wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 05:03 AM GMT

PDB ID	:	2OTL
Title	:	Girodazole bound to the large subunit of Haloarcula marismortui
Authors	:	Blaha, G.; Schroeder, S.J.; Tirado-Rives, J.
Deposited on	:	2007-02-08
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:

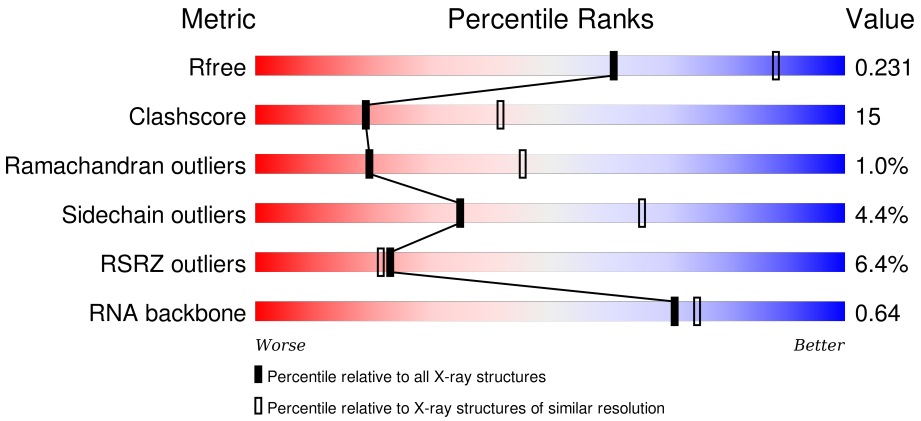
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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))
R_{free}	91344	2103 (2.70-2.70)
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	2% 49% 39% 6% 6%
2	9	122	3% 43% 44% 12%
3	A	239	12% 70% 26%
4	B	337	% 61% 35%

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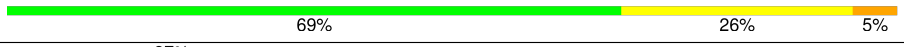
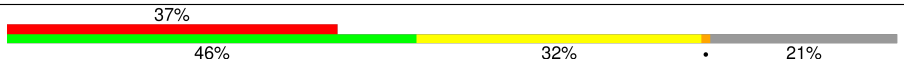
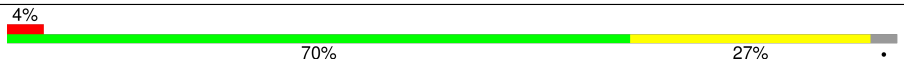
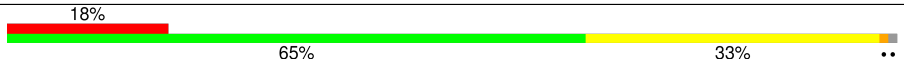
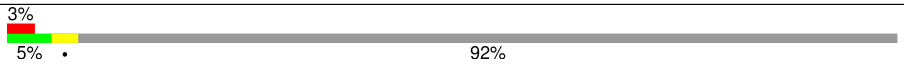
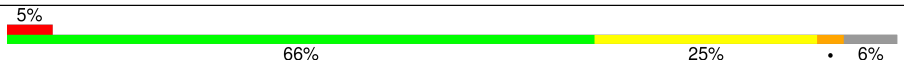
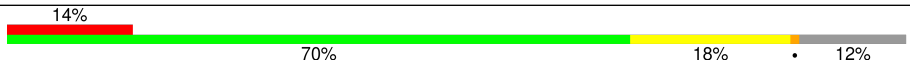
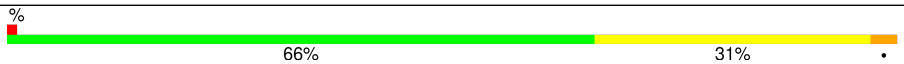
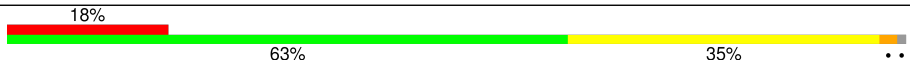
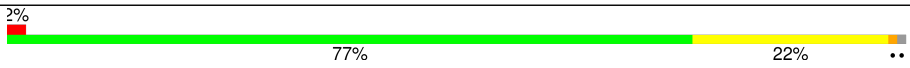
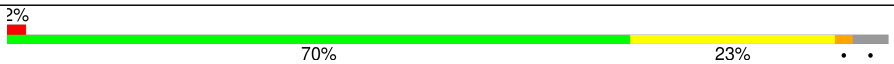
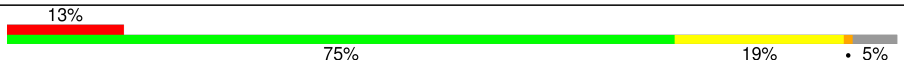
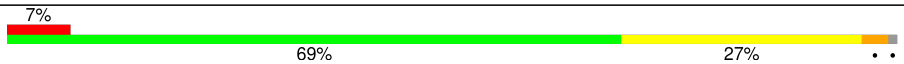
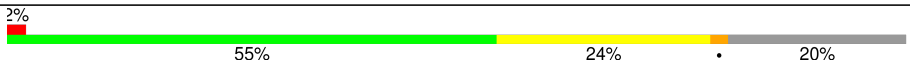
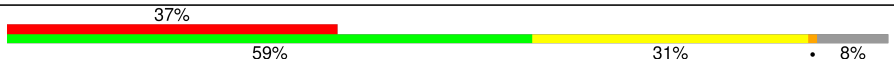
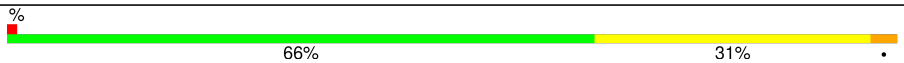
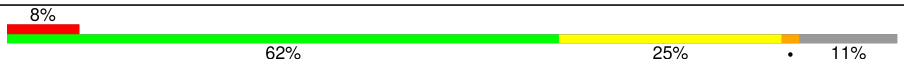
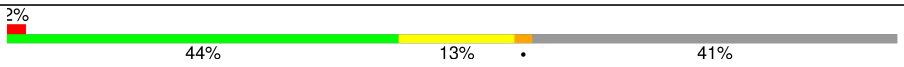
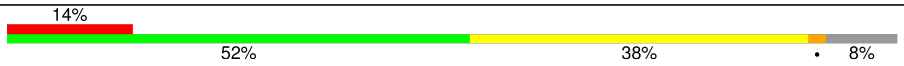
Mol	Chain	Length	Quality of chain
5	C	246	
6	D	177	
7	E	178	
8	F	120	
9	G	348	
10	H	171	
11	J	145	
12	K	132	
13	L	165	
14	M	194	
15	N	187	
16	O	116	
17	P	149	
18	Q	96	
19	R	155	
20	S	85	
21	T	120	
22	U	66	
23	V	71	
24	W	154	
25	X	92	
26	Y	241	
27	Z	73	
28	1	57	
29	2	50	

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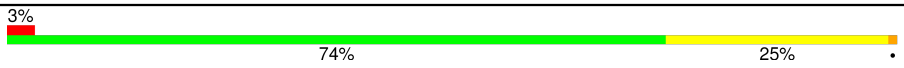
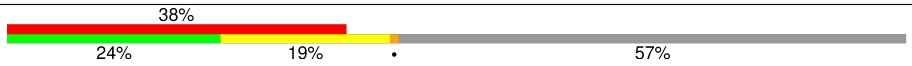
Mol	Chain	Length	Quality of chain
30	3	92	
31	I	162	

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	8060	-	-	-	X
35	NA	0	8502	-	-	-	X
35	NA	0	8503	-	-	-	X
35	NA	0	8514	-	-	-	X
35	NA	0	8521	-	-	-	X
35	NA	0	8526	-	-	-	X
35	NA	0	8529	-	-	-	X
35	NA	0	8532	-	-	-	X
35	NA	0	8535	-	-	-	X
35	NA	0	8550	-	-	-	X
35	NA	0	8555	-	-	-	X
35	NA	0	8556	-	-	-	X
35	NA	0	8561	-	-	-	X
35	NA	0	8562	-	-	-	X
35	NA	0	8564	-	-	-	X
35	NA	0	8565	-	-	-	X
35	NA	0	8566	-	-	-	X
35	NA	0	8568	-	-	-	X
35	NA	0	8569	-	-	-	X
35	NA	0	8571	-	-	-	X
35	NA	0	8572	-	-	-	X
35	NA	0	8573	-	-	-	X
35	NA	0	8574	-	-	-	X
35	NA	0	8576	-	-	-	X
35	NA	0	8577	-	-	-	X
35	NA	0	8578	-	-	-	X
35	NA	0	8582	-	-	-	X
35	NA	9	8583	-	-	-	X
35	NA	L	8580	-	-	-	X
35	NA	R	8537	-	-	-	X
35	NA	R	8586	-	-	-	X
36	CL	0	8705	-	-	-	X
36	CL	0	8713	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
36	CL	0	8715	-	-	-	X
36	CL	J	8701	-	-	X	-
36	CL	M	8718	-	-	X	-

2 Entry composition (i)

There are 38 unique types of molecules in this entry. The entry contains 99016 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
			Total	C	N	O	P			
1	0	2754	59021	26350	10878	19048	2745	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
0	560	C	U	CONFLICT	GB 3377779
0	628	1MA	A	MODIFIED RESIDUE	GB 3377779
0	2587	OMU	U	MODIFIED RESIDUE	GB 3377779
0	2588	OMG	G	MODIFIED RESIDUE	GB 3377779
0	2619	UR3	U	MODIFIED RESIDUE	GB 3377779
0	2621	PSU	U	MODIFIED RESIDUE	GB 3377779

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

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

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

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

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

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

- 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
			1859	1131	344	383	1			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	73	LEU	GLN	CONFLICT	UNP P12735

- 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			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	248	ASP	ALA	CONFLICT	UNP P15825

- 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
			1266	785	237	238	6			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	164	ASP	-	INSERTION	UNP P60617
H	165	SER	-	INSERTION	UNP P60617
H	166	SER	-	INSERTION	UNP P60617
H	167	PRO	-	INSERTION	UNP P60617
H	168	ALA	-	INSERTION	UNP P60617
H	169	GLY	-	INSERTION	UNP P60617
H	170	ASN	-	INSERTION	UNP P60617
H	171	ALA	-	INSERTION	UNP P60617

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	J	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	K	132	Total	C	N	O	S	0	0	0
			992	609	187	192	4			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	44	LEU	HIS	CONFLICT	UNP P22450

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	L	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	M	194	Total	C	N	O	S	0	0	0
			1560	943	332	284	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	13	GLU	LYS	CONFLICT	UNP P60618
M	194	ALA	-	INSERTION	UNP P60618

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	N	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	O	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	P	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	Q	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	R	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	S	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	T	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	U	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	V	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	W	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	X	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	Y	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	Z	73	Total	C	N	O	S	0	0	0
			579	346	116	112	5			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Z	10	ARG	-	INSERTION	UNP P60619

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	1	56	Total	C	N	O	S	0	0	0
			430	258	86	82	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	2	46	Total	C	N	O	S	0	0	0
			396	239	89	67	1			

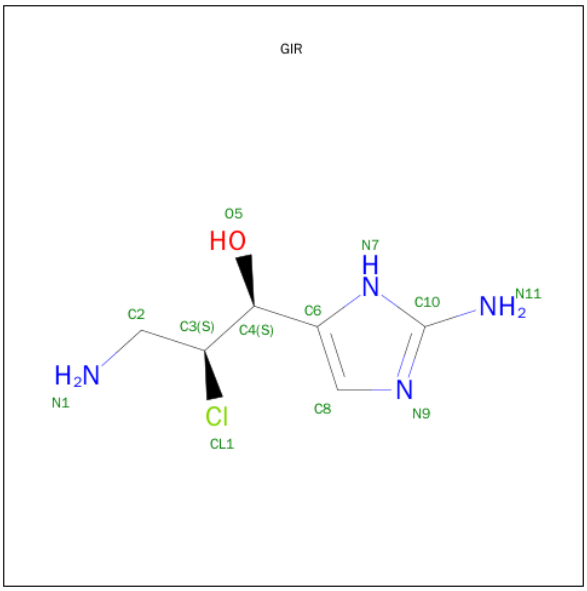
- Molecule 30 is a protein called 50S ribosomal protein L44E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	3	92	Total	C	N	O	S	0	0	0
			755	458	153	137	7			

- Molecule 31 is a protein called 50S ribosomal protein L11P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	I	70	Total	C	N	O	S	0	0	0
			519	323	81	114	1			

