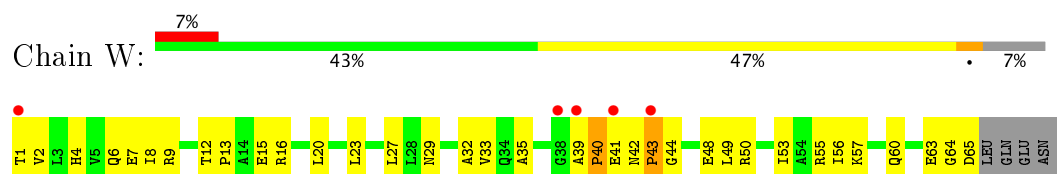
- Molecule 22: 50S ribosomal protein L24P



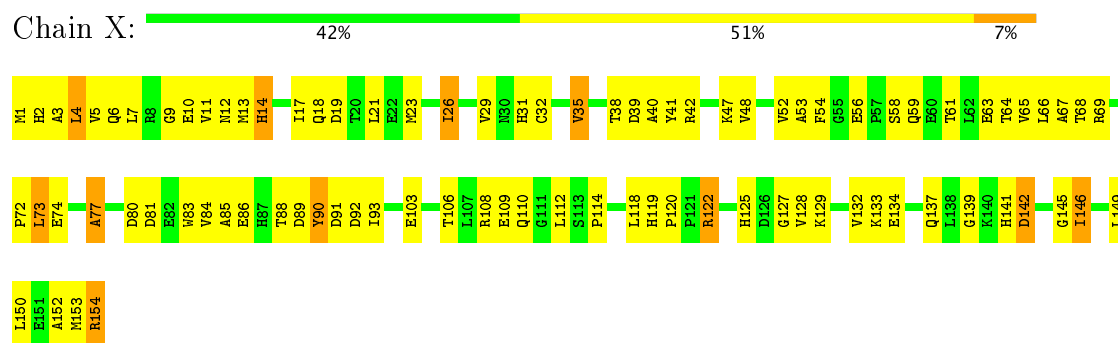
- Molecule 23: 50S ribosomal protein L24E



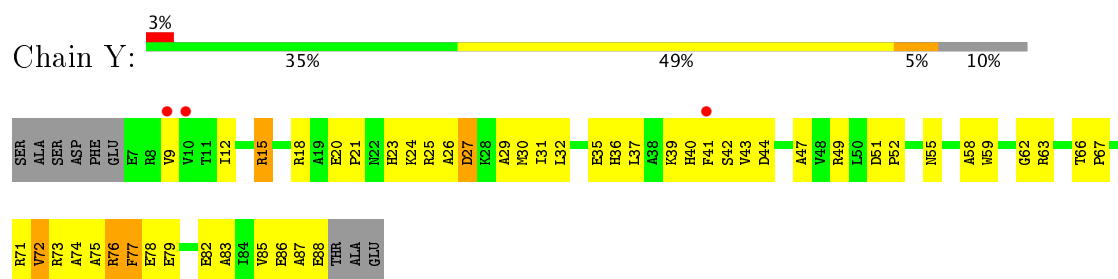
- Molecule 24: 50S ribosomal protein L29P



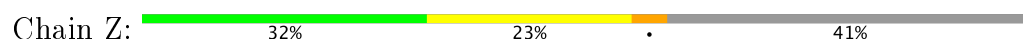
- Molecule 25: 50S ribosomal protein L30P

