wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 08:04 AM GMT

PDB ID	:	3CPW
Title	:	The structure of the antibiotic LINEZOLID bound to the large ribosomal subunit of HALOARCULA MARISMORTUI
Authors	:	Ippolito, J.A.; Kanyo, Z.K.; Wang, D.; Franceschi, F.J.; Moore, P.B.; Steitz, T.A.; Duffy, E.M.
Deposited on	:	2008-04-01
Resolution	:	2.70 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

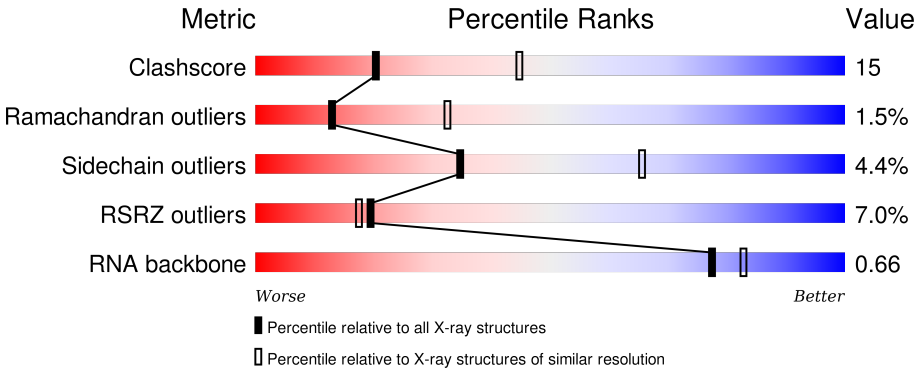
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)
RNA backbone	2183	1069 (3.10-2.30)

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 <=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	2922	4% 55% 34% 5% 6%
2	9	122	11% 48% 39% 11% •
3	A	240	5% 60% 33% 6% •
4	B	338	2% 61% 36% •
5	C	246	2% 66% 30% •

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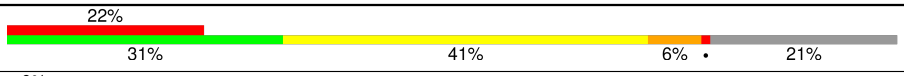
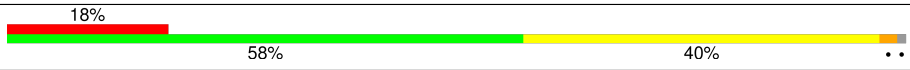
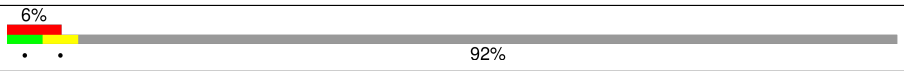
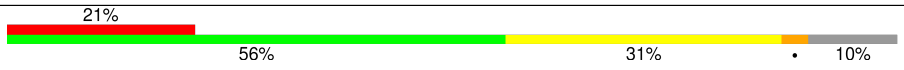
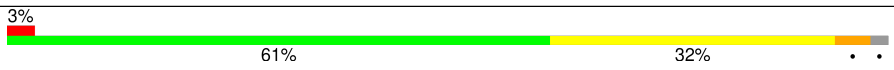
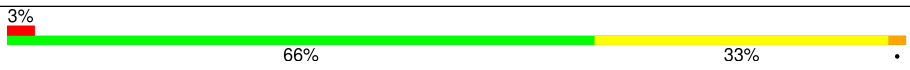
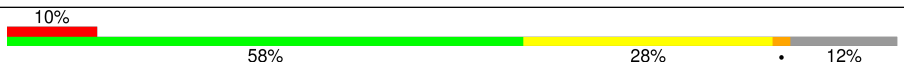
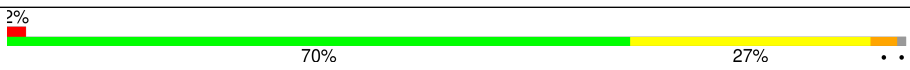
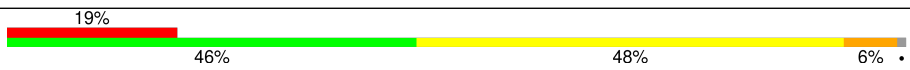
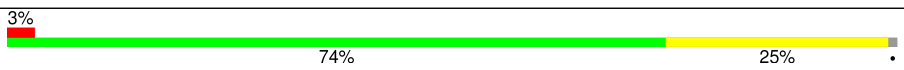
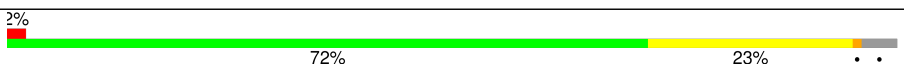
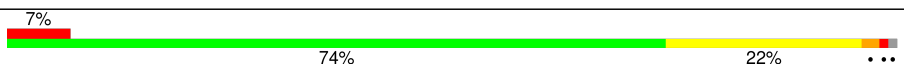
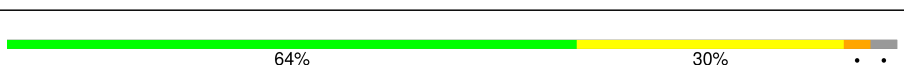
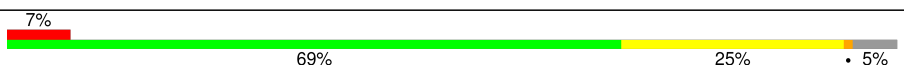
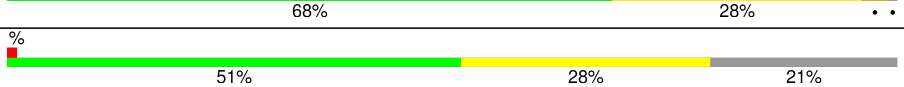
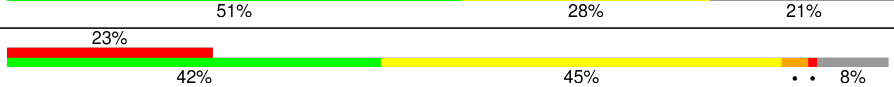
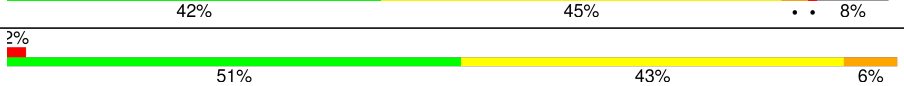
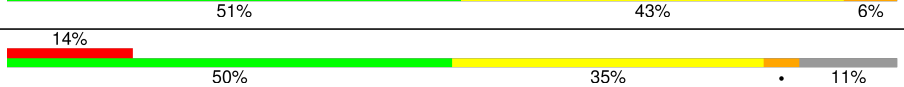
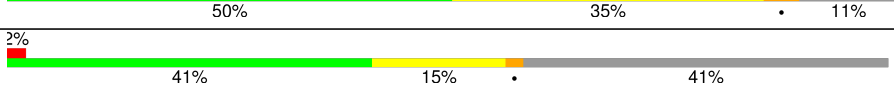
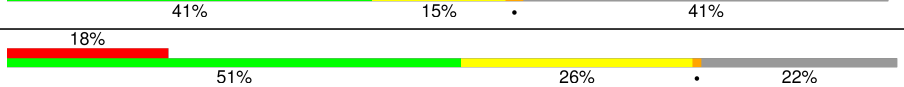
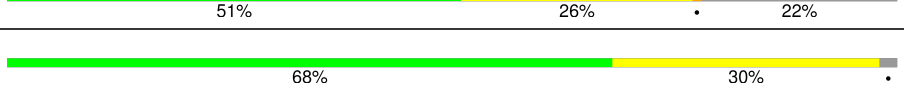
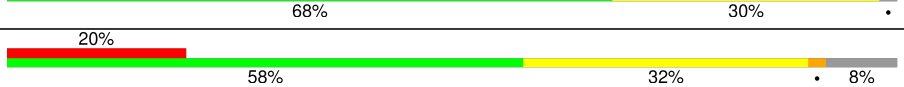
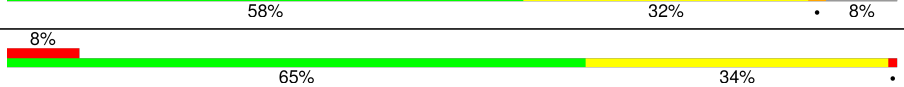
Mol	Chain	Length	Quality of chain
6	D	177	
7	E	178	
8	F	120	
9	G	348	
10	H	177	
11	I	145	
12	J	132	
13	K	165	
14	L	196	
15	M	187	
16	N	116	
17	O	149	
18	P	96	
19	Q	155	
20	R	85	
21	S	120	
22	T	67	
23	U	71	
24	V	154	
25	W	92	
26	X	241	
27	Y	92	
28	Z	57	
29	1	50	
30	2	92	

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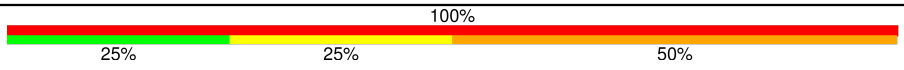
Mol	Chain	Length	Quality of chain
31	4	4	

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
33	MG	0	8001	-	-	-	X
33	MG	0	8002	-	-	-	X
33	MG	0	8006	-	-	-	X
33	MG	0	8009	-	-	-	X
33	MG	0	8028	-	-	-	X
33	MG	0	8043	-	-	-	X
33	MG	0	8044	-	-	-	X
33	MG	0	8047	-	-	-	X
33	MG	0	8062	-	-	-	X
33	MG	0	8065	-	-	-	X
33	MG	0	8076	-	-	-	X
33	MG	0	8085	-	-	-	X
33	MG	A	8050	-	-	-	X
34	K	0	8401	-	-	-	X
35	NA	0	8504	-	-	-	X
35	NA	0	8512	-	-	-	X
35	NA	0	8517	-	-	-	X
35	NA	0	8519	-	-	-	X
35	NA	0	8521	-	-	-	X
35	NA	0	8522	-	-	-	X
35	NA	0	8523	-	-	-	X
35	NA	0	8527	-	-	-	X
35	NA	0	8528	-	-	-	X
35	NA	0	8535	-	-	-	X
35	NA	0	8542	-	-	-	X
35	NA	0	8545	-	-	-	X
35	NA	0	8547	-	-	-	X
35	NA	0	8550	-	-	-	X
35	NA	0	8553	-	-	-	X
35	NA	0	8555	-	-	-	X
35	NA	0	8556	-	-	-	X
35	NA	0	8557	-	-	-	X
35	NA	0	8559	-	-	-	X
35	NA	0	8562	-	-	-	X
35	NA	0	8563	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
35	NA	0	8564	-	-	-	X
35	NA	0	8565	-	-	-	X
35	NA	0	8569	-	-	-	X
35	NA	0	8571	-	-	-	X
35	NA	0	8575	-	-	-	X
35	NA	9	8572	-	-	-	X
35	NA	B	8552	-	-	-	X
35	NA	L	8539	-	-	-	X
36	CL	B	8819	-	-	-	X
36	CL	N	8808	-	-	-	X
37	SR	0	8902	-	-	-	X
37	SR	0	8926	-	-	-	X
37	SR	0	8947	-	-	-	X
37	SR	0	8985	-	-	-	X
37	SR	B	8987	-	-	-	X

2 Entry composition

There are 40 unique types of molecules in this entry. The entry contains 98629 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	0	2754	Total	C	N	O	P	0	0	0
			59016	26346	10879	19046	2745			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
0	559	C	U	CONFLICT	GB 3377779
0	560	C	U	CONFLICT	GB 3377779
0	2099	A	G	ENGINEERED	GB 3377779

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	9	122	Total	C	N	O	P	0	0	0
			2600	1160	472	847	121			

- Molecule 3 is a protein called 50S ribosomal protein L2P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	237	Total	C	N	O	S	0	0	0
			1753	1072	352	324	5			

- Molecule 4 is a protein called 50S ribosomal protein L3P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	337	Total	C	N	O	S	0	0	0
			2625	1616	493	511	5			

- Molecule 5 is a protein called 50S ribosomal protein L4P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	C	246	Total	C	N	O	S	0	0	0
			1860	1130	345	384	1			

- Molecule 6 is a protein called 50S ribosomal protein L5P.

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

- Molecule 7 is a protein called 50S ribosomal protein L6P.

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

- Molecule 8 is a protein called 50S ribosomal protein L7Ae.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	F	119	Total	C	N	O	S	0	0	0
			890	551	141	197	1			

- Molecule 9 is a protein called 50S ribosomal protein L10E.

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

- Molecule 10 is a protein called 50S ribosomal protein L10e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	H	160	Total	C	N	O	S	0	0	0
			1282	798	240	238	6			

- Molecule 11 is a protein called 50S ribosomal protein L13P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	I	142	Total	C	N	O	S	0	0	0
			1120	696	199	222	3			

- Molecule 12 is a protein called 50S ribosomal protein L14P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	J	132	Total	C	N	O	S	0	0	0
			994	609	189	192	4			

- Molecule 13 is a protein called 50S ribosomal protein L15P.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	K	145	Total	C	N	O	0	0	0
			1118	670	222	226			

- Molecule 14 is a protein called 50S ribosomal protein L15e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	L	194	Total	C	N	O	S	0	0	0
			1558	943	333	281	1			

- Molecule 15 is a protein called 50S ribosomal protein L18P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	M	186	Total	C	N	O	S	0	0	0
			1445	895	262	286	2			

- Molecule 16 is a protein called 50S ribosomal protein L18e.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
16	N	115	Total	C	N	O	0	0	0
			865	529	161	175			

- Molecule 17 is a protein called 50S ribosomal protein L19e.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
17	O	143	Total	C	N	O	0	0	0
			1136	683	229	224			

- Molecule 18 is a protein called 50S ribosomal protein L21e.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	P	95	Total	C	N	O	0	0	0
			735	450	141	144			

- Molecule 19 is a protein called 50S ribosomal protein L22P.

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

- Molecule 20 is a protein called 50S ribosomal protein L23P.

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

- Molecule 21 is a protein called 50S ribosomal protein L24P.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	S	119	Total	C	N	O	0	0	0
			950	568	180	202			

- Molecule 22 is a protein called 50S ribosomal protein L24e.

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

- Molecule 23 is a protein called 50S ribosomal protein L29P.