- Molecule 32 is GIRODAZOLE (three-letter code: GIR) (formula: $C_6H_{11}ClN_4O$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
32	0	1	Total	C	Cl	N	O	0	0
			12	6	1	4	1		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	0	107	Total	Mg	0	0
			107	107		
33	Y	1	Total	Mg	0	0
			1	1		
33	K	1	Total	Mg	0	0
			1	1		
33	B	2	Total	Mg	0	0
			2	2		
33	A	2	Total	Mg	0	0
			2	2		
33	T	1	Total	Mg	0	0
			1	1		
33	9	1	Total	Mg	0	0
			1	1		
33	3	1	Total	Mg	0	0
			1	1		

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

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	0	71	Total	Na	0	0
			71	71		
35	J	1	Total	Na	0	0
			1	1		
35	Q	1	Total	Na	0	0
			1	1		
35	H	2	Total	Na	0	0
			2	2		
35	C	1	Total	Na	0	0
			1	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	A	1	Total Na 1 1	0	0
35	R	3	Total Na 3 3	0	0
35	9	2	Total Na 2 2	0	0
35	L	1	Total Na 1 1	0	0
35	S	1	Total Na 1 1	0	0
35	M	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	3	Total Cl 3 3	0	0
36	Q	1	Total Cl 1 1	0	0
36	B	1	Total Cl 1 1	0	0
36	A	1	Total Cl 1 1	0	0
36	N	1	Total Cl 1 1	0	0
36	O	1	Total Cl 1 1	0	0
36	R	1	Total Cl 1 1	0	0
36	Y	1	Total Cl 1 1	0	0
36	L	1	Total Cl 1 1	0	0
36	3	1	Total Cl 1 1	0	0
36	M	1	Total Cl 1 1	0	0

- Molecule 37 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	O	1	Total Cd 1 1	0	0
37	Z	1	Total Cd 1 1	0	0
37	1	1	Total Cd 1 1	0	0
37	3	1	Total Cd 1 1	0	0
37	U	1	Total Cd 1 1	0	0

- Molecule 38 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
38	0	5893	Total O 5893 5893	0	0
38	9	145	Total O 145 145	0	0
38	A	118	Total O 118 118	0	0
38	B	147	Total O 147 147	0	0
38	C	163	Total O 163 163	0	0
38	D	48	Total O 48 48	0	0
38	E	46	Total O 46 46	0	0
38	F	23	Total O 23 23	0	0
38	G	19	Total O 19 19	0	0
38	H	69	Total O 69 69	0	0
38	J	58	Total O 58 58	0	0
38	K	58	Total O 58 58	0	0
38	L	81	Total O 81 81	0	0
38	M	115	Total O 115 115	0	0
38	N	58	Total O 58 58	0	0

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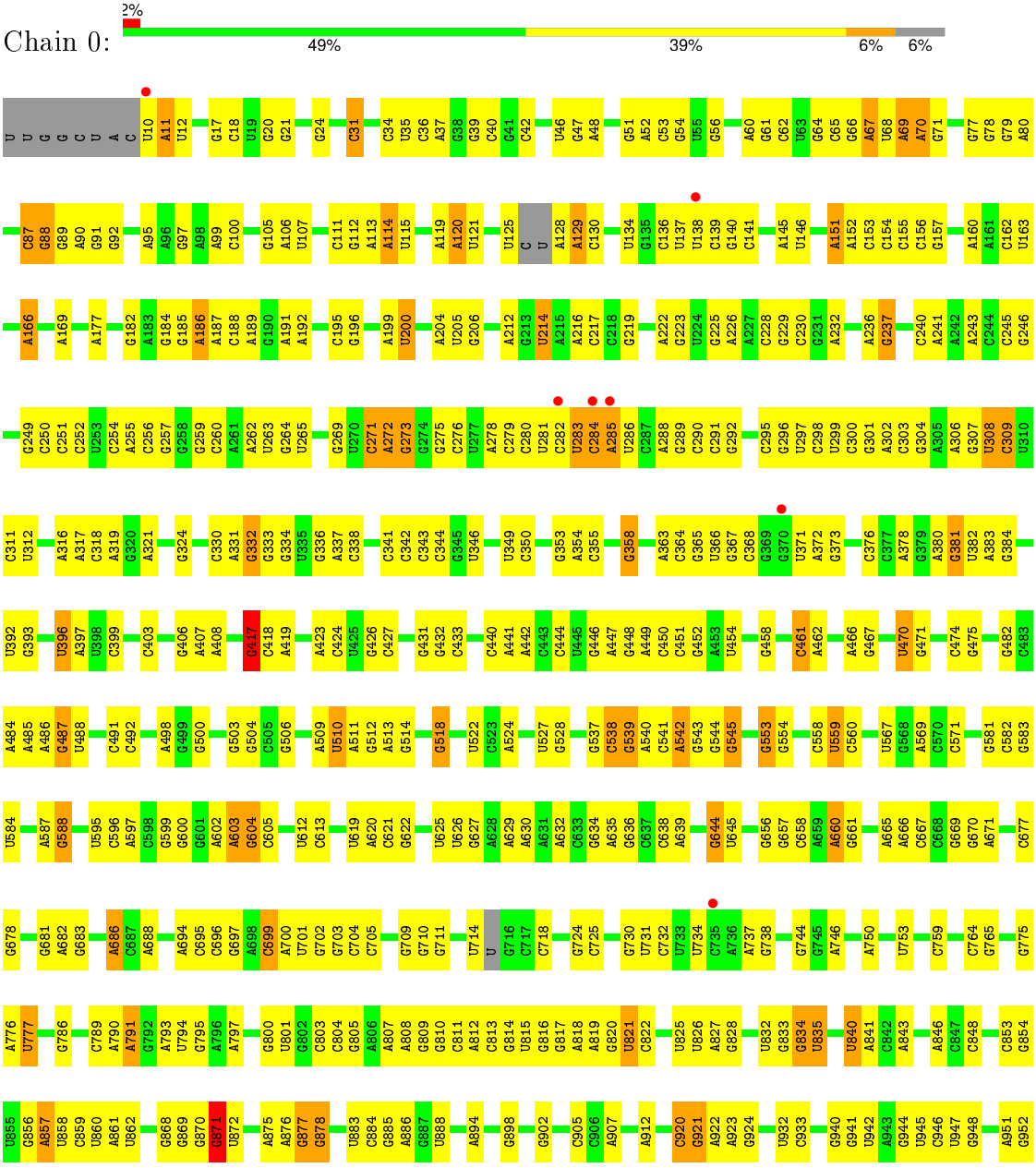
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
38	O	44	Total O 44 44	0	0
38	P	61	Total O 61 61	0	0
38	Q	55	Total O 55 55	0	0
38	R	81	Total O 81 81	0	0
38	S	37	Total O 37 37	0	0
38	T	39	Total O 39 39	0	0
38	U	28	Total O 28 28	0	0
38	V	11	Total O 11 11	0	0
38	W	70	Total O 70 70	0	0
38	X	26	Total O 26 26	0	0
38	Y	99	Total O 99 99	0	0
38	Z	32	Total O 32 32	0	0
38	1	56	Total O 56 56	0	0
38	2	40	Total O 40 40	0	0
38	3	66	Total O 66 66	0	0
38	I	4	Total O 4 4	0	0

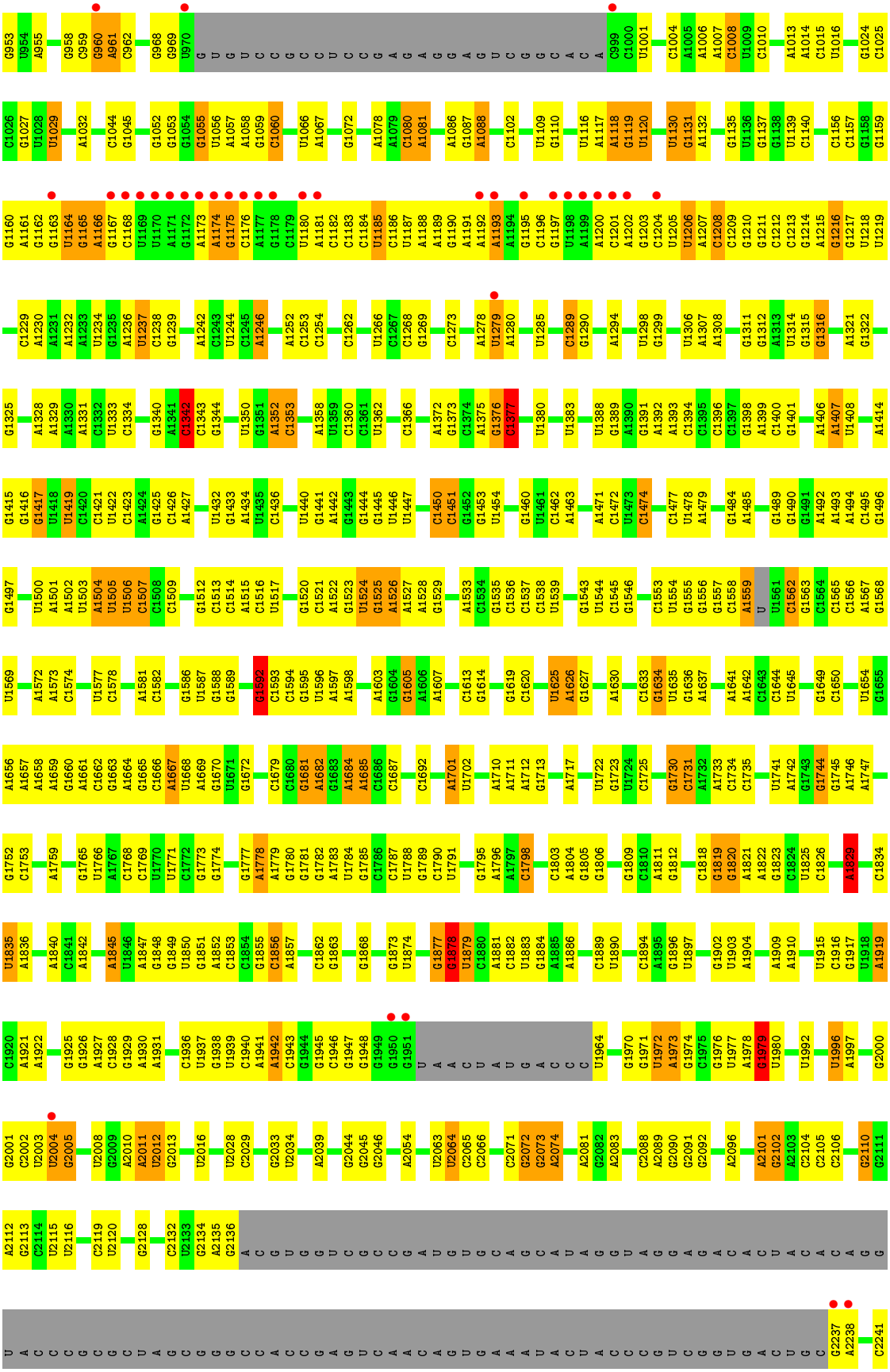
3 Residue-property plots (i)

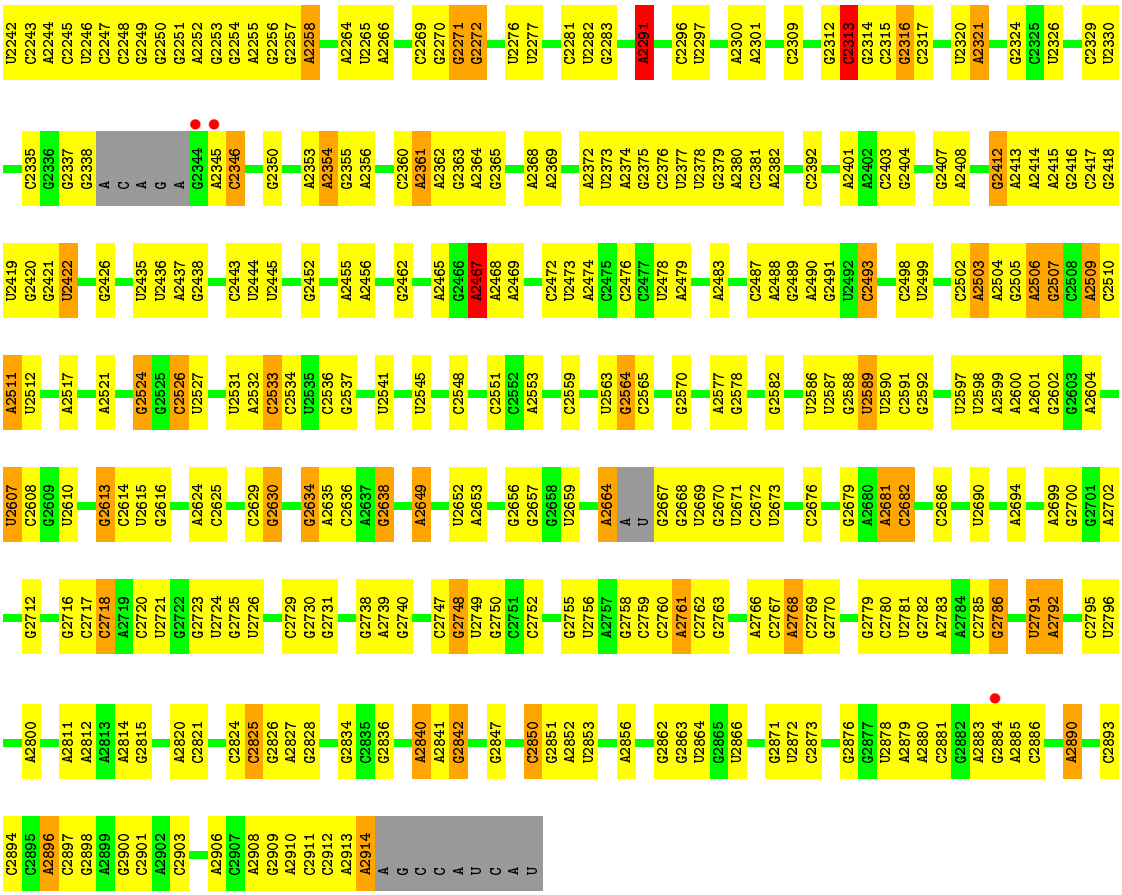
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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:

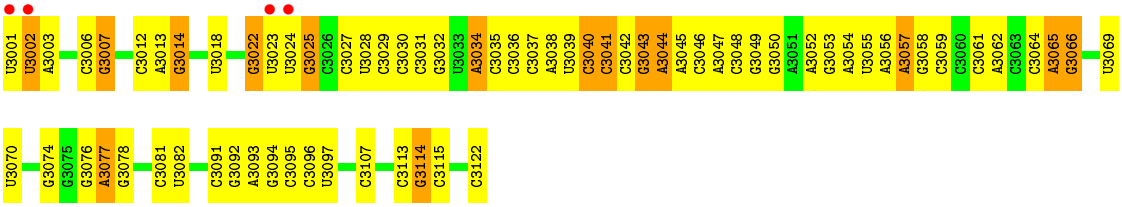



G953 U954 A955 G958 C959 G960 A961 C962 G968 G969 U970 C999 C1000 U1001 C1004 A1005 A1006 A1007 C1008 U1009 C1010 A1013 A1014 C1015 U1016 G1024 C1025
C1026 G1027 U1028 U1029 A1032 C1044 G1045 G1052 G1053 G1054 G1055 U1056 A1057 A1058 G1059 C1060 U1066 A1067 G1072 A1078 A1079 C1080 A1081 A1086 G1087 A1088 C1102 U1109 G1110 U1116 A1117 A1118 G1119 U1120 U1130 G1131 A1132 G1135 U1136 G1137 G1138 U1139 C1140 C1156 C1157 G1158 G1159
G1160 A1161 G1162 G1163 U1164 G1165 A1166 G1167 C1168 U1169 U1170 A1171 G1172 A1173 A1174 G1175 C1176 A1177 G1178 C1179 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 A1205 U1206 A1207 C1208 C1209 G1210 G1211 C1212 C1213 G1214 A1215 G1216 A1217 U1218 U1219
C1229 A1230 A1231 A1232 A1233 U1234 G1235 A1236 U1237 C1238 G1239 A1242 C1243 U1244 C1245 A1246 A1252 C1253 C1254 C1262 U1266 C1267 C1268 G1269 C1273 A1278 U1279 A1280 U1285 C1289 G1290 A1294 U1298 G1299 U1306 A1307 A1308 G1311 G1312 A1313 U1314 G1315 G1316 A1321 G1322
G1325 A1328 A1329 A1330 A1331 C1332 U1333 C1334 G1340 A1341 C1342 C1343 G1344 U1350 G1351 A1352 C1353 A1358 U1359 C1360 C1361 U1362 C1366 A1372 G1373 C1374 A1375 G1376 C1377 U1380 U1383 U1388 G1389 A1390 G1391 A1392 A1393 C1394 C1395 C1396 C1397 G1398 A1399 C1400 G1401 A1406 A1407 U1408 A1414
G1415 G1416 G1417 U1418 U1419 C1420 C1421 U1422 C1423 A1424 G1425 C1426 A1427 U1432 G1433 A1434 U1435 C1436 U1440 G1441 A1442 G1443 G1444 G1445 U1446 U1447 C1450 C1451 G1452 G1453 U1454 G1460 U1461 C1462 A1463 A1471 C1472 U1473 C1474 C1477 U1478 A1479 G1484 A1485 G1489 G1490 G1491 A1492 A1493 A1494 C1495 G1496
G1497 U1500 A1501 A1502 U1503 A1504 U1505 U1506 C1507 C1508 C1509 G1512 C1513 C1514 A1515 C1516 U1517 G1520 C1521 A1522 G1523 U1524 G1525 A1526 A1527 A1528 G1529 A1533 C1534 G1535 C1536 C1537 C1538 U1539 G1543 U1544 C1545 G1546 C1553 U1554 G1555 G1556 G1557 C1558 A1559 U1561 C1562 G1563 C1564 C1565 C1566 A1567 G1568
U1569 A1572 A1573 C1574 U1577 C1578 A1581 C1582 G1586 U1587 G1588 G1589 G1592 C1593 C1594 G1595 U1596 A1597 A1598 A1603 G1604 G1605 A1606 A1607 C1613 G1614 G1619 C1620 U1625 A1626 G1627 A1630 C1633 G1634 U1635 G1636 A1637 A1641 A1642 C1643 C1644 U1645 G1649 C1650 U1654 G1655
A1656 A1657 A1658 A1659 G1660 A1661 C1662 G1663 A1664 G1665 C1666 A1667 U1668 A1669 G1670 U1671 G1672 C1679 C1680 G1681 A1682 G1683 A1684 A1685 C1686 C1687 C1692 A1701 U1702 A1710 A1711 A1712 G1713 A1717 U1722 G1723 U1724 C1725 G1730 C1731 A1732 A1733 C1734 C1735 U1741 A1742 G1743 G1744 G1745 A1746 A1747
G1752 C1753 A1759 G1765 U1766 A1767 C1768 C1769 U1770 U1771 C1772 G1773 G1774 G1777 A1778 A1779 G1780 G1781 G1782 A1783 U1784 G1785 C1786 C1787 U1788 G1789 C1790 U1791 G1795 A1796 A1797 C1798 C1803 A1804 G1805 G1806 G1809 C1810 A1811 G1812 C1818 G1819 G1820 A1821 A1822 G1823 C1824 U1825 C1826 A1829 C1834
U1835 A1836 A1840 C1841 A1842 A1845 U1846 A1847 G1848 G1849 U1850 G1851 A1852 C1853 C1854 G1855 C1856 A1857 C1862 G1863 G1868 G1873 U1874 G1877 G1878 U1879 C1880 A1881 C1882 U1883 G1884 A1885 A1886 C1889 U1890 C1894 A1895 G1896 U1897 G1902 U1903 A1904 A1909 A1910 U1915 C1916 G1917 U1918 A1919
C1920 A1921 A1922 G1925 G1926 A1927 C1928 G1929 A1930 A1931 C1936 U1937 G1938 U1939 C1940 A1941 A1942 G1943 G1944 G1945 C1946 G1947 G1948 G1949 G1950 G1951 U1964 G1970 G1971 U1972 A1973 G1974 C1975 G1976 U1977 A1978 G1979 U1980 U1992 U1996 A1997 G2000
G2001 C2002 U2003 U2004 G2005 U2008 G2009 A2010 A2011 U2012 G2013 U2016 U2028 C2029 G2033 U2034 A2039 G2044 G2045 G2046 A2054 U2063 U2064 C2065 C2066 C2071 G2072 G2073 A2074 A2081 G2082 A2083 C2088 A2089 G2090 G2091 G2092 A2096 A2101 G2102 A2103 C2104 C2105 C2106 G2110 G2111
A2112 G2113 C2114 U2115 U2116 C2119 U2120 G2128 C2132 U2133 G2134 A2135 G2136
G2237 A2238 C2241



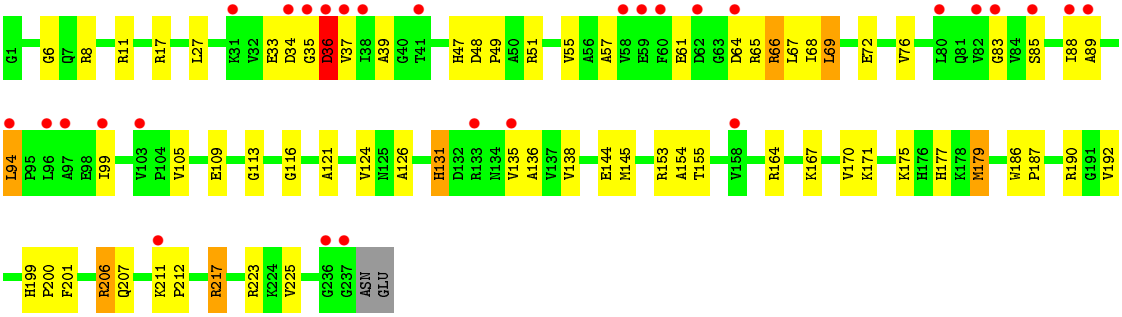
- Molecule 2: 5S ribosomal RNA

Chain 9:



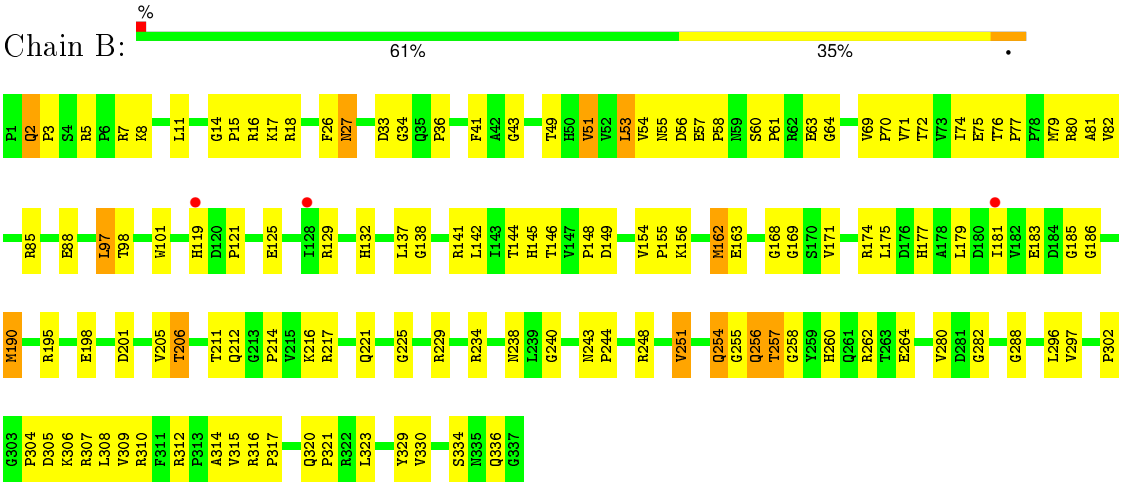
- Molecule 3: 50S ribosomal protein L2P

Chain A:



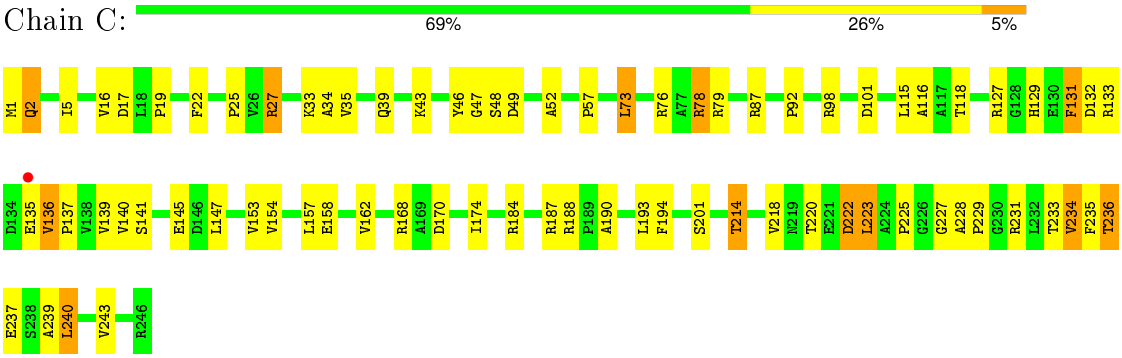
- Molecule 4: 50S ribosomal protein L3P

Chain B:



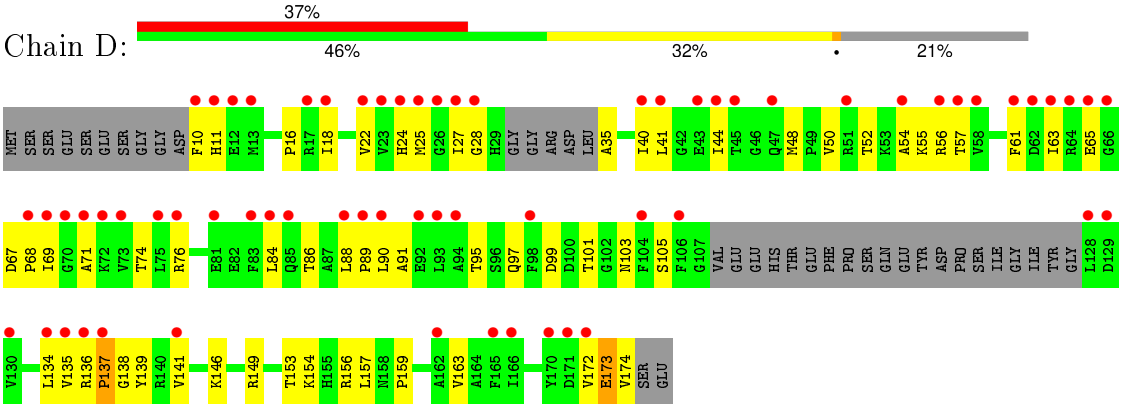
- Molecule 5: 50S ribosomal protein L4P

Chain C:



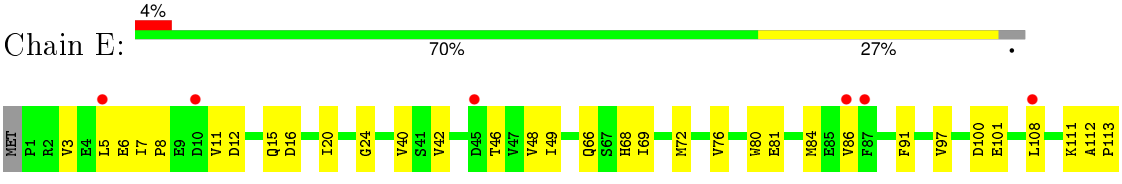
- Molecule 6: 50S ribosomal protein L5P

Chain D:

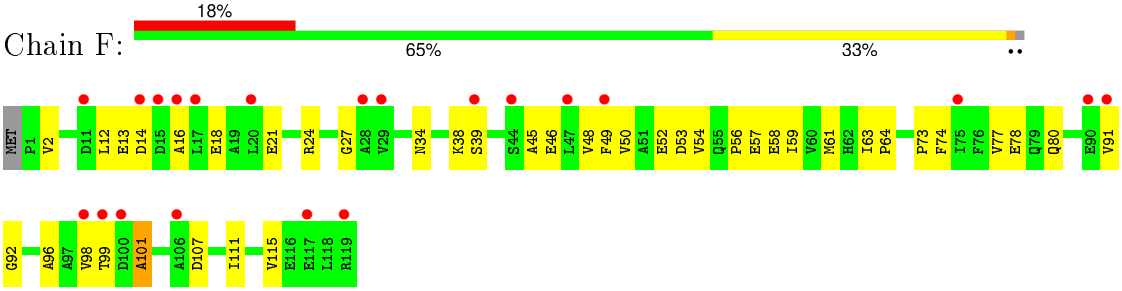


- Molecule 7: 50S ribosomal protein L6P

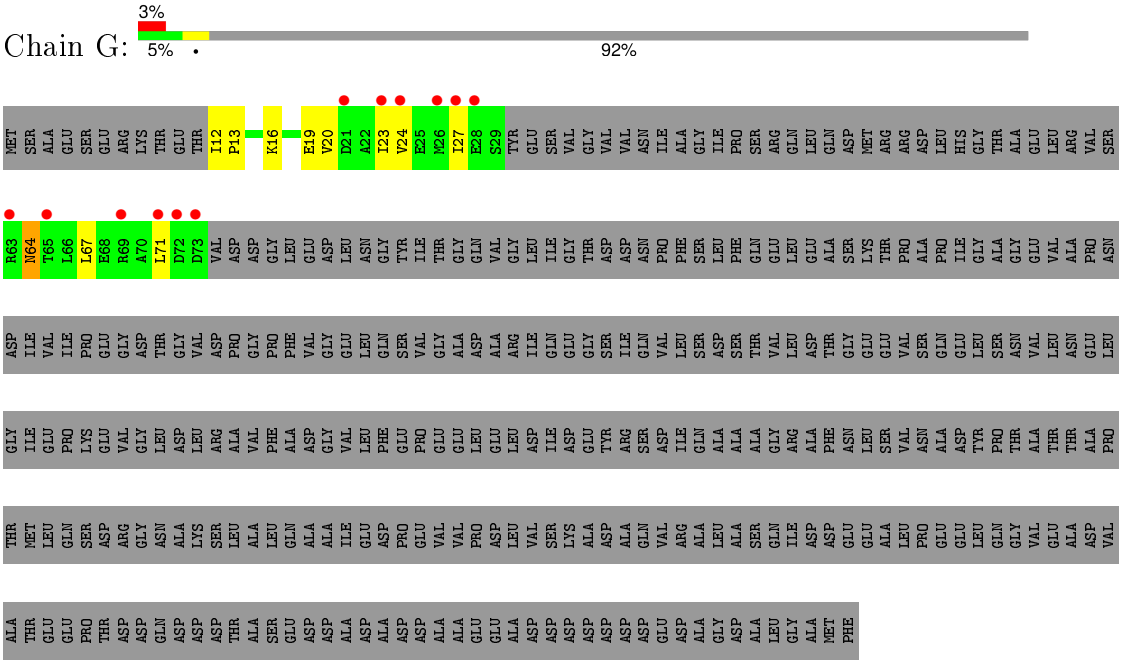
Chain E:



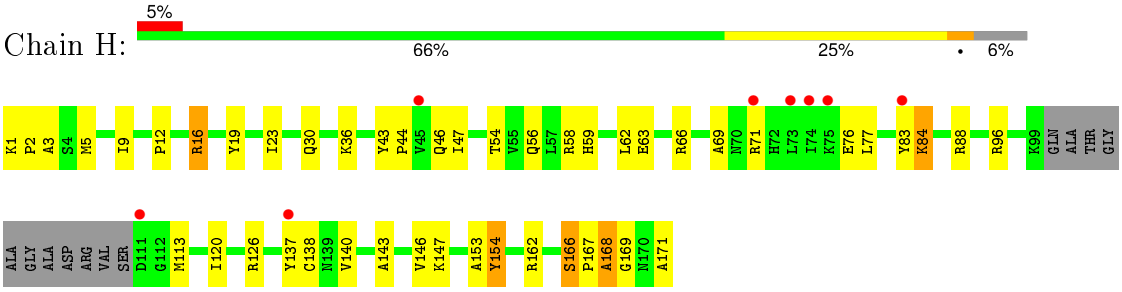
• Molecule 8: 50S ribosomal protein L7Ae



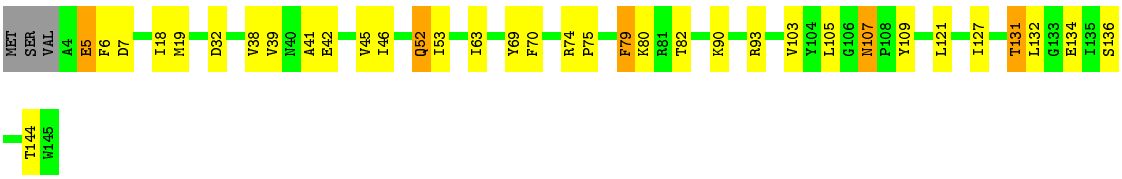
• Molecule 9: 50S ribosomal protein L10E



• Molecule 10: 50S ribosomal protein L10e

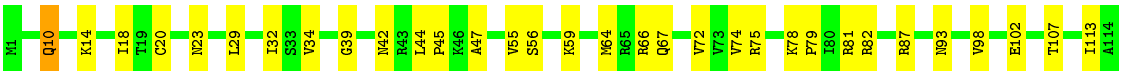


• Molecule 11: 50S ribosomal protein L13P



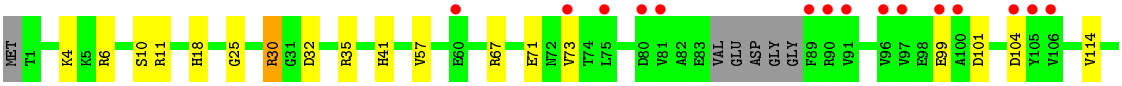
- Molecule 12: 50S ribosomal protein L14P

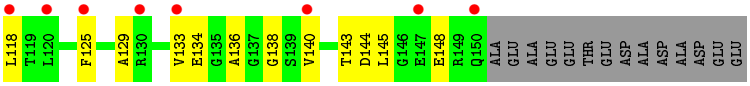
Chain K:



- Molecule 13: 50S ribosomal protein L15P

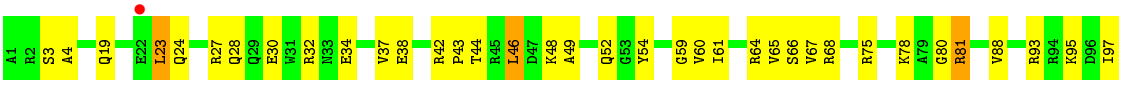
Chain L:

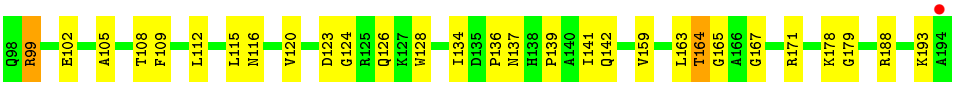




- Molecule 14: 50S ribosomal protein L15e

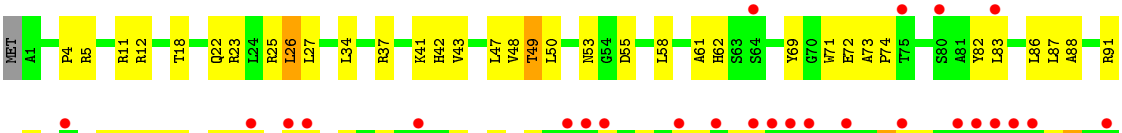
Chain M:

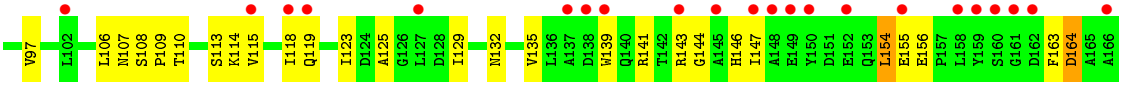


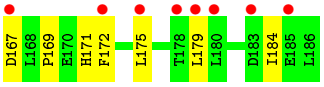


- Molecule 15: 50S ribosomal protein L18P

Chain N:

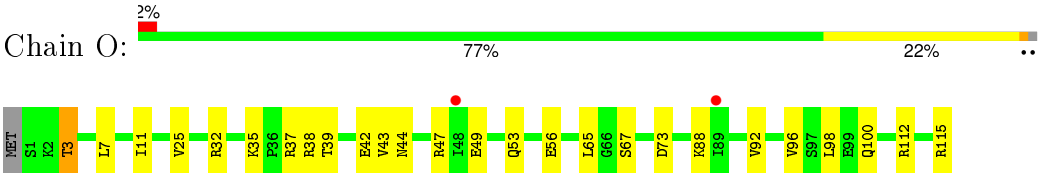






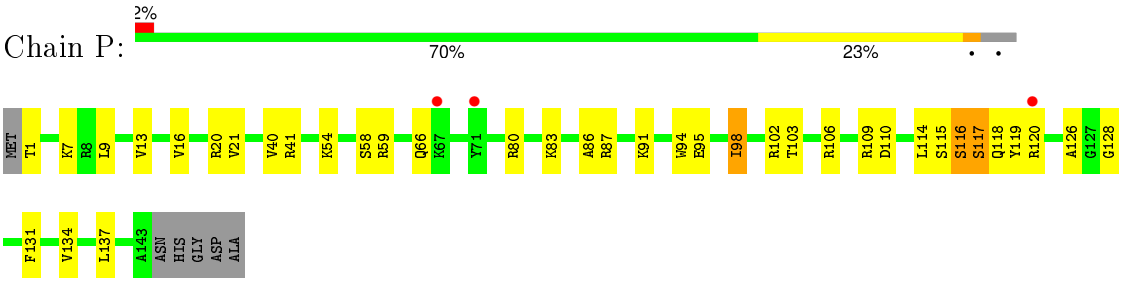
- Molecule 16: 50S ribosomal protein L18e