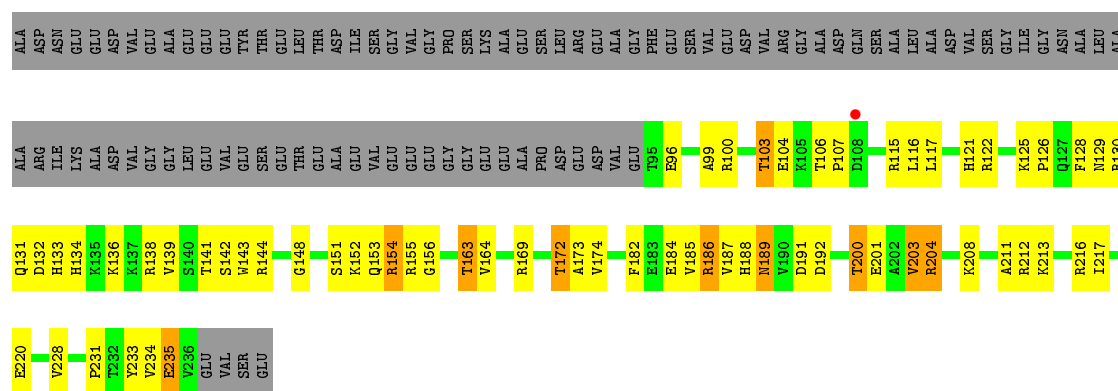


- Molecule 26: 50S ribosomal protein L31e

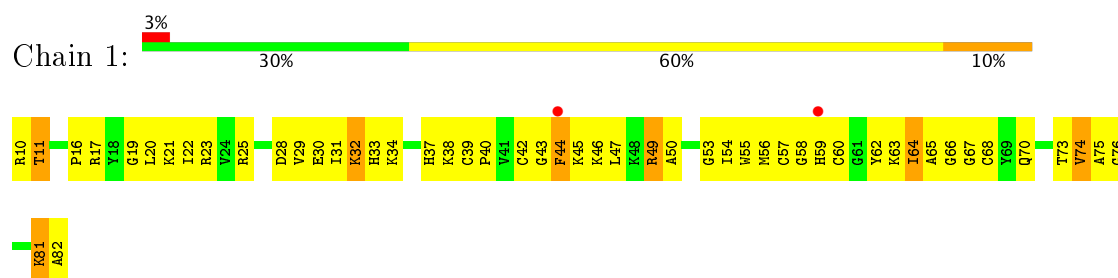


- Molecule 27: 50S ribosomal protein L32E

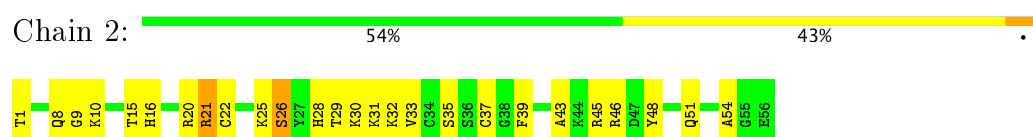




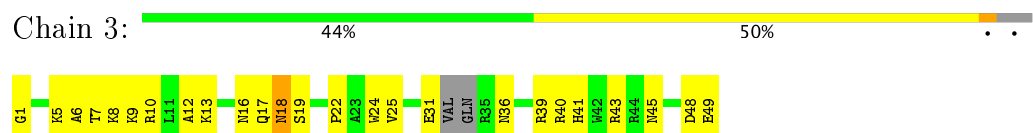
• Molecule 28: L37Ae 50S ribosomal protein



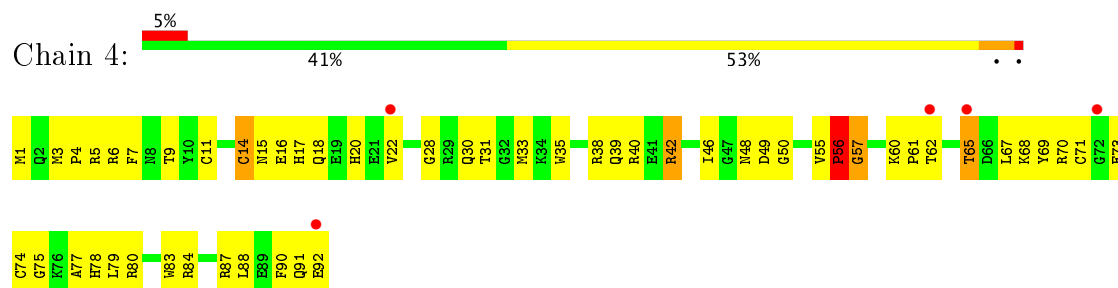
• Molecule 29: 50S ribosomal protein L37e



• Molecule 30: 50S ribosomal protein L39e



• Molecule 31: 50S ribosomal protein L44E





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	212.90Å 300.47Å 575.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.99 – 3.20 49.89 – 2.98	Depositor EDS
% Data completeness (in resolution range)	92.1 (19.99-3.20) 88.4 (49.89-2.98)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.47 (at 2.96Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.225 , 0.280 0.211 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	55.2	Xtriage
Anisotropy	0.709	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 59.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	98616	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.45% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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, CL, NA, PO4, CD, PUY, K

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	A	1.03	52/66076 (0.1%)	0.96	138/103052 (0.1%)
2	B	0.91	0/2905	0.95	10/4528 (0.2%)
3	5	1.87	0/64	1.14	0/97
4	C	0.76	0/1787	0.95	1/2409 (0.0%)
5	D	0.73	0/2689	0.96	1/3652 (0.0%)
6	E	0.77	0/1883	0.97	1/2551 (0.0%)
7	F	0.63	0/1111	0.79	0/1498
8	G	0.71	0/1382	0.85	1/1880 (0.1%)
9	H	0.69	0/896	0.85	0/1219
10	I	0.99	0/241	0.91	0/324
11	J	0.79	0/1246	1.05	4/1686 (0.2%)
12	K	0.76	0/1135	0.89	0/1530
13	L	0.80	1/1003 (0.1%)	1.00	0/1351
14	M	0.75	0/1126	1.00	1/1504 (0.1%)
15	N	0.89	0/1633	1.04	2/2180 (0.1%)
16	O	0.70	0/1473	0.94	0/1999
17	P	0.78	0/873	0.97	2/1181 (0.2%)
18	Q	0.74	0/1143	0.91	0/1521
19	R	0.77	0/748	1.00	2/1005 (0.2%)
20	S	0.81	0/1172	0.99	1/1578 (0.1%)
21	T	0.79	0/648	0.94	0/875
22	U	0.76	0/957	0.95	0/1289
23	V	0.74	0/417	0.88	0/562
24	W	0.66	0/502	0.81	0/675
25	X	0.75	1/1218 (0.1%)	0.94	0/1655
26	Y	0.74	0/664	0.94	0/895
27	Z	0.74	0/1146	0.93	0/1536
28	1	0.79	0/575	0.98	0/763
29	2	0.87	0/437	1.08	0/578
30	3	0.70	0/398	0.86	0/527
31	4	0.81	1/771 (0.1%)	0.97	1/1024 (0.1%)
All	All	0.95	55/98319 (0.1%)	0.96	165/147124 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	1	386
2	B	1	12
5	D	0	2
6	E	0	1
25	X	0	1
29	2	0	1
All	All	2	403

The worst 5 of 55 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2638	G	P-OP2	12.82	1.70	1.49
1	A	2636	C	C3'-O3'	11.93	1.58	1.42
1	A	2619	U	C3'-O3'	10.66	1.57	1.42
1	A	2620	U	C5'-C4'	-10.62	1.38	1.51
1	A	2619	U	C2'-O2'	-10.44	1.28	1.41

The worst 5 of 165 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1164	U	OP1-P-O3'	-19.52	62.25	105.20
1	A	1164	U	OP2-P-O3'	-16.77	68.31	105.20
1	A	1165	G	O5'-P-OP1	-15.53	91.72	105.70
1	A	1563	G	C2'-C3'-O3'	10.27	132.10	109.50
1	A	1942	A	C5'-C4'-C3'	9.66	131.46	116.00

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	1563	G	C3'
2	B	3024	U	C3'

5 of 403 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	16	A	Sidechain
1	A	30	U	Sidechain
1	A	44	G	Sidechain

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Mol	Chain	Res	Type	Group
1	A	55	U	Sidechain
1	A	57	C	Sidechain