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

- Molecule 24 is a protein called 50S ribosomal protein L30P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	V	154	Total	C	N	O	S	0	0	0
			1196	737	209	244	6			

- Molecule 25 is a protein called 50S ribosomal protein L31e.

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

- Molecule 26 is a protein called 50S ribosomal protein L32e.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
26	X	142	Total	C	N	O	0	0	0
			1130	686	228	216			

- Molecule 27 is a protein called 50S ribosomal protein L37Ae.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	Y	72	Total	C	N	O	S	0	0	0
			567	340	112	110	5			

- Molecule 28 is a protein called 50S ribosomal protein L37e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	Z	56	Total	C	N	O	S	0	0	0
			431	258	86	83	4			

- Molecule 29 is a protein called 50S ribosomal protein L39e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	1	46	Total	C	N	O	S	0	0	0
			396	239	89	67	1			

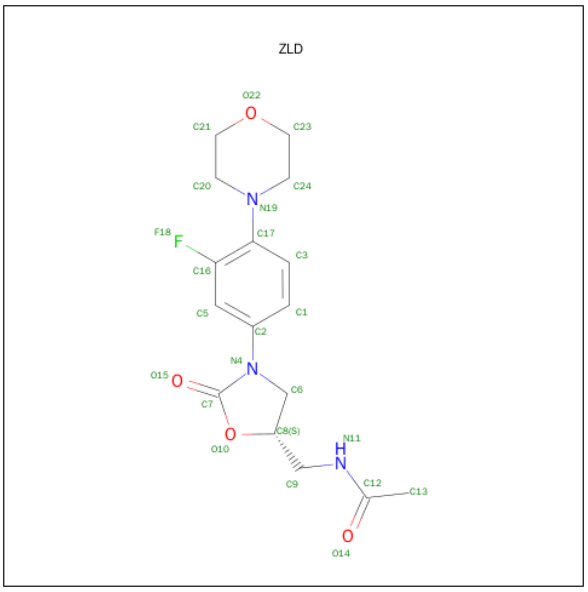
- Molecule 30 is a protein called 50S ribosomal protein L44E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	2	92	Total	C	N	O	S	0	0	0
			755	458	153	137	7			

- Molecule 31 is a RNA chain called 5'-R(*CP*CP*AP*(PHE)*(ACA))-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	4	4	Total	C	N	O	P	0	0	0
			70	37	12	19	2			

- Molecule 32 is N-{[(5S)-3-(3-FLUORO-4-MORPHOLIN-4-YLPHENYL)-2-OXO-1,3-OXAZOLIDIN-5-YL]METHYL}ACETAMIDE (three-letter code: ZLD) (formula: $C_{16}H_{20}FN_3O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	0	1	Total C F N O 24 16 1 3 4	0	0

- Molecule 33 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	0	84	Total Mg 84 84	0	0
33	J	1	Total Mg 1 1	0	0
33	1	1	Total Mg 1 1	0	0
33	B	1	Total Mg 1 1	0	0
33	A	2	Total Mg 2 2	0	0
33	X	1	Total Mg 1 1	0	0
33	9	1	Total Mg 1 1	0	0
33	S	1	Total Mg 1 1	0	0

- Molecule 34 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	0	2	Total K 2 2	0	0

- Molecule 35 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	0	64	Total Na 64 64	0	0
35	P	1	Total Na 1 1	0	0
35	Q	2	Total Na 2 2	0	0
35	K	1	Total Na 1 1	0	0
35	B	1	Total Na 1 1	0	0
35	I	1	Total Na 1 1	0	0
35	C	1	Total Na 1 1	0	0
35	R	1	Total Na 1 1	0	0
35	9	2	Total Na 2 2	0	0
35	L	1	Total Na 1 1	0	0

- Molecule 36 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	0	9	Total Cl 9 9	0	0
36	J	1	Total Cl 1 1	0	0
36	Q	1	Total Cl 1 1	0	0
36	K	1	Total Cl 1 1	0	0
36	B	1	Total Cl 1 1	0	0
36	I	3	Total Cl 3 3	0	0
36	A	1	Total Cl 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	N	1	Total Cl 1 1	0	0
36	X	1	Total Cl 1 1	0	0
36	2	1	Total Cl 1 1	0	0
36	L	1	Total Cl 1 1	0	0
36	M	1	Total Cl 1 1	0	0

- Molecule 37 is STRONTIUM ION (three-letter code: SR) (formula: Sr).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	0	92	Total Sr 92 92	0	0
37	Q	1	Total Sr 1 1	0	0
37	H	1	Total Sr 1 1	0	0
37	B	2	Total Sr 2 2	0	0
37	Z	2	Total Sr 2 2	0	0
37	A	3	Total Sr 3 3	0	0
37	2	1	Total Sr 1 1	0	0
37	R	1	Total Sr 1 1	0	0
37	9	3	Total Sr 3 3	0	0
37	S	1	Total Sr 1 1	0	0
37	F	1	Total Sr 1 1	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
38	Z	1	Total Cd 1 1	0	0

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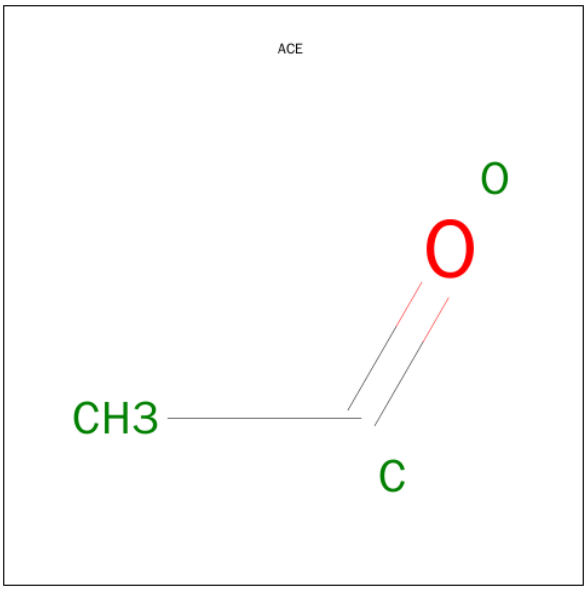
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
38	Y	1	Total Cd 1 1	0	0
38	T	1	Total Cd 1 1	0	0
38	2	1	Total Cd 1 1	0	0
38	N	1	Total Cd 1 1	0	0

- Molecule 39 is ACETYL GROUP (three-letter code: ACE) (formula: C_2H_4O).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
39	4	1	Total C O 3 2 1	0	0

- Molecule 40 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
40	0	5757	Total O 5757 5757	0	0
40	9	144	Total O 144 144	0	0
40	A	129	Total O 129 129	0	0
40	B	158	Total O 158 158	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
40	C	183	Total O 183 183	0	0
40	D	53	Total O 53 53	0	0
40	E	50	Total O 50 50	0	0
40	F	25	Total O 25 25	0	0
40	G	22	Total O 22 22	0	0
40	H	66	Total O 66 66	0	0
40	I	57	Total O 57 57	0	0
40	J	59	Total O 59 59	0	0
40	K	84	Total O 84 84	0	0
40	L	136	Total O 136 136	0	0
40	M	66	Total O 66 66	0	0
40	N	45	Total O 45 45	0	0
40	O	70	Total O 70 70	0	0
40	P	51	Total O 51 51	0	0
40	Q	84	Total O 84 84	0	0
40	R	38	Total O 38 38	0	0
40	S	43	Total O 43 43	0	0
40	T	28	Total O 28 28	0	0
40	U	15	Total O 15 15	0	0
40	V	75	Total O 75 75	0	0
40	W	28	Total O 28 28	0	0

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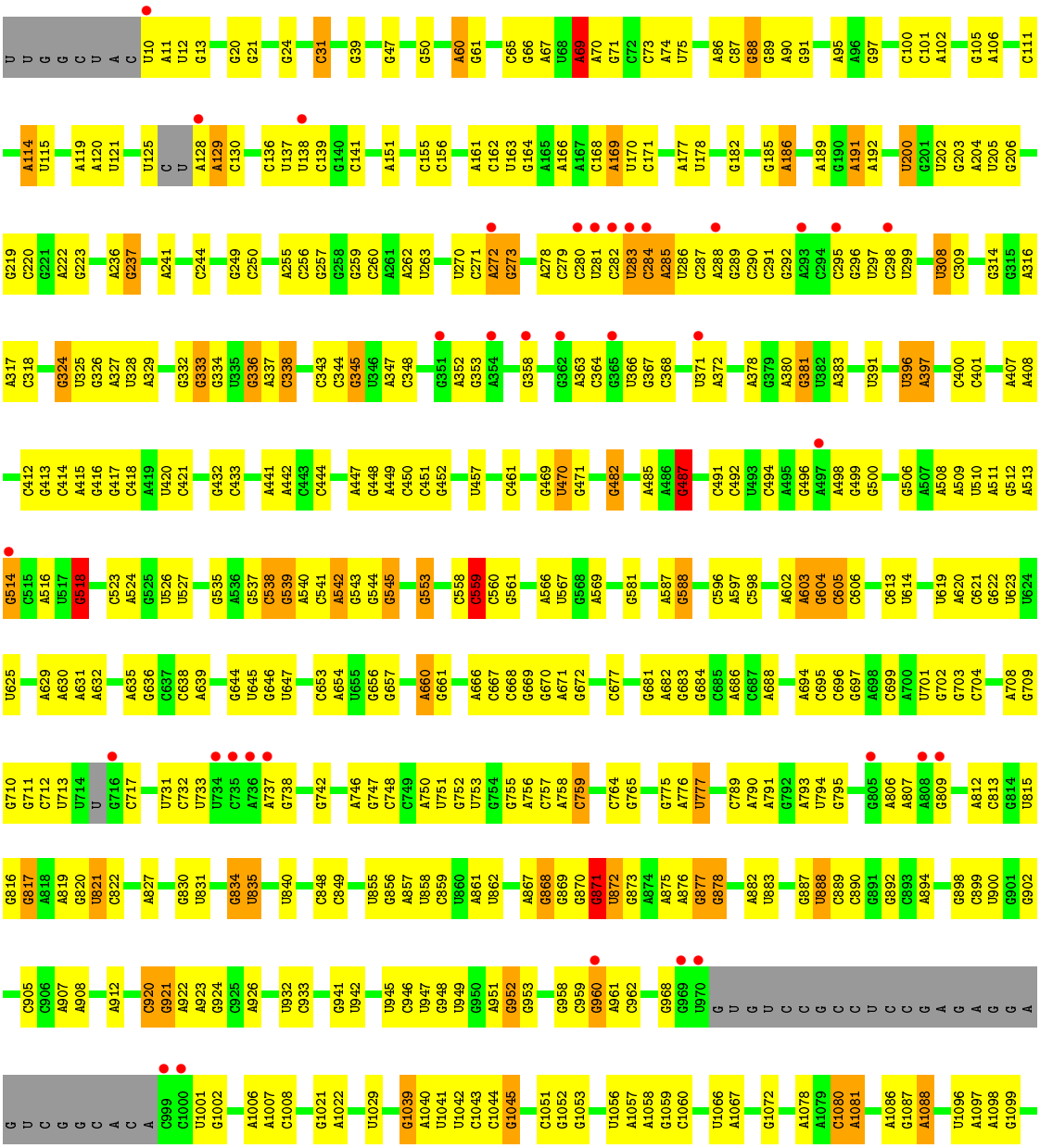
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
40	X	99	Total O 99 99	0	0
40	Y	23	Total O 23 23	0	0
40	Z	58	Total O 58 58	0	0
40	1	40	Total O 40 40	0	0
40	2	73	Total O 73 73	0	0
40	4	3	Total O 3 3	0	0

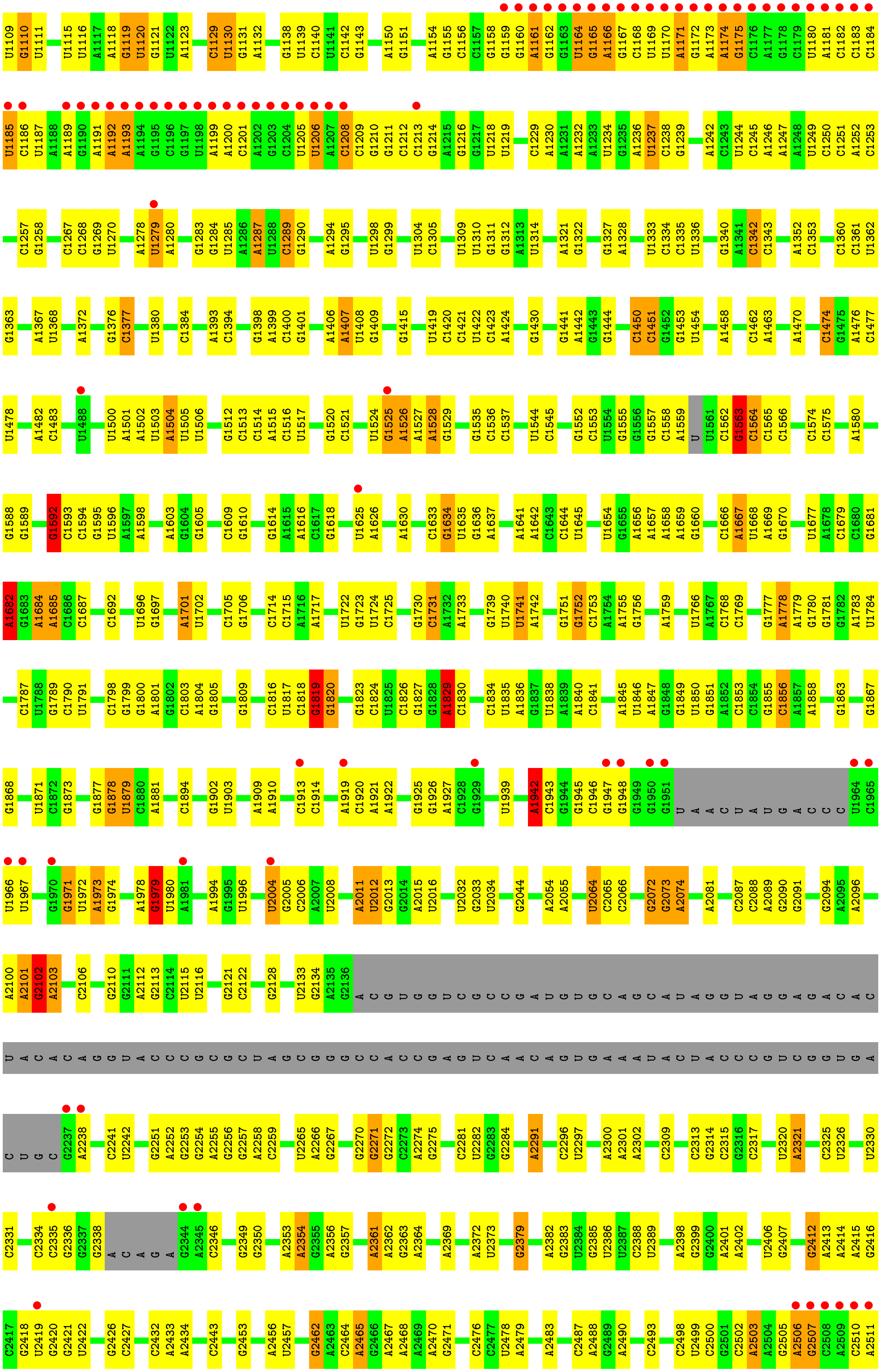
3 Residue-property plots (i)