Chain O:



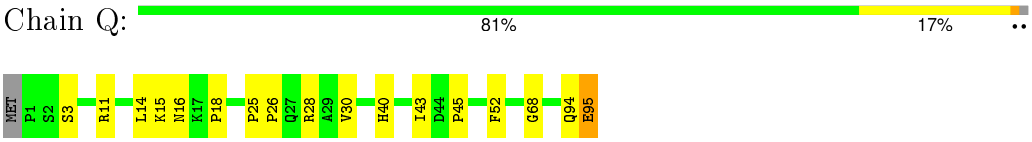
- Molecule 17: 50S ribosomal protein L19e

Chain P:



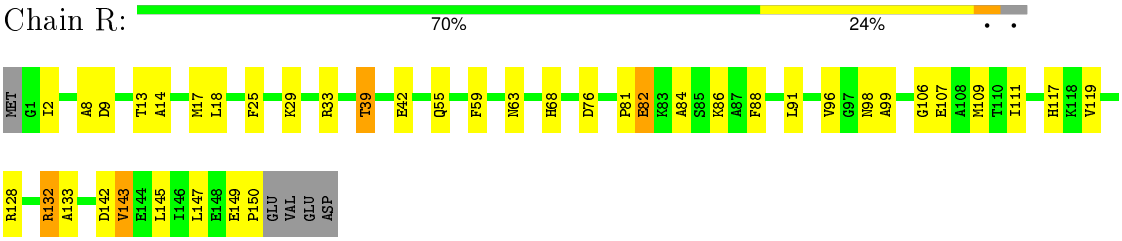
- Molecule 18: 50S ribosomal protein L21e

Chain Q:



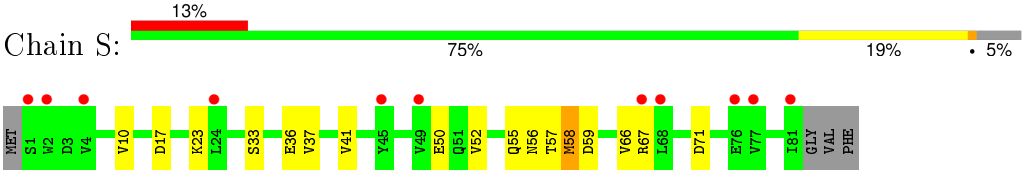
- Molecule 19: 50S ribosomal protein L22P

Chain R:



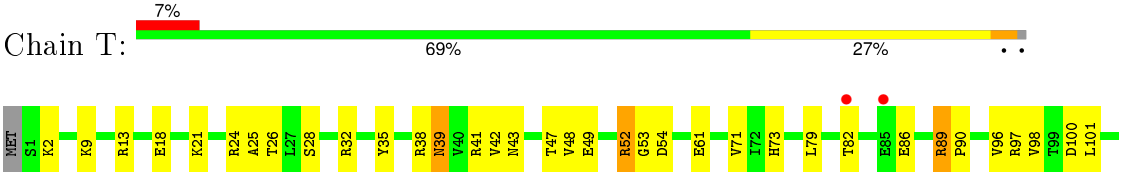
- Molecule 20: 50S ribosomal protein L23P

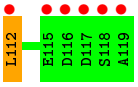
Chain S:



- Molecule 21: 50S ribosomal protein L24P

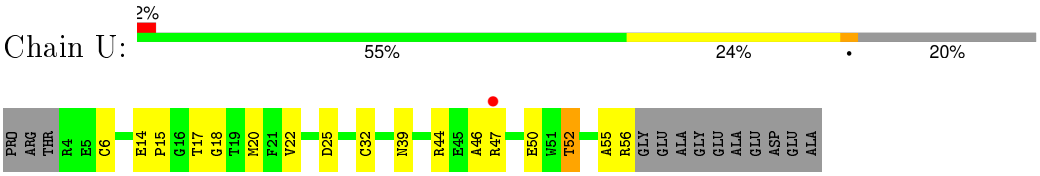
Chain T:





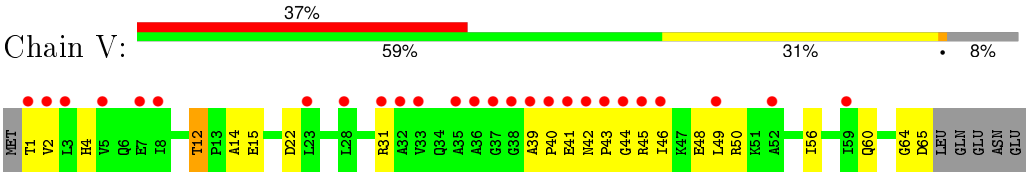
- Molecule 22: 50S ribosomal protein L24e

Chain U:



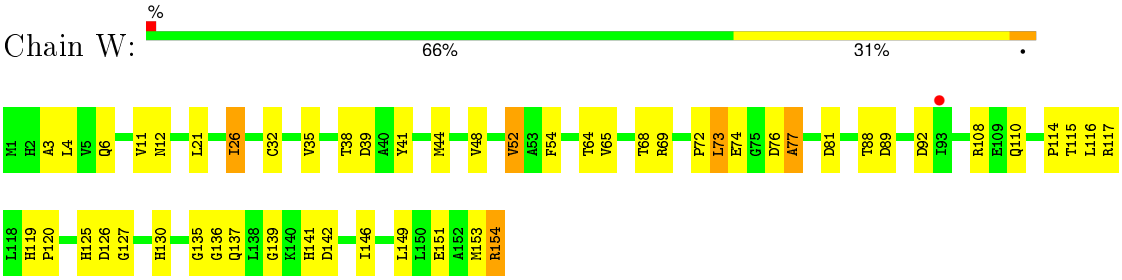
- Molecule 23: 50S ribosomal protein L29P

Chain V:



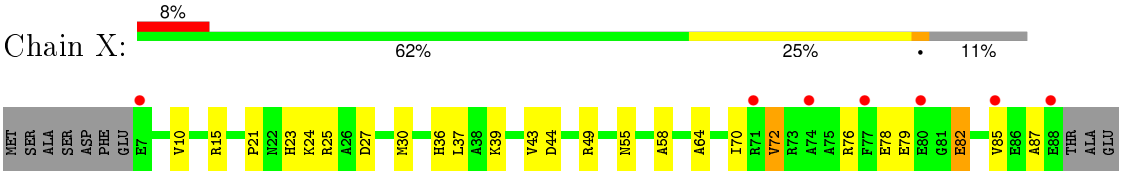
- Molecule 24: 50S ribosomal protein L30P

Chain W:



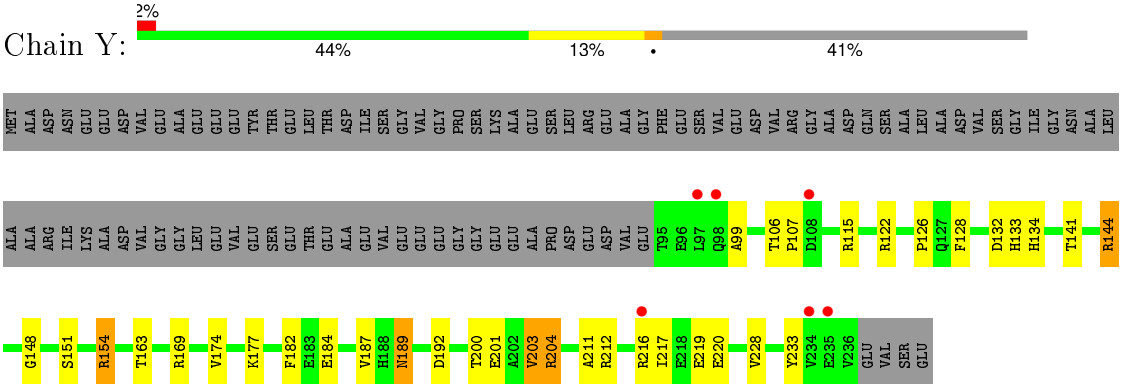
- Molecule 25: 50S ribosomal protein L31e

Chain X:



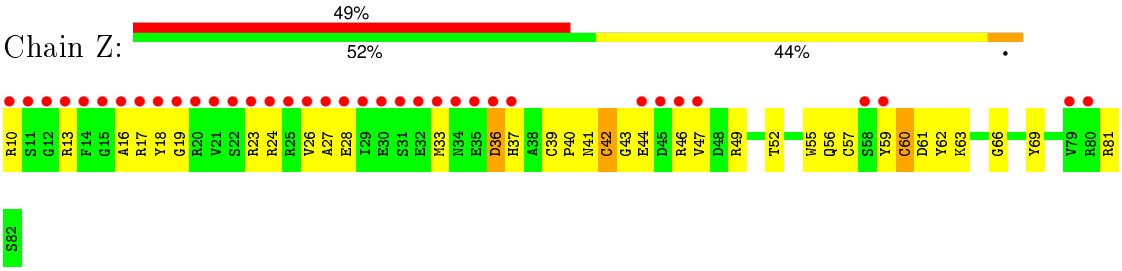
- Molecule 26: 50S ribosomal protein L32e

Chain Y:



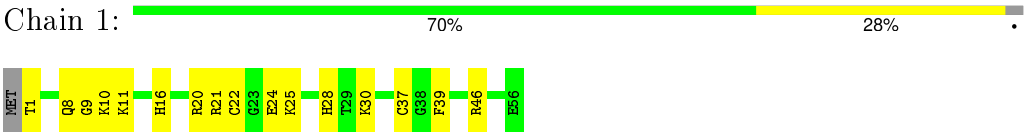
- Molecule 27: 50S ribosomal protein L37Ae

Chain Z:



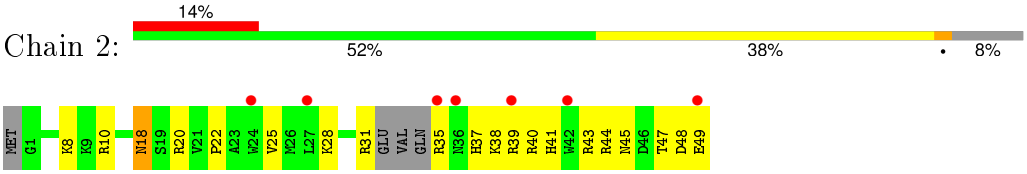
• Molecule 28: 50S ribosomal protein L37e

Chain 1:



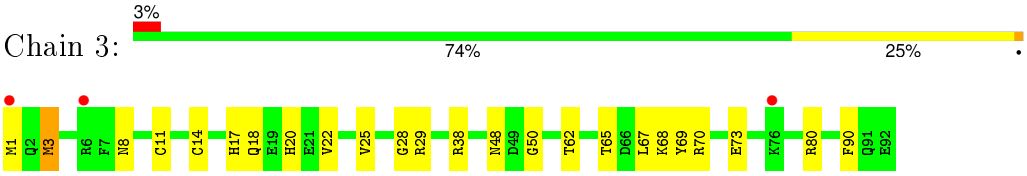
• Molecule 29: 50S ribosomal protein L39e

Chain 2:



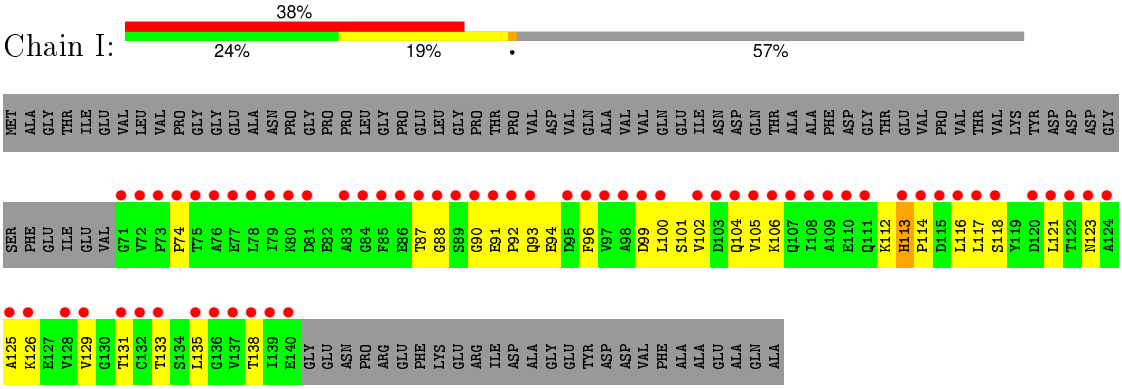
• Molecule 30: 50S ribosomal protein L44E

Chain 3:



• Molecule 31: 50S ribosomal protein L11P

Chain I:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	213.08Å 300.60Å 575.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.36 – 2.70 85.94 – 2.41	Depositor EDS
% Data completeness (in resolution range)	99.4 (49.36-2.70) 90.7 (85.94-2.41)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.70 (at 2.69Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.204 , 0.248 0.192 , 0.231	Depositor DCC
R_{free} test set	4912 reflections (1.10%)	DCC
Wilson B-factor (Å^2)	49.9	Xtriage
Anisotropy	0.260	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 55.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	0 of 496615 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	99016	wwPDB-VP
Average B, all atoms (Å^2)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.51% 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: MG, OMG, GIR, CL, NA, K, CD, OMU, UR3, 1MA, PSU

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	0.40	0/65959	0.69	14/102870 (0.0%)
2	9	0.34	0/2905	0.68	0/4528
3	A	0.36	0/1786	0.66	0/2408
4	B	0.33	0/2690	0.65	0/3652
5	C	0.39	0/1884	0.69	1/2551 (0.0%)
6	D	0.33	0/1111	0.55	0/1498
7	E	0.33	0/1382	0.57	0/1880
8	F	0.38	0/901	0.58	0/1224
9	G	0.30	0/241	0.47	0/324
10	H	0.35	0/1287	0.66	0/1725
11	J	0.36	0/1136	0.61	0/1530
12	K	0.36	0/1001	0.68	0/1347
13	L	0.38	0/1130	0.67	0/1509
14	M	0.38	0/1584	0.64	0/2119
15	N	0.33	0/1474	0.64	0/1999
16	O	0.35	0/874	0.59	0/1181
17	P	0.36	0/1147	0.55	0/1528
18	Q	0.36	0/749	0.70	0/1005
19	R	0.38	0/1172	0.65	0/1578
20	S	0.34	0/648	0.59	0/875
21	T	0.35	0/958	0.64	1/1289 (0.1%)
22	U	0.37	0/417	0.55	0/562
23	V	0.35	0/502	0.57	0/675
24	W	0.38	0/1219	0.64	0/1655
25	X	0.35	0/664	0.60	0/895
26	Y	0.38	0/1146	0.65	0/1536
27	Z	0.54	0/590	0.66	0/787
28	1	0.39	0/437	0.63	0/578
29	2	0.39	0/401	0.54	0/529
30	3	0.39	0/771	0.59	0/1024
31	I	0.33	0/526	0.55	0/716
All	All	0.39	0/98692	0.67	16/147577 (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	52

There are no bond length outliers.

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	0	1878	G	N9-C1'-C2'	-6.83	104.49	112.00
1	0	1979	G	C2'-C3'-O3'	6.63	124.31	113.70
1	0	1504	A	C1'-O4'-C4'	-6.20	104.94	109.90
1	0	1559	A	C2'-C3'-O3'	5.63	122.71	113.70
1	0	2313	C	C5'-C4'-O4'	5.55	115.76	109.10

There are no chirality outliers.

5 of 52 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	214	U	Sidechain
1	0	332	G	Sidechain
1	0	396	U	Sidechain
1	0	417	G	Sidechain
1	0	48	A	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	0	59021	0	29810	1361	0
2	9	2600	0	1326	97	0
3	A	1753	0	1766	74	0
4	B	2625	0	2533	110	0
5	C	1859	0	1816	70	0
6	D	1094	0	1085	45	0
7	E	1357	0	1266	33	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	F	890	0	843	36	0
9	G	240	0	231	10	0
10	H	1266	0	1268	41	0
11	J	1120	0	1098	41	0
12	K	992	0	1031	38	0
13	L	1118	0	1076	24	0
14	M	1560	0	1568	55	0
15	N	1445	0	1401	64	0
16	O	865	0	873	21	0
17	P	1136	0	1123	35	0
18	Q	735	0	729	13	0
19	R	1149	0	1122	40	0
20	S	641	0	605	12	0
21	T	950	0	923	38	0
22	U	410	0	364	17	0
23	V	499	0	511	20	0
24	W	1196	0	1137	54	0
25	X	654	0	653	23	0
26	Y	1130	0	1133	37	0
27	Z	579	0	540	46	0
28	1	430	0	426	20	0
29	2	396	0	413	25	0
30	3	755	0	729	27	0
31	I	519	0	500	27	0
32	0	12	0	10	0	0
33	0	107	0	0	0	0
33	3	1	0	0	0	0
33	9	1	0	0	0	0
33	A	2	0	0	0	0
33	B	2	0	0	0	0
33	K	1	0	0	0	0
33	T	1	0	0	0	0
33	Y	1	0	0	0	0
34	0	2	0	0	0	0
35	0	71	0	0	0	0
35	9	2	0	0	0	0
35	A	1	0	0	0	0
35	C	1	0	0	0	0
35	H	2	0	0	0	0
35	J	1	0	0	0	0
35	L	1	0	0	0	0
35	M	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	Q	1	0	0	0	0
35	R	3	0	0	0	0
35	S	1	0	0	0	0
36	0	9	0	0	4	0
36	3	1	0	0	0	0
36	A	1	0	0	0	0
36	B	1	0	0	0	0
36	J	3	0	0	4	0
36	L	1	0	0	0	0
36	M	1	0	0	2	0
36	N	1	0	0	1	0
36	O	1	0	0	0	0
36	Q	1	0	0	0	0
36	R	1	0	0	0	0
36	Y	1	0	0	0	0
37	1	1	0	0	0	0
37	3	1	0	0	0	0
37	O	1	0	0	0	0
37	U	1	0	0	0	0
37	Z	1	0	0	0	0
38	0	5893	0	0	185	0
38	1	56	0	0	1	0
38	2	40	0	0	3	0
38	3	66	0	0	5	0
38	9	145	0	0	9	0
38	A	118	0	0	10	0
38	B	147	0	0	15	0
38	C	163	0	0	14	0
38	D	48	0	0	8	0
38	E	46	0	0	4	0
38	F	23	0	0	3	0
38	G	19	0	0	0	0
38	H	69	0	0	6	0
38	I	4	0	0	1	0
38	J	58	0	0	4	0
38	K	58	0	0	4	0
38	L	81	0	0	8	0
38	M	115	0	0	5	0
38	N	58	0	0	5	0
38	O	44	0	0	6	0
38	P	61	0	0	1	0
38	Q	55	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	R	81	0	0	4	0
38	S	37	0	0	0	0
38	T	39	0	0	3	0
38	U	28	0	0	2	0
38	V	11	0	0	3	0
38	W	70	0	0	5	0
38	X	26	0	0	2	0
38	Y	99	0	0	10	0
38	Z	32	0	0	5	0
All	All	99016	0	59909	2306	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 2306 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)
10:H:46:GLN:HB3	10:H:167:PRO:HD2	1.29	1.15
1:0:871:G:H8	1:0:871:G:H5'	1.06	1.12
1:0:656:G:H5'	16:O:3:THR:HG22	1.16	1.12
2:9:3056:A:H2'	2:9:3057:A:H5"	1.31	1.10
5:C:236:THR:HG22	5:C:239:ALA:H	1.16	1.09

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	235/239 (98%)	209 (89%)	23 (10%)	3 (1%)	15 37
4	B	335/337 (99%)	305 (91%)	24 (7%)	6 (2%)	11 27

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
5	C	244/246 (99%)	228 (93%)	15 (6%)	1 (0%)	39 69
6	D	134/177 (76%)	107 (80%)	23 (17%)	4 (3%)	5 13
7	E	170/178 (96%)	163 (96%)	7 (4%)	0	100 100
8	F	117/120 (98%)	106 (91%)	10 (8%)	1 (1%)	21 49
9	G	25/348 (7%)	25 (100%)	0	0	100 100
10	H	156/171 (91%)	143 (92%)	9 (6%)	4 (3%)	7 16
11	J	140/145 (97%)	128 (91%)	11 (8%)	1 (1%)	26 55
12	K	130/132 (98%)	122 (94%)	8 (6%)	0	100 100
13	L	141/165 (86%)	127 (90%)	14 (10%)	0	100 100
14	M	192/194 (99%)	178 (93%)	13 (7%)	1 (0%)	34 63
15	N	184/187 (98%)	168 (91%)	13 (7%)	3 (2%)	12 30
16	O	113/116 (97%)	109 (96%)	4 (4%)	0	100 100
17	P	141/149 (95%)	136 (96%)	3 (2%)	2 (1%)	14 35
18	Q	93/96 (97%)	87 (94%)	5 (5%)	1 (1%)	17 42
19	R	148/155 (96%)	138 (93%)	9 (6%)	1 (1%)	26 55
20	S	79/85 (93%)	76 (96%)	2 (2%)	1 (1%)	15 37
21	T	117/120 (98%)	109 (93%)	8 (7%)	0	100 100
22	U	51/66 (77%)	49 (96%)	2 (4%)	0	100 100
23	V	63/71 (89%)	59 (94%)	3 (5%)	1 (2%)	12 30
24	W	152/154 (99%)	146 (96%)	4 (3%)	2 (1%)	15 37
25	X	80/92 (87%)	74 (92%)	4 (5%)	2 (2%)	7 18
26	Y	140/241 (58%)	140 (100%)	0	0	100 100
27	Z	71/73 (97%)	58 (82%)	9 (13%)	4 (6%)	2 3
28	1	54/57 (95%)	51 (94%)	3 (6%)	0	100 100
29	2	42/50 (84%)	42 (100%)	0	0	100 100
30	3	90/92 (98%)	87 (97%)	3 (3%)	0	100 100
31	I	68/162 (42%)	65 (96%)	3 (4%)	0	100 100
All	All	3705/4418 (84%)	3435 (93%)	232 (6%)	38 (1%)	19 45

5 of 38 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	D	137	PRO

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Mol	Chain	Res	Type
6	D	173	GLU
8	F	101	ALA
10	H	166	SER
10	H	168	ALA

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	179/181 (99%)	169 (94%)	10 (6%)	26	54
4	B	282/282 (100%)	264 (94%)	18 (6%)	22	47
5	C	193/193 (100%)	177 (92%)	16 (8%)	14	31
6	D	117/148 (79%)	113 (97%)	4 (3%)	44	75
7	E	152/156 (97%)	149 (98%)	3 (2%)	63	87
8	F	93/94 (99%)	92 (99%)	1 (1%)	80	94
9	G	27/283 (10%)	26 (96%)	1 (4%)	41	72
10	H	132/138 (96%)	125 (95%)	7 (5%)	28	57
11	J	118/121 (98%)	110 (93%)	8 (7%)	20	43
12	K	106/106 (100%)	105 (99%)	1 (1%)	84	95
13	L	113/127 (89%)	107 (95%)	6 (5%)	28	57
14	M	158/158 (100%)	150 (95%)	8 (5%)	29	59
15	N	149/150 (99%)	145 (97%)	4 (3%)	52	82
16	O	93/94 (99%)	89 (96%)	4 (4%)	35	66
17	P	113/117 (97%)	108 (96%)	5 (4%)	35	65
18	Q	79/80 (99%)	77 (98%)	2 (2%)	55	84
19	R	117/122 (96%)	112 (96%)	5 (4%)	35	66
20	S	71/74 (96%)	69 (97%)	2 (3%)	51	81
21	T	105/106 (99%)	100 (95%)	5 (5%)	31	62
22	U	44/52 (85%)	43 (98%)	1 (2%)	58	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
23	V	51/57 (90%)	49 (96%)	2 (4%)	39 70
24	W	130/130 (100%)	124 (95%)	6 (5%)	33 64
25	X	66/74 (89%)	62 (94%)	4 (6%)	23 49
26	Y	120/196 (61%)	114 (95%)	6 (5%)	30 60
27	Z	60/60 (100%)	58 (97%)	2 (3%)	45 76
28	1	46/47 (98%)	46 (100%)	0	100 100
29	2	42/46 (91%)	40 (95%)	2 (5%)	31 62
30	3	79/79 (100%)	77 (98%)	2 (2%)	55 84
31	I	58/130 (45%)	57 (98%)	1 (2%)	68 90
All	All	3093/3601 (86%)	2957 (96%)	136 (4%)	35 65

5 of 136 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	J	32	ASP
14	M	46	LEU
26	Y	163	THR
11	J	46	ILE
13	L	30	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 78 such sidechains are listed below:

Mol	Chain	Res	Type
14	M	170	ASN
17	P	118	GLN
29	2	41	HIS
15	N	53	ASN
15	N	119	GLN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2746/2922 (93%)	235 (8%)	35 (1%)
2	9	121/122 (99%)	18 (14%)	1 (0%)
All	All	2867/3044 (94%)	253 (8%)	36 (1%)

5 of 253 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 36 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	1352	A
1	0	1667	A
1	0	2791	U
1	0	1450	C
1	0	1685	A