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	59017	0	29801	2017	0
2	B	2600	0	1326	128	0
3	5	58	0	34	2	0
4	C	1754	0	1763	155	0
5	D	2624	0	2533	238	0
6	E	1858	0	1816	194	0
7	F	1094	0	1085	172	0
8	G	1357	0	1266	103	0
9	H	885	0	854	74	0
10	I	240	0	231	33	0
11	J	1215	0	1215	194	0
12	K	1119	0	1098	80	0
13	L	993	0	1027	88	0
14	M	1114	0	1072	85	0
15	N	1605	0	1676	207	0
16	O	1444	0	1401	182	0
17	P	864	0	873	65	0
18	Q	1133	0	1127	74	0
19	R	734	0	728	62	0
20	S	1149	0	1122	87	0
21	T	641	0	605	27	0
22	U	949	0	923	87	0
23	V	410	0	364	44	0
24	W	499	0	511	40	0
25	X	1195	0	1137	120	0
26	Y	654	0	653	64	0
27	Z	1130	0	1133	81	0
28	1	563	0	599	76	0
29	2	430	0	427	38	0
30	3	393	0	406	34	0
31	4	755	0	730	64	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	1	1	0	0	0	0
32	4	1	0	0	0	0
32	5	1	0	0	0	0
32	A	109	0	0	0	0
32	B	1	0	0	0	0
32	C	1	0	0	0	0
32	L	1	0	0	0	0
32	U	1	0	0	0	0
32	Z	1	0	0	0	0
33	A	2	0	0	0	0
34	A	72	0	0	0	0
34	B	2	0	0	0	0
34	C	1	0	0	1	0
34	E	1	0	0	0	0
34	J	2	0	0	0	0
34	K	1	0	0	0	0
34	M	1	0	0	0	0
34	N	1	0	0	0	0
34	R	1	0	0	0	0
34	S	3	0	0	0	0
34	T	1	0	0	0	0
35	4	1	0	0	0	0
35	A	11	0	0	2	0
35	C	1	0	0	1	0
35	D	1	0	0	0	0
35	K	3	0	0	2	0
35	N	1	0	0	1	0
35	O	1	0	0	1	0
35	P	1	0	0	1	0
35	S	1	0	0	0	0
35	Z	1	0	0	0	0
36	5	3	0	0	1	0
37	5	34	0	28	0	0
38	1	1	0	0	0	0
38	2	1	0	0	0	0
38	4	1	0	0	2	0
38	P	1	0	0	0	0
38	V	1	0	0	0	0
39	1	36	0	0	15	0
39	2	63	0	0	13	0
39	3	42	0	0	7	0
39	4	73	0	0	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
39	5	6	0	0	0	0
39	A	5861	0	0	566	2
39	B	154	0	0	27	0
39	C	123	0	0	34	0
39	D	149	0	0	35	0
39	E	178	0	0	56	0
39	F	50	0	0	34	0
39	G	46	0	0	17	0
39	H	27	0	0	14	0
39	I	20	0	0	5	0
39	J	75	0	0	34	0
39	K	56	0	0	10	0
39	L	60	0	0	20	0
39	M	90	0	0	27	0
39	N	128	0	0	35	0
39	O	63	0	0	41	0
39	P	45	0	0	21	0
39	Q	62	0	0	11	0
39	R	53	0	0	10	0
39	S	86	0	0	15	0
39	T	36	0	0	6	0
39	U	42	0	0	14	0
39	V	30	0	0	10	0
39	W	15	0	0	5	1
39	X	73	0	0	20	0
39	Y	30	0	0	11	0
39	Z	99	0	0	19	0
All	All	98616	0	59564	4529	2

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 30.

The worst 5 of 4529 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)
1:A:871:G:H5'	1:A:871:G:C8	1.74	1.23
30:3:39:ARG:HG2	39:3:3143:HOH:O	1.36	1.22
2:B:3006:C:H5''	16:O:37:ARG:NH1	1.55	1.19
1:A:1702:U:H5''	39:A:6685:HOH:O	1.35	1.19
1:A:871:G:H5'	1:A:871:G:H8	1.02	1.18

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:A:5574:HOH:O	39:W:2786:HOH:O[4_565]	2.14	0.06
39:A:3438:HOH:O	39:A:9956:HOH:O[5_445]	2.17	0.03

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	C	235/239 (98%)	204 (87%)	23 (10%)	8 (3%)	4	28
5	D	335/337 (99%)	297 (89%)	28 (8%)	10 (3%)	5	32
6	E	244/246 (99%)	206 (84%)	34 (14%)	4 (2%)	11	50
7	F	134/176 (76%)	95 (71%)	26 (19%)	13 (10%)	1	4
8	G	170/177 (96%)	160 (94%)	9 (5%)	1 (1%)	28	72
9	H	117/119 (98%)	105 (90%)	10 (8%)	2 (2%)	11	48
10	I	25/348 (7%)	23 (92%)	2 (8%)	0	100	100
11	J	152/167 (91%)	130 (86%)	13 (9%)	9 (6%)	2	15
12	K	140/145 (97%)	125 (89%)	11 (8%)	4 (3%)	5	33
13	L	130/132 (98%)	110 (85%)	15 (12%)	5 (4%)	4	25
14	M	141/164 (86%)	114 (81%)	25 (18%)	2 (1%)	13	53
15	N	192/194 (99%)	167 (87%)	22 (12%)	3 (2%)	11	50
16	O	184/186 (99%)	153 (83%)	23 (12%)	8 (4%)	3	23
17	P	113/115 (98%)	107 (95%)	4 (4%)	2 (2%)	10	47
18	Q	141/148 (95%)	129 (92%)	12 (8%)	0	100	100
19	R	93/95 (98%)	89 (96%)	3 (3%)	1 (1%)	17	58
20	S	148/154 (96%)	132 (89%)	15 (10%)	1 (1%)	25	68
21	T	79/84 (94%)	75 (95%)	3 (4%)	1 (1%)	14	55