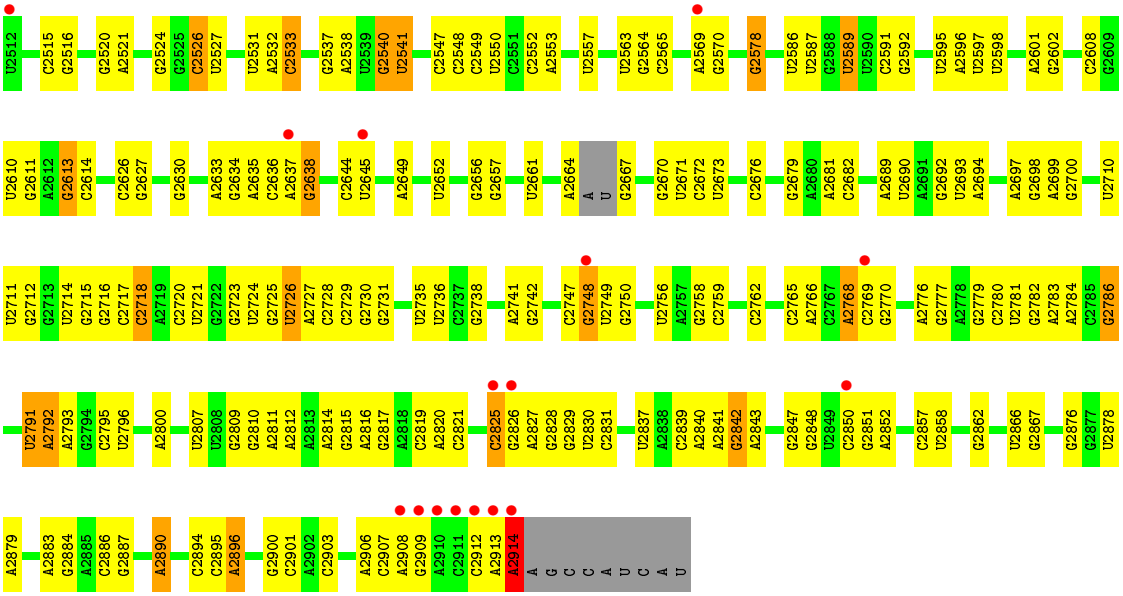
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: 23S RIBOSOMAL RNA

Chain 0:

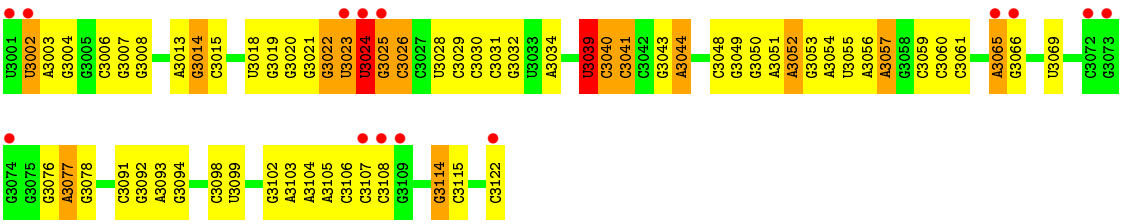



U1109 G1110 U1111 U1115 U1116 A1117 A1118 G1119 U1120 G1121 U1122 A1123 C1129 U1130 G1131 A1132 G1138 U1139 C1140 U1141 C1142 G1143 A1150 G1151 A1154 G1155 C1156 C1157 G1158 G1159 G1160 A1161 G1162 G1163 U1164 G1165 A1166 G1167 C1168 U1169 U1170 A1171 G1172 A1173 A1174 G1175 C1176 A1177 G1178 G1179 U1180 A1181 C1182 C1183 C1184
U1185 C1186 U1187 A1188 A1189 G1190 A1191 A1192 A1193 A1194 G1195 C1196 G1197 U1198 A1199 A1200 C1201 A1202 G1203 C1204 U1205 U1206 A1207 C1208 C1209 G1210 G1211 C1212 C1213 G1214 A1215 G1216 G1217 U1218 U1219 C1229 A1230 A1231 A1232 A1233 U1234 G1235 A1236 U1237 C1238 G1239 A1242 C1243 U1244 C1245 A1246 A1247 A1248 U1249 C1250 C1251 A1252 C1253
C1257 G1258 C1267 C1268 G1269 U1270 A1278 U1279 A1280 G1283 G1284 G1285 A1286 A1287 U1288 C1289 G1290 A1294 G1295 U1298 G1299 U1304 C1305 U1309 U1310 G1311 G1312 A1313 U1314 A1321 G1322 G1327 A1328 U1333 C1334 C1335 U1336 G1340 A1341 C1342 C1343 A1352 C1353 C1360 C1361 U1362
G1363 A1367 U1368 A1372 G1376 C1377 U1380 C1384 A1393 C1394 G1398 A1399 C1400 G1401 A1406 A1407 U1408 G1409 G1415 U1419 C1420 C1421 U1422 C1423 A1424 G1430 G1441 A1442 G1443 G1444 C1450 C1451 G1452 G1453 U1454 A1458 C1462 A1463 A1470 C1474 G1475 A1476 C1477
U1478 A1482 C1483 U1488 U1500 A1501 A1502 U1503 A1504 U1505 U1506 G1512 C1513 C1514 A1515 C1516 U1517 G1520 C1521 U1524 G1525 A1526 A1527 A1528 G1529 G1535 C1536 C1537 U1544 C1545 G1552 C1553 U1554 G1555 G1556 G1557 C1558 A1559 U U1561 C1562 G1563 C1564 C1565 C1566 C1574 C1575 A1580
G1588 G1589 G1592 C1593 C1594 G1595 U1596 A1597 A1598 A1603 G1604 G1605 C1609 G1610 G1614 A1615 A1616 C1617 G1618 U1625 A1626 A1630 C1633 G1634 U1635 G1636 A1637 A1641 A1642 C1643 C1644 U1645 U1654 G1655 A1656 A1657 A1658 A1659 G1660 C1666 A1667 U1668 A1669 G1670 U1677 A1678 C1679 C1680 G1681
A1682 G1683 A1684 A1685 C1686 C1687 C1692 U1696 G1697 A1701 U1702 C1705 G1706 C1714 C1715 A1716 A1717 U1722 G1723 U1724 C1725 G1730 C1731 A1732 A1733 G1739 U1740 U1741 A1742 G1751 G1752 C1753 A1754 A1755 G1756 A1759 U1766 G1767 C1768 C1769 G1777 A1778 A1779 G1780 G1781 G1782 A1783 U1784
C1787 U1788 G1789 C1790 U1791 C1798 G1799 G1800 A1801 G1802 C1803 A1804 G1805 G1809 C1816 U1817 C1818 G1819 G1820 G1823 C1824 U1825 C1826 G1827 G1828 A1829 C1830 C1834 U1835 A1836 G1837 U1838 A1839 A1840 C1841 A1845 U1846 A1847 G1848 G1849 U1850 G1851 A1852 C1853 G1854 G1855 C1856 A1857 A1858 G1863 G1867
G1868 U1871 C1872 G1873 G1877 G1878 U1879 C1880 A1881 C1894 G1902 U1903 A1909 A1910 C1913 C1914 A1919 C1920 A1921 A1922 G1925 G1926 A1927 C1928 G1929 U1939 A1942 C1943 G1944 G1945 C1946 G1947 G1948 G1949 G1950 G1951 U A A C U A U G A C C U1964 C1965
U1966 U1967 G1970 G1971 U1972 A1973 G1974 A1978 G1979 U1980 A1981 A1994 G1995 U1996 U2004 G2005 C2006 A2007 U2008 A2011 U2012 G2013 G2014 A2015 U2016 U2032 G2033 U2034 G2044 A2054 A2055 U2064 C2065 C2066 G2072 G2073 A2074 A2081 C2087 C2088 A2089 G2090 G2091 G2094 A2095 A2096
A2100 A2101 G2102 A2103 C2106 G2110 G2111 A2112 G2113 C2114 U2115 U2116 G2121 C2122 G2128 U2133 G2134 A2135 G2136 A C G U G G U C G C C G A U G U G C A G C A U A G G U A G G A G A C A C
U A C A C A G G U A C C C G C G C U A G C G G G C C A C C G A G U C A A C A G U G A A A U A C U A C C C G U C G G U G A
C U G C G2237 A2238 C2241 U2242 G2251 A2252 G2253 G2254 A2255 G2256 G2257 A2258 C2259 U2265 A2266 G2267 G2270 G2271 G2272 C2273 A2274 G2275 C2281 U2282 G2283 G2284 A2291 C2296 U2297 A2300 A2301 A2302 C2309 C2313 G2314 C2315 G2316 C2317 U2320 A2321 C2325 U2326 U2330
C2331 C2334 C2335 G2336 G2337 G2338 A C A G A G2344 A2345 C2346 G2349 G2350 A2353 A2354 G2355 A2356 G2357 A2361 A2362 G2363 A2364 A2369 A2372 U2373 G2379 A2382 G2383 U2384 G2385 U2386 U2387 C2388 U2389 A2398 G2399 G2400 A2401 A2402 U2406 G2407 G2412 A2413 A2414 A2415 G2416
C2417 G2418 U2419 G2420 G2421 U2422 G2426 C2427 C2432 A2433 A2434 C2443 G2453 A2456 U2457 G2462 A2463 C2464 A2465 G2466 A2467 A2468 A2469 A2470 G2471 C2476 C2477 U2478 A2479 A2483 C2487 A2488 G2489 A2490 C2493 C2498 U2499 C2500 G2501 C2502 A2503 A2504 G2505 A2506 G2507 C2508 A2509 C2510 A2511



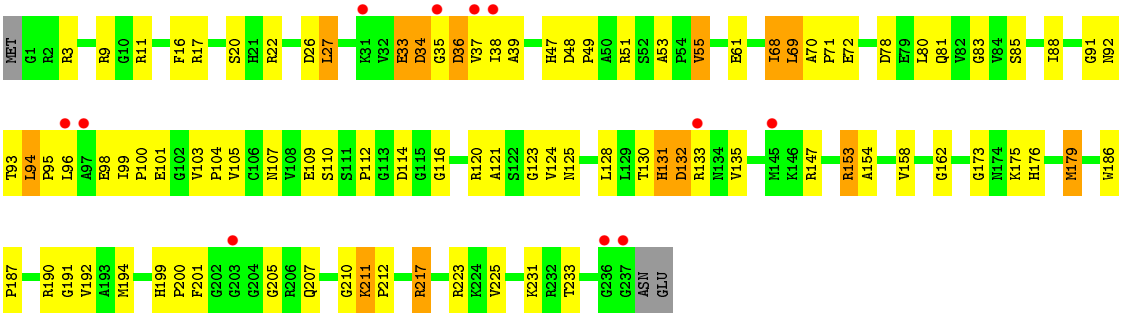
• Molecule 2: 5S RIBOSOMAL RNA

Chain 9:



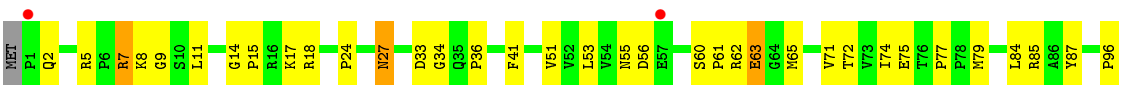
• Molecule 3: 50S ribosomal protein L2P

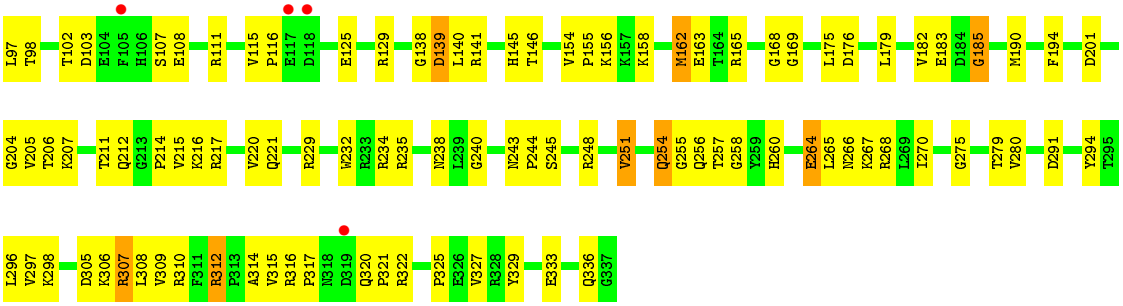
Chain A:



• Molecule 4: 50S ribosomal protein L3P

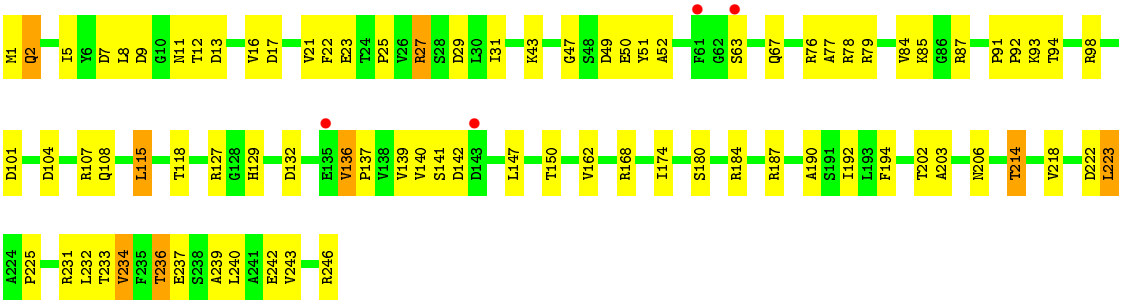
Chain B:





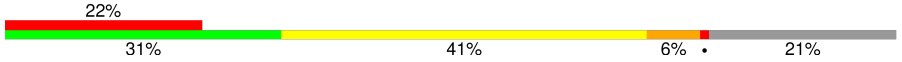
• Molecule 5: 50S ribosomal protein L4P

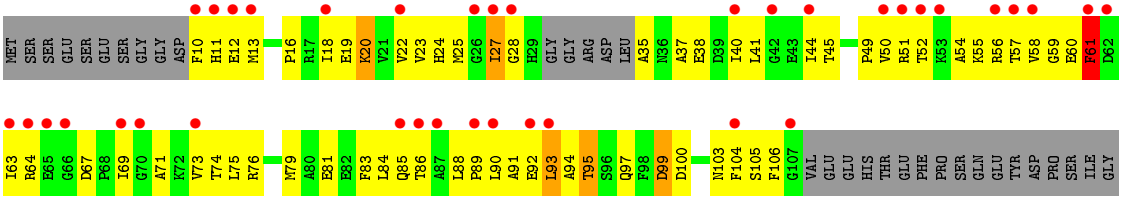
Chain C:

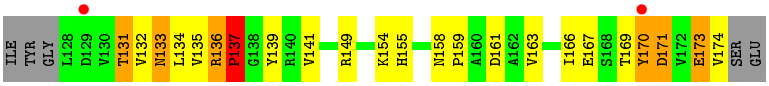


• Molecule 6: 50S ribosomal protein L5P

Chain D:

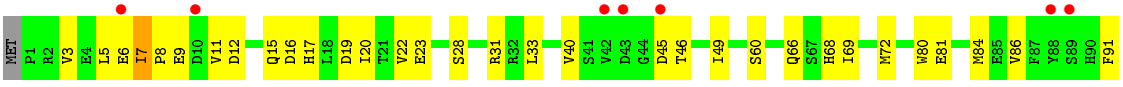






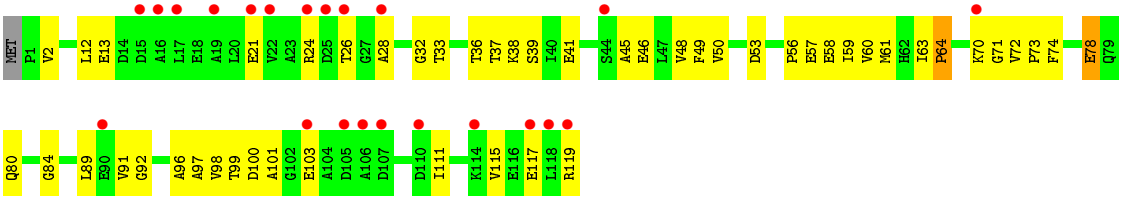
• Molecule 7: 50S ribosomal protein L6P

Chain E:



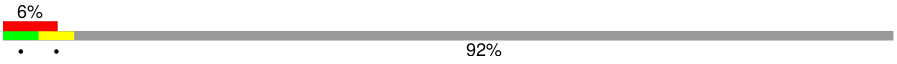
• Molecule 8: 50S ribosomal protein L7Ae

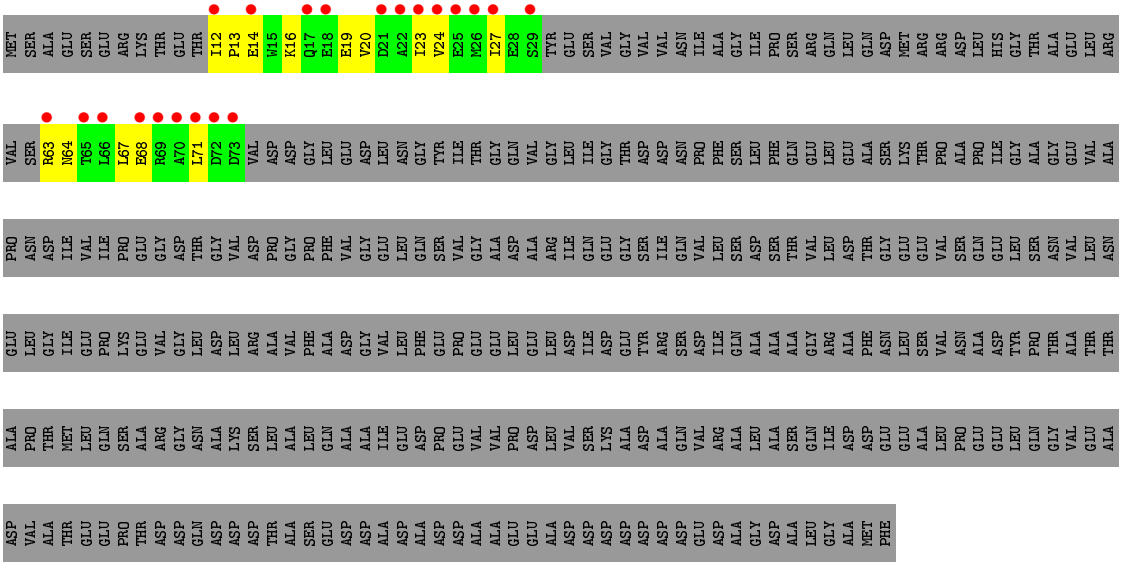
Chain F:



• Molecule 9: 50S ribosomal protein L10E

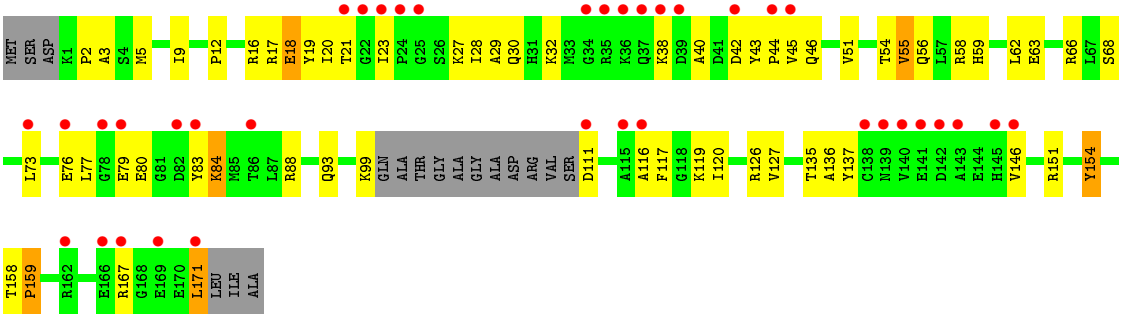
Chain G:





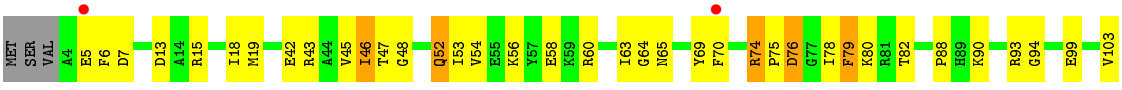
• Molecule 10: 50S ribosomal protein L10e

Chain H:



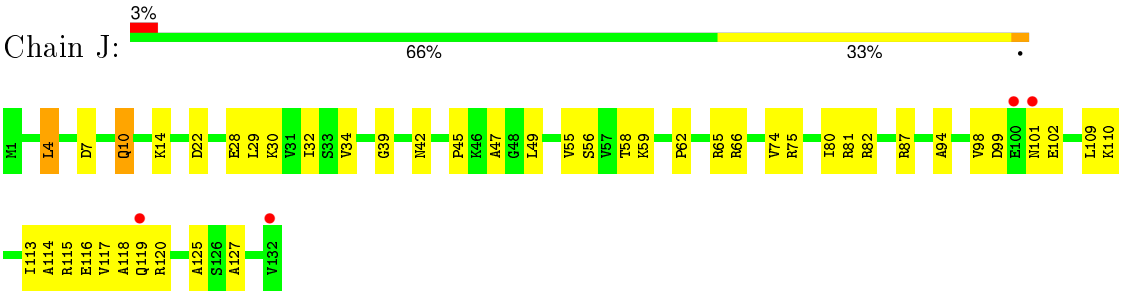
• Molecule 11: 50S ribosomal protein L13P

Chain I:



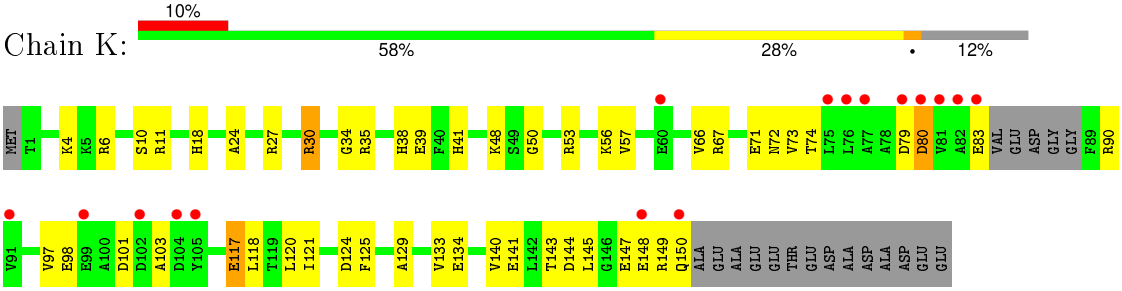
- Molecule 12: 50S ribosomal protein L14P

Chain J:



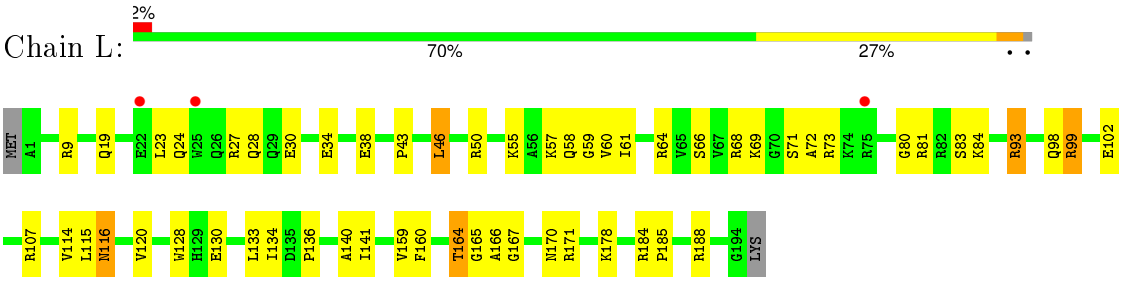
- Molecule 13: 50S ribosomal protein L15P

Chain K:



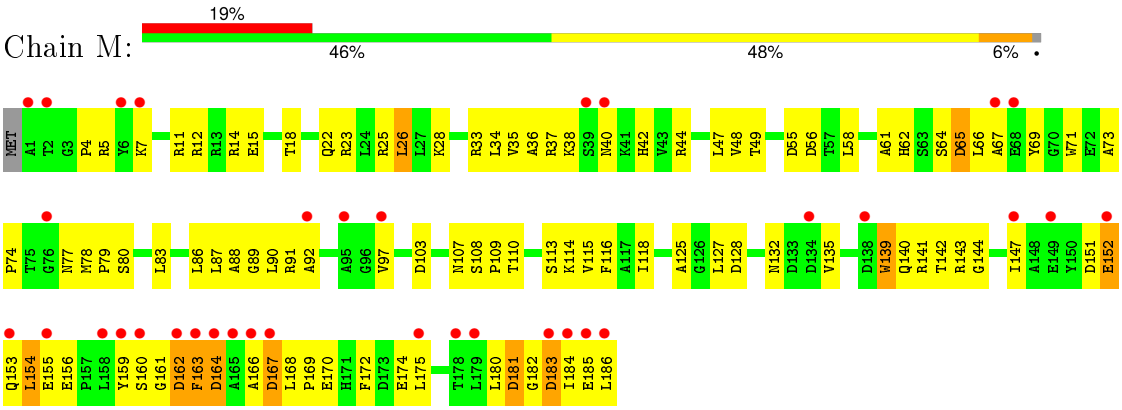
- Molecule 14: 50S ribosomal protein L15e

Chain L:



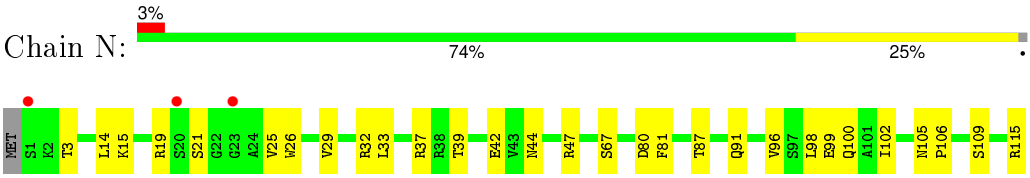
- Molecule 15: 50S ribosomal protein L18P

Chain M:



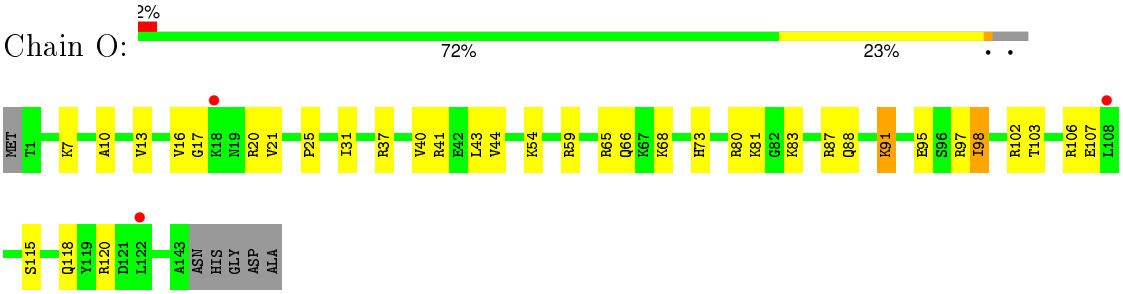
- Molecule 16: 50S ribosomal protein L18e