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

5 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	OMU	0	2587	1	12,22,23	0.92	1 (8%)	19,31,34	3.16	2 (10%)
1	OMG	0	2588	1	17,26,27	1.05	1 (5%)	21,38,41	2.52	3 (14%)
1	UR3	0	2619	1	12,22,23	0.69	0	16,32,35	0.77	0
1	PSU	0	2621	1	13,21,22	1.71	2 (15%)	18,30,33	6.18	4 (22%)
1	1MA	0	628	1,35	14,25,26	0.97	1 (7%)	15,37,40	1.11	1 (6%)

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
1	OMU	0	2587	1	-	0/5/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMG	0	2588	1	-	0/5/27/28	0/3/3/3
1	UR3	0	2619	1	-	0/3/25/26	0/2/2/2
1	PSU	0	2621	1	-	0/7/25/26	0/2/2/2
1	1MA	0	628	1,35	-	0/3/25/26	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	0	2621	PSU	C5-C1'	-5.13	1.47	1.52
1	0	2587	OMU	C4-N3	2.09	1.37	1.33
1	0	2621	PSU	C4-N3	2.53	1.37	1.33
1	0	628	1MA	C6-N6	2.63	1.33	1.29
1	0	2588	OMG	C6-N1	3.39	1.39	1.33

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	0	2621	PSU	N1-C2-N3	-21.81	114.42	128.33
1	0	2588	OMG	C5-C6-N1	-8.72	111.67	123.59
1	0	628	1MA	C2-N3-C4	-3.59	110.84	116.40
1	0	2587	OMU	C5-C4-N3	-3.31	114.62	123.12
1	0	2621	PSU	C5-C1'-C2'	-2.53	111.02	115.52

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	0	2587	OMU	2	0
1	0	2588	OMG	1	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 231 ligands modelled in this entry, 230 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
32	GIR	0	9000	-	9,12,12	0.82	0	6,16,16	0.98	0

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	GIR	0	9000	-	-	0/4/10/10	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (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^{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	2749/2922 (94%)	-0.23	44 (1%) 74 75	24, 49, 93, 153	0
2	9	122/122 (100%)	-0.23	4 (3%) 50 50	38, 64, 91, 149	0
3	A	237/239 (99%)	0.66	29 (12%) 5 4	30, 58, 99, 119	0
4	B	337/337 (100%)	0.19	3 (0%) 85 86	28, 56, 84, 95	0
5	C	246/246 (100%)	0.26	1 (0%) 93 94	25, 49, 74, 80	0
6	D	140/177 (79%)	2.17	65 (46%) 0 0	61, 105, 127, 136	0
7	E	172/178 (96%)	0.49	7 (4%) 41 41	46, 68, 87, 93	0
8	F	119/120 (99%)	1.00	21 (17%) 2 1	53, 78, 99, 117	0
9	G	29/348 (8%)	2.05	12 (41%) 0 0	77, 94, 105, 107	0
10	H	160/171 (93%)	0.45	8 (5%) 32 31	40, 58, 92, 100	0
11	J	142/145 (97%)	0.01	0 100 100	35, 50, 74, 90	0
12	K	132/132 (100%)	0.12	1 (0%) 87 88	36, 54, 77, 87	0
13	L	145/165 (87%)	0.92	23 (15%) 3 2	29, 71, 118, 130	0
14	M	194/194 (100%)	0.05	2 (1%) 84 85	35, 47, 63, 73	0
15	N	186/187 (99%)	1.01	34 (18%) 2 1	41, 68, 115, 120	0
16	O	115/116 (99%)	0.29	2 (1%) 73 74	41, 57, 75, 80	0
17	P	143/149 (95%)	0.30	3 (2%) 67 68	43, 59, 78, 83	0
18	Q	95/96 (98%)	0.04	0 100 100	37, 48, 62, 78	0
19	R	150/155 (96%)	0.00	0 100 100	33, 47, 66, 74	0
20	S	81/85 (95%)	0.89	11 (13%) 4 3	47, 67, 87, 94	0
21	T	119/120 (99%)	0.58	8 (6%) 21 19	41, 61, 88, 108	0
22	U	53/66 (80%)	0.46	1 (1%) 70 70	44, 61, 77, 83	0
23	V	65/71 (91%)	2.01	26 (40%) 0 0	60, 84, 118, 121	0
24	W	154/154 (100%)	0.09	1 (0%) 90 91	34, 49, 66, 76	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
25	X	82/92 (89%)	0.46	7 (8%) 13 10	45, 61, 87, 102	0
26	Y	142/241 (58%)	0.21	6 (4%) 40 39	28, 47, 71, 92	0
27	Z	73/73 (100%)	2.98	36 (49%) 0 0	61, 98, 111, 115	0
28	1	56/57 (98%)	0.04	0 100 100	29, 37, 43, 50	0
29	2	46/50 (92%)	0.65	7 (15%) 3 2	39, 68, 101, 114	0
30	3	92/92 (100%)	0.52	3 (3%) 50 50	40, 62, 75, 83	0
31	I	70/162 (43%)	4.02	62 (88%) 0 0	105, 124, 141, 141	0
All	All	6646/7462 (89%)	0.25	427 (6%) 23 21	24, 55, 105, 153	0

The worst 5 of 427 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
23	V	1	THR	13.0
27	Z	26	VAL	13.0
27	Z	20	ARG	11.2
27	Z	11	SER	9.9
27	Z	34	ASN	9.4

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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^{th} 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
1	1MA	0	628	23/24	0.99	0.18	-	28,32,33,35	0
1	OMU	0	2587	21/22	0.98	0.13	-	34,36,37,39	0
1	UR3	0	2619	21/22	0.98	0.16	-	36,39,42,48	0
1	PSU	0	2621	20/21	0.99	0.14	-	28,30,33,34	0
1	OMG	0	2588	24/25	0.98	0.15	-	33,36,38,39	0