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
22	U	117/119 (98%)	103 (88%)	11 (9%)	3 (3%)	6	36
23	V	51/66 (77%)	45 (88%)	5 (10%)	1 (2%)	9	44
24	W	63/70 (90%)	56 (89%)	5 (8%)	2 (3%)	5	30
25	X	152/154 (99%)	141 (93%)	8 (5%)	3 (2%)	9	44
26	Y	80/91 (88%)	69 (86%)	8 (10%)	3 (4%)	4	25
27	Z	140/240 (58%)	133 (95%)	7 (5%)	0	100	100
28	1	71/73 (97%)	58 (82%)	11 (16%)	2 (3%)	6	34
29	2	54/56 (96%)	47 (87%)	7 (13%)	0	100	100
30	3	42/48 (88%)	42 (100%)	0	0	100	100
31	4	90/92 (98%)	81 (90%)	7 (8%)	2 (2%)	8	41
All	All	3633/4235 (86%)	3196 (88%)	347 (10%)	90 (2%)	6	38

5 of 90 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	D	139	ASP
7	F	11	HIS
7	F	93	LEU
7	F	95	THR
7	F	173	GLU

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	C	179/181 (99%)	167 (93%)	12 (7%)	19	56
5	D	282/282 (100%)	264 (94%)	18 (6%)	20	59
6	E	193/193 (100%)	173 (90%)	20 (10%)	8	33
7	F	117/147 (80%)	107 (92%)	10 (8%)	12	44
8	G	152/155 (98%)	145 (95%)	7 (5%)	31	70
9	H	92/92 (100%)	89 (97%)	3 (3%)	43	78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	I	27/283 (10%)	26 (96%)	1 (4%)	39	75
11	J	122/122 (100%)	112 (92%)	10 (8%)	13	47
12	K	118/121 (98%)	107 (91%)	11 (9%)	10	38
13	L	106/106 (100%)	102 (96%)	4 (4%)	38	74
14	M	112/126 (89%)	108 (96%)	4 (4%)	40	76
15	N	166/166 (100%)	156 (94%)	10 (6%)	22	61
16	O	149/149 (100%)	142 (95%)	7 (5%)	30	69
17	P	93/93 (100%)	88 (95%)	5 (5%)	26	65
18	Q	113/116 (97%)	108 (96%)	5 (4%)	33	70
19	R	79/79 (100%)	75 (95%)	4 (5%)	28	66
20	S	117/121 (97%)	112 (96%)	5 (4%)	33	71
21	T	71/73 (97%)	70 (99%)	1 (1%)	71	90
22	U	105/105 (100%)	100 (95%)	5 (5%)	30	68
23	V	44/52 (85%)	44 (100%)	0	100	100
24	W	51/56 (91%)	51 (100%)	0	100	100
25	X	130/130 (100%)	122 (94%)	8 (6%)	21	60
26	Y	66/73 (90%)	61 (92%)	5 (8%)	15	51
27	Z	120/195 (62%)	109 (91%)	11 (9%)	11	38
28	1	56/56 (100%)	50 (89%)	6 (11%)	8	31
29	2	46/46 (100%)	44 (96%)	2 (4%)	33	71
30	3	42/44 (96%)	41 (98%)	1 (2%)	54	84
31	4	79/79 (100%)	76 (96%)	3 (4%)	38	74
All	All	3027/3441 (88%)	2849 (94%)	178 (6%)	23	62

5 of 178 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	J	150	LYS
14	M	117	GLU
27	Z	231	PRO
12	K	47	THR
12	K	127	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 96 such sidechains are listed below:

Mol	Chain	Res	Type
14	M	41	HIS
18	Q	50	GLN
29	2	28	HIS
14	M	58	GLN
16	O	107	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2747/2922 (94%)	259 (9%)	44 (1%)
2	B	121/122 (99%)	19 (15%)	5 (4%)
3	5	1/3 (33%)	0	0
All	All	2869/3047 (94%)	278 (9%)	49 (1%)

5 of 278 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	11	A
1	A	31	C
1	A	60	A
1	A	67	A
1	A	69	A

5 of 49 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	1246	A
1	A	1450	C
2	B	3024	U
1	A	1377	C
1	A	1504	A

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 234 ligands modelled in this entry, 232 are monoatomic - leaving 2 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
36	PO4	5	77	3,37	0,2,4	0.00	-	0,1,6	0.00	-
37	PUY	5	78	36	31,37,37	3.09	11 (35%)	34,53,53	2.10	10 (29%)

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
36	PO4	5	77	3,37	-	0/0/0/0	0/0/0/0
37	PUY	5	78	36	-	0/20/40/40	0/4/4/4

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	5	78	PUY	OM-CMZ	-4.77	1.28	1.42
37	5	78	PUY	C9-N6	-4.00	1.36	1.45
37	5	78	PUY	C10-N6	-3.53	1.37	1.45
37	5	78	PUY	C8-N7	-2.09	1.30	1.34
37	5	78	PUY	CB-CG	2.55	1.57	1.51

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	5	78	PUY	CG-CB-CA	-5.36	103.18	114.33
37	5	78	PUY	O-C-N3'	-4.10	115.18	122.90
37	5	78	PUY	CB-CA-C	-3.69	101.63	108.37
37	5	78	PUY	C3'-N3'-C	-2.90	118.83	123.21
37	5	78	PUY	CE1-CD1-CG	-2.71	117.27	121.02