Chain N:



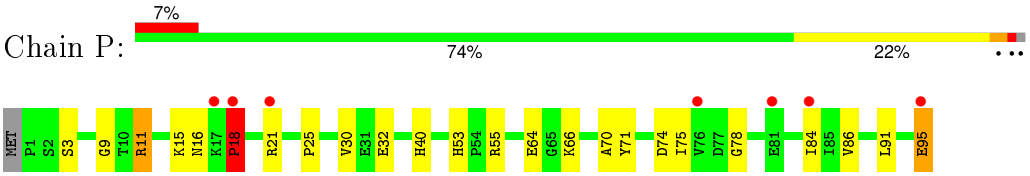
• Molecule 17: 50S ribosomal protein L19e

Chain O:



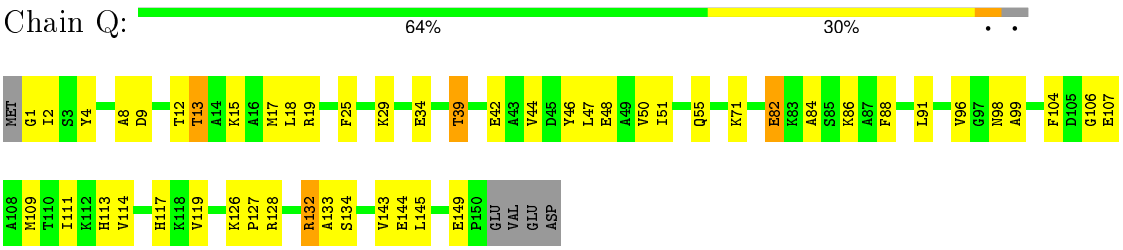
• Molecule 18: 50S ribosomal protein L21e

Chain P:



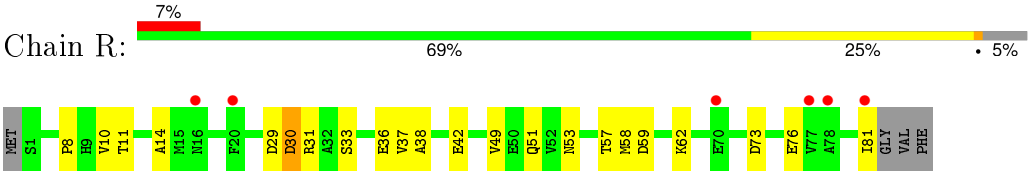
• Molecule 19: 50S ribosomal protein L22P

Chain Q:



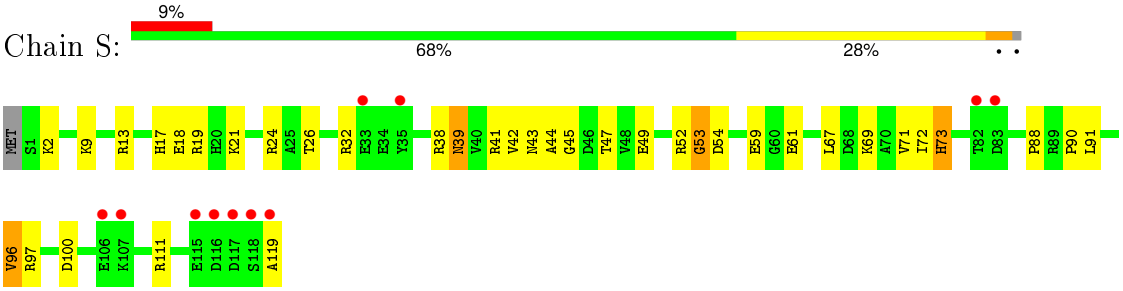
• Molecule 20: 50S ribosomal protein L23P

Chain R:



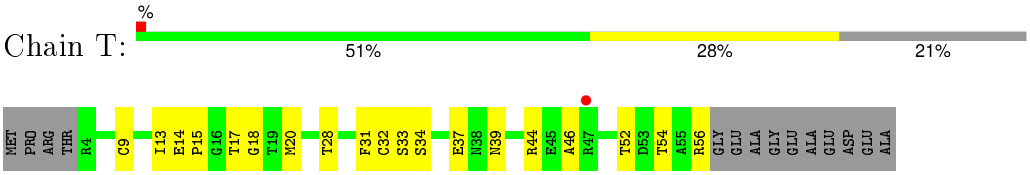
• Molecule 21: 50S ribosomal protein L24P

Chain S:



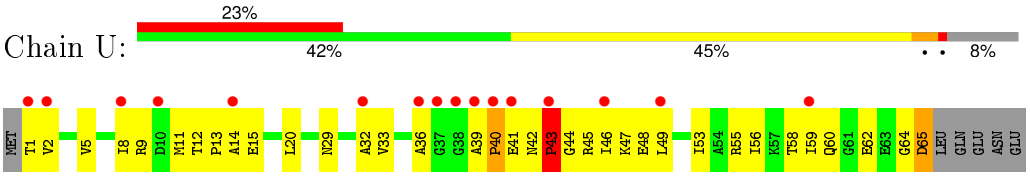
- Molecule 22: 50S ribosomal protein L24e

Chain T:



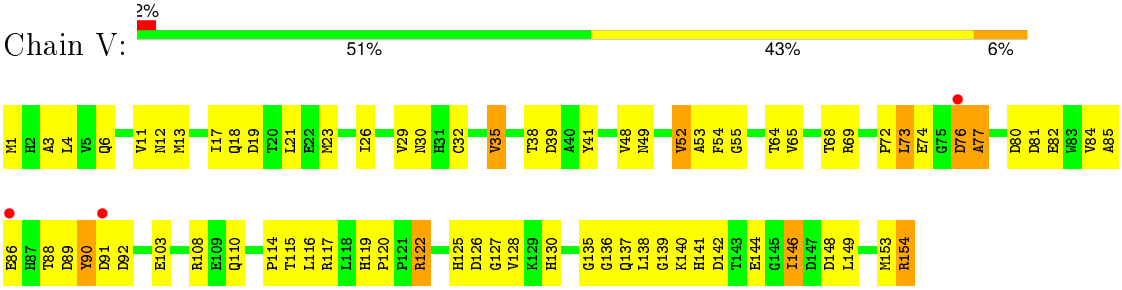
- Molecule 23: 50S ribosomal protein L29P

Chain U:



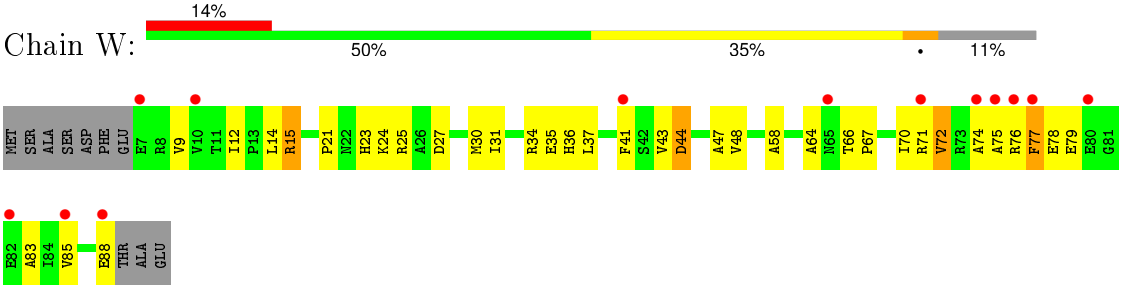
- Molecule 24: 50S ribosomal protein L30P

Chain V:



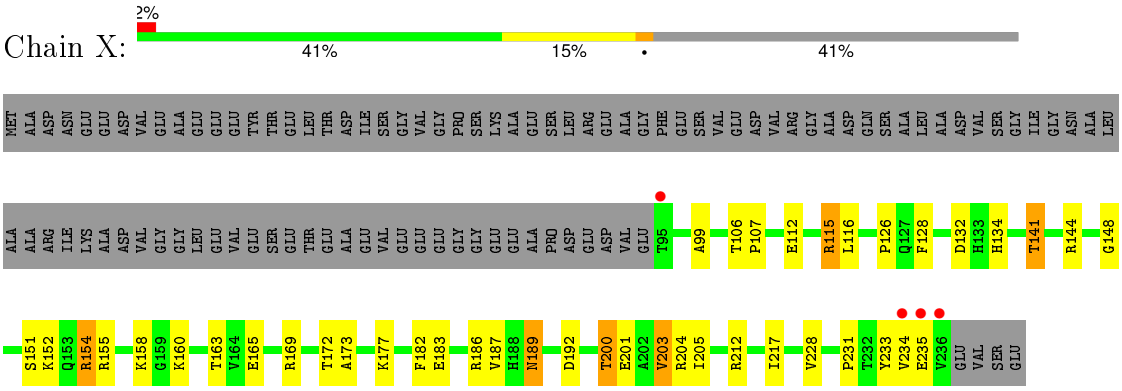
- Molecule 25: 50S ribosomal protein L31e

Chain W:



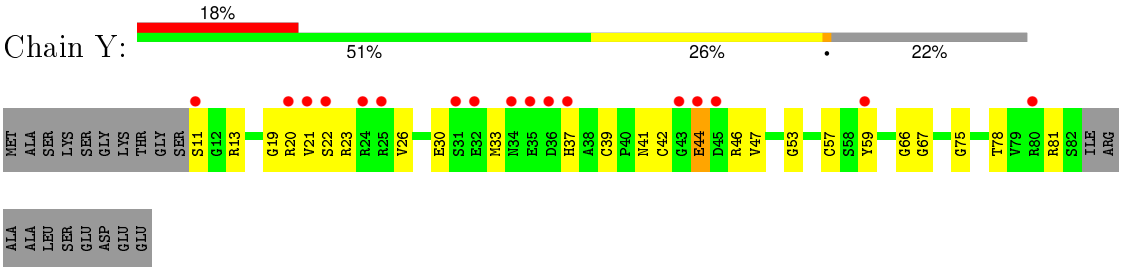
- Molecule 26: 50S ribosomal protein L32e

Chain X:



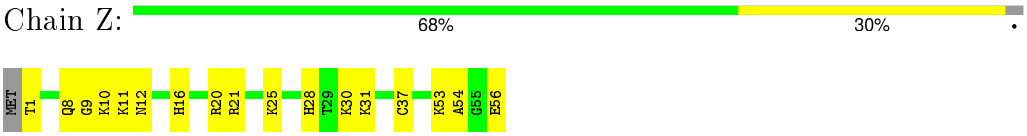
- Molecule 27: 50S ribosomal protein L37Ae

Chain Y:



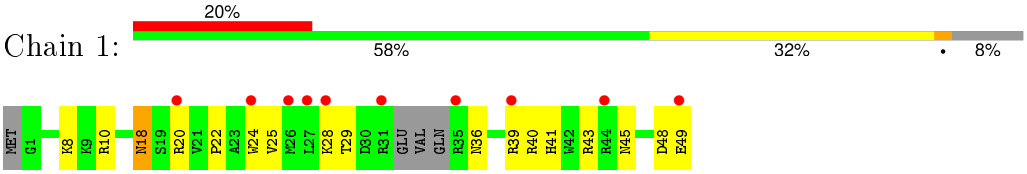
• Molecule 28: 50S ribosomal protein L37e

Chain Z:



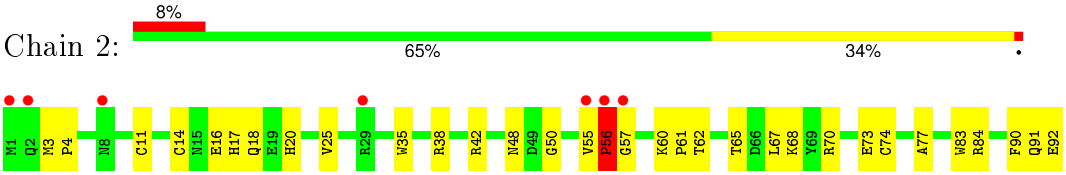
• Molecule 29: 50S ribosomal protein L39e

Chain 1:



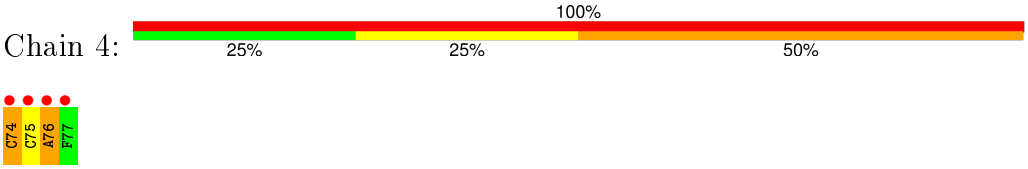
• Molecule 30: 50S ribosomal protein L44E

Chain 2:



• Molecule 31: 5'-R(*CP*CP*AP*(PHE)*(ACA))-3'

Chain 4:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	211.73Å 298.58Å 575.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.70 39.62 – 2.70	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-2.70) 91.4 (39.62-2.70)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.06 (at 2.69Å)	Xtriage
Refinement program	CNX	Depositor
R, R_{free}	0.191 , 0.230 0.193 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	58.0	Xtriage
Anisotropy	0.119	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 74.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 470025 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	98629	wwPDB-VP
Average B, all atoms (Å^2)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.06% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZLD, MG, ACE, CL, NA, K, CD, SR

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	0	0.37	2/66075 (0.0%)	0.69	25/103050 (0.0%)
2	9	0.34	0/2905	0.75	2/4528 (0.0%)
3	A	0.35	0/1786	0.65	0/2408
4	B	0.33	0/2690	0.64	0/3652
5	C	0.37	0/1885	0.63	0/2552
6	D	0.31	0/1111	0.57	0/1498
7	E	0.32	0/1382	0.57	0/1880
8	F	0.38	0/901	0.57	0/1224
9	G	0.28	0/241	0.48	0/324
10	H	0.51	0/1302	0.70	1/1743 (0.1%)
11	I	0.35	0/1136	0.59	0/1530
12	J	0.32	0/1004	0.65	0/1351
13	K	0.33	0/1130	0.65	0/1509
14	L	0.48	0/1582	0.67	0/2116
15	M	0.29	0/1474	0.62	0/1999
16	N	0.32	0/874	0.59	0/1181
17	O	0.35	0/1147	0.56	0/1528
18	P	0.33	0/749	0.65	0/1005
19	Q	0.34	0/1172	0.64	0/1578
20	R	0.31	0/648	0.57	0/875
21	S	0.31	0/958	0.62	0/1289
22	T	0.34	0/417	0.54	0/562
23	U	0.28	0/502	0.53	0/675
24	V	0.34	0/1219	0.62	0/1655
25	W	0.33	0/664	0.58	0/895
26	X	0.34	0/1146	0.64	0/1536
27	Y	0.46	0/578	0.69	0/773
28	Z	0.40	0/438	0.66	0/578
29	1	0.35	0/401	0.59	0/529
30	2	0.37	0/771	0.58	0/1024
31	4	1.99	3/76 (3.9%)	1.29	1/112 (0.9%)
All	All	0.37	5/98364 (0.0%)	0.68	29/147159 (0.0%)

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	0	0	54
2	9	0	2
24	V	0	1
All	All	0	57

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	0	559	C	C4-N4	-11.17	1.23	1.33
1	0	559	C	N3-C4	6.65	1.38	1.33
31	4	74	C	N1-C6	6.21	1.40	1.37
31	4	75	C	N1-C6	5.85	1.40	1.37
31	4	76	A	N3-C4	5.43	1.38	1.34

The worst 5 of 29 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	0	559	C	N3-C4-C5	-18.22	114.61	121.90
1	0	559	C	C2-N3-C4	14.39	127.10	119.90
2	9	3024	U	C2'-C3'-O3'	8.50	128.19	109.50
1	0	559	C	C5-C4-N4	7.84	125.69	120.20
1	0	871	G	C5'-C4'-O4'	-7.72	99.84	109.10

There are no chirality outliers.