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, 95^{th} 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	8574	1/1	0.82	0.54	31.81	66,66,66,66	0
35	NA	0	8529	1/1	0.55	0.45	20.44	77,77,77,77	0
35	NA	R	8586	1/1	0.48	0.79	20.05	95,95,95,95	0
35	NA	0	8503	1/1	0.90	0.36	18.55	47,47,47,47	0
35	NA	0	8571	1/1	0.78	0.42	15.79	65,65,65,65	0
35	NA	9	8583	1/1	0.86	0.43	15.38	65,65,65,65	0
35	NA	0	8577	1/1	0.80	0.38	13.98	71,71,71,71	0
35	NA	0	8526	1/1	0.89	0.64	13.85	58,58,58,58	0
35	NA	0	8532	1/1	0.90	0.30	13.35	49,49,49,49	0
35	NA	0	8566	1/1	0.87	0.29	11.53	66,66,66,66	0
35	NA	0	8569	1/1	0.90	0.37	10.70	74,74,74,74	0
36	CL	0	8715	1/1	0.93	0.24	9.67	86,86,86,86	0
35	NA	0	8502	1/1	0.97	0.21	8.71	51,51,51,51	0
35	NA	0	8572	1/1	0.95	0.28	8.43	54,54,54,54	0
35	NA	0	8573	1/1	0.93	0.29	8.41	69,69,69,69	0
35	NA	0	8550	1/1	0.93	0.26	8.16	45,45,45,45	0
35	NA	0	8514	1/1	0.96	0.27	8.07	38,38,38,38	0
35	NA	0	8564	1/1	0.93	0.29	7.64	53,53,53,53	0
35	NA	0	8578	1/1	0.97	0.28	7.06	51,51,51,51	0
35	NA	0	8521	1/1	0.94	0.28	5.98	61,61,61,61	0
35	NA	0	8582	1/1	0.78	0.21	5.33	79,79,79,79	0
35	NA	0	8561	1/1	0.92	0.23	5.12	56,56,56,56	0
35	NA	L	8580	1/1	0.97	0.28	5.12	57,57,57,57	0
35	NA	0	8576	1/1	0.98	0.24	4.85	46,46,46,46	0
35	NA	0	8555	1/1	0.97	0.34	4.50	57,57,57,57	0
33	MG	0	8060	1/1	0.99	0.27	4.33	40,40,40,40	0
36	CL	0	8705	1/1	0.89	0.20	4.23	67,67,67,67	0
35	NA	0	8568	1/1	0.69	0.18	3.24	71,71,71,71	0
35	NA	R	8537	1/1	0.89	0.25	2.82	48,48,48,48	0
35	NA	0	8535	1/1	0.95	0.22	2.55	56,56,56,56	0
35	NA	0	8556	1/1	0.92	0.20	2.46	49,49,49,49	0
35	NA	0	8565	1/1	0.93	0.38	2.24	40,40,40,40	0
35	NA	0	8562	1/1	0.92	0.20	2.12	60,60,60,60	0
33	MG	0	8080	1/1	0.97	0.20	1.92	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
35	NA	0	8527	1/1	0.92	0.17	1.91	44,44,44,44	0
35	NA	C	8504	1/1	0.83	0.27	1.81	49,49,49,49	0
35	NA	0	8579	1/1	0.97	0.19	1.21	64,64,64,64	0
35	NA	0	8524	1/1	0.95	0.19	1.18	62,62,62,62	0
32	GIR	0	9000	12/12	0.91	0.21	1.17	23,40,50,53	0
34	K	0	8401	1/1	0.96	0.18	1.09	85,85,85,85	0
35	NA	M	8547	1/1	0.94	0.18	1.03	34,34,34,34	0
35	NA	0	8543	1/1	0.96	0.19	0.74	39,39,39,39	0
36	CL	O	8708	1/1	0.91	0.21	0.59	73,73,73,73	0
33	MG	0	8057	1/1	0.97	0.18	0.48	45,45,45,45	0
35	NA	0	8505	1/1	0.95	0.18	0.12	33,33,33,33	0
33	MG	0	8054	1/1	0.97	0.17	-0.57	37,37,37,37	0
35	NA	A	8545	1/1	0.96	0.16	-0.70	62,62,62,62	0
33	MG	0	8010	1/1	1.00	0.17	-0.91	33,33,33,33	0
37	CD	Z	8603	1/1	0.97	0.09	-1.02	98,98,98,98	0
36	CL	M	8718	1/1	0.99	0.13	-1.19	47,47,47,47	0
33	MG	0	8008	1/1	0.97	0.14	-1.24	37,37,37,37	0
35	NA	0	8533	1/1	0.85	0.14	-1.27	39,39,39,39	0
35	NA	0	8531	1/1	0.97	0.15	-1.28	50,50,50,50	0
35	NA	0	8523	1/1	0.95	0.17	-1.30	43,43,43,43	0
33	MG	0	8018	1/1	0.98	0.14	-1.38	50,50,50,50	0
33	MG	0	8076	1/1	0.98	0.12	-1.39	55,55,55,55	0
36	CL	3	8704	1/1	0.93	0.16	-1.43	71,71,71,71	0
35	NA	J	8546	1/1	0.93	0.13	-1.46	53,53,53,53	0
33	MG	0	8017	1/1	0.98	0.13	-1.53	26,26,26,26	0
35	NA	0	8544	1/1	0.97	0.10	-1.55	28,28,28,28	0
37	CD	3	8604	1/1	0.99	0.08	-1.59	68,68,68,68	0
33	MG	0	8053	1/1	0.94	0.16	-1.65	45,45,45,45	0
33	MG	0	8014	1/1	0.96	0.16	-1.68	32,32,32,32	0
33	MG	0	8038	1/1	0.99	0.13	-1.70	34,34,34,34	0
36	CL	0	8716	1/1	0.96	0.10	-1.81	56,56,56,56	0
35	NA	0	8510	1/1	0.92	0.12	-1.95	36,36,36,36	0
37	CD	U	8601	1/1	1.00	0.09	-1.99	62,62,62,62	0
33	MG	0	8012	1/1	0.97	0.10	-2.02	39,39,39,39	0
35	NA	0	8525	1/1	0.96	0.15	-2.05	56,56,56,56	0
36	CL	J	8721	1/1	0.98	0.10	-2.16	58,58,58,58	0
35	NA	0	8539	1/1	0.96	0.15	-2.25	30,30,30,30	0
33	MG	T	8073	1/1	0.85	0.12	-2.32	71,71,71,71	0
35	NA	H	8509	1/1	0.95	0.10	-2.36	39,39,39,39	0
36	CL	0	8712	1/1	0.98	0.08	-2.46	49,49,49,49	0
33	MG	0	8015	1/1	0.97	0.14	-2.50	35,35,35,35	0
34	K	0	8402	1/1	0.99	0.14	-2.50	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
35	NA	R	8538	1/1	0.85	0.08	-2.58	60,60,60,60	0
35	NA	0	8517	1/1	0.93	0.06	-2.62	51,51,51,51	0
33	MG	0	8112	1/1	0.99	0.12	-2.63	42,42,42,42	0
33	MG	0	8021	1/1	0.98	0.12	-2.63	30,30,30,30	0
33	MG	0	8007	1/1	0.98	0.13	-2.68	22,22,22,22	0
33	MG	0	8058	1/1	0.97	0.06	-2.98	39,39,39,39	0
35	NA	Q	8548	1/1	0.95	0.06	-3.01	42,42,42,42	0
35	NA	0	8520	1/1	0.97	0.14	-3.02	34,34,34,34	0
33	MG	0	8074	1/1	0.98	0.05	-3.04	36,36,36,36	0
33	MG	0	8107	1/1	0.98	0.07	-3.05	36,36,36,36	0
33	MG	0	8004	1/1	0.98	0.09	-3.05	29,29,29,29	0
33	MG	0	8039	1/1	0.94	0.11	-3.06	52,52,52,52	0
33	MG	0	8067	1/1	0.97	0.12	-3.15	52,52,52,52	0
33	MG	0	8013	1/1	0.97	0.12	-3.23	38,38,38,38	0
33	MG	B	8055	1/1	0.94	0.05	-3.30	48,48,48,48	0
33	MG	0	8096	1/1	0.87	0.11	-3.41	52,52,52,52	0
33	MG	Y	8109	1/1	0.99	0.09	-3.42	37,37,37,37	0
33	MG	B	8056	1/1	0.98	0.05	-3.45	55,55,55,55	0
36	CL	0	8713	1/1	0.93	0.08	-3.49	65,65,65,65	0
36	CL	B	8719	1/1	0.98	0.12	-3.65	51,51,51,51	0
37	CD	1	8602	1/1	0.99	0.10	-3.66	63,63,63,63	0
33	MG	0	8001	1/1	0.99	0.14	-3.86	36,36,36,36	0
33	MG	0	8032	1/1	0.97	0.06	-4.41	28,28,28,28	0
33	MG	0	8091	1/1	0.96	0.07	-4.76	51,51,51,51	0
33	MG	0	8077	1/1	0.98	0.14	-5.13	33,33,33,33	0
33	MG	3	8078	1/1	0.98	0.05	-5.22	43,43,43,43	0
33	MG	0	8108	1/1	0.99	0.09	-5.55	70,70,70,70	0
33	MG	0	8044	1/1	0.91	0.10	-5.58	46,46,46,46	0
33	MG	0	8110	1/1	0.97	0.11	-5.65	27,27,27,27	0
35	NA	0	8553	1/1	0.97	0.11	-5.89	30,30,30,30	0
33	MG	0	8052	1/1	0.98	0.07	-7.12	54,54,54,54	0
33	MG	A	8065	1/1	0.99	0.06	-7.63	41,41,41,41	0
33	MG	0	8019	1/1	0.98	0.06	-8.09	35,35,35,35	0
33	MG	0	8020	1/1	0.98	0.09	-8.52	33,33,33,33	0
33	MG	0	8022	1/1	0.98	0.10	-8.67	38,38,38,38	0
33	MG	0	8006	1/1	0.99	0.06	-9.02	33,33,33,33	0
33	MG	0	8084	1/1	0.95	0.05	-9.19	47,47,47,47	0
33	MG	0	8035	1/1	0.97	0.05	-9.96	46,46,46,46	0
33	MG	0	8033	1/1	0.97	0.09	-10.68	31,31,31,31	0
33	MG	0	8003	1/1	0.99	0.09	-11.24	35,35,35,35	0
33	MG	0	8064	1/1	0.97	0.07	-11.92	30,30,30,30	0
33	MG	0	8002	1/1	0.98	0.09	-16.72	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
35	NA	0	8536	1/1	0.95	0.10	-	55,55,55,55	0
33	MG	0	8011	1/1	0.98	0.18	-	27,27,27,27	0
33	MG	0	8036	1/1	0.98	0.06	-	33,33,33,33	0
33	MG	0	8090	1/1	0.68	0.75	-	69,69,69,69	0
33	MG	0	8075	1/1	0.95	0.06	-	44,44,44,44	0
33	MG	0	8027	1/1	0.97	0.04	-	44,44,44,44	0
35	NA	0	8575	1/1	0.96	0.27	-	61,61,61,61	0
33	MG	0	8115	1/1	0.98	0.08	-	52,52,52,52	0
35	NA	0	8563	1/1	0.85	0.46	-	57,57,57,57	0
33	MG	0	8059	1/1	0.99	0.06	-	43,43,43,43	0
33	MG	0	8063	1/1	0.97	0.21	-	60,60,60,60	0
36	CL	R	8706	1/1	0.96	0.15	-	46,46,46,46	0
33	MG	0	8079	1/1	0.98	0.17	-	37,37,37,37	0
33	MG	0	8106	1/1	0.98	0.09	-	65,65,65,65	0
35	NA	0	8567	1/1	0.89	0.29	-	59,59,59,59	0
33	MG	0	8046	1/1	0.92	0.09	-	53,53,53,53	0
33	MG	0	8116	1/1	0.88	0.07	-	58,58,58,58	0
33	MG	0	8083	1/1	0.99	0.12	-	43,43,43,43	0
36	CL	0	8717	1/1	0.91	0.11	-	65,65,65,65	0
33	MG	0	8072	1/1	0.97	0.07	-	63,63,63,63	0
33	MG	0	8031	1/1	0.96	0.12	-	34,34,34,34	0
35	NA	0	8518	1/1	0.97	0.19	-	42,42,42,42	0
33	MG	0	8048	1/1	0.98	0.12	-	54,54,54,54	0
35	NA	S	8512	1/1	0.87	0.09	-	43,43,43,43	0
33	MG	0	8093	1/1	0.97	0.09	-	56,56,56,56	0
33	MG	0	8111	1/1	0.98	0.09	-	42,42,42,42	0
36	CL	A	8709	1/1	0.93	0.24	-	77,77,77,77	0
36	CL	0	8714	1/1	0.96	0.14	-	54,54,54,54	0
35	NA	0	8515	1/1	0.97	0.20	-	42,42,42,42	0
33	MG	0	8034	1/1	0.99	0.09	-	33,33,33,33	0
33	MG	A	8066	1/1	0.91	0.04	-	72,72,72,72	0
33	MG	0	8088	1/1	0.97	0.14	-	38,38,38,38	0
36	CL	0	8703	1/1	0.98	0.08	-	58,58,58,58	0
35	NA	0	8540	1/1	0.78	0.21	-	58,58,58,58	0
33	MG	0	8098	1/1	0.98	0.08	-	40,40,40,40	0
33	MG	0	8117	1/1	0.98	0.06	-	32,32,32,32	0
36	CL	J	8701	1/1	0.94	0.22	-	66,66,66,66	0
33	MG	0	8041	1/1	0.91	0.19	-	56,56,56,56	0
36	CL	0	8722	1/1	0.87	0.37	-	81,81,81,81	0
35	NA	0	8584	1/1	0.88	0.14	-	62,62,62,62	0
33	MG	0	8045	1/1	0.98	0.07	-	53,53,53,53	0
33	MG	0	8026	1/1	0.98	0.17	-	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
33	MG	0	8042	1/1	0.96	0.10	-	38,38,38,38	0
35	NA	0	8552	1/1	0.78	0.21	-	62,62,62,62	0
33	MG	0	8089	1/1	0.97	0.14	-	74,74,74,74	0
33	MG	0	8087	1/1	0.88	0.12	-	66,66,66,66	0
35	NA	0	8528	1/1	0.98	0.32	-	42,42,42,42	0
35	NA	0	8511	1/1	0.90	0.15	-	50,50,50,50	0
33	MG	0	8101	1/1	0.93	0.19	-	69,69,69,69	0
33	MG	0	8071	1/1	0.96	0.04	-	69,69,69,69	0
35	NA	0	8558	1/1	0.95	0.35	-	82,82,82,82	0
33	MG	0	8103	1/1	0.93	0.18	-	82,82,82,82	0
35	NA	0	8541	1/1	0.94	0.10	-	50,50,50,50	0
33	MG	0	8099	1/1	0.96	0.16	-	45,45,45,45	0
33	MG	0	8092	1/1	0.79	0.13	-	89,89,89,89	0
33	MG	0	8016	1/1	0.98	0.09	-	40,40,40,40	0
33	MG	0	8062	1/1	0.98	0.09	-	54,54,54,54	0
33	MG	0	8081	1/1	0.94	0.10	-	49,49,49,49	0
33	MG	K	8069	1/1	0.97	0.05	-	58,58,58,58	0
33	MG	0	8086	1/1	0.95	0.07	-	52,52,52,52	0
35	NA	0	8559	1/1	0.94	0.24	-	49,49,49,49	0
33	MG	0	8050	1/1	0.90	0.08	-	59,59,59,59	0
33	MG	0	8114	1/1	0.86	0.65	-	67,67,67,67	0
35	NA	0	8516	1/1	0.92	0.25	-	54,54,54,54	0
35	NA	0	8542	1/1	0.90	0.39	-	47,47,47,47	0
36	CL	Q	8711	1/1	0.98	0.08	-	55,55,55,55	0
33	MG	0	8068	1/1	0.96	0.04	-	61,61,61,61	0
33	MG	9	8095	1/1	0.89	0.12	-	76,76,76,76	0
33	MG	0	8040	1/1	0.97	0.13	-	60,60,60,60	0
35	NA	0	8506	1/1	0.90	0.37	-	48,48,48,48	0
33	MG	0	8030	1/1	0.99	0.10	-	25,25,25,25	0
35	NA	0	8501	1/1	0.95	0.21	-	32,32,32,32	0
33	MG	0	8049	1/1	0.75	0.19	-	92,92,92,92	0
35	NA	0	8554	1/1	0.98	0.16	-	40,40,40,40	0
33	MG	0	8082	1/1	0.88	0.14	-	63,63,63,63	0
36	CL	N	8707	1/1	0.95	0.11	-	66,66,66,66	0
35	NA	0	8581	1/1	0.95	0.08	-	48,48,48,48	0
35	NA	0	8534	1/1	0.95	0.07	-	45,45,45,45	0
33	MG	0	8061	1/1	0.97	0.17	-	41,41,41,41	0
33	MG	0	8113	1/1	0.91	0.12	-	53,53,53,53	0
36	CL	Y	8720	1/1	0.98	0.13	-	46,46,46,46	0
33	MG	0	8051	1/1	0.97	0.05	-	59,59,59,59	0
33	MG	0	8028	1/1	0.97	0.05	-	38,38,38,38	0
37	CD	O	8605	1/1	0.96	0.08	-	93,93,93,93	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
33	MG	0	8009	1/1	0.99	0.17	-	35,35,35,35	0
33	MG	0	8085	1/1	0.94	0.12	-	54,54,54,54	0
36	CL	J	8702	1/1	0.97	0.10	-	57,57,57,57	0
36	CL	L	8710	1/1	0.95	0.19	-	60,60,60,60	0
35	NA	0	8513	1/1	0.90	0.09	-	62,62,62,62	0
35	NA	0	8570	1/1	0.95	0.34	-	69,69,69,69	0
35	NA	9	8551	1/1	0.71	0.19	-	50,50,50,50	0
35	NA	0	8549	1/1	0.96	0.18	-	51,51,51,51	0
33	MG	0	8097	1/1	0.94	0.10	-	34,34,34,34	0
33	MG	0	8043	1/1	0.96	0.08	-	48,48,48,48	0
35	NA	0	8557	1/1	0.92	0.12	-	61,61,61,61	0
33	MG	0	8094	1/1	0.97	0.07	-	77,77,77,77	0
33	MG	0	8029	1/1	0.98	0.07	-	35,35,35,35	0
33	MG	0	8102	1/1	0.91	0.29	-	73,73,73,73	0
35	NA	0	8507	1/1	0.94	0.32	-	59,59,59,59	0
33	MG	0	8104	1/1	0.91	0.23	-	65,65,65,65	0
33	MG	0	8100	1/1	0.91	0.18	-	66,66,66,66	0
35	NA	0	8560	1/1	0.95	0.30	-	51,51,51,51	0
33	MG	0	8024	1/1	0.98	0.13	-	21,21,21,21	0
33	MG	0	8070	1/1	0.97	0.16	-	50,50,50,50	0
33	MG	0	8037	1/1	0.98	0.09	-	43,43,43,43	0
35	NA	H	8522	1/1	0.83	0.33	-	67,67,67,67	0
35	NA	0	8530	1/1	0.97	0.15	-	50,50,50,50	0
33	MG	0	8047	1/1	0.93	0.13	-	74,74,74,74	0
35	NA	0	8585	1/1	0.86	0.26	-	51,51,51,51	0
33	MG	0	8005	1/1	0.99	0.16	-	33,33,33,33	0
33	MG	0	8023	1/1	0.97	0.27	-	41,41,41,41	0
33	MG	0	8025	1/1	0.97	0.09	-	37,37,37,37	0
35	NA	0	8508	1/1	0.92	0.15	-	56,56,56,56	0

6.5 Other polymers (i)

There are no such residues in this entry.