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
36	5	77	PO4	1	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	2754/2922 (94%)	-0.19	32 (1%) 79 67	24, 50, 96, 142	0
2	B	122/122 (100%)	0.04	4 (3%) 47 31	36, 65, 94, 147	0
3	5	3/3 (100%)	0.00	0 100 100	53, 53, 56, 62	0
4	C	237/239 (99%)	0.11	10 (4%) 37 24	29, 59, 91, 111	0
5	D	337/337 (100%)	-0.20	1 (0%) 93 92	23, 55, 83, 90	0
6	E	246/246 (100%)	-0.21	0 100 100	29, 54, 76, 85	0
7	F	140/176 (79%)	1.04	26 (18%) 1 1	62, 101, 118, 131	0
8	G	172/177 (97%)	0.31	4 (2%) 61 46	40, 69, 91, 96	0
9	H	119/119 (100%)	0.55	10 (8%) 12 7	58, 81, 101, 106	0
10	I	29/348 (8%)	1.62	11 (37%) 0 0	82, 96, 102, 103	0
11	J	156/167 (93%)	-0.08	1 (0%) 89 83	33, 54, 85, 93	0
12	K	142/145 (97%)	-0.26	0 100 100	32, 48, 71, 87	0
13	L	132/132 (100%)	-0.28	0 100 100	28, 51, 73, 82	0
14	M	145/164 (88%)	0.67	28 (19%) 1 1	24, 76, 110, 119	0
15	N	194/194 (100%)	-0.23	0 100 100	37, 52, 69, 78	0
16	O	186/186 (100%)	0.37	13 (6%) 17 10	43, 70, 109, 120	0
17	P	115/115 (100%)	-0.11	0 100 100	48, 61, 81, 85	0
18	Q	143/148 (96%)	0.03	1 (0%) 87 80	40, 62, 75, 80	0
19	R	95/95 (100%)	-0.15	0 100 100	29, 49, 59, 74	0
20	S	150/154 (97%)	-0.30	0 100 100	31, 47, 66, 72	0
21	T	81/84 (96%)	0.10	3 (3%) 42 27	53, 70, 85, 90	0
22	U	119/119 (100%)	0.46	4 (3%) 46 30	48, 63, 85, 94	0
23	V	53/66 (80%)	-0.13	0 100 100	43, 57, 74, 81	0
24	W	65/70 (92%)	0.73	5 (7%) 14 8	61, 81, 110, 114	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
25	X	154/154 (100%)	-0.39	0 100 100	37, 49, 67, 76	0
26	Y	82/91 (90%)	0.11	3 (3%) 42 27	38, 62, 81, 97	0
27	Z	142/240 (59%)	-0.12	1 (0%) 87 80	30, 51, 74, 89	0
28	1	73/73 (100%)	-0.04	2 (2%) 55 40	52, 66, 80, 84	0
29	2	56/56 (100%)	-0.31	0 100 100	25, 40, 46, 48	0
30	3	46/48 (95%)	0.09	0 100 100	43, 65, 86, 95	0
31	4	92/92 (100%)	0.30	5 (5%) 26 15	36, 62, 72, 78	0
All	All	6580/7282 (90%)	-0.05	164 (2%) 58 43	23, 56, 97, 147	0

The worst 5 of 164 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
14	M	104	ASP	6.4
16	O	186	LEU	5.5
10	I	27	ILE	5.3
14	M	105	TYR	5.0
2	B	3001	U	4.5