5 of 57 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	182	G	Sidechain
1	0	270	U	Sidechain
1	0	324	G	Sidechain
1	0	332	G	Sidechain
1	0	50	G	Sidechain

5.2 Too-close contacts (i)

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	59016	0	29807	894	0
2	9	2600	0	1326	75	0
3	A	1753	0	1766	102	0
4	B	2625	0	2532	132	0
5	C	1860	0	1813	85	0
6	D	1094	0	1085	92	0
7	E	1357	0	1266	62	0
8	F	890	0	843	46	0
9	G	240	0	231	15	0
10	H	1282	0	1295	61	0
11	I	1120	0	1098	56	0
12	J	994	0	1027	48	0
13	K	1118	0	1076	47	0
14	L	1558	0	1573	57	0
15	M	1445	0	1401	113	0
16	N	865	0	873	28	0
17	O	1136	0	1123	38	0
18	P	735	0	728	19	0
19	Q	1149	0	1122	49	0
20	R	641	0	605	21	0
21	S	950	0	923	37	0
22	T	410	0	364	21	0
23	U	499	0	511	36	0
24	V	1196	0	1137	87	0
25	W	654	0	653	35	0
26	X	1130	0	1133	43	0
27	Y	567	0	526	18	0
28	Z	431	0	426	26	0
29	1	396	0	413	25	0
30	2	755	0	728	29	0
31	4	70	0	42	4	0
32	0	24	0	20	0	0
33	0	84	0	0	0	0
33	1	1	0	0	0	0
33	9	1	0	0	0	0
33	A	2	0	0	0	0
33	B	1	0	0	0	0
33	J	1	0	0	0	0
33	S	1	0	0	0	0
33	X	1	0	0	0	0
34	0	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	0	64	0	0	0	0
35	9	2	0	0	0	0
35	B	1	0	0	0	0
35	C	1	0	0	0	0
35	I	1	0	0	0	0
35	K	1	0	0	0	0
35	L	1	0	0	0	0
35	P	1	0	0	0	0
35	Q	2	0	0	0	0
35	R	1	0	0	0	0
36	0	9	0	0	0	0
36	2	1	0	0	0	0
36	A	1	0	0	0	0
36	B	1	0	0	0	0
36	I	3	0	0	1	0
36	J	1	0	0	0	0
36	K	1	0	0	0	0
36	L	1	0	0	1	0
36	M	1	0	0	0	0
36	N	1	0	0	0	0
36	Q	1	0	0	0	0
36	X	1	0	0	0	0
37	0	92	0	0	0	0
37	2	1	0	0	0	0
37	9	3	0	0	0	0
37	A	3	0	0	0	0
37	B	2	0	0	0	0
37	F	1	0	0	0	0
37	H	1	0	0	0	0
37	Q	1	0	0	0	0
37	R	1	0	0	0	0
37	S	1	0	0	0	0
37	Z	2	0	0	0	0
38	2	1	0	0	0	0
38	N	1	0	0	0	0
38	T	1	0	0	0	0
38	Y	1	0	0	0	0
38	Z	1	0	0	0	0
39	4	3	0	3	0	0
40	0	5757	0	0	72	0
40	1	40	0	0	1	0
40	2	73	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
40	4	3	0	0	0	0
40	9	144	0	0	5	0
40	A	129	0	0	10	0
40	B	158	0	0	12	0
40	C	183	0	0	12	0
40	D	53	0	0	4	0
40	E	50	0	0	4	0
40	F	25	0	0	2	0
40	G	22	0	0	2	0
40	H	66	0	0	6	0
40	I	57	0	0	3	0
40	J	59	0	0	4	0
40	K	84	0	0	9	0
40	L	136	0	0	5	0
40	M	66	0	0	10	0
40	N	45	0	0	3	0
40	O	70	0	0	1	0
40	P	51	0	0	2	0
40	Q	84	0	0	1	0
40	R	38	0	0	0	0
40	S	43	0	0	4	0
40	T	28	0	0	1	0
40	U	15	0	0	1	0
40	V	75	0	0	4	0
40	W	28	0	0	1	0
40	X	99	0	0	4	0
40	Y	23	0	0	2	0
40	Z	58	0	0	1	0
All	All	98629	0	59469	2191	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 15.

The worst 5 of 2191 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)
1:0:1160:G:H5'	1:0:1161:A:H5'	1.21	1.14
5:C:236:THR:HG22	5:C:239:ALA:H	1.07	1.11
2:9:3023:U:H3'	2:9:3024:U:H5"	1.29	1.09
1:0:156:C:H5"	14:L:171:ARG:HD3	1.37	1.04
1:0:2637:A:H2'	31:4:74:C:H5"	1.35	1.04

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
3	A	235/240 (98%)	210 (89%)	19 (8%)	6 (3%)	7 16
4	B	335/338 (99%)	311 (93%)	18 (5%)	6 (2%)	11 27
5	C	244/246 (99%)	227 (93%)	17 (7%)	0	100 100
6	D	134/177 (76%)	99 (74%)	25 (19%)	10 (8%)	1 1
7	E	170/178 (96%)	161 (95%)	9 (5%)	0	100 100
8	F	117/120 (98%)	104 (89%)	10 (8%)	3 (3%)	7 16
9	G	25/348 (7%)	25 (100%)	0	0	100 100
10	H	156/177 (88%)	140 (90%)	15 (10%)	1 (1%)	30 59
11	I	140/145 (97%)	128 (91%)	8 (6%)	4 (3%)	6 14
12	J	130/132 (98%)	120 (92%)	9 (7%)	1 (1%)	24 51
13	K	141/165 (86%)	120 (85%)	20 (14%)	1 (1%)	26 55
14	L	192/196 (98%)	179 (93%)	12 (6%)	1 (0%)	34 63
15	M	184/187 (98%)	162 (88%)	15 (8%)	7 (4%)	4 9
16	N	113/116 (97%)	111 (98%)	2 (2%)	0	100 100
17	O	141/149 (95%)	137 (97%)	4 (3%)	0	100 100
18	P	93/96 (97%)	87 (94%)	4 (4%)	2 (2%)	8 22
19	Q	148/155 (96%)	140 (95%)	8 (5%)	0	100 100
20	R	79/85 (93%)	77 (98%)	1 (1%)	1 (1%)	15 37
21	S	117/120 (98%)	108 (92%)	7 (6%)	2 (2%)	11 29
22	T	51/67 (76%)	47 (92%)	4 (8%)	0	100 100
23	U	63/71 (89%)	57 (90%)	4 (6%)	2 (3%)	5 12
24	V	152/154 (99%)	145 (95%)	5 (3%)	2 (1%)	15 37

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
25	W	80/92 (87%)	72 (90%)	7 (9%)	1 (1%)	15 37
26	X	140/241 (58%)	138 (99%)	2 (1%)	0	100 100
27	Y	70/92 (76%)	61 (87%)	6 (9%)	3 (4%)	3 7
28	Z	54/57 (95%)	52 (96%)	2 (4%)	0	100 100
29	1	42/50 (84%)	41 (98%)	1 (2%)	0	100 100
30	2	90/92 (98%)	86 (96%)	2 (2%)	2 (2%)	8 22
All	All	3636/4286 (85%)	3345 (92%)	236 (6%)	55 (2%)	13 32

5 of 55 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	27	LEU
4	B	139	ASP
6	D	93	LEU
6	D	95	THR
6	D	137	PRO

5.3.2 Protein sidechains (i)

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
3	A	179/182 (98%)	167 (93%)	12 (7%)	20 44
4	B	282/283 (100%)	268 (95%)	14 (5%)	30 60
5	C	193/193 (100%)	178 (92%)	15 (8%)	16 35
6	D	117/148 (79%)	107 (92%)	10 (8%)	13 30
7	E	152/156 (97%)	149 (98%)	3 (2%)	63 87
8	F	93/94 (99%)	91 (98%)	2 (2%)	60 86
9	G	27/282 (10%)	27 (100%)	0	100 100
10	H	134/145 (92%)	127 (95%)	7 (5%)	29 58
11	I	118/121 (98%)	108 (92%)	10 (8%)	13 30
12	J	106/106 (100%)	102 (96%)	4 (4%)	40 71

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
13	K	113/127 (89%)	108 (96%)	5 (4%)	35 65
14	L	158/160 (99%)	152 (96%)	6 (4%)	40 71
15	M	149/150 (99%)	144 (97%)	5 (3%)	44 75
16	N	93/94 (99%)	92 (99%)	1 (1%)	80 94
17	O	113/117 (97%)	111 (98%)	2 (2%)	66 89
18	P	79/80 (99%)	75 (95%)	4 (5%)	29 59
19	Q	117/122 (96%)	113 (97%)	4 (3%)	44 75
20	R	71/74 (96%)	71 (100%)	0	100 100
21	S	105/106 (99%)	102 (97%)	3 (3%)	50 80
22	T	44/53 (83%)	44 (100%)	0	100 100
23	U	51/57 (90%)	49 (96%)	2 (4%)	39 70
24	V	130/130 (100%)	122 (94%)	8 (6%)	23 49
25	W	66/74 (89%)	62 (94%)	4 (6%)	23 49
26	X	120/196 (61%)	111 (92%)	9 (8%)	17 38
27	Y	59/74 (80%)	58 (98%)	1 (2%)	68 90
28	Z	46/47 (98%)	46 (100%)	0	100 100
29	1	42/46 (91%)	41 (98%)	1 (2%)	57 85
30	2	79/79 (100%)	78 (99%)	1 (1%)	76 92
All	All	3036/3496 (87%)	2903 (96%)	133 (4%)	35 65

5 of 133 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
10	H	154	TYR
12	J	7	ASP
26	X	141	THR
10	H	159	PRO
11	I	79	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 77 such sidechains are listed below:

Mol	Chain	Res	Type
14	L	77	HIS
17	O	118	GLN
29	1	18	ASN

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Mol	Chain	Res	Type
14	L	143	ASN
17	O	50	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2746/2922 (93%)	239 (8%)	29 (1%)
2	9	121/122 (99%)	17 (14%)	2 (1%)
31	4	2/4 (50%)	1 (50%)	0
All	All	2869/3048 (94%)	257 (8%)	31 (1%)

5 of 257 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	0	11	A
1	0	31	C
1	0	60	A
1	0	67	A
1	0	69	A

5 of 31 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	1164	U
1	0	1352	A
1	0	2791	U
1	0	1232	A
1	0	1450	C

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 306 ligands modelled in this entry, 304 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	$\#\|Z\| > 2$
32	ZLD	0	9500	-	26,26,26	3.03	14 (53%)	35,36,36	3.14	14 (40%)
39	ACE	4	78	31	2,2,2	0.83	0	0,1,1	0.00	-

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	ZLD	0	9500	-	-	0/13/33/33	0/3/3/3
39	ACE	4	78	31	-	0/0/0/0	0/0/0/0

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	0	9500	ZLD	O10-C8	-2.31	1.43	1.46
32	0	9500	ZLD	C24-N19	-2.25	1.43	1.46
32	0	9500	ZLD	C2-N4	2.13	1.48	1.43
32	0	9500	ZLD	O10-C7	2.23	1.38	1.35
32	0	9500	ZLD	O15-C7	2.49	1.25	1.21

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	0	9500	ZLD	C6-N4-C7	-9.92	105.60	111.24
32	0	9500	ZLD	O15-C7-N4	-6.23	123.88	128.87
32	0	9500	ZLD	F18-C16-C5	-3.25	112.47	118.59
32	0	9500	ZLD	C3-C17-C16	-2.71	110.98	116.98
32	0	9500	ZLD	C8-O10-C7	-2.66	108.01	110.20

