Full wwPDB X-ray Structure Validation 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 Full wwPDB X-ray Structure Validation 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:

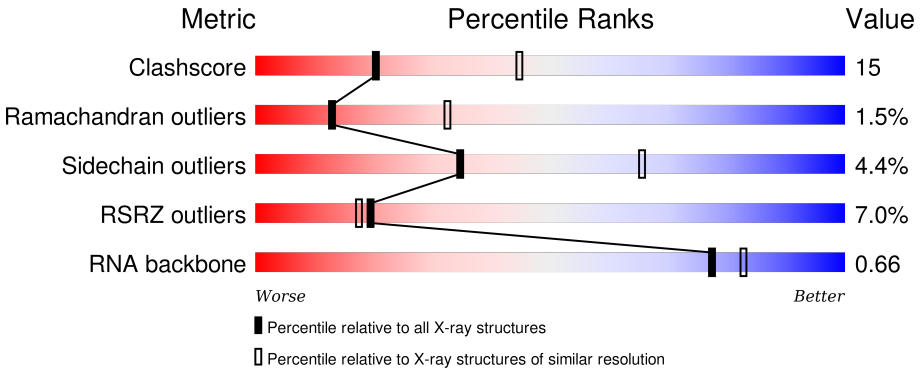
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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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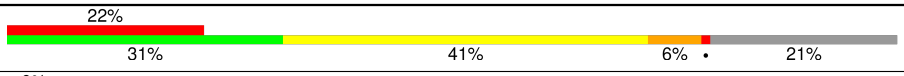
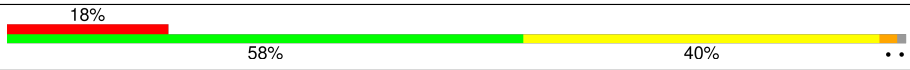
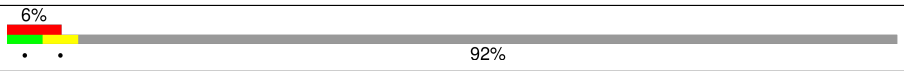
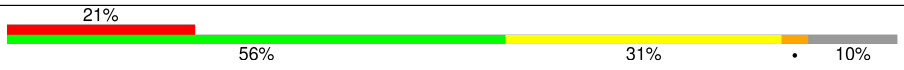
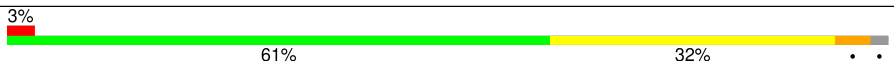
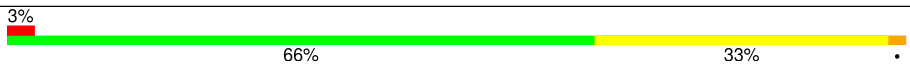
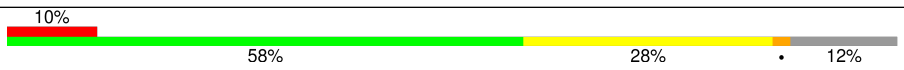
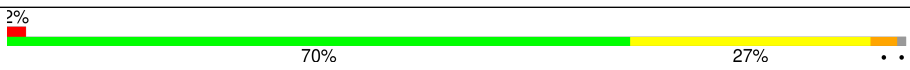
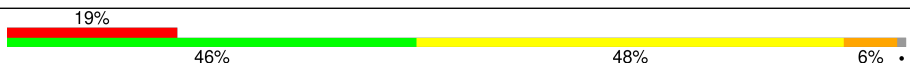
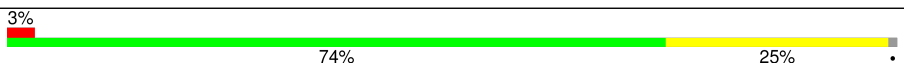
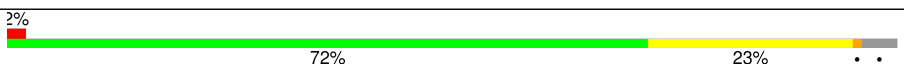
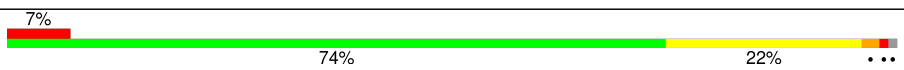
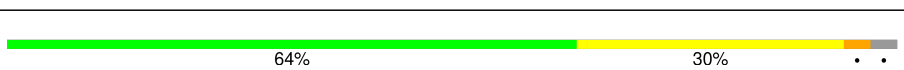
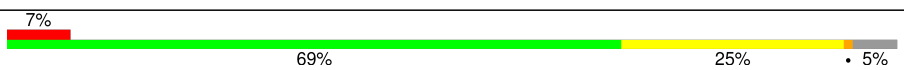
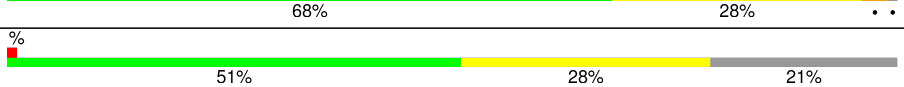
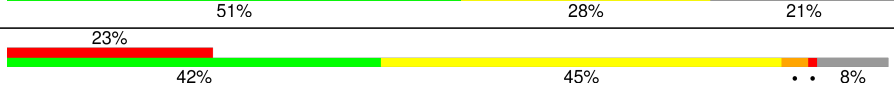
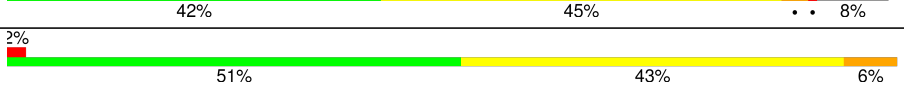
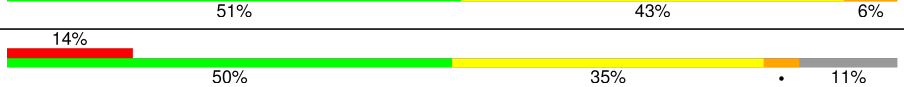
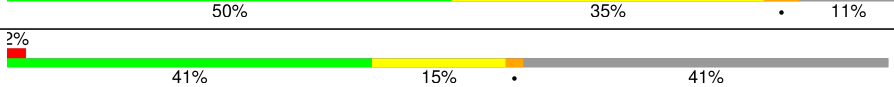
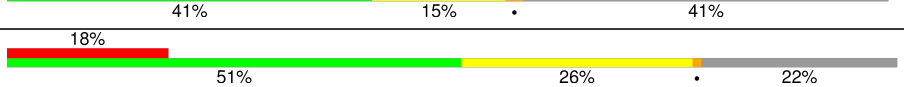
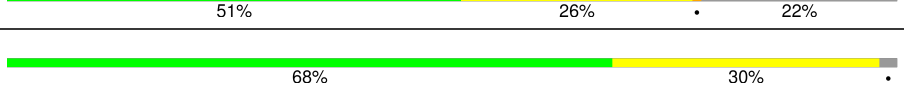
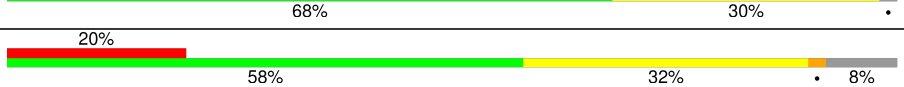
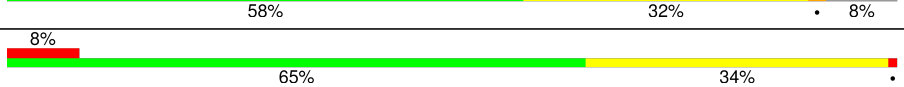
Mol	Chain	Length	Quality of chain
6	D	177	
7	E	178	
8	F	120	
9	G	348	
10	H	177	
11	I	145	
12	J	132	
13	K	165	
14	L	196	
15	M	187	
16	N	116	
17	O	149	
18	P	96	
19	Q	155	
20	R	85	
21	S	120	
22	T	67	
23	U	71	
24	V	154	
25	W	92	
26	X	241	
27	Y	92	
28	Z	57	
29	1	50	
30	2	92	

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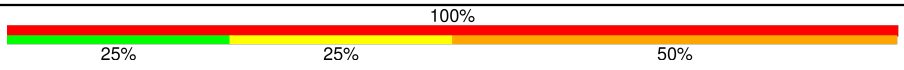
Mol	Chain	Length	Quality of chain
31	4	4	

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
			Total	C	N	O	P			
1	0	2754	59016	26346	10879	19046	2745	0	0	0

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
			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
			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			

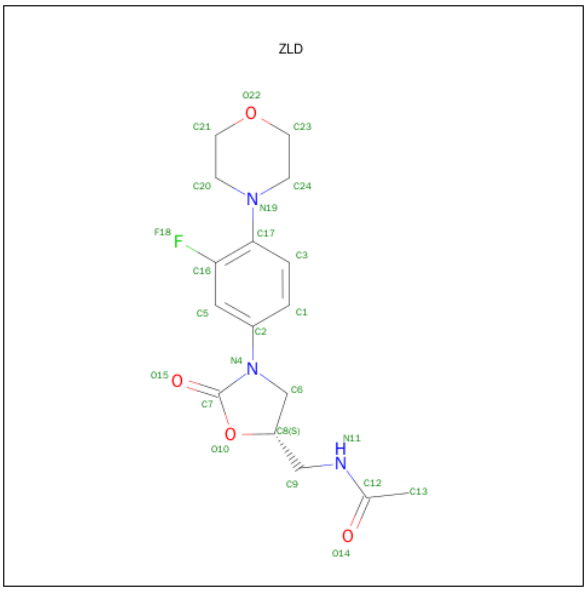
- Molecule 30 is a protein called 50S ribosomal protein L44E.

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	0	0
			24	16	1	3	4		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	0	84	Total	Mg	0	0
			84	84		
33	J	1	Total	Mg	0	0
			1	1		
33	1	1	Total	Mg	0	0
			1	1		
33	B	1	Total	Mg	0	0
			1	1		
33	A	2	Total	Mg	0	0
			2	2		
33	X	1	Total	Mg	0	0
			1	1		
33	9	1	Total	Mg	0	0
			1	1		
33	S	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 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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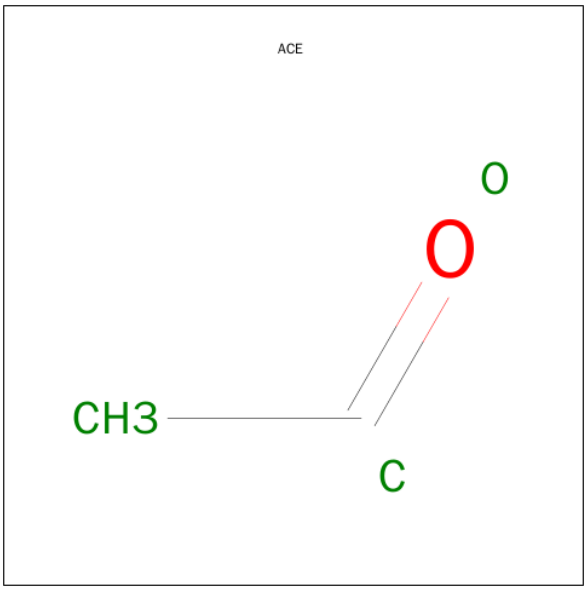
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
38	Y	1	Total Cd 1 1	0	0
38	T	1	Total Cd 1 1	0	0
38	2	1	Total Cd 1 1	0	0
38	N	1	Total Cd 1 1	0	0