## 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. 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
34	NA	A	8356	1/1	0.92	0.60	76.89	86,86,86,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
34	NA	A	8303	1/1	0.76	0.41	26.22	42,42,42,42	0
34	NA	A	8323	1/1	0.71	0.49	23.80	62,62,62,62	0
35	CL	A	8515	1/1	0.85	0.46	16.64	131,131,131,131	0
34	NA	A	8362	1/1	0.90	0.27	12.58	38,38,38,38	0
34	NA	A	8377	1/1	0.93	0.36	11.03	70,70,70,70	0
32	MG	A	8049	1/1	0.96	0.30	9.14	49,49,49,49	0
35	CL	P	8508	1/1	0.72	0.62	9.08	113,113,113,113	0
34	NA	A	8332	1/1	0.90	0.26	8.69	37,37,37,37	0
35	CL	A	8513	1/1	0.86	0.35	8.59	81,81,81,81	0
34	NA	B	8383	1/1	0.60	0.26	7.88	63,63,63,63	0
34	NA	A	8374	1/1	0.95	0.30	7.65	46,46,46,46	0
34	NA	A	8335	1/1	0.98	0.23	7.38	43,43,43,43	0
34	NA	S	8386	1/1	0.51	0.47	7.17	48,48,48,48	0
34	NA	M	8380	1/1	0.95	0.35	7.12	73,73,73,73	0
34	NA	A	8371	1/1	0.78	0.23	6.58	32,32,32,32	0
34	NA	A	8340	1/1	0.95	0.23	6.43	29,29,29,29	0
37	PUY	5	78	34/34	0.88	0.37	6.36	66,69,74,75	0
34	NA	A	8321	1/1	0.97	0.22	6.29	52,52,52,52	0
35	CL	D	8519	1/1	0.95	0.33	4.55	55,55,55,55	0
34	NA	A	8361	1/1	0.97	0.22	4.32	35,35,35,35	0
35	CL	A	8505	1/1	0.67	0.30	4.24	65,65,65,65	0
33	K	A	8201	1/1	0.86	0.22	4.19	76,76,76,76	0
34	NA	A	8350	1/1	0.95	0.22	3.73	18,18,18,18	0
34	NA	A	8369	1/1	0.92	0.30	3.45	49,49,49,49	0
35	CL	A	8510	1/1	0.81	0.70	3.42	101,101,101,101	0
32	MG	A	8060	1/1	0.94	0.23	3.37	43,43,43,43	0
32	MG	1	8105	1/1	0.85	0.33	3.24	32,32,32,32	0
32	MG	A	8110	1/1	0.97	0.17	2.86	54,54,54,54	0
35	CL	A	8511	1/1	0.77	0.42	2.60	92,92,92,92	0
34	NA	A	8331	1/1	0.97	0.19	2.55	35,35,35,35	0
32	MG	A	8044	1/1	0.92	0.23	2.42	68,68,68,68	0
34	NA	A	8327	1/1	0.94	0.19	1.91	24,24,24,24	0
34	NA	A	8355	1/1	0.91	0.23	1.72	60,60,60,60	0
34	NA	A	8372	1/1	0.92	0.18	1.49	25,25,25,25	0
34	NA	A	8378	1/1	0.97	0.21	1.40	18,18,18,18	0
32	MG	A	8064	1/1	0.90	0.17	0.95	31,31,31,31	0
34	NA	S	8337	1/1	0.89	0.28	0.85	70,70,70,70	0
34	NA	A	8366	1/1	0.82	0.19	0.65	58,58,58,58	0
35	CL	4	8504	1/1	0.71	0.35	0.42	69,69,69,69	0
34	NA	S	8338	1/1	0.98	0.21	0.18	65,65,65,65	0
32	MG	5	8114	1/1	0.94	0.19	0.00	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
33	K	A	8202	1/1	0.93	0.16	-0.01	56,56,56,56	0
32	MG	A	8112	1/1	0.96	0.18	-0.08	58,58,58,58	0
34	NA	A	8365	1/1	0.89	0.20	-0.09	29,29,29,29	0
35	CL	K	8521	1/1	0.94	0.18	-0.13	47,47,47,47	0
32	MG	A	8056	1/1	0.95	0.20	-0.21	75,75,75,75	0
34	NA	A	8326	1/1	0.89	0.17	-0.28	35,35,35,35	0
32	MG	A	8096	1/1	0.96	0.16	-0.39	33,33,33,33	0
34	NA	J	8309	1/1	0.97	0.15	-0.40	21,21,21,21	0
34	NA	A	8379	1/1	0.97	0.14	-0.67	33,33,33,33	0
34	NA	C	8345	1/1	0.95	0.17	-0.72	68,68,68,68	0
32	MG	A	8052	1/1	0.84	0.14	-1.00	24,24,24,24	0
32	MG	A	8013	1/1	0.98	0.15	-1.10	21,21,21,21	0
32	MG	A	8101	1/1	0.96	0.13	-1.13	49,49,49,49	0
38	CD	1	8403	1/1	0.99	0.07	-1.26	88,88,88,88	0
32	MG	A	8055	1/1	0.95	0.12	-1.39	29,29,29,29	0
32	MG	A	8086	1/1	0.98	0.11	-1.46	75,75,75,75	0
35	CL	A	8512	1/1	0.93	0.13	-1.50	30,30,30,30	0
32	MG	A	8018	1/1	0.89	0.13	-1.59	24,24,24,24	0
34	NA	A	8314	1/1	0.93	0.12	-1.64	29,29,29,29	0
38	CD	4	8404	1/1	0.99	0.08	-1.66	67,67,67,67	0
38	CD	V	8401	1/1	0.98	0.11	-1.66	70,70,70,70	0
32	MG	U	8073	1/1	0.95	0.14	-1.70	21,21,21,21	0
32	MG	A	8053	1/1	0.94	0.12	-1.70	85,85,85,85	0
34	NA	K	8346	1/1	0.97	0.14	-1.76	7,7,7,7	0
34	NA	A	8333	1/1	0.86	0.10	-1.84	14,14,14,14	0
34	NA	A	8325	1/1	0.96	0.12	-1.95	48,48,48,48	0
32	MG	A	8008	1/1	0.98	0.12	-2.02	40,40,40,40	0
35	CL	N	8518	1/1	0.98	0.15	-2.11	50,50,50,50	0
34	NA	E	8304	1/1	0.94	0.09	-2.28	4,4,4,4	0
32	MG	Z	8109	1/1	0.82	0.12	-2.28	32,32,32,32	0
32	MG	A	8012	1/1	0.99	0.10	-2.33	35,35,35,35	0
32	MG	A	8067	1/1	0.97	0.12	-2.34	22,22,22,22	0