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

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^{th} 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	2754/2922 (94%)	-0.14	129 (4%) 35 34	29, 53, 97, 144	0
2	9	122/122 (100%)	0.64	14 (11%) 6 5	45, 75, 98, 149	0
3	A	237/240 (98%)	0.17	11 (4%) 36 35	34, 58, 90, 107	0
4	B	337/338 (99%)	0.10	6 (1%) 71 72	35, 60, 86, 96	0
5	C	246/246 (100%)	-0.09	4 (1%) 74 75	28, 53, 75, 86	0
6	D	140/177 (79%)	1.55	39 (27%) 1 1	67, 101, 122, 127	0
7	E	172/178 (96%)	0.53	11 (6%) 23 21	48, 74, 93, 98	0
8	F	119/120 (99%)	0.74	22 (18%) 2 1	57, 78, 99, 108	0
9	G	29/348 (8%)	2.71	21 (72%) 0 0	79, 99, 105, 109	0
10	H	160/177 (90%)	0.87	37 (23%) 1 1	41, 55, 80, 88	0
11	I	142/145 (97%)	0.03	4 (2%) 56 57	43, 56, 75, 94	0
12	J	132/132 (100%)	-0.04	4 (3%) 54 54	40, 54, 78, 90	0
13	K	145/165 (87%)	0.58	16 (11%) 7 5	34, 73, 107, 120	0
14	L	194/196 (98%)	-0.20	3 (1%) 76 76	33, 42, 65, 70	0
15	M	186/187 (99%)	0.92	35 (18%) 2 1	52, 72, 110, 121	0
16	N	115/116 (99%)	0.21	3 (2%) 59 59	45, 62, 77, 82	0
17	O	143/149 (95%)	0.40	3 (2%) 67 68	47, 59, 71, 82	0
18	P	95/96 (98%)	0.18	7 (7%) 17 15	46, 55, 72, 84	0
19	Q	150/155 (96%)	-0.10	0 100 100	37, 51, 70, 76	0
20	R	81/85 (95%)	0.29	6 (7%) 17 15	50, 65, 85, 90	0
21	S	119/120 (99%)	0.58	11 (9%) 11 9	47, 61, 87, 108	0
22	T	53/67 (79%)	0.37	1 (1%) 70 70	47, 59, 78, 86	0
23	U	65/71 (91%)	1.54	16 (24%) 1 1	59, 79, 115, 121	0
24	V	154/154 (100%)	0.21	3 (1%) 70 70	43, 58, 76, 81	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
25	W	82/92 (89%)	0.78	13 (15%) 3 2	48, 64, 88, 106	0
26	X	142/241 (58%)	0.01	4 (2%) 56 57	32, 49, 71, 91	0
27	Y	72/92 (78%)	0.80	17 (23%) 1 1	43, 59, 70, 76	0
28	Z	56/57 (98%)	-0.17	0 100 100	33, 40, 46, 57	0
29	1	46/50 (92%)	1.00	10 (21%) 1 1	41, 62, 87, 99	0
30	2	92/92 (100%)	0.40	7 (7%) 17 15	47, 64, 77, 86	0
31	4	4/4 (100%)	3.36	4 (100%) 0 0	78, 83, 85, 88	0
All	All	6584/7334 (89%)	0.17	461 (7%) 19 17	28, 57, 98, 149	0

The worst 5 of 461 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	9	3001	U	13.3
15	M	186	LEU	10.3
23	U	39	ALA	10.2
23	U	1	THR	10.1
21	S	119	ALA	10.1