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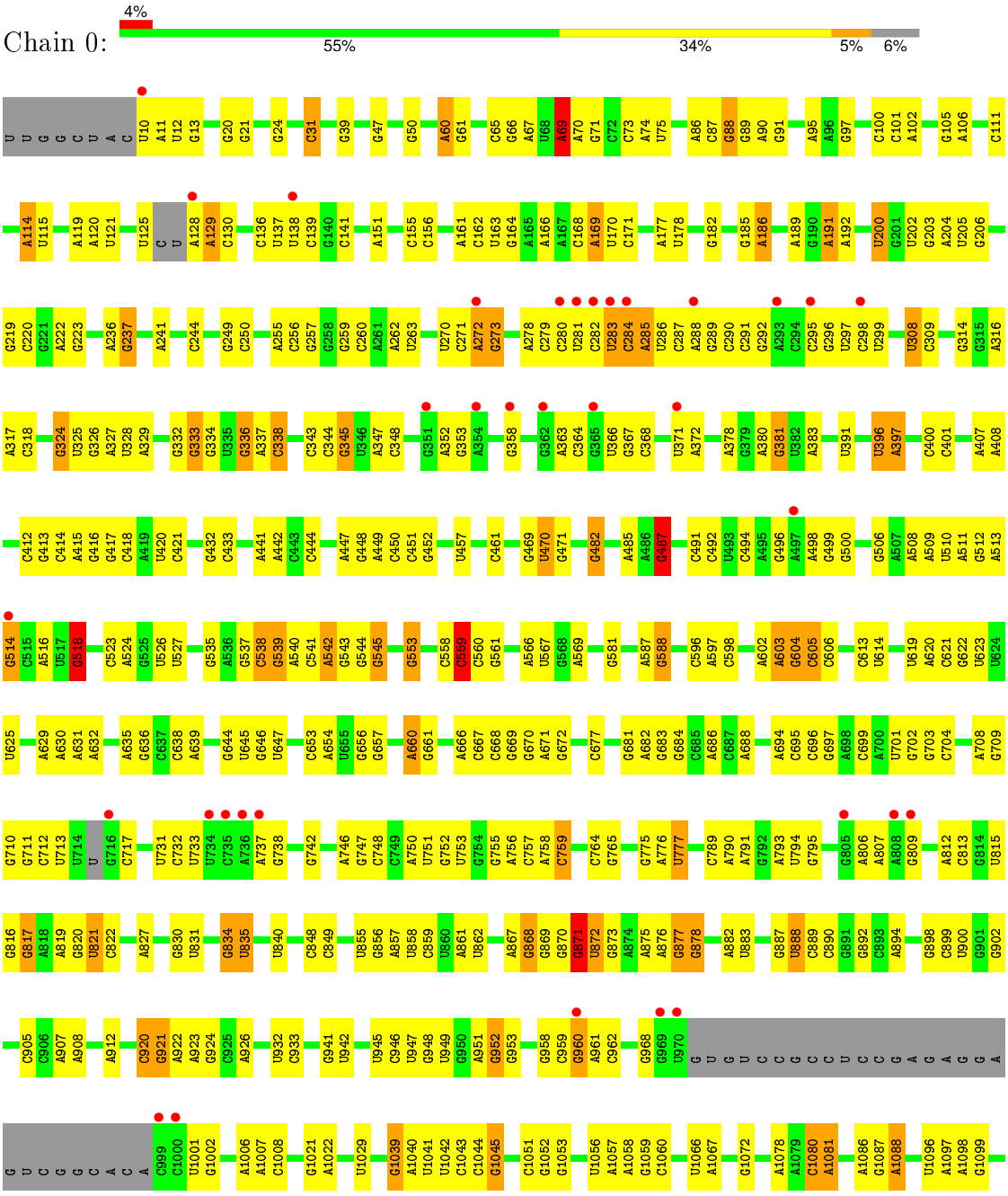
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
40	X	99	Total O 99 99	0	0
40	Y	23	Total O 23 23	0	0
40	Z	58	Total O 58 58	0	0
40	1	40	Total O 40 40	0	0
40	2	73	Total O 73 73	0	0
40	4	3	Total O 3 3	0	0

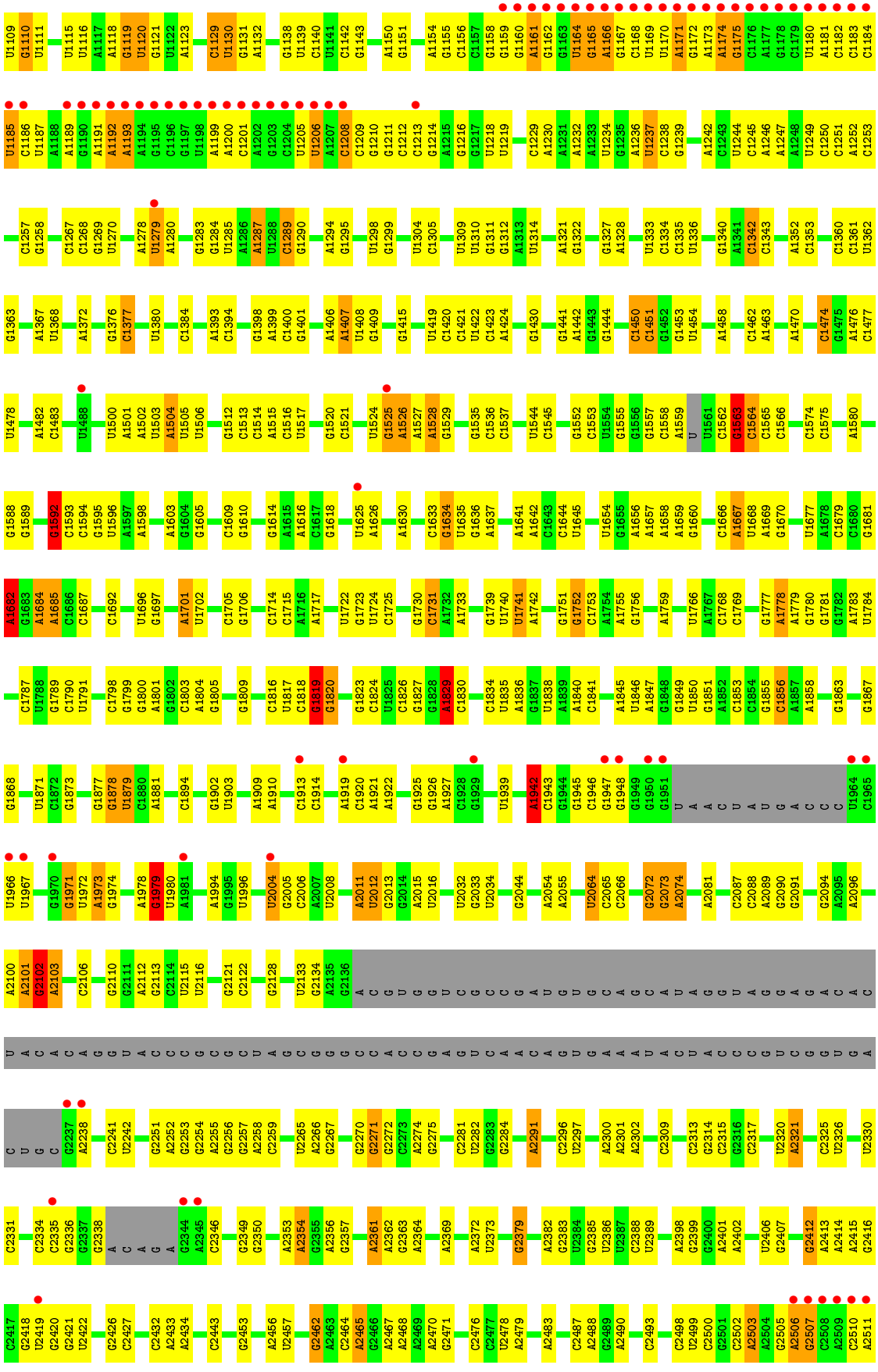
3 Residue-property plots (i)

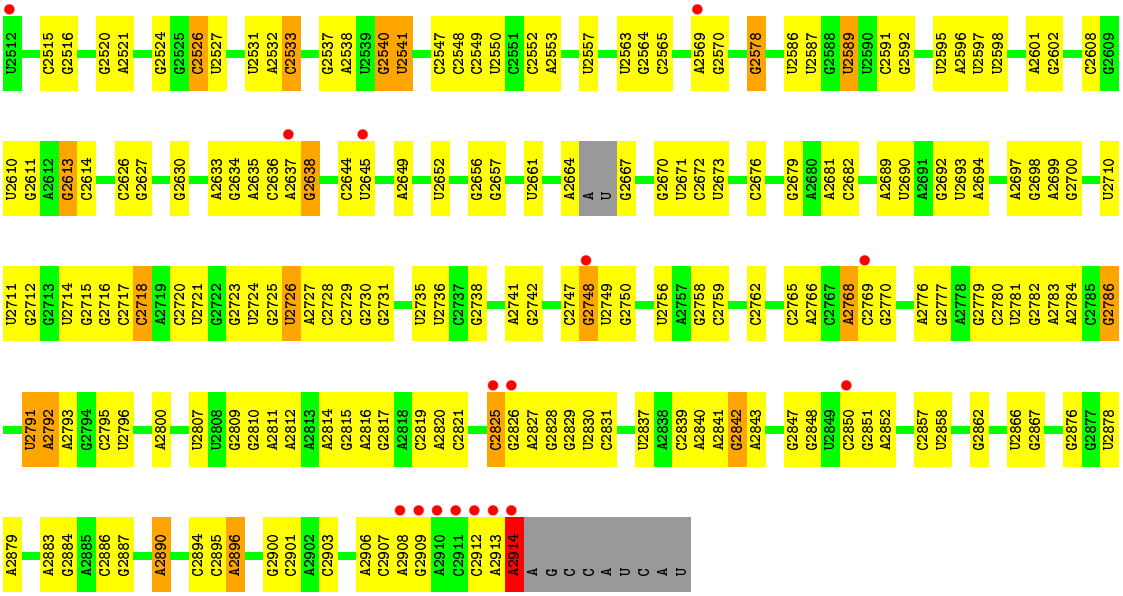
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

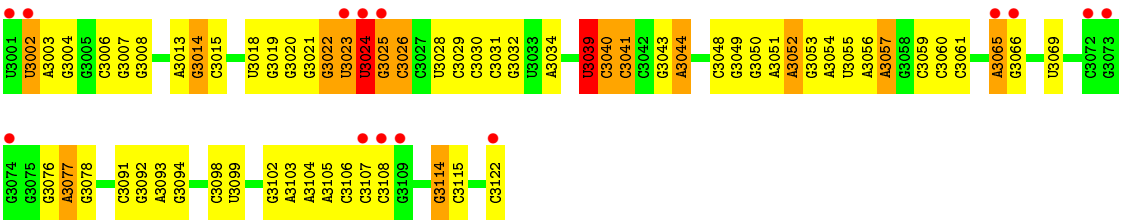



U1109 G1110 U1111 U1115 U1116 A1117 A1118 G1119 U1120 G1121 U1122 A1123 C1129 U1130 G1131 A1132 G1138 U1139 C1140 U1141 C1142 G1143 A1150 G1151 A1154 G1155 C1156 C1157 G1158 G1159 G1160 A1161 G1162 G1163 U1164 G1165 A1166 G1167 C1168 U1169 U1170 A1171 G1172 A1173 A1174 G1175 C1176 A1177 G1178 C1179 U1180 A1181 C1182 C1183 C1184
U1185 C1186 U1187 A1188 A1189 G1190 A1191 A1192 A1193 A1194 G1195 C1196 G1197 U1198 A1199 A1200 C1201 A1202 G1203 C1204 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 U1285 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 A1767 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 C1854 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 G A C C C C U U A A C G G G G U U U



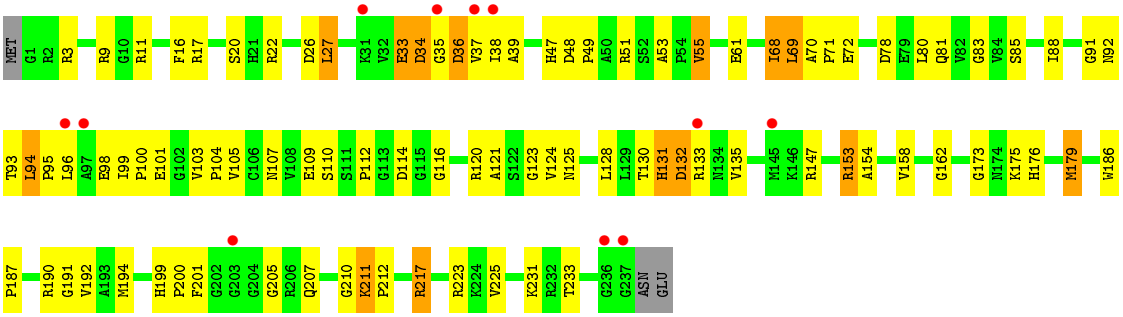
• Molecule 2: 5S RIBOSOMAL RNA

Chain 9:



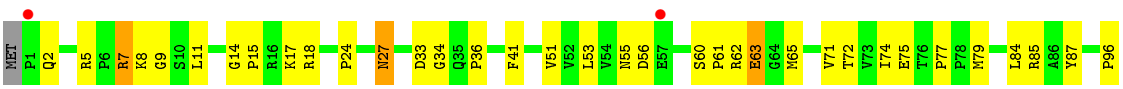
• Molecule 3: 50S ribosomal protein L2P

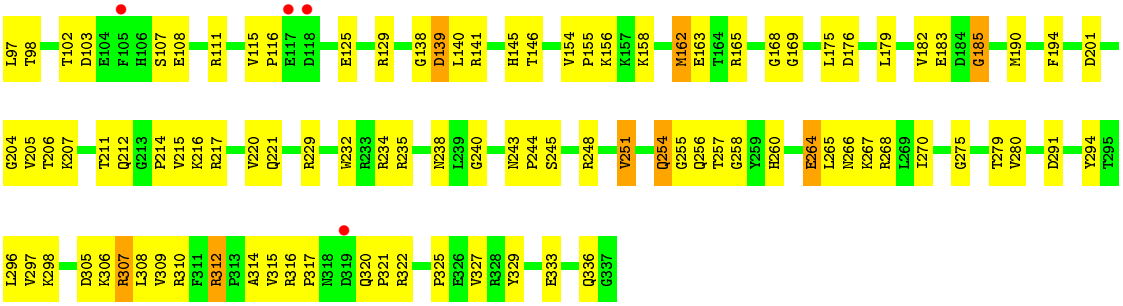
Chain A:



• Molecule 4: 50S ribosomal protein L3P

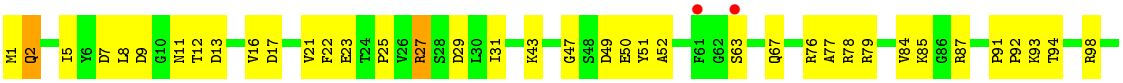
Chain B:





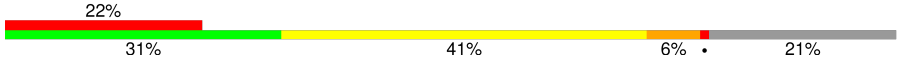
• Molecule 5: 50S ribosomal protein L4P

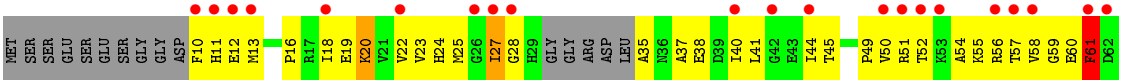
Chain C:



• Molecule 6: 50S ribosomal protein L5P

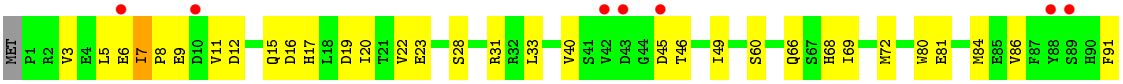
Chain D:





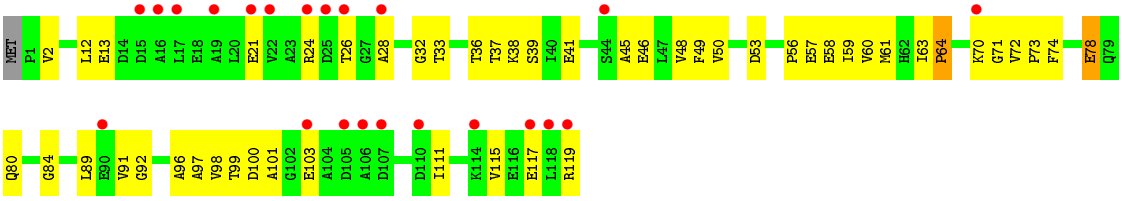
• Molecule 7: 50S ribosomal protein L6P

Chain E:



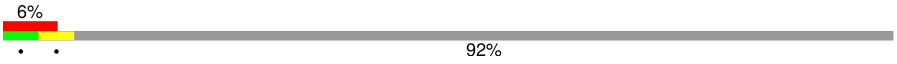
• Molecule 8: 50S ribosomal protein L7Ae

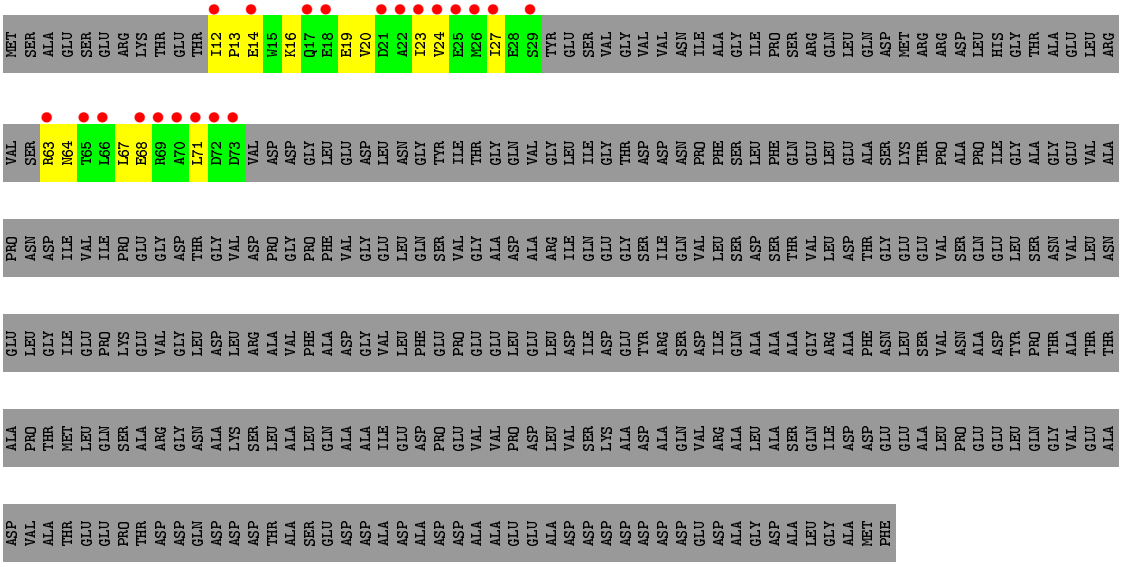
Chain F:



• Molecule 9: 50S ribosomal protein L10E

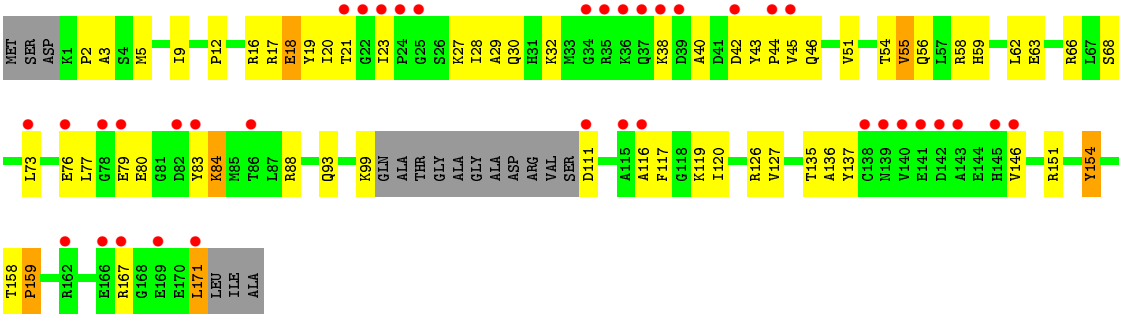
Chain G:





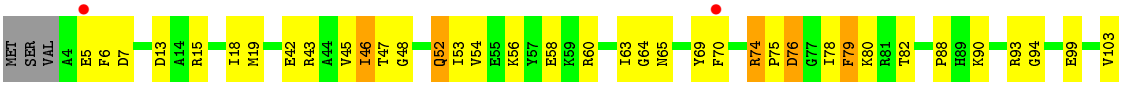
• Molecule 10: 50S ribosomal protein L10e

Chain H:

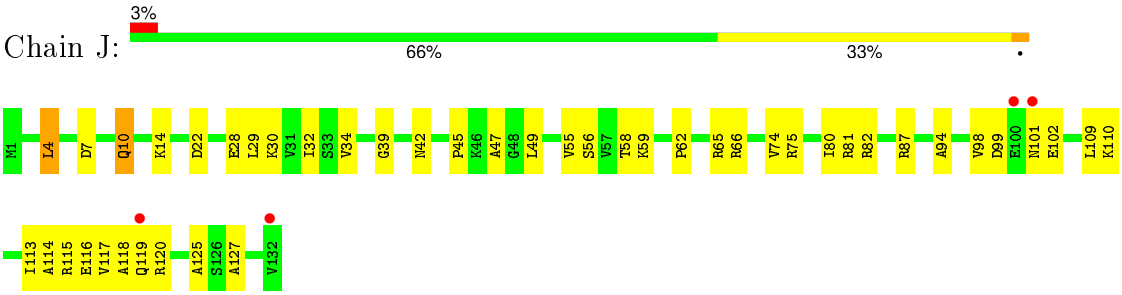


• Molecule 11: 50S ribosomal protein L13P

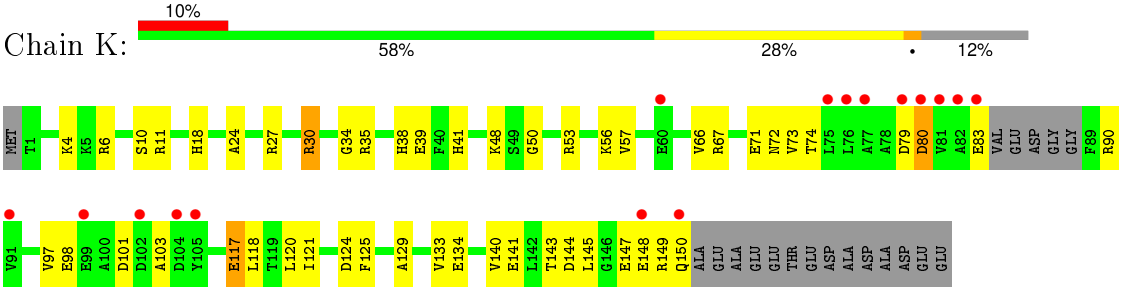
Chain I:



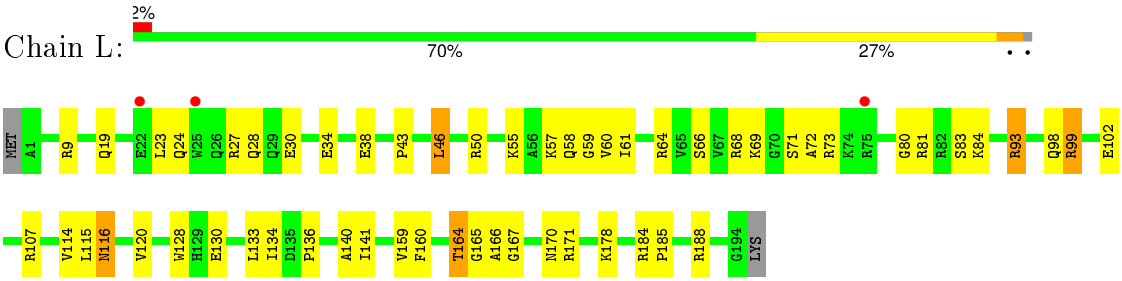
• Molecule 12: 50S ribosomal protein L14P



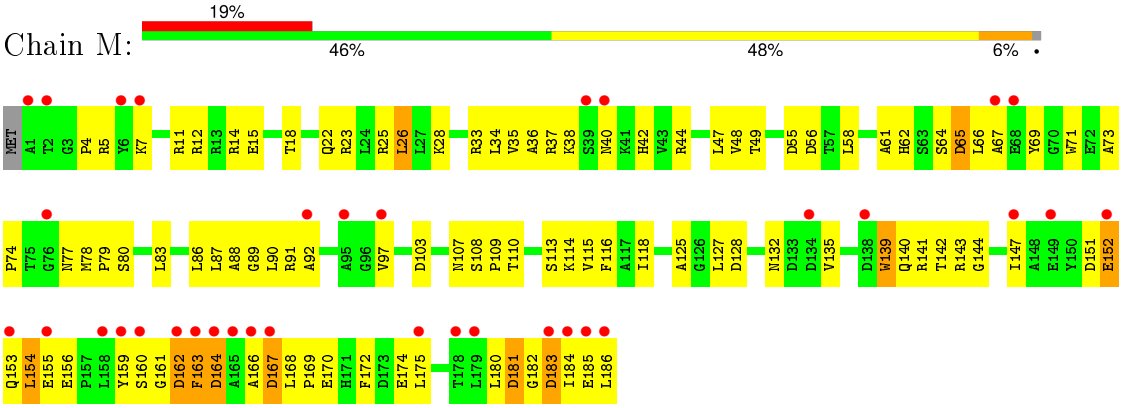
• Molecule 13: 50S ribosomal protein L15P



• Molecule 14: 50S ribosomal protein L15e

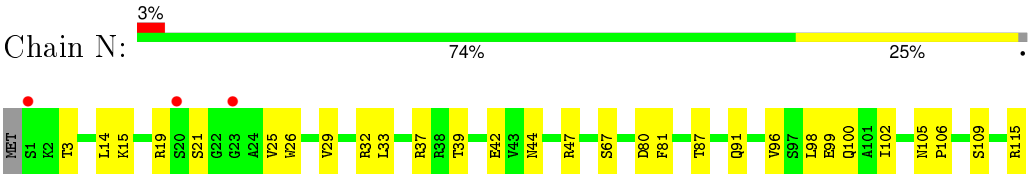


• Molecule 15: 50S ribosomal protein L18P



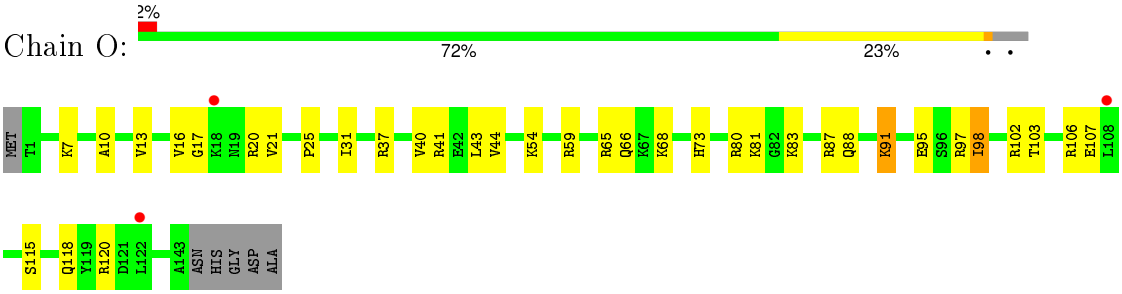
• Molecule 16: 50S ribosomal protein L18e