32	MG	A	8077	1/1	0.99	0.11	-2.35	39,39,39,39	0
32	MG	A	8058	1/1	0.98	0.11	-2.50	33,33,33,33	0
32	MG	A	8032	1/1	0.96	0.07	-2.55	23,23,23,23	0
32	MG	A	8003	1/1	0.98	0.13	-2.57	30,30,30,30	0
32	MG	A	8039	1/1	0.96	0.10	-2.59	57,57,57,57	0
32	MG	A	8015	1/1	0.97	0.07	-2.61	66,66,66,66	0
32	MG	A	8074	1/1	0.99	0.07	-2.62	16,16,16,16	0
38	CD	2	8402	1/1	0.99	0.07	-2.73	72,72,72,72	0
32	MG	C	8065	1/1	0.95	0.09	-2.83	85,85,85,85	0
34	NA	A	8353	1/1	0.95	0.07	-2.93	13,13,13,13	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	A	8057	1/1	0.96	0.11	-3.03	15,15,15,15	0
32	MG	A	8108	1/1	0.90	0.10	-3.27	50,50,50,50	0
34	NA	A	8368	1/1	0.90	0.08	-3.32	35,35,35,35	0
34	NA	A	8376	1/1	0.98	0.12	-3.34	27,27,27,27	0
32	MG	A	8010	1/1	0.98	0.09	-3.77	26,26,26,26	0
34	NA	A	8381	1/1	0.96	0.11	-3.90	51,51,51,51	0
34	NA	N	8347	1/1	0.97	0.10	-4.03	19,19,19,19	0
32	MG	A	8017	1/1	0.97	0.04	-4.25	40,40,40,40	0
32	MG	A	8014	1/1	0.96	0.10	-4.29	18,18,18,18	0
32	MG	A	8093	1/1	0.98	0.10	-4.36	16,16,16,16	0
32	MG	A	8022	1/1	0.98	0.05	-4.40	22,22,22,22	0
32	MG	4	8078	1/1	0.95	0.07	-4.45	23,23,23,23	0
34	NA	R	8348	1/1	0.98	0.07	-4.46	18,18,18,18	0
32	MG	A	8019	1/1	0.98	0.07	-4.59	31,31,31,31	0
32	MG	A	8027	1/1	0.95	0.06	-4.63	60,60,60,60	0
32	MG	A	8004	1/1	0.97	0.05	-4.69	43,43,43,43	0
32	MG	A	8007	1/1	0.99	0.08	-4.79	9,9,9,9	0
34	NA	A	8373	1/1	0.95	0.07	-4.89	36,36,36,36	0
32	MG	A	8054	1/1	0.98	0.11	-5.26	46,46,46,46	0
34	NA	A	8343	1/1	0.94	0.07	-5.27	9,9,9,9	0
34	NA	A	8317	1/1	0.95	0.06	-5.33	25,25,25,25	0
32	MG	A	8020	1/1	0.99	0.07	-5.37	36,36,36,36	0
32	MG	A	8006	1/1	0.96	0.05	-5.64	33,33,33,33	0
32	MG	A	8038	1/1	0.99	0.08	-5.81	43,43,43,43	0
32	MG	A	8033	1/1	0.91	0.10	-6.03	42,42,42,42	0
32	MG	A	8002	1/1	0.98	0.06	-6.18	15,15,15,15	0
32	MG	A	8035	1/1	0.95	0.07	-6.44	70,70,70,70	0
34	NA	A	8344	1/1	0.95	0.06	-6.53	11,11,11,11	0
32	MG	A	8001	1/1	0.93	0.09	-6.57	31,31,31,31	0
32	MG	A	8091	1/1	0.98	0.05	-6.67	65,65,65,65	0
32	MG	A	8080	1/1	0.99	0.07	-7.42	38,38,38,38	0
34	NA	A	8305	1/1	0.96	0.08	-7.75	10,10,10,10	0
34	NA	A	8339	1/1	0.93	0.08	-8.29	30,30,30,30	0
34	NA	A	8320	1/1	0.96	0.09	-8.88	29,29,29,29	0
32	MG	A	8084	1/1	0.99	0.03	-17.18	34,34,34,34	0
35	CL	K	8501	1/1	0.95	0.12	-	55,55,55,55	0
35	CL	A	8517	1/1	0.91	0.24	-	61,61,61,61	0
32	MG	A	8083	1/1	0.97	0.04	-	32,32,32,32	0
32	MG	A	8090	1/1	0.95	0.22	-	46,46,46,46	0
34	NA	A	8358	1/1	0.96	0.50	-	109,109,109,109	0
34	NA	A	8328	1/1	0.90	0.26	-	52,52,52,52	0
34	NA	A	8319	1/1	0.95	0.11	-	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
34	NA	A	8329	1/1	0.90	0.10	-	40,40,40,40	0
32	MG	A	8087	1/1	0.93	0.19	-	41,41,41,41	0
34	NA	A	8324	1/1	0.97	0.10	-	32,32,32,32	0
34	NA	A	8375	1/1	0.86	0.56	-	42,42,42,42	0
34	NA	A	8354	1/1	0.93	0.17	-	16,16,16,16	0
32	MG	A	8061	1/1	0.98	0.06	-	33,33,33,33	0
32	MG	A	8016	1/1	0.98	0.08	-	23,23,23,23	0
34	NA	A	8367	1/1	0.94	0.09	-	22,22,22,22	0
32	MG	A	8062	1/1	0.98	0.07	-	38,38,38,38	0
32	MG	A	8046	1/1	0.85	0.13	-	62,62,62,62	0
34	NA	A	8302	1/1	0.93	0.17	-	25,25,25,25	0
32	MG	A	8048	1/1	0.98	0.08	-	33,33,33,33	0
34	NA	A	8352	1/1	0.97	0.16	-	17,17,17,17	0
34	NA	A	8306	1/1	0.98	0.40	-	35,35,35,35	0
32	MG	A	8028	1/1	0.93	0.10	-	75,75,75,75	0
34	NA	A	8384	1/1	0.22	0.80	-	103,103,103,103	0
34	NA	A	8360	1/1	0.87	0.43	-	37,37,37,37	0
32	MG	A	8036	1/1	0.98	0.06	-	29,29,29,29	0
32	MG	A	8029	1/1	0.98	0.12	-	34,34,34,34	0
32	MG	A	8068	1/1	0.95	0.09	-	44,44,44,44	0
34	NA	A	8336	1/1	0.93	0.09	-	51,51,51,51	0
32	MG	A	8031	1/1	0.97	0.05	-	29,29,29,29	0
34	NA	A	8313	1/1	0.94	0.14	-	47,47,47,47	0
35	CL	A	8514	1/1	0.98	0.15	-	45,45,45,45	0
32	MG	A	8037	1/1	0.98	0.09	-	41,41,41,41	0
35	CL	A	8516	1/1	0.99	0.10	-	37,37,37,37	0
32	MG	A	8102	1/1	0.88	0.18	-	83,83,83,83	0