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
35	NA	0	8555	1/1	0.71	0.66	67.14	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
33	MG	0	8065	1/1	0.91	0.79	57.02	100,100,100,100	0
35	NA	0	8522	1/1	0.77	0.82	40.65	77,77,77,77	0
35	NA	0	8553	1/1	0.88	0.44	37.85	63,63,63,63	0
35	NA	0	8512	1/1	0.70	0.57	34.29	72,72,72,72	0
35	NA	0	8527	1/1	0.93	0.30	33.85	51,51,51,51	0
35	NA	0	8562	1/1	0.85	0.84	33.31	78,78,78,78	0
33	MG	0	8047	1/1	0.93	0.40	28.09	98,98,98,98	0
35	NA	0	8521	1/1	0.91	0.44	27.34	110,110,110,110	0
35	NA	0	8559	1/1	0.89	0.36	25.32	85,85,85,85	0
35	NA	0	8545	1/1	0.95	0.45	24.48	57,57,57,57	0
35	NA	0	8563	1/1	0.82	0.68	24.28	69,69,69,69	0
35	NA	0	8535	1/1	0.74	0.50	22.96	79,79,79,79	0
35	NA	0	8517	1/1	0.83	0.35	21.78	53,53,53,53	0
33	MG	0	8002	1/1	0.91	0.37	21.09	82,82,82,82	0
36	CL	B	8819	1/1	0.88	0.38	21.06	72,72,72,72	0
34	K	0	8401	1/1	0.64	0.91	20.43	129,129,129,129	0
35	NA	0	8547	1/1	0.96	0.32	17.78	75,75,75,75	0
35	NA	0	8571	1/1	0.40	0.80	17.30	103,103,103,103	0
35	NA	0	8542	1/1	0.86	0.58	16.62	68,68,68,68	0
35	NA	0	8528	1/1	0.86	0.28	16.29	57,57,57,57	0
35	NA	B	8552	1/1	0.97	0.41	15.46	59,59,59,59	0
35	NA	0	8565	1/1	0.88	0.42	14.98	66,66,66,66	0
33	MG	0	8001	1/1	0.93	0.32	14.33	31,31,31,31	0
33	MG	0	8044	1/1	0.94	0.53	13.76	79,79,79,79	0
35	NA	0	8564	1/1	0.92	0.37	12.10	74,74,74,74	0
35	NA	L	8539	1/1	0.93	0.35	11.67	43,43,43,43	0
37	SR	B	8987	1/1	0.81	0.40	10.91	150,150,150,150	0
35	NA	0	8519	1/1	0.94	0.33	10.53	49,49,49,49	0
35	NA	9	8572	1/1	0.59	0.55	10.34	99,99,99,99	0
35	NA	0	8550	1/1	0.81	0.29	9.36	66,66,66,66	0
33	MG	A	8050	1/1	0.98	0.47	7.95	93,93,93,93	0
35	NA	0	8575	1/1	0.73	0.56	7.81	104,104,104,104	0
33	MG	0	8006	1/1	0.99	0.25	7.29	27,27,27,27	0
33	MG	0	8028	1/1	0.98	0.23	5.65	29,29,29,29	0
35	NA	0	8556	1/1	0.83	0.34	5.54	66,66,66,66	0
35	NA	0	8504	1/1	0.87	0.21	5.33	42,42,42,42	0
33	MG	0	8009	1/1	0.98	0.28	5.31	23,23,23,23	0
33	MG	0	8076	1/1	0.92	0.21	4.63	68,68,68,68	0
37	SR	0	8902	1/1	0.99	0.21	4.14	49,49,49,49	0
33	MG	0	8043	1/1	0.93	0.27	4.14	72,72,72,72	0
33	MG	0	8085	1/1	0.89	0.25	3.70	105,105,105,105	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
33	MG	0	8062	1/1	0.90	0.20	3.37	61,61,61,61	0
35	NA	0	8523	1/1	0.95	0.20	3.30	51,51,51,51	0
37	SR	0	8985	1/1	0.89	0.24	3.27	116,116,116,116	0
37	SR	0	8947	1/1	0.91	0.24	3.02	109,109,109,109	0
36	CL	N	8808	1/1	0.98	0.27	2.66	76,76,76,76	0
35	NA	0	8569	1/1	0.83	0.20	2.60	61,61,61,61	0
37	SR	0	8926	1/1	0.97	0.19	2.26	82,82,82,82	0
35	NA	0	8557	1/1	0.94	0.19	2.08	67,67,67,67	0
37	SR	0	8948	1/1	0.94	0.16	1.87	102,102,102,102	0
35	NA	K	8568	1/1	0.98	0.23	1.83	57,57,57,57	0
36	CL	L	8818	1/1	0.98	0.21	1.54	48,48,48,48	0
32	ZLD	0	9500	24/24	0.86	0.37	1.24	69,77,79,80	0
39	ACE	4	78	3/3	0.88	0.39	1.00	79,79,80,81	0
37	SR	0	8910	1/1	0.97	0.18	0.93	59,59,59,59	0
37	SR	Q	8912	1/1	1.00	0.17	0.91	75,75,75,75	0
35	NA	0	8530	1/1	0.96	0.17	0.82	56,56,56,56	0
37	SR	0	8904	1/1	0.99	0.17	0.76	52,52,52,52	0
33	MG	0	8058	1/1	0.95	0.22	0.66	28,28,28,28	0
33	MG	0	8014	1/1	0.99	0.20	0.61	37,37,37,37	0
33	MG	0	8040	1/1	0.70	0.18	0.39	97,97,97,97	0
37	SR	0	8936	1/1	0.99	0.15	0.31	70,70,70,70	0
33	MG	0	8075	1/1	0.96	0.16	-0.04	50,50,50,50	0
33	MG	0	8087	1/1	0.89	0.17	-0.20	61,61,61,61	0
37	SR	0	8964	1/1	0.91	0.13	-0.20	101,101,101,101	0
35	NA	0	8520	1/1	0.98	0.14	-0.42	61,61,61,61	0
37	SR	0	8943	1/1	0.84	0.14	-0.49	110,110,110,110	0
35	NA	0	8534	1/1	0.94	0.15	-0.51	61,61,61,61	0
36	CL	I	8821	1/1	0.93	0.16	-0.54	67,67,67,67	0
33	MG	0	8003	1/1	0.98	0.17	-0.61	35,35,35,35	0
35	NA	P	8540	1/1	0.92	0.13	-0.82	73,73,73,73	0
33	MG	0	8052	1/1	0.95	0.20	-0.84	49,49,49,49	0
37	SR	Z	8913	1/1	0.99	0.14	-0.85	52,52,52,52	0
35	NA	0	8515	1/1	0.98	0.15	-0.86	34,34,34,34	0
33	MG	0	8008	1/1	0.97	0.13	-0.94	34,34,34,34	0
33	MG	0	8084	1/1	0.95	0.10	-1.04	66,66,66,66	0
36	CL	J	8812	1/1	0.99	0.13	-1.07	54,54,54,54	0
37	SR	0	8942	1/1	0.99	0.12	-1.09	89,89,89,89	0
33	MG	S	8057	1/1	0.92	0.19	-1.13	55,55,55,55	0
35	NA	0	8529	1/1	0.89	0.11	-1.17	46,46,46,46	0
37	SR	0	8922	1/1	0.99	0.12	-1.17	77,77,77,77	0
38	CD	2	8704	1/1	1.00	0.07	-1.22	65,65,65,65	0
38	CD	T	8701	1/1	0.99	0.10	-1.24	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
37	SR	H	8972	1/1	0.91	0.10	-1.32	148,148,148,148	0
35	NA	I	8538	1/1	0.92	0.12	-1.35	51,51,51,51	0
35	NA	C	8503	1/1	0.94	0.14	-1.44	34,34,34,34	0
37	SR	2	8932	1/1	0.99	0.12	-1.45	76,76,76,76	0
38	CD	Y	8703	1/1	1.00	0.08	-1.45	59,59,59,59	0
36	CL	2	8804	1/1	0.93	0.12	-1.57	88,88,88,88	0
36	CL	0	8815	1/1	0.90	0.13	-1.59	61,61,61,61	0
37	SR	0	8969	1/1	0.94	0.12	-1.81	127,127,127,127	0
33	MG	A	8051	1/1	0.89	0.15	-1.83	71,71,71,71	0
35	NA	Q	8533	1/1	0.92	0.09	-1.87	68,68,68,68	0
37	SR	0	8949	1/1	0.98	0.12	-1.89	80,80,80,80	0
38	CD	Z	8702	1/1	0.99	0.09	-1.89	67,67,67,67	0
33	MG	X	8086	1/1	0.96	0.14	-1.91	51,51,51,51	0
37	SR	0	8981	1/1	0.92	0.10	-2.03	150,150,150,150	0
37	SR	A	8929	1/1	0.96	0.10	-2.14	103,103,103,103	0
33	MG	0	8012	1/1	0.98	0.10	-2.35	30,30,30,30	0
37	SR	0	8991	1/1	0.85	0.10	-2.57	150,150,150,150	0
33	MG	0	8004	1/1	0.97	0.11	-2.80	36,36,36,36	0
36	CL	0	8805	1/1	0.95	0.10	-2.87	65,65,65,65	0
33	MG	0	8041	1/1	0.98	0.13	-2.89	44,44,44,44	0
37	SR	0	8970	1/1	0.97	0.10	-2.90	80,80,80,80	0
37	SR	0	8992	1/1	0.98	0.09	-2.98	115,115,115,115	0
37	SR	0	8984	1/1	0.96	0.10	-3.00	109,109,109,109	0
37	SR	0	8975	1/1	0.90	0.08	-3.04	133,133,133,133	0
37	SR	0	8945	1/1	0.94	0.11	-3.10	92,92,92,92	0
33	MG	0	8025	1/1	0.96	0.08	-3.18	43,43,43,43	0
37	SR	0	8990	1/1	0.91	0.10	-3.25	131,131,131,131	0
37	SR	0	8959	1/1	0.90	0.07	-3.25	150,150,150,150	0
35	NA	0	8537	1/1	0.97	0.09	-3.48	43,43,43,43	0
33	MG	0	8011	1/1	0.91	0.08	-3.79	33,33,33,33	0
33	MG	0	8088	1/1	0.95	0.07	-4.45	57,57,57,57	0
34	K	0	8402	1/1	0.98	0.09	-4.51	70,70,70,70	0
37	SR	0	8962	1/1	0.97	0.06	-4.93	108,108,108,108	0
35	NA	0	8558	1/1	0.96	0.08	-5.39	63,63,63,63	0
33	MG	0	8034	1/1	0.98	0.07	-7.09	44,44,44,44	0
33	MG	0	8070	1/1	0.97	0.07	-8.09	62,62,62,62	0
33	MG	0	8093	1/1	0.98	0.07	-	41,41,41,41	0
35	NA	9	8543	1/1	-0.00	0.94	-	116,116,116,116	0
35	NA	0	8544	1/1	0.57	0.52	-	86,86,86,86	0
37	SR	0	8994	1/1	0.91	0.82	-	150,150,150,150	0
33	MG	0	8023	1/1	0.98	0.16	-	39,39,39,39	0
33	MG	0	8037	1/1	0.60	0.48	-	102,102,102,102	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
37	SR	9	8980	1/1	0.74	0.07	-	137,137,137,137	0
37	SR	0	8989	1/1	0.76	0.14	-	150,150,150,150	0
37	SR	0	8914	1/1	0.99	0.25	-	84,84,84,84	0
37	SR	0	8958	1/1	0.88	0.07	-	96,96,96,96	0
36	CL	X	8820	1/1	0.96	0.08	-	49,49,49,49	0
37	SR	0	8951	1/1	0.95	0.14	-	113,113,113,113	0
35	NA	0	8525	1/1	0.69	0.28	-	92,92,92,92	0
33	MG	0	8089	1/1	0.76	0.10	-	49,49,49,49	0
37	SR	0	8960	1/1	0.83	0.10	-	116,116,116,116	0
36	CL	I	8802	1/1	0.89	0.19	-	71,71,71,71	0
38	CD	N	8705	1/1	0.89	0.41	-	150,150,150,150	0
33	MG	0	8024	1/1	0.97	0.21	-	81,81,81,81	0
33	MG	0	8081	1/1	0.54	0.34	-	82,82,82,82	0
35	NA	0	8526	1/1	0.94	0.15	-	50,50,50,50	0
37	SR	0	8928	1/1	0.97	0.12	-	91,91,91,91	0
36	CL	I	8801	1/1	0.96	0.13	-	61,61,61,61	0
35	NA	0	8549	1/1	0.93	0.32	-	75,75,75,75	0
33	MG	0	8019	1/1	0.95	0.23	-	37,37,37,37	0
33	MG	0	8073	1/1	0.78	0.69	-	105,105,105,105	0
33	MG	0	8029	1/1	0.92	0.27	-	100,100,100,100	0
37	SR	0	9001	1/1	0.85	0.08	-	150,150,150,150	0
37	SR	0	8905	1/1	0.99	0.21	-	59,59,59,59	0
37	SR	A	8930	1/1	0.98	0.19	-	81,81,81,81	0
33	MG	0	8091	1/1	0.95	0.05	-	54,54,54,54	0
35	NA	0	8505	1/1	0.93	0.37	-	51,51,51,51	0
33	MG	0	8063	1/1	0.82	0.34	-	94,94,94,94	0
37	SR	0	8971	1/1	0.67	0.13	-	150,150,150,150	0
35	NA	0	8567	1/1	0.77	0.69	-	83,83,83,83	0
33	MG	0	8083	1/1	0.99	0.16	-	55,55,55,55	0
37	SR	0	8920	1/1	0.92	0.09	-	96,96,96,96	0
37	SR	9	8968	1/1	0.96	0.12	-	132,132,132,132	0
33	MG	0	8036	1/1	0.89	0.08	-	58,58,58,58	0
37	SR	0	8983	1/1	0.91	0.15	-	150,150,150,150	0
33	MG	0	8080	1/1	0.96	0.07	-	78,78,78,78	0
33	MG	0	8016	1/1	0.97	0.20	-	94,94,94,94	0
33	MG	0	8079	1/1	0.93	0.14	-	72,72,72,72	0
35	NA	0	8516	1/1	0.87	0.73	-	52,52,52,52	0
37	SR	9	9003	1/1	0.93	0.34	-	150,150,150,150	0
33	MG	0	8064	1/1	0.86	0.12	-	69,69,69,69	0
37	SR	0	8946	1/1	0.86	0.17	-	99,99,99,99	0
37	SR	0	8956	1/1	0.85	0.07	-	128,128,128,128	0
33	MG	0	8048	1/1	0.98	0.07	-	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
37	SR	0	8903	1/1	0.99	0.14	-	59,59,59,59	0
36	CL	0	8803	1/1	0.96	0.20	-	61,61,61,61	0
36	CL	Q	8806	1/1	0.95	0.12	-	49,49,49,49	0
33	MG	0	8030	1/1	0.77	0.44	-	99,99,99,99	0
37	SR	0	8979	1/1	0.95	0.28	-	150,150,150,150	0
37	SR	0	9000	1/1	0.92	0.08	-	111,111,111,111	0
37	SR	0	8921	1/1	0.99	0.17	-	70,70,70,70	0
35	NA	0	8513	1/1	0.94	0.21	-	50,50,50,50	0
33	MG	B	8042	1/1	0.59	0.19	-	85,85,85,85	0
33	MG	J	8054	1/1	0.99	0.20	-	37,37,37,37	0
37	SR	0	8923	1/1	0.98	0.13	-	83,83,83,83	0
37	SR	0	8993	1/1	0.94	0.08	-	139,139,139,139	0
37	SR	0	9008	1/1	0.93	0.13	-	91,91,91,91	0
36	CL	0	8822	1/1	0.95	0.26	-	69,69,69,69	0
36	CL	M	8807	1/1	0.94	0.35	-	71,71,71,71	0
35	NA	0	8554	1/1	0.77	0.28	-	63,63,63,63	0
37	SR	0	8938	1/1	0.95	0.26	-	105,105,105,105	0
37	SR	0	8917	1/1	0.98	0.16	-	81,81,81,81	0
35	NA	0	8511	1/1	0.93	0.18	-	71,71,71,71	0
33	MG	0	8045	1/1	0.91	0.61	-	71,71,71,71	0
35	NA	0	8518	1/1	0.57	0.67	-	107,107,107,107	0
36	CL	0	8816	1/1	0.96	0.19	-	77,77,77,77	0
33	MG	0	8017	1/1	0.55	0.52	-	121,121,121,121	0
33	MG	0	8010	1/1	0.83	0.42	-	70,70,70,70	0
35	NA	0	8524	1/1	0.98	0.37	-	56,56,56,56	0
37	SR	F	9005	1/1	0.95	0.21	-	116,116,116,116	0
37	SR	0	8925	1/1	0.98	0.21	-	79,79,79,79	0
33	MG	0	8007	1/1	0.86	0.25	-	53,53,53,53	0
33	MG	0	8018	1/1	0.98	0.29	-	44,44,44,44	0
36	CL	0	8817	1/1	0.98	0.13	-	56,56,56,56	0
33	MG	0	8061	1/1	0.99	0.17	-	36,36,36,36	0
33	MG	0	8022	1/1	0.95	0.27	-	46,46,46,46	0
37	SR	0	8918	1/1	0.99	0.21	-	59,59,59,59	0
35	NA	0	8566	1/1	0.96	0.59	-	54,54,54,54	0
35	NA	0	8531	1/1	0.95	0.08	-	41,41,41,41	0
37	SR	0	8955	1/1	0.81	0.08	-	122,122,122,122	0
33	MG	0	8072	1/1	0.99	0.14	-	47,47,47,47	0
33	MG	0	8026	1/1	0.97	0.11	-	61,61,61,61	0
37	SR	0	8939	1/1	0.88	0.14	-	100,100,100,100	0
33	MG	0	8039	1/1	0.89	0.37	-	68,68,68,68	0
36	CL	0	8811	1/1	0.95	0.14	-	83,83,83,83	0
33	MG	0	8071	1/1	0.77	1.23	-	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
37	SR	0	8999	1/1	0.99	0.09	-	88,88,88,88	0
35	NA	0	8541	1/1	0.83	0.37	-	62,62,62,62	0
37	SR	0	8997	1/1	0.86	0.12	-	142,142,142,142	0
33	MG	0	8066	1/1	0.42	0.33	-	103,103,103,103	0
37	SR	0	8978	1/1	0.97	0.06	-	85,85,85,85	0
33	MG	0	8032	1/1	0.96	0.09	-	56,56,56,56	0
37	SR	Z	8952	1/1	0.97	0.11	-	71,71,71,71	0
33	MG	0	8077	1/1	0.95	0.08	-	47,47,47,47	0
37	SR	0	8996	1/1	0.96	0.50	-	150,150,150,150	0
37	SR	0	8988	1/1	0.85	0.07	-	125,125,125,125	0
33	MG	0	8035	1/1	0.79	0.28	-	80,80,80,80	0
37	SR	0	8973	1/1	0.91	0.13	-	101,101,101,101	0
35	NA	0	8506	1/1	0.92	0.38	-	66,66,66,66	0
35	NA	Q	8532	1/1	0.93	0.09	-	49,49,49,49	0
37	SR	0	8935	1/1	0.99	0.18	-	80,80,80,80	0
36	CL	K	8810	1/1	0.94	0.14	-	55,55,55,55	0
35	NA	0	8502	1/1	0.87	0.32	-	75,75,75,75	0
37	SR	0	8963	1/1	0.97	0.12	-	83,83,83,83	0
37	SR	0	8909	1/1	0.98	0.17	-	74,74,74,74	0
37	SR	0	8916	1/1	0.98	0.17	-	85,85,85,85	0
33	MG	1	8060	1/1	0.90	0.13	-	58,58,58,58	0
33	MG	0	8055	1/1	0.99	0.16	-	40,40,40,40	0
35	NA	0	8507	1/1	0.89	0.17	-	51,51,51,51	0
37	SR	0	8944	1/1	0.87	0.34	-	135,135,135,135	0
33	MG	0	8020	1/1	0.97	0.17	-	52,52,52,52	0
37	SR	0	8919	1/1	0.78	0.15	-	131,131,131,131	0
37	SR	0	8940	1/1	0.99	0.10	-	77,77,77,77	0
37	SR	0	8976	1/1	0.89	0.24	-	139,139,139,139	0
37	SR	0	8937	1/1	0.96	0.13	-	80,80,80,80	0
33	MG	0	8068	1/1	0.92	0.60	-	86,86,86,86	0
36	CL	0	8813	1/1	0.94	0.09	-	59,59,59,59	0
33	MG	0	8053	1/1	0.93	0.20	-	64,64,64,64	0
37	SR	0	8967	1/1	0.88	0.12	-	113,113,113,113	0
37	SR	0	8927	1/1	0.94	0.15	-	90,90,90,90	0
35	NA	0	8514	1/1	0.92	0.23	-	51,51,51,51	0
36	CL	A	8809	1/1	0.95	0.20	-	65,65,65,65	0
35	NA	0	8570	1/1	0.81	0.30	-	57,57,57,57	0
35	NA	0	8508	1/1	0.83	0.66	-	55,55,55,55	0
33	MG	0	8082	1/1	0.77	0.42	-	78,78,78,78	0
33	MG	0	8067	1/1	0.92	0.06	-	58,58,58,58	0
33	MG	0	8069	1/1	0.82	0.34	-	78,78,78,78	0
37	SR	0	9007	1/1	0.86	0.44	-	150,150,150,150	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
35	NA	0	8573	1/1	0.64	1.09	-	92,92,92,92	0
37	SR	A	8977	1/1	0.93	0.19	-	99,99,99,99	0
33	MG	9	8074	1/1	0.94	0.20	-	64,64,64,64	0
33	MG	0	8005	1/1	0.99	0.07	-	39,39,39,39	0
33	MG	0	8049	1/1	0.93	0.22	-	85,85,85,85	0
37	SR	R	8961	1/1	0.91	0.16	-	122,122,122,122	0
35	NA	R	8510	1/1	0.34	0.38	-	127,127,127,127	0
36	CL	0	8814	1/1	0.99	0.19	-	57,57,57,57	0
37	SR	0	9004	1/1	0.95	0.15	-	150,150,150,150	0
37	SR	S	8911	1/1	0.97	0.15	-	72,72,72,72	0
33	MG	0	8078	1/1	0.91	0.20	-	64,64,64,64	0
37	SR	0	9002	1/1	0.84	0.12	-	125,125,125,125	0
33	MG	0	8038	1/1	0.49	0.80	-	88,88,88,88	0
33	MG	0	8059	1/1	0.95	0.08	-	56,56,56,56	0
35	NA	0	8501	1/1	0.91	0.15	-	46,46,46,46	0
33	MG	0	8090	1/1	0.94	0.38	-	83,83,83,83	0
33	MG	0	8027	1/1	0.96	0.24	-	53,53,53,53	0
37	SR	0	8933	1/1	0.94	0.08	-	103,103,103,103	0
35	NA	0	8548	1/1	0.72	0.14	-	59,59,59,59	0
37	SR	0	8924	1/1	0.93	0.24	-	112,112,112,112	0
37	SR	0	8931	1/1	0.88	0.15	-	94,94,94,94	0
37	SR	B	8950	1/1	0.92	0.17	-	106,106,106,106	0
37	SR	0	8998	1/1	0.98	0.11	-	133,133,133,133	0
37	SR	0	8901	1/1	0.99	0.14	-	75,75,75,75	0
33	MG	0	8092	1/1	0.84	0.15	-	72,72,72,72	0
35	NA	0	8546	1/1	0.94	0.29	-	77,77,77,77	0
37	SR	0	8965	1/1	0.92	0.11	-	108,108,108,108	0
33	MG	0	8015	1/1	0.98	0.13	-	62,62,62,62	0
37	SR	0	9006	1/1	0.75	0.71	-	150,150,150,150	0
33	MG	0	8021	1/1	0.98	0.15	-	38,38,38,38	0
33	MG	0	8046	1/1	0.93	0.41	-	65,65,65,65	0
35	NA	0	8560	1/1	0.96	0.47	-	88,88,88,88	0
35	NA	0	8574	1/1	0.70	0.53	-	66,66,66,66	0
35	NA	0	8536	1/1	0.79	0.33	-	71,71,71,71	0
35	NA	0	8551	1/1	0.94	0.35	-	46,46,46,46	0
35	NA	0	8509	1/1	0.91	0.39	-	83,83,83,83	0
33	MG	0	8031	1/1	0.87	0.09	-	57,57,57,57	0
37	SR	0	8982	1/1	0.77	0.22	-	144,144,144,144	0
37	SR	0	8995	1/1	0.95	0.21	-	107,107,107,107	0
37	SR	0	8953	1/1	0.98	0.17	-	96,96,96,96	0
35	NA	0	8561	1/1	0.69	0.17	-	122,122,122,122	0
37	SR	0	8941	1/1	0.98	0.15	-	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
37	SR	0	8908	1/1	0.89	0.16	-	90,90,90,90	0
33	MG	0	8056	1/1	0.93	0.38	-	83,83,83,83	0
37	SR	0	8954	1/1	0.97	0.15	-	94,94,94,94	0
37	SR	0	8966	1/1	0.94	0.09	-	98,98,98,98	0
37	SR	0	8915	1/1	0.95	0.08	-	93,93,93,93	0
37	SR	0	8907	1/1	0.98	0.14	-	63,63,63,63	0
37	SR	0	8974	1/1	0.93	0.23	-	134,134,134,134	0
33	MG	0	8033	1/1	0.93	0.07	-	58,58,58,58	0
37	SR	0	8957	1/1	0.90	0.13	-	120,120,120,120	0
37	SR	0	8986	1/1	0.75	0.08	-	131,131,131,131	0
37	SR	0	8906	1/1	0.98	0.18	-	56,56,56,56	0
37	SR	0	8934	1/1	0.98	0.17	-	90,90,90,90	0

6.5 Other polymers (i)

There are no such residues in this entry.