Chain N:



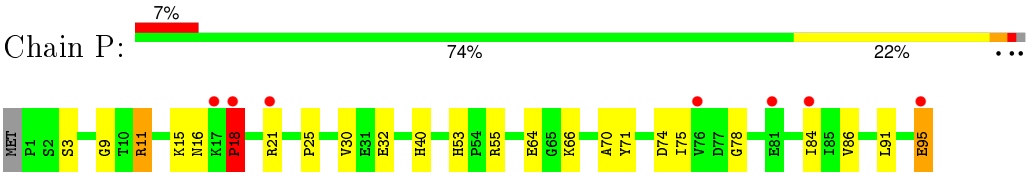
• Molecule 17: 50S ribosomal protein L19e

Chain O:



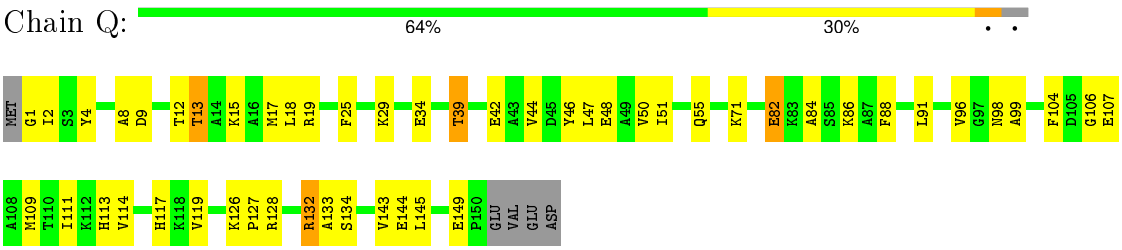
• Molecule 18: 50S ribosomal protein L21e

Chain P:



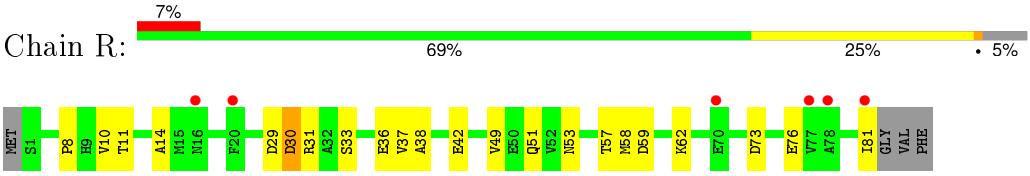
• Molecule 19: 50S ribosomal protein L22P

Chain Q:



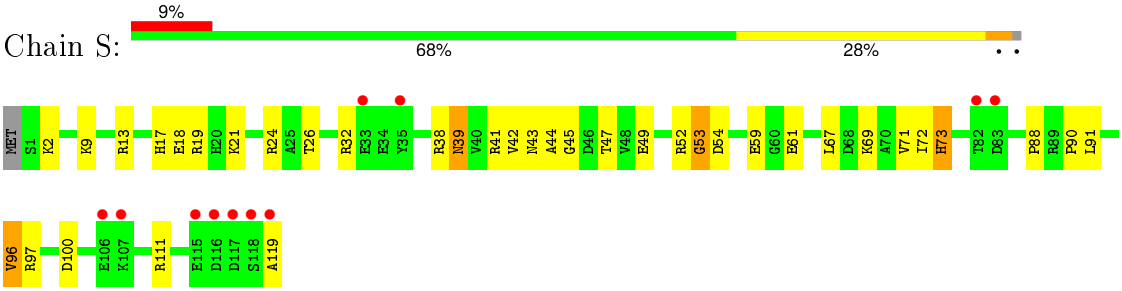
• Molecule 20: 50S ribosomal protein L23P

Chain R:



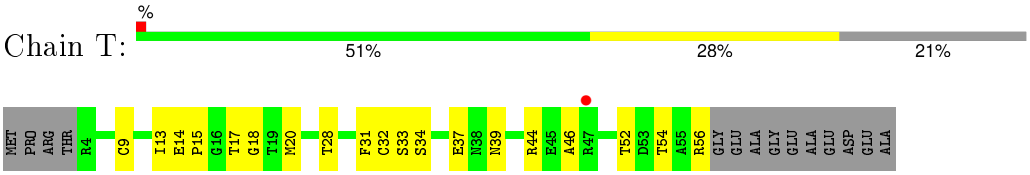
• Molecule 21: 50S ribosomal protein L24P

Chain S:



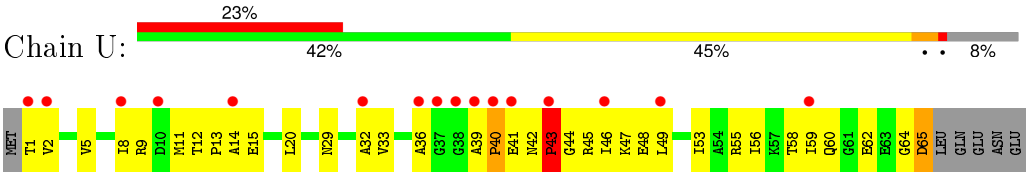
• Molecule 22: 50S ribosomal protein L24e

Chain T:



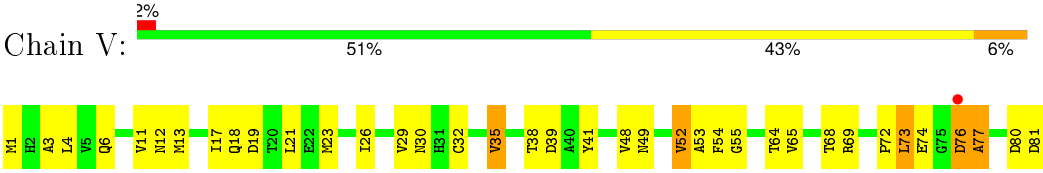
• Molecule 23: 50S ribosomal protein L29P

Chain U:



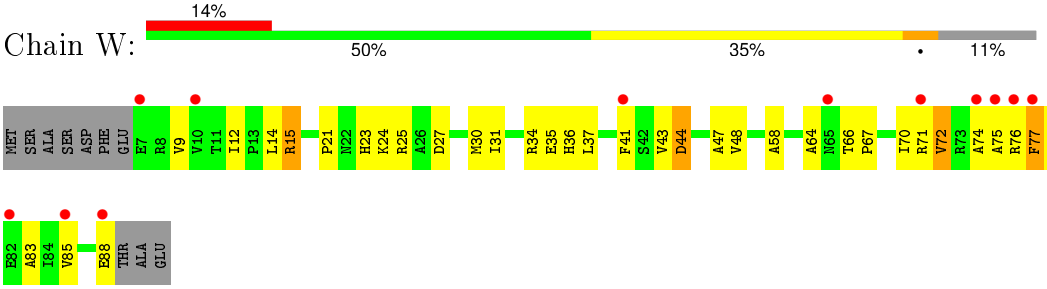
• Molecule 24: 50S ribosomal protein L30P

Chain V:



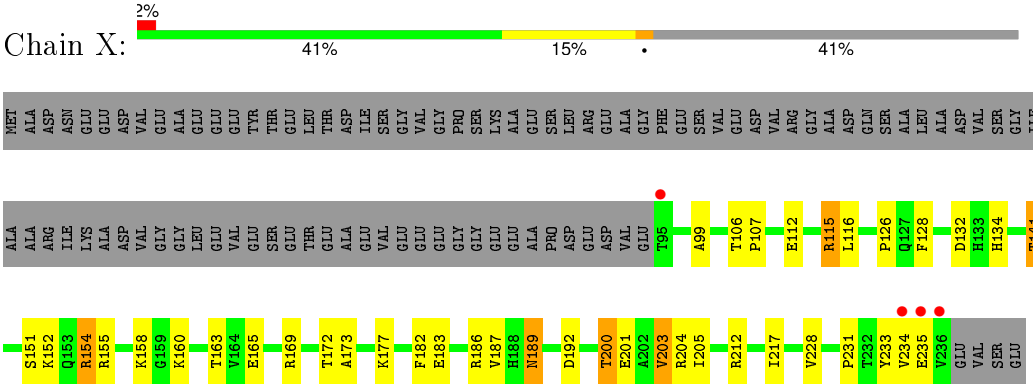
• Molecule 25: 50S ribosomal protein L31e

Chain W:



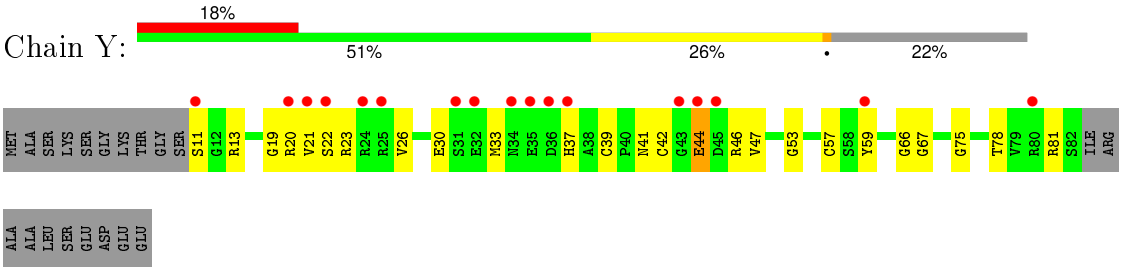
• Molecule 26: 50S ribosomal protein L32e

Chain X:



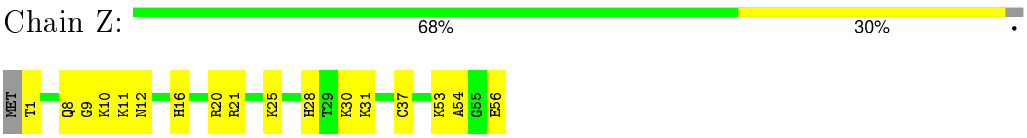
• Molecule 27: 50S ribosomal protein L37Ae

Chain Y:



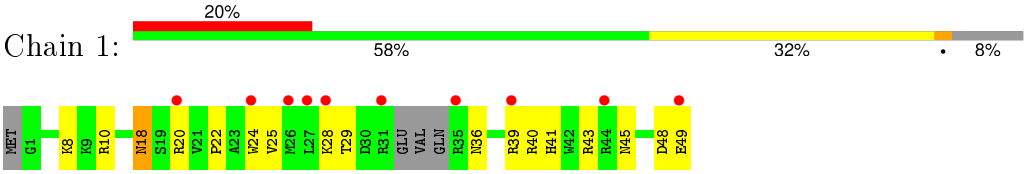
• Molecule 28: 50S ribosomal protein L37e

Chain Z:



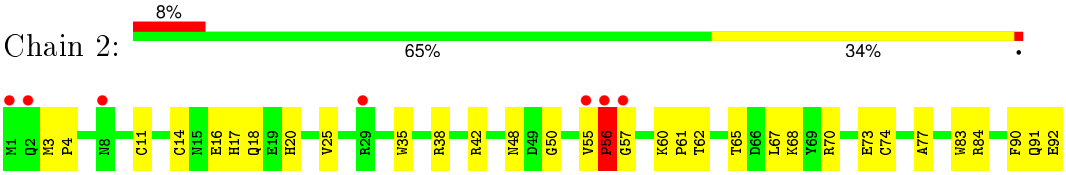
• Molecule 29: 50S ribosomal protein L39e

Chain 1:



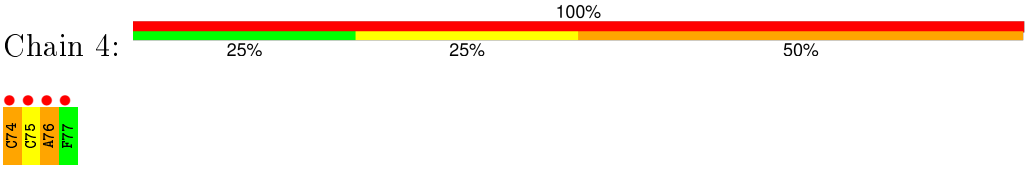
• Molecule 30: 50S ribosomal protein L44E

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

All (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
1	0	1563	G	C2'-C3'-O3'	7.43	125.84	109.50
1	0	1979	G	C2'-C3'-O3'	7.17	125.27	109.50
1	0	559	C	N1-C2-O2	7.08	123.14	118.90
1	0	1559	A	C2'-C3'-O3'	7.07	125.05	109.50
1	0	777	U	O4'-C1'-N1	6.73	113.58	108.20
31	4	76	A	C3'-C2'-C1'	6.58	106.77	101.50
2	9	3039	U	N1-C1'-C2'	6.24	122.11	114.00
1	0	559	C	N1-C2-N3	-6.22	114.84	119.20
1	0	2338	G	C2'-C3'-O3'	6.20	123.61	113.70
1	0	1120	U	C5'-C4'-C3'	-6.00	106.41	116.00
1	0	1592	G	N9-C1'-C2'	5.99	121.79	114.00
1	0	69	A	C5'-C4'-O4'	-5.94	101.97	109.10
1	0	1829	A	N9-C1'-C2'	-5.87	105.54	112.00
1	0	1942	A	C5'-C4'-C3'	5.68	125.08	116.00
1	0	2726	U	N1-C1'-C2'	5.61	121.30	114.00
1	0	1819	G	C5'-C4'-C3'	5.48	124.77	116.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	0	206	G	C5'-C4'-C3'	-5.46	107.27	116.00
1	0	2313	C	C5'-C4'-C3'	5.33	124.53	116.00
1	0	2914	A	C2'-C3'-O3'	5.30	122.19	113.70
1	0	2313	C	C5'-C4'-O4'	5.23	115.38	109.10
10	H	171	LEU	CB-CG-CD2	-5.23	102.11	111.00
1	0	1504	A	N9-C1'-C2'	5.13	120.67	114.00
1	0	535	G	N9-C1'-C2'	5.08	120.61	114.00
1	0	518	G	O4'-C1'-N9	5.03	112.22	108.20

There are no chirality outliers.

All (57) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	1039	G	Sidechain
1	0	1078	A	Sidechain
1	0	1327	G	Sidechain
1	0	1340	G	Sidechain
1	0	1376	G	Sidechain
1	0	1430	G	Sidechain
1	0	1458	A	Sidechain
1	0	1592	G	Sidechain
1	0	1682	A	Sidechain
1	0	1696	U	Sidechain
1	0	1741	U	Sidechain
1	0	1777	G	Sidechain
1	0	1809	G	Sidechain
1	0	182	G	Sidechain
1	0	1829	A	Sidechain
1	0	1863	G	Sidechain
1	0	1867	G	Sidechain
1	0	1877	G	Sidechain
1	0	1878	G	Sidechain
1	0	1979	G	Sidechain
1	0	2102	G	Sidechain
1	0	2412	G	Sidechain
1	0	2465	A	Sidechain
1	0	2493	C	Sidechain
1	0	2503	A	Sidechain
1	0	2506	A	Sidechain
1	0	2552	C	Sidechain
1	0	2557	U	Sidechain
1	0	2630	G	Sidechain

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Mol	Chain	Res	Type	Group
1	0	2679	G	Sidechain
1	0	270	U	Sidechain
1	0	2714	U	Sidechain
1	0	2793	A	Sidechain
1	0	2842	G	Sidechain
1	0	324	G	Sidechain
1	0	332	G	Sidechain
1	0	333	G	Sidechain
1	0	396	U	Sidechain
1	0	469	G	Sidechain
1	0	470	U	Sidechain
1	0	471	G	Sidechain
1	0	482	G	Sidechain
1	0	487	G	Sidechain
1	0	50	G	Sidechain
1	0	518	G	Sidechain
1	0	619	U	Sidechain
1	0	742	G	Sidechain
1	0	795	G	Sidechain
1	0	817	G	Sidechain
1	0	867	A	Sidechain
1	0	868	G	Sidechain
1	0	888	U	Sidechain
1	0	900	U	Sidechain
1	0	952	G	Sidechain
2	9	3039	U	Sidechain
2	9	3065	A	Sidechain
24	V	90	TYR	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	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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.

All (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
2:9:3076:G:H3'	2:9:3077:A:H5"	1.38	1.03
21:S:71:VAL:HG11	21:S:90:PRO:HB3	1.34	1.03
25:W:37:LEU:HD13	25:W:85:VAL:HG21	1.38	1.02
2:9:3006:C:H5"	15:M:37:ARG:HH12	1.25	1.02
2:9:3006:C:H5"	15:M:37:ARG:NH1	1.74	1.02
23:U:12:THR:HG22	23:U:15:GLU:HG3	1.39	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:264:GLU:HG2	4:B:267:LYS:HE2	1.40	1.00
17:O:115:SER:H	17:O:118:GLN:HE21	1.06	1.00
12:J:29:LEU:HB3	12:J:55:VAL:HG11	1.43	1.00
24:V:88:THR:HG22	24:V:89:ASP:H	1.24	0.99
14:L:107:ARG:HG3	14:L:107:ARG:HH11	1.25	0.98
6:D:134:LEU:HD11	6:D:166:ILE:HD11	1.45	0.98
1:0:1242:A:H5'	11:I:82:THR:HG23	1.44	0.96
24:V:137:GLN:HE21	24:V:141:HIS:HE1	1.09	0.96
5:C:78:ARG:HG3	5:C:78:ARG:HH11	1.29	0.96
20:R:57:THR:HG22	20:R:59:ASP:H	1.26	0.96
1:0:870:G:H2'	1:0:871:G:H5"	1.45	0.95
12:J:10:GLN:NE2	12:J:10:GLN:H	1.62	0.95
15:M:144:GLY:O	15:M:147:ILE:HG22	1.65	0.94
12:J:10:GLN:N	12:J:10:GLN:HE21	1.65	0.94
1:0:871:G:C8	1:0:871:G:H5'	2.01	0.94
1:0:871:G:H8	1:0:871:G:H5'	1.31	0.94
2:9:3056:A:H2'	2:9:3057:A:H5"	1.50	0.93
5:C:127:ARG:NH2	5:C:225:PRO:HG2	1.83	0.93
1:0:2812:A:H2	1:0:2814:A:H62	1.16	0.92
24:V:4:LEU:HD22	24:V:52:VAL:HG21	1.51	0.92
19:Q:99:ALA:HB1	19:Q:109:MET:HE1	1.51	0.91
15:M:47:LEU:HD11	15:M:127:LEU:HD21	1.52	0.91
24:V:122:ARG:HH11	24:V:122:ARG:HG2	1.35	0.91
6:D:25:MET:HE1	6:D:37:ALA:HB1	1.50	0.91
3:A:153:ARG:HH11	3:A:153:ARG:HB2	1.33	0.91
10:H:27:LYS:H	10:H:59:HIS:HD2	1.19	0.90
5:C:5:ILE:HD11	5:C:16:VAL:HG23	1.51	0.90
1:0:1166:A:H1'	1:0:1192:A:C2	2.08	0.89
15:M:113:SER:HB2	40:M:8860:HOH:O	1.72	0.89
19:Q:8:ALA:HB1	19:Q:13:THR:HG21	1.54	0.88
14:L:99:ARG:HH21	14:L:170:ASN:HD22	1.18	0.88
1:0:1701:A:H4'	1:0:1702:U:H5"	1.53	0.88
3:A:211:LYS:HB3	3:A:212:PRO:HD2	1.54	0.88
6:D:154:LYS:HD2	6:D:154:LYS:H	1.39	0.87
12:J:39:GLY:HA2	40:J:4183:HOH:O	1.72	0.87
11:I:93:ARG:HB3	11:I:93:ARG:HH11	1.39	0.87
5:C:115:LEU:HD21	5:C:243:VAL:HG13	1.55	0.87
8:F:91:VAL:HG12	8:F:92:GLY:H	1.40	0.87
1:0:542:A:H5'	1:0:542:A:H8	1.38	0.87
26:X:200:THR:HG22	26:X:201:GLU:HG3	1.54	0.86
1:0:21:G:H5'	19:Q:2:ILE:HA	1.58	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:2:70:ARG:HG2	30:2:77:ALA:HB2	1.58	0.86
4:B:238:ASN:HD22	4:B:240:GLY:H	1.24	0.86
15:M:83:LEU:HD13	15:M:175:LEU:HD23	1.56	0.86
5:C:236:THR:HG22	5:C:239:ALA:N	1.90	0.86
6:D:27:ILE:HG22	6:D:28:GLY:H	1.41	0.85
20:R:51:GLN:HE21	20:R:53:ASN:HD21	1.24	0.85
24:V:6:GLN:HB2	24:V:26:ILE:HD12	1.58	0.85
1:0:2506:A:O2'	1:0:2507:G:H8	1.60	0.85
12:J:74:VAL:HG13	12:J:113:ILE:HG23	1.56	0.85
5:C:104:ASP:HA	5:C:107:ARG:HH12	1.40	0.85
1:0:2586:U:H3	1:0:2592:G:H22	1.23	0.85
5:C:115:LEU:HD13	5:C:223:LEU:HD21	1.58	0.85
4:B:190:MET:HE2	4:B:194:PHE:CD1	2.13	0.84
24:V:88:THR:HG22	24:V:89:ASP:N	1.91	0.84
14:L:102:GLU:OE1	14:L:164:THR:HG21	1.77	0.84
28:Z:25:LYS:HD2	29:1:49:GLU:H	1.42	0.83
1:0:2717:C:C2'	1:0:2718:C:H5"	2.08	0.83
1:0:2840:A:OP1	4:B:211:THR:HG23	1.78	0.83
1:0:1160:G:H5'	1:0:1161:A:C5'	2.06	0.83
10:H:167:ARG:HD2	40:H:8990:HOH:O	1.78	0.83
4:B:162:MET:HE3	4:B:308:LEU:HD21	1.60	0.83
16:N:47:ARG:HH11	16:N:47:ARG:HG3	1.44	0.83
1:0:2637:A:H2'	31:4:74:C:C5'	2.09	0.82
8:F:58:GLU:HA	8:F:61:MET:HE2	1.60	0.82
7:E:15:GLN:HG3	7:E:20:ILE:HG12	1.59	0.82
1:0:1603:A:H5'	1:0:1605:G:O4'	1.79	0.82
1:0:560:C:H42	1:0:597:A:H61	1.26	0.82
12:J:4:LEU:HD22	12:J:116:GLU:HB3	1.61	0.82
1:0:1835:U:H5	1:0:1840:A:N7	1.78	0.82
6:D:20:LYS:HA	6:D:75:LEU:O	1.80	0.82
1:0:541:C:C2'	1:0:542:A:H5"	2.10	0.82
23:U:1:THR:HG23	23:U:2:VAL:H	1.45	0.82
1:0:289:G:H22	1:0:363:A:H2	1.28	0.81
11:I:74:ARG:HB3	11:I:74:ARG:HH11	1.45	0.81
24:V:88:THR:HB	40:V:6679:HOH:O	1.81	0.81
7:E:20:ILE:HD11	7:E:40:VAL:HG11	1.63	0.81
2:9:3023:U:C3'	2:9:3024:U:H5"	2.11	0.80
24:V:88:THR:HG23	24:V:110:GLN:NE2	1.95	0.80
1:0:1119:G:N2	1:0:1246:A:C2	2.50	0.80
5:C:5:ILE:HD11	5:C:16:VAL:CG2	2.11	0.80
2:9:3025:G:H3'	2:9:3026:C:C5'	2.12	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:105:SER:HB2	6:D:131:THR:HG23	1.63	0.80
6:D:25:MET:HE2	6:D:41:LEU:HG	1.63	0.80
1:0:2694:A:H4'	7:E:91:PHE:HE1	1.47	0.80
3:A:88:ILE:HD13	3:A:100:PRO:HD3	1.64	0.80
15:M:38:LYS:HE2	15:M:107:ASN:ND2	1.96	0.80
1:0:1160:G:C5'	1:0:1161:A:H5'	2.07	0.79
1:0:541:C:H2'	1:0:542:A:H5"	1.64	0.79
1:0:2506:A:HO2'	1:0:2507:G:H8	0.80	0.79
1:0:870:G:C2'	1:0:871:G:H5"	2.10	0.79
1:0:962:C:H1'	15:M:5:ARG:NH1	1.96	0.79
12:J:74:VAL:HG11	12:J:113:ILE:HG12	1.65	0.79
1:0:2054:A:N3	19:Q:128:ARG:NH2	2.30	0.79
4:B:36:PRO:HA	4:B:168:GLY:HA3	1.65	0.79
1:0:288:A:H61	1:0:364:C:H42	1.31	0.79
24:V:88:THR:HG23	24:V:110:GLN:HE21	1.47	0.79
21:S:9:LYS:HE3	21:S:13:ARG:NH1	1.98	0.78
26:X:187:VAL:HG23	26:X:192:ASP:HB2	1.63	0.78
24:V:137:GLN:HE21	24:V:141:HIS:CE1	1.99	0.78
15:M:87:LEU:HD12	15:M:186:LEU:HD21	1.66	0.78
16:N:32:ARG:O	16:N:32:ARG:HD3	1.82	0.78
14:L:107:ARG:HG3	14:L:107:ARG:NH1	1.98	0.78
29:1:41:HIS:H	29:1:45:ASN:HD22	1.28	0.78
28:Z:21:ARG:HD2	28:Z:37:CYS:SG	2.24	0.78
2:9:3023:U:H3'	2:9:3024:U:C5'	2.13	0.78
2:9:3051:A:H5'	15:M:160:SER:HB3	1.64	0.78
10:H:45:VAL:HA	10:H:167:ARG:O	1.83	0.77
3:A:191:GLY:HA2	3:A:194:MET:CE	2.13	0.77
25:W:15:ARG:HH11	25:W:15:ARG:HB3	1.49	0.77
24:V:21:LEU:HD21	24:V:48:VAL:HG11	1.65	0.77
1:0:2717:C:O2'	1:0:2718:C:H5"	1.84	0.77
20:R:57:THR:HG22	20:R:59:ASP:N	1.98	0.77
12:J:10:GLN:H	12:J:10:GLN:HE21	0.82	0.77
14:L:134:ILE:HG23	14:L:141:ILE:HD13	1.65	0.77
4:B:212:GLN:HB2	4:B:257:THR:HG21	1.66	0.77
3:A:199:HIS:HD2	3:A:201:PHE:H	1.33	0.77
1:0:21:G:C5'	19:Q:2:ILE:HA	2.15	0.76
3:A:35:GLY:O	3:A:36:ASP:HB3	1.85	0.76
1:0:1474:C:H5'	1:0:1474:C:H6	1.50	0.76
24:V:84:VAL:HG12	40:V:6679:HOH:O	1.85	0.76
1:0:1116:U:H3	1:0:1246:A:H62	1.32	0.76
9:G:12:ILE:N	9:G:13:PRO:HD3	2.00	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:9:3024:U:O2'	2:9:3025:G:H4'	1.85	0.76
2:9:3025:G:H3'	2:9:3026:C:H5'	1.66	0.76
30:2:25:VAL:HG22	30:2:68:LYS:HG3	1.67	0.76
1:0:1209:C:H2'	1:0:1210:G:H8	1.50	0.76
17:O:115:SER:OG	17:O:118:GLN:HG3	1.86	0.76
1:0:2694:A:H4'	7:E:91:PHE:CE1	2.22	0.75
1:0:2676:C:H4'	11:I:70:PHE:CE1	2.20	0.75
2:9:3092:G:H2'	2:9:3093:A:C8	2.21	0.75
6:D:22:VAL:HG22	6:D:74:THR:HG22	1.67	0.75
1:0:2780:C:H1'	7:E:143:GLN:HE21	1.51	0.75
19:Q:9:ASP:O	19:Q:13:THR:HB	1.87	0.75
6:D:54:ALA:HB2	6:D:69:ILE:HD12	1.67	0.75
3:A:153:ARG:CB	3:A:153:ARG:HH11	2.00	0.74
1:0:544:G:H2'	1:0:545:G:H5"	1.69	0.74
1:0:545:G:H8	1:0:545:G:H5'	1.52	0.74
7:E:6:GLU:HA	7:E:46:THR:HG22	1.70	0.74
11:I:45:VAL:HG23	11:I:130:VAL:O	1.87	0.74
12:J:32:ILE:HD11	12:J:56:SER:HB3	1.68	0.74
8:F:50:VAL:HG13	8:F:60:VAL:HG11	1.70	0.74
12:J:14:LYS:HB2	12:J:45:PRO:HG2	1.68	0.74
1:0:506:G:H22	1:0:509:A:C5'	2.00	0.74
1:0:1751:G:H2'	1:0:1752:G:H5"	1.69	0.74
1:0:1165:G:H4'	1:0:1174:A:O2'	1.88	0.73
8:F:91:VAL:HG12	8:F:92:GLY:N	2.02	0.73
1:0:871:G:H8	1:0:871:G:C5'	2.02	0.73
1:0:2890:A:H1'	22:T:56:ARG:NH2	2.03	0.73
3:A:200:PRO:HG2	3:A:225:VAL:HG21	1.70	0.73
24:V:21:LEU:HD22	24:V:26:ILE:CD1	2.19	0.73
1:0:2420:G:O2'	1:0:2421:G:H5'	1.87	0.73
23:U:39:ALA:N	23:U:40:PRO:HD2	2.03	0.73
10:H:21:THR:O	10:H:120:ILE:HD12	1.89	0.73
19:Q:18:LEU:HD12	19:Q:143:VAL:HG11	1.70	0.73
1:0:284:C:H4'	1:0:285:A:O5'	1.89	0.72
29:1:18:ASN:HD21	29:1:40:ARG:H	1.34	0.72
15:M:48:VAL:CG1	15:M:55:ASP:HB3	2.19	0.72
24:V:80:ASP:O	24:V:84:VAL:HG23	1.88	0.72
10:H:27:LYS:N	10:H:59:HIS:HD2	1.86	0.72
15:M:38:LYS:HE2	15:M:107:ASN:HD21	1.54	0.72
24:V:21:LEU:HD22	24:V:26:ILE:HD11	1.72	0.72
2:9:3039:U:H1'	2:9:3044:A:H61	1.53	0.72
1:0:657:G:OP1	5:C:27:ARG:NH2	2.21	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:9:3006:C:C5'	15:M:37:ARG:HH12	2.01	0.72
1:0:2505:G:O2'	1:0:2506:A:H5'	1.90	0.72
2:9:3029:C:H2'	2:9:3030:C:H5'	1.71	0.72
1:0:2716:G:H5"	4:B:206:THR:HG21	1.71	0.72
15:M:49:THR:HG22	15:M:56:ASP:HB2	1.72	0.72
13:K:143:THR:HG22	13:K:144:ASP:N	2.05	0.72
1:0:877:G:H5'	1:0:878:G:OP1	1.90	0.72
17:O:91:LYS:O	17:O:95:GLU:HG3	1.90	0.72
3:A:153:ARG:NH1	3:A:153:ARG:HB2	2.05	0.71
1:0:2831:C:O3'	19:Q:71:LYS:HE2	1.90	0.71
1:0:1164:U:H4'	1:0:1165:G:OP1	1.89	0.71
1:0:1182:C:H1'	1:0:1192:A:H8	1.56	0.71
15:M:183:ASP:OD2	15:M:186:LEU:HD12	1.88	0.71
15:M:80:SER:HB2	40:M:8837:HOH:O	1.90	0.71
4:B:275:GLY:O	4:B:291:ASP:HA	1.90	0.71
24:V:13:MET:HE3	24:V:17:ILE:HG22	1.72	0.71
1:0:2717:C:H2'	1:0:2718:C:H5"	1.73	0.71
1:0:1116:U:HO2'	1:0:1118:A:H2	1.36	0.71
1:0:282:C:H1'	1:0:368:C:N4	2.05	0.71
24:V:68:THR:HG23	24:V:69:ARG:HG2	1.73	0.71
2:9:3056:A:C2'	2:9:3057:A:H5"	2.21	0.71
1:0:1666:C:H2'	1:0:1667:A:H5'	1.73	0.71
1:0:1819:G:H2'	1:0:1820:G:H4'	1.72	0.71
24:V:88:THR:CG2	24:V:89:ASP:H	1.99	0.71
21:S:49:GLU:OE2	21:S:97:ARG:HD2	1.90	0.71
10:H:56:GLN:NE2	10:H:126:ARG:HE	1.89	0.71
25:W:72:VAL:HG22	25:W:85:VAL:HG12	1.72	0.70
30:2:62:THR:HB	40:2:8981:HOH:O	1.90	0.70
1:0:1244:U:OP1	11:I:18:ILE:HD13	1.91	0.70
4:B:179:LEU:O	4:B:183:GLU:HG2	1.90	0.70
17:O:115:SER:H	17:O:118:GLN:NE2	1.85	0.70
1:0:1119:G:H2'	11:I:52:GLN:NE2	2.05	0.70
6:D:54:ALA:CB	6:D:69:ILE:HD12	2.21	0.70
1:0:2468:A:H61	30:2:48:ASN:HD21	1.40	0.70
1:0:371:U:H2'	1:0:372:A:H8	1.55	0.70
1:0:1701:A:H4'	1:0:1702:U:C5'	2.20	0.70
1:0:541:C:H2'	1:0:542:A:C5'	2.21	0.70
10:H:20:ILE:HG23	10:H:120:ILE:HD11	1.73	0.70
1:0:1641:A:H2'	1:0:1642:A:H5'	1.73	0.70
23:U:55:ARG:O	23:U:59:ILE:HG12	1.91	0.70
1:0:2827:A:H2'	1:0:2828:G:O4'	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:104:ASP:HA	5:C:107:ARG:NH1	2.06	0.70
3:A:192:VAL:HG12	3:A:207:GLN:HB3	1.72	0.70
1:0:2769:C:H2'	1:0:2770:G:O4'	1.92	0.70
13:K:67:ARG:O	13:K:71:GLU:HG3	1.92	0.69
1:0:1189:A:H1'	1:0:1209:C:O4'	1.92	0.69
27:Y:11:SER:HB3	27:Y:23:ARG:HB2	1.71	0.69
4:B:7:ARG:HG2	4:B:7:ARG:HH11	1.57	0.69
2:9:3006:C:C5'	15:M:37:ARG:NH1	2.53	0.69
5:C:76:ARG:HG2	5:C:78:ARG:NH1	2.07	0.69
11:I:74:ARG:O	11:I:78:ILE:HG12	1.92	0.69
24:V:137:GLN:NE2	24:V:141:HIS:HE1	1.87	0.69
3:A:33:GLU:O	3:A:34:ASP:HB2	1.92	0.69
24:V:141:HIS:HB2	24:V:146:ILE:HG12	1.75	0.69
1:0:1116:U:O2'	1:0:1118:A:H2	1.76	0.69
3:A:199:HIS:CD2	3:A:201:PHE:H	2.09	0.69
1:0:506:G:H22	1:0:509:A:H5'	1.56	0.69
1:0:470:U:O2'	28:Z:16:HIS:HD2	1.76	0.69
1:0:2851:G:O2'	1:0:2852:A:H5'	1.92	0.69
17:O:80:ARG:HG2	17:O:87:ARG:CZ	2.22	0.69
24:V:125:HIS:CD2	24:V:127:GLY:H	2.11	0.69
13:K:90:ARG:NH2	13:K:121:ILE:HD11	2.08	0.69
23:U:12:THR:HG22	23:U:15:GLU:CG	2.18	0.69
3:A:191:GLY:HA2	3:A:194:MET:HE2	1.73	0.69
19:Q:18:LEU:HB2	19:Q:143:VAL:HG12	1.73	0.69
24:V:125:HIS:HD2	24:V:127:GLY:H	1.39	0.69
8:F:53:ASP:OD1	8:F:80:GLN:HB2	1.93	0.69
1:0:1209:C:H2'	1:0:1210:G:C8	2.28	0.69
1:0:2502:C:C2'	1:0:2503:A:H5'	2.23	0.69
19:Q:25:PHE:CE2	19:Q:29:LYS:HE2	2.28	0.68
12:J:81:ARG:HB2	12:J:87:ARG:NH1	2.09	0.68
2:9:3023:U:H4'	2:9:3024:U:OP2	1.93	0.68
19:Q:106:GLY:HA2	19:Q:109:MET:HE3	1.76	0.68
12:J:81:ARG:HB2	12:J:87:ARG:HH11	1.57	0.68
26:X:187:VAL:HG23	26:X:192:ASP:CB	2.23	0.68
14:L:80:GLY:O	14:L:81:ARG:HD2	1.94	0.68
25:W:78:GLU:HG2	25:W:79:GLU:H	1.59	0.68
1:0:2005:G:H3'	1:0:2005:G:OP2	1.94	0.68
24:V:6:GLN:HB2	24:V:26:ILE:CD1	2.23	0.68
30:2:65:THR:HG23	30:2:67:LEU:HG	1.74	0.68
1:0:2346:C:O2'	6:D:52:THR:HG21	1.93	0.68
25:W:71:ARG:HB3	25:W:88:GLU:OE1	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2908:A:H2'	1:0:2909:G:O4'	1.92	0.68
7:E:154:ILE:HD11	7:E:157:LYS:HB2	1.76	0.68
5:C:236:THR:CG2	5:C:239:ALA:H	1.96	0.68
1:0:544:G:C2'	1:0:545:G:H5"	2.23	0.67
2:9:3006:C:OP1	15:M:37:ARG:NH1	2.27	0.67
7:E:68:HIS:O	7:E:72:MET:HG3	1.95	0.67
4:B:258:GLY:H	4:B:260:HIS:CE1	2.12	0.67
26:X:154:ARG:HH12	26:X:155:ARG:HG3	1.59	0.67
6:D:99:ASP:HB2	6:D:103:ASN:HB2	1.74	0.67
5:C:78:ARG:HG3	5:C:78:ARG:NH1	2.02	0.67
6:D:86:THR:O	6:D:90:LEU:HG	1.94	0.67
24:V:122:ARG:NH2	24:V:154:ARG:OXT	2.27	0.67
3:A:192:VAL:CG1	3:A:207:GLN:HB3	2.24	0.67
17:O:59:ARG:NH2	17:O:66:GLN:HE22	1.91	0.67
1:0:432:G:O2'	1:0:433:C:H5'	1.95	0.67
1:0:1116:U:O2'	1:0:1118:A:C2	2.48	0.67
3:A:105:VAL:CG1	3:A:154:ALA:HB1	2.25	0.67
17:O:10:ALA:HA	17:O:13:VAL:HG12	1.76	0.67
7:E:81:GLU:HG2	7:E:134:SER:HB3	1.76	0.67
3:A:101:GLU:OE2	3:A:131:HIS:HB2	1.95	0.67
14:L:24:GLN:NE2	14:L:27:ARG:HH11	1.92	0.67
1:0:20:G:H21	19:Q:117:HIS:HD2	1.42	0.67
28:Z:25:LYS:HD2	29:1:49:GLU:N	2.10	0.67
10:H:167:ARG:CD	40:H:8990:HOH:O	2.38	0.67
5:C:1:MET:HG2	5:C:2:GLN:H	1.60	0.67
6:D:170:TYR:O	6:D:171:ASP:HB3	1.95	0.67
3:A:125:ASN:HB3	3:A:158:VAL:HG12	1.77	0.67
5:C:47:GLY:HA2	5:C:92:PRO:HB2	1.77	0.67
21:S:41:ARG:HH11	21:S:41:ARG:HG2	1.60	0.67
1:0:1450:C:H4'	1:0:1451:C:OP2	1.95	0.67
1:0:450:C:OP1	5:C:184:ARG:NH2	2.26	0.67
24:V:21:LEU:HD21	24:V:48:VAL:CG1	2.25	0.66
6:D:19:GLU:O	6:D:20:LYS:HG2	1.95	0.66
1:0:1118:A:H3'	1:0:1118:A:H8	1.60	0.66
4:B:53:LEU:HD11	4:B:327:VAL:HG22	1.75	0.66
22:T:17:THR:HG22	22:T:18:GLY:N	2.10	0.66
6:D:25:MET:CE	6:D:37:ALA:HB1	2.25	0.66
6:D:88:LEU:HB2	6:D:89:PRO:HD3	1.76	0.66
2:9:3020:G:O2'	2:9:3021:G:H5'	1.95	0.66
10:H:29:ALA:HB3	10:H:66:ARG:HH12	1.60	0.66
21:S:9:LYS:HE3	21:S:13:ARG:HH11	1.57	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:H:58:ARG:HG3	10:H:58:ARG:HH11	1.60	0.66
1:0:1377:C:H6	1:0:1377:C:H5'	1.60	0.66
26:X:189:ASN:HA	26:X:217:ILE:HD11	1.75	0.66
7:E:5:LEU:HD21	7:E:66:GLN:HG3	1.76	0.66
15:M:61:ALA:HB3	15:M:88:ALA:HB2	1.77	0.66
24:V:122:ARG:HH11	24:V:122:ARG:CG	2.07	0.66
5:C:27:ARG:HG3	5:C:29:ASP:OD1	1.94	0.66
23:U:20:LEU:HD22	23:U:60:GLN:HE22	1.60	0.66
21:S:61:GLU:HG3	40:S:3851:HOH:O	1.95	0.66
15:M:71:TRP:CE3	15:M:175:LEU:HD22	2.31	0.66
8:F:37:THR:O	8:F:41:GLU:HG3	1.95	0.66
3:A:36:ASP:HA	3:A:83:GLY:HA3	1.78	0.65
1:0:2547:C:OP2	4:B:5:ARG:NH1	2.29	0.65
21:S:47:THR:HB	21:S:100:ASP:HB3	1.78	0.65
20:R:51:GLN:NE2	20:R:53:ASN:HD21	1.94	0.65
12:J:49:LEU:HD12	12:J:80:ILE:HG21	1.79	0.65
12:J:34:VAL:HG22	12:J:47:ALA:HB2	1.79	0.65
8:F:58:GLU:OE1	14:L:27:ARG:NH2	2.28	0.65
11:I:107:ASN:ND2	11:I:109:TYR:H	1.94	0.65
1:0:1201:C:H5"	40:0:6599:HOH:O	1.96	0.65
19:Q:99:ALA:HB1	19:Q:109:MET:CE	2.26	0.65
2:9:3039:U:H1'	2:9:3044:A:N6	2.10	0.65
1:0:2526:C:O2'	1:0:2527:U:H5'	1.97	0.65
20:R:10:VAL:HG11	23:U:36:ALA:HA	1.76	0.65
1:0:2414:A:H2'	1:0:2415:A:C8	2.32	0.65
1:0:559:C:H6	1:0:559:C:H5'	1.62	0.65
25:W:66:THR:HG23	25:W:67:PRO:HD2	1.77	0.65
15:M:155:GLU:O	15:M:156:GLU:HG3	1.97	0.65
8:F:63:ILE:HB	8:F:64:PRO:HD3	1.78	0.65
6:D:64:ARG:HG2	6:D:67:ASP:HB3	1.78	0.65
6:D:57:THR:HG23	6:D:63:ILE:HG22	1.79	0.65
5:C:162:VAL:HG12	5:C:192:ILE:HD11	1.76	0.65
2:9:3025:G:C3'	2:9:3026:C:H5'	2.27	0.65
11:I:74:ARG:CB	11:I:74:ARG:HH11	2.10	0.64
21:S:9:LYS:CE	21:S:13:ARG:NH1	2.59	0.64
1:0:2502:C:H2'	1:0:2503:A:H5'	1.79	0.64
3:A:131:HIS:O	3:A:132:ASP:HB2	1.95	0.64
23:U:56:ILE:O	23:U:60:GLN:HG3	1.96	0.64
4:B:62:ARG:HA	4:B:65:MET:CE	2.26	0.64
1:0:1462:C:H2'	1:0:1463:A:C8	2.32	0.64
25:W:74:ALA:HB2	25:W:85:VAL:HG13	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:T:39:ASN:ND2	22:T:44:ARG:HH11	1.94	0.64
1:0:558:C:O2'	1:0:559:C:H5"	1.96	0.64
1:0:289:G:N2	1:0:363:A:H2	1.93	0.64
1:0:281:U:H2'	1:0:282:C:O4'	1.97	0.64
27:Y:11:SER:CB	27:Y:23:ARG:HB2	2.27	0.64
28:Z:10:LYS:HG3	40:Z:8984:HOH:O	1.97	0.64
10:H:46:GLN:HE21	10:H:137:TYR:HE2	1.43	0.64
1:0:1234:U:N3	4:B:244:PRO:HB3	2.12	0.64
21:S:32:ARG:NH1	21:S:38:ARG:HH12	1.96	0.64
14:L:164:THR:HG22	14:L:167:GLY:H	1.63	0.64
8:F:2:VAL:HG22	8:F:57:GLU:OE1	1.97	0.64
4:B:201:ASP:HB2	4:B:312:ARG:HD2	1.78	0.64
4:B:18:ARG:HG3	4:B:256:GLN:HG3	1.79	0.64
27:Y:53:GLY:HA2	27:Y:67:GLY:O	1.98	0.64
1:0:1942:A:H3'	40:0:7683:HOH:O	1.98	0.64
3:A:100:PRO:HG2	3:A:103:VAL:HG21	1.79	0.64
1:0:1878:G:O2'	1:0:1879:U:C6	2.51	0.64
1:0:1118:A:H3'	1:0:1118:A:C8	2.33	0.64
1:0:775:G:OP1	28:Z:16:HIS:HE1	1.81	0.64
8:F:96:ALA:HA	40:F:3111:HOH:O	1.96	0.64
1:0:1170:U:O2'	1:0:1172:G:N7	2.29	0.64
1:0:1118:A:H8	1:0:1119:G:H5"	1.64	0.63
11:I:45:VAL:HG21	11:I:129:PHE:CD1	2.33	0.63
15:M:169:PRO:O	15:M:172:PHE:HB3	1.97	0.63
1:0:2878:U:H2'	1:0:2879:A:O4'	1.99	0.63
21:S:71:VAL:HG11	21:S:90:PRO:CB	2.21	0.63
10:H:27:LYS:H	10:H:59:HIS:CD2	2.08	0.63
26:X:154:ARG:NH1	26:X:155:ARG:HG3	2.13	0.63
4:B:238:ASN:HD22	4:B:240:GLY:N	1.96	0.63
1:0:2548:C:OP2	4:B:5:ARG:NH2	2.32	0.63
1:0:2426:G:H1'	40:0:6457:HOH:O	1.96	0.63
15:M:7:LYS:HE3	18:P:21:ARG:O	1.99	0.63
1:0:371:U:H2'	1:0:372:A:C8	2.32	0.63
7:E:31:ARG:HH12	7:E:68:HIS:CD2	2.16	0.63
1:0:2064:U:H5'	1:0:2652:U:H4'	1.81	0.63
9:G:12:ILE:HG22	9:G:12:ILE:O	1.99	0.63
7:E:133:VAL:HG12	7:E:141:VAL:HG13	1.81	0.63
1:0:1766:U:O2	1:0:1778:A:H5'	1.99	0.63
6:D:69:ILE:O	6:D:69:ILE:HG22	1.98	0.63
17:O:59:ARG:HH22	17:O:66:GLN:HE22	1.46	0.63
4:B:140:LEU:HA	40:B:9055:HOH:O	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1183:C:N4	1:0:1184:C:H41	1.97	0.63
24:V:4:LEU:HD23	24:V:54:PHE:HB3	1.79	0.63
6:D:44:ILE:HG12	6:D:83:PHE:HE1	1.63	0.63
1:0:2533:C:H5'	1:0:2533:C:H6	1.64	0.63
3:A:121:ALA:O	3:A:124:VAL:HG22	1.99	0.63
6:D:135:VAL:HG21	6:D:139:TYR:CD1	2.34	0.63
4:B:24:PRO:CG	4:B:204:GLY:HA2	2.29	0.63
15:M:62:HIS:HB3	15:M:65:ASP:OD1	1.99	0.63
1:0:542:A:H5'	1:0:542:A:C8	2.28	0.62
8:F:50:VAL:CG1	8:F:60:VAL:HG11	2.29	0.62
11:I:74:ARG:NH1	11:I:76:ASP:HB2	2.13	0.62
16:N:39:THR:O	16:N:115:ARG:NH2	2.33	0.62
12:J:74:VAL:CG1	12:J:113:ILE:HG12	2.29	0.62
1:0:1206:U:H6	1:0:1206:U:H5'	1.62	0.62
1:0:1333:U:H2'	1:0:1334:C:C6	2.34	0.62
1:0:1080:C:H4'	1:0:1081:A:OP1	1.97	0.62
12:J:29:LEU:HB3	12:J:55:VAL:CG1	2.26	0.62
1:0:285:A:H2'	1:0:286:U:O4'	1.99	0.62
1:0:282:C:O2'	1:0:283:U:H5'	1.99	0.62
4:B:51:VAL:HG23	4:B:329:TYR:O	2.00	0.62
1:0:603:A:H5"	1:0:604:G:OP1	1.99	0.62
5:C:246:ARG:NH1	5:C:246:ARG:HB3	2.14	0.62
5:C:104:ASP:O	5:C:108:GLN:HG3	1.99	0.62
1:0:121:U:OP2	29:1:10:ARG:NH2	2.32	0.62
7:E:23:GLU:HG2	7:E:28:SER:HB3	1.82	0.62
6:D:38:GLU:HB3	6:D:49:PRO:HG2	1.80	0.62
4:B:139:ASP:HB2	4:B:165:ARG:HE	1.65	0.62
13:K:73:VAL:HG23	13:K:74:THR:H	1.64	0.62
21:S:69:LYS:O	21:S:71:VAL:HG23	2.00	0.62
12:J:115:ARG:HG3	12:J:116:GLU:N	2.14	0.62
1:0:2676:C:H4'	11:I:70:PHE:HE1	1.63	0.62
7:E:11:VAL:HG12	7:E:12:ASP:N	2.14	0.62
1:0:119:A:H2'	1:0:120:A:H5"	1.80	0.62
15:M:139:TRP:HA	15:M:139:TRP:CE3	2.35	0.62
1:0:2346:C:O5'	1:0:2346:C:H6	1.83	0.62
24:V:21:LEU:HD13	24:V:26:ILE:HD11	1.82	0.62
15:M:11:ARG:O	15:M:15:GLU:HG3	2.00	0.62
7:E:116:THR:HG22	7:E:151:LEU:HD22	1.80	0.62
1:0:1191:A:H3'	1:0:1192:A:H5"	1.81	0.61
1:0:1189:A:H1'	1:0:1209:C:C1'	2.30	0.61
3:A:135:VAL:HG21	3:A:147:ARG:NH1	2.15	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1299:G:O6	13:K:6:ARG:HD3	2.00	0.61
1:0:1165:G:H1'	1:0:1174:A:H1'	1.82	0.61
19:Q:44:VAL:O	19:Q:48:GLU:HG3	2.00	0.61
15:M:164:ASP:CG	15:M:167:ASP:HA	2.19	0.61
30:2:73:GLU:HB3	40:2:8990:HOH:O	2.00	0.61
1:0:1189:A:H3'	40:0:8098:HOH:O	2.01	0.61
15:M:49:THR:CG2	15:M:56:ASP:HB2	2.31	0.61
3:A:109:GLU:HG2	3:A:116:GLY:N	2.14	0.61
3:A:81:GLN:HB2	3:A:92:ASN:ND2	2.14	0.61
3:A:51:ARG:NH1	3:A:120:ARG:O	2.34	0.61
1:0:1730:G:H5'	1:0:1731:C:C5	2.36	0.61
25:W:37:LEU:CD1	25:W:85:VAL:HG21	2.22	0.61
1:0:2768:A:H2'	1:0:2769:C:O4'	2.01	0.61
19:Q:39:THR:HG23	19:Q:107:GLU:O	1.99	0.61
19:Q:18:LEU:HB2	19:Q:143:VAL:CG1	2.30	0.61
11:I:75:PRO:HG2	11:I:105:LEU:HD21	1.83	0.61
29:1:22:PRO:HG2	29:1:25:VAL:HG23	1.81	0.61
12:J:55:VAL:HG12	12:J:56:SER:N	2.15	0.61
6:D:44:ILE:HG23	6:D:45:THR:HG23	1.83	0.61
1:0:2851:G:C2'	1:0:2852:A:H5'	2.30	0.61
1:0:1701:A:H5"	1:0:1702:U:H3'	1.83	0.61
3:A:191:GLY:HA2	3:A:194:MET:HE3	1.82	0.61
3:A:125:ASN:CB	3:A:158:VAL:HG12	2.31	0.61
14:L:57:LYS:HE2	14:L:140:ALA:O	2.01	0.61
1:0:1328:A:OP1	26:X:169:ARG:HD2	2.00	0.61
30:2:70:ARG:HB3	40:2:9001:HOH:O	2.00	0.61
19:Q:18:LEU:HG	19:Q:91:LEU:HD13	1.83	0.61
4:B:248:ARG:O	4:B:251:VAL:HG13	2.01	0.61
6:D:41:LEU:HA	6:D:44:ILE:HG22	1.82	0.61
4:B:321:PRO:HA	40:B:9136:HOH:O	2.01	0.61
1:0:1714:C:O2'	1:0:1715:C:H5'	2.01	0.61
11:I:19:MET:CE	11:I:132:LEU:HD11	2.31	0.61
1:0:338:C:H4'	5:C:174:ILE:HD11	1.82	0.61
5:C:76:ARG:HG2	5:C:78:ARG:HH12	1.65	0.60
6:D:23:VAL:HG21	6:D:45:THR:HG21	1.81	0.60
4:B:51:VAL:CG2	4:B:327:VAL:HG13	2.30	0.60
24:V:4:LEU:HD22	24:V:52:VAL:CG2	2.27	0.60
2:9:3114:G:O6	15:M:11:ARG:HD3	2.00	0.60
1:0:2862:G:H4'	4:B:336:GLN:O	2.00	0.60
11:I:19:MET:HE3	11:I:132:LEU:HD11	1.82	0.60
24:V:149:LEU:HG	24:V:153:MET:CE	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:E:20:ILE:CD1	7:E:40:VAL:HG11	2.30	0.60
1:0:1441:G:O2'	1:0:1442:A:H5'	2.01	0.60
1:0:1477:C:O2'	1:0:1478:U:H5'	2.01	0.60
6:D:95:THR:C	6:D:97:GLN:H	2.05	0.60
1:0:1926:G:H2'	1:0:1927:A:C8	2.36	0.60
5:C:118:THR:HG22	5:C:137:PRO:HB3	1.83	0.60
24:V:13:MET:HE1	24:V:18:GLN:HA	1.82	0.60
5:C:139:VAL:HG13	40:C:8656:HOH:O	2.02	0.60
9:G:64:ASN:O	9:G:68:GLU:HG3	2.01	0.60
2:9:3023:U:H6	2:9:3023:U:H5"	1.67	0.60
1:0:871:G:C8	1:0:871:G:C5'	2.78	0.60
15:M:152:GLU:C	15:M:154:LEU:H	2.03	0.60
1:0:155:C:OP2	14:L:188:ARG:HD3	2.00	0.60
15:M:110:THR:HB	15:M:113:SER:OG	2.02	0.60
1:0:1667:A:H8	1:0:1667:A:H5'	1.67	0.60
18:P:53:HIS:ND1	18:P:55:ARG:HB2	2.16	0.60
1:0:1120:U:H5'	1:0:1121:G:OP2	2.02	0.60
24:V:13:MET:CE	24:V:17:ILE:HG22	2.31	0.60
5:C:246:ARG:HB3	5:C:246:ARG:HH11	1.67	0.60
3:A:69:LEU:HD21	3:A:120:ARG:HB3	1.83	0.60
27:Y:37:HIS:HB2	27:Y:47:VAL:HB	1.84	0.60
8:F:58:GLU:CD	14:L:27:ARG:HH22	2.04	0.59
27:Y:19:GLY:O	27:Y:23:ARG:HG2	2.02	0.59
1:0:1878:G:O2'	1:0:1879:U:P	2.60	0.59
12:J:28:GLU:HB3	12:J:59:LYS:HB2	1.84	0.59
4:B:154:VAL:HG12	4:B:156:LYS:HG2	1.84	0.59
1:0:645:U:OP2	13:K:4:LYS:HE2	2.02	0.59
10:H:30:GLN:H	10:H:66:ARG:NH1	1.99	0.59
1:0:2779:G:H21	7:E:143:GLN:NE2	2.00	0.59
29:1:18:ASN:ND2	29:1:40:ARG:H	2.00	0.59
15:M:114:LYS:O	15:M:118:ILE:HG13	2.02	0.59
5:C:16:VAL:HG12	5:C:17:ASP:N	2.17	0.59
4:B:108:GLU:HB3	4:B:111:ARG:HD2	1.85	0.59
27:Y:22:SER:O	27:Y:26:VAL:HG23	2.03	0.59
1:0:1973:A:H5'	1:0:1973:A:H8	1.67	0.59
5:C:233:THR:HG22	5:C:234:VAL:N	2.17	0.59
4:B:297:VAL:HB	40:B:9084:HOH:O	2.03	0.59
4:B:41:PHE:HA	4:B:79:MET:HE2	1.84	0.59
1:0:2676:C:H4'	11:I:70:PHE:CD1	2.37	0.59
29:1:22:PRO:HG2	29:1:25:VAL:CG2	2.32	0.59
1:0:111:C:O2'	28:Z:20:ARG:HG2	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:X:126:PRO:HG2	26:X:128:PHE:CE1	2.38	0.59
4:B:162:MET:CE	4:B:310:ARG:HD3	2.33	0.59
23:U:39:ALA:N	23:U:40:PRO:CD	2.65	0.59
25:W:25:ARG:HD3	25:W:64:ALA:O	2.02	0.59
24:V:81:ASP:OD1	24:V:92:ASP:HB2	2.03	0.59
4:B:307:ARG:CG	4:B:307:ARG:HH11	2.15	0.59
8:F:46:GLU:OE1	8:F:100:ASP:HA	2.03	0.59
5:C:236:THR:H	5:C:239:ALA:HB3	1.68	0.59
11:I:107:ASN:HD22	11:I:107:ASN:C	2.06	0.59
9:G:23:ILE:O	9:G:27:ILE:HG13	2.03	0.59
15:M:47:LEU:HD13	15:M:97:VAL:HG11	1.83	0.59
30:2:60:LYS:HG3	30:2:61:PRO:HD2	1.83	0.59
1:0:259:G:H21	14:L:58:GLN:NE2	2.00	0.59
10:H:56:GLN:HE21	10:H:126:ARG:HE	1.47	0.58
4:B:72:THR:HB	40:B:9084:HOH:O	2.03	0.58
23:U:1:THR:HG23	23:U:2:VAL:N	2.17	0.58
14:L:134:ILE:CG2	14:L:141:ILE:HD13	2.31	0.58
1:0:2478:U:O2'	1:0:2479:A:H5'	2.03	0.58
6:D:158:ASN:HB2	6:D:161:ASP:OD2	2.03	0.58
1:0:558:C:H2'	1:0:559:C:H5'	1.85	0.58
9:G:12:ILE:N	9:G:13:PRO:CD	2.65	0.58
4:B:329:TYR:CE2	22:T:15:PRO:HG2	2.37	0.58
25:W:9:VAL:HG22	25:W:88:GLU:OE2	2.04	0.58
1:0:926:A:H5'	13:K:39:GLU:OE2	2.04	0.58
1:0:902:G:N7	13:K:18:HIS:HD2	2.01	0.58
1:0:156:C:H5"	14:L:171:ARG:CD	2.24	0.58
6:D:64:ARG:CG	6:D:67:ASP:HB3	2.34	0.58
19:Q:18:LEU:HD12	19:Q:143:VAL:CG1	2.34	0.58
4:B:141:ARG:HG2	4:B:165:ARG:HA	1.85	0.58
24:V:130:HIS:O	24:V:136:GLY:HA3	2.03	0.58
20:R:8:PRO:HD2	23:U:32:ALA:HA	1.85	0.58
12:J:34:VAL:CG2	12:J:47:ALA:HB2	2.34	0.58
3:A:190:ARG:NH2	3:A:207:GLN:OE1	2.36	0.58
4:B:62:ARG:HA	4:B:65:MET:HE3	1.85	0.58
1:0:962:C:H1'	15:M:5:ARG:HH12	1.69	0.58
4:B:24:PRO:HG3	4:B:204:GLY:HA2	1.86	0.58
8:F:46:GLU:O	8:F:73:PRO:HD2	2.04	0.58
1:0:1236:A:H2'	1:0:1237:U:O4'	2.04	0.58
1:0:656:G:OP2	16:N:37:ARG:HD2	2.03	0.58
8:F:36:THR:HG23	8:F:97:ALA:HB2	1.86	0.58
15:M:89:GLY:O	15:M:92:ALA:HB3	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1175:G:H1'	1:0:1193:A:H2'	1.86	0.58
12:J:82:ARG:NH2	12:J:115:ARG:HG2	2.18	0.58
6:D:64:ARG:CD	6:D:67:ASP:HB3	2.32	0.58
6:D:97:GLN:HG2	6:D:97:GLN:O	2.04	0.58
1:0:1755:A:H2'	1:0:1756:G:O4'	2.03	0.58
17:O:98:ILE:HD12	17:O:102:ARG:NE	2.19	0.58
4:B:305:ASP:O	4:B:306:LYS:HB2	2.04	0.58
1:0:1594:C:OP2	17:O:120:ARG:HD2	2.04	0.58
1:0:396:U:O2'	1:0:418:C:H4'	2.04	0.58
1:0:21:G:H5"	19:Q:1:GLY:O	2.04	0.58
3:A:88:ILE:HD13	3:A:100:PRO:CD	2.33	0.58
1:0:280:C:H2'	1:0:281:U:O4'	2.04	0.58
11:I:107:ASN:HD22	11:I:109:TYR:H	1.49	0.58
1:0:338:C:H4'	5:C:174:ILE:CD1	2.34	0.58
6:D:95:THR:O	6:D:97:GLN:N	2.31	0.58
23:U:64:GLY:O	23:U:65:ASP:HB2	2.03	0.58
1:0:512:G:O3'	1:0:513:A:H8	1.87	0.58
2:9:3004:G:H21	15:M:44:ARG:NH1	2.01	0.58
14:L:164:THR:CG2	14:L:165:GLY:N	2.66	0.58
1:0:2768:A:O2'	1:0:2769:C:H5'	2.04	0.58
1:0:2270:G:H4'	3:A:223:ARG:HH12	1.69	0.58
1:0:949:U:O2'	18:P:40:HIS:HE1	1.87	0.58
4:B:265:LEU:HD21	4:B:316:ARG:HD3	1.86	0.58
20:R:29:ASP:OD1	20:R:31:ARG:NH1	2.37	0.58
1:0:2265:U:H2'	1:0:2266:A:C8	2.38	0.58
1:0:2670:G:O2'	1:0:2671:U:H5'	2.04	0.58
2:9:3029:C:C2'	2:9:3030:C:H5'	2.34	0.57
13:K:143:THR:HG22	13:K:144:ASP:H	1.68	0.57
1:0:960:G:H2'	1:0:960:G:N3	2.19	0.57
8:F:117:GLU:C	8:F:119:ARG:H	2.07	0.57
1:0:272:A:H5'	1:0:273:G:OP2	2.04	0.57
2:9:3014:G:H8	2:9:3014:G:H5'	1.68	0.57
24:V:52:VAL:HG22	24:V:53:ALA:H	1.69	0.57
24:V:65:VAL:HA	24:V:68:THR:HG22	1.86	0.57
1:0:1342:C:O2'	1:0:1343:C:H5'	2.04	0.57
14:L:164:THR:HG22	14:L:166:ALA:N	2.20	0.57
7:E:15:GLN:HG2	7:E:19:ASP:O	2.04	0.57
23:U:39:ALA:C	23:U:41:GLU:H	2.08	0.57
25:W:9:VAL:HG13	25:W:88:GLU:OE2	2.04	0.57
4:B:254:GLN:HG2	4:B:255:GLY:N	2.17	0.57
1:0:1185:U:H2'	1:0:1186:C:C6	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:95:PRO:HG2	3:A:98:GLU:HG2	1.85	0.57
11:I:107:ASN:HD21	11:I:109:TYR:HB2	1.68	0.57
1:0:1878:G:O2'	1:0:1879:U:H6	1.88	0.57
17:O:103:THR:HA	17:O:106:ARG:NH1	2.19	0.57
4:B:221:GLN:HE22	12:J:42:ASN:HD22	1.53	0.57
2:9:3054:A:O2'	2:9:3055:U:H5'	2.04	0.57
14:L:34:GLU:HB3	14:L:38:GLU:HG3	1.86	0.57
2:9:3076:G:C3'	2:9:3077:A:H5"	2.25	0.57
15:M:139:TRP:HA	15:M:139:TRP:HE3	1.69	0.57
16:N:87:THR:O	16:N:91:GLN:HG3	2.05	0.57
17:O:40:VAL:