32	MG	A	8089	1/1	0.79	0.24	-	104,104,104,104	0
38	CD	P	8405	1/1	0.93	0.33	-	196,196,196,196	0
34	NA	A	8315	1/1	0.94	0.11	-	25,25,25,25	0
34	NA	A	8341	1/1	0.84	0.14	-	40,40,40,40	0
32	MG	A	8082	1/1	0.98	0.07	-	16,16,16,16	0
32	MG	A	8045	1/1	0.96	0.14	-	63,63,63,63	0
34	NA	A	8364	1/1	0.96	0.18	-	12,12,12,12	0
32	MG	A	8059	1/1	0.95	0.13	-	119,119,119,119	0
32	MG	A	8050	1/1	0.94	0.11	-	41,41,41,41	0
34	NA	A	8310	1/1	0.97	0.15	-	22,22,22,22	0
32	MG	A	8021	1/1	0.96	0.10	-	46,46,46,46	0
34	NA	A	8382	1/1	0.81	0.46	-	52,52,52,52	0
36	PO4	5	77	3/5	0.96	0.13	-	67,67,68,68	0
32	MG	A	8076	1/1	0.93	0.44	-	134,134,134,134	0
32	MG	A	8116	1/1	0.86	0.24	-	95,95,95,95	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	A	8023	1/1	0.98	0.07	-	35,35,35,35	0
34	NA	A	8318	1/1	0.97	0.15	-	65,65,65,65	0
32	MG	A	8106	1/1	0.95	0.12	-	69,69,69,69	0
32	MG	L	8069	1/1	0.88	0.13	-	105,105,105,105	0
32	MG	A	8063	1/1	0.98	0.12	-	64,64,64,64	0
32	MG	A	8071	1/1	0.94	0.07	-	52,52,52,52	0
32	MG	A	8005	1/1	0.96	0.10	-	68,68,68,68	0
35	CL	C	8509	1/1	0.92	0.20	-	66,66,66,66	0
32	MG	A	8072	1/1	0.95	0.26	-	55,55,55,55	0
32	MG	A	8075	1/1	0.91	0.07	-	42,42,42,42	0
32	MG	A	8026	1/1	0.99	0.13	-	45,45,45,45	0
34	NA	A	8311	1/1	0.96	0.19	-	43,43,43,43	0
32	MG	A	8113	1/1	0.94	0.10	-	29,29,29,29	0
35	CL	Z	8520	1/1	0.93	0.21	-	64,64,64,64	0
32	MG	A	8079	1/1	0.98	0.09	-	25,25,25,25	0
34	NA	A	8359	1/1	0.87	0.46	-	47,47,47,47	0
32	MG	A	8070	1/1	0.81	0.80	-	101,101,101,101	0
32	MG	A	8030	1/1	0.92	0.13	-	68,68,68,68	0
32	MG	A	8097	1/1	0.94	0.52	-	64,64,64,64	0
32	MG	A	8034	1/1	0.92	0.04	-	50,50,50,50	0
34	NA	A	8308	1/1	0.93	0.09	-	40,40,40,40	0
32	MG	A	8100	1/1	0.84	0.13	-	51,51,51,51	0
34	NA	A	8334	1/1	0.96	0.06	-	30,30,30,30	0
34	NA	A	8349	1/1	0.98	0.21	-	25,25,25,25	0
32	MG	A	8117	1/1	0.96	0.08	-	1,1,1,1	0
35	CL	A	8503	1/1	0.89	0.24	-	62,62,62,62	0
32	MG	A	8088	1/1	0.96	0.10	-	12,12,12,12	0
32	MG	A	8066	1/1	0.75	0.27	-	84,84,84,84	0
32	MG	A	8025	1/1	0.98	0.05	-	12,12,12,12	0
32	MG	A	8099	1/1	0.94	0.14	-	43,43,43,43	0
34	NA	A	8363	1/1	0.88	0.40	-	100,100,100,100	0
32	MG	A	8092	1/1	0.91	0.20	-	58,58,58,58	0
32	MG	A	8040	1/1	0.98	0.07	-	33,33,33,33	0
32	MG	A	8098	1/1	0.96	0.24	-	47,47,47,47	0
34	NA	T	8312	1/1	0.72	0.57	-	122,122,122,122	0
32	MG	A	8051	1/1	0.96	0.10	-	93,93,93,93	0
32	MG	A	8009	1/1	0.99	0.05	-	14,14,14,14	0
32	MG	A	8047	1/1	0.99	0.09	-	62,62,62,62	0
32	MG	A	8041	1/1	0.93	0.18	-	80,80,80,80	0
32	MG	A	8094	1/1	0.95	0.09	-	50,50,50,50	0
34	NA	A	8357	1/1	0.85	0.07	-	43,43,43,43	0
34	NA	A	8370	1/1	0.46	0.40	-	93,93,93,93	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
34	NA	A	8330	1/1	0.91	0.14	-	36,36,36,36	0
32	MG	A	8024	1/1	0.93	1.03	-	108,108,108,108	0
35	CL	A	8522	1/1	0.92	0.45	-	57,57,57,57	0
34	NA	A	8385	1/1	0.92	0.26	-	22,22,22,22	0
34	NA	J	8322	1/1	0.86	0.17	-	26,26,26,26	0
35	CL	O	8507	1/1	0.71	0.51	-	102,102,102,102	0
34	NA	A	8307	1/1	0.87	0.17	-	34,34,34,34	0
32	MG	A	8104	1/1	0.93	0.11	-	31,31,31,31	0
32	MG	A	8103	1/1	0.75	0.39	-	57,57,57,57	0
32	MG	A	8115	1/1	0.88	0.17	-	51,51,51,51	0
35	CL	S	8506	1/1	0.86	0.30	-	77,77,77,77	0
34	NA	A	8342	1/1	0.96	0.18	-	30,30,30,30	0
32	MG	A	8107	1/1	0.95	0.03	-	46,46,46,46	0
34	NA	B	8351	1/1	0.54	0.26	-	67,67,67,67	0
34	NA	A	8301	1/1	0.95	0.14	-	22,22,22,22	0
32	MG	A	8042	1/1	0.91	0.10	-	25,25,25,25	0
34	NA	A	8316	1/1	0.91	0.23	-	42,42,42,42	0
32	MG	A	8043	1/1	0.96	0.07	-	50,50,50,50	0
32	MG	A	8011	1/1	0.97	0.05	-	27,27,27,27	0
32	MG	B	8095	1/1	0.95	0.17	-	85,85,85,85	0
32	MG	A	8085	1/1	0.90	0.12	-	39,39,39,39	0
32	MG	A	8111	1/1	0.95	0.27	-	82,82,82,82	0
35	CL	K	8502	1/1	0.92	0.26	-	91,91,91,91	0
32	MG	A	8081	1/1	0.96	0.15	-	29,29,29,29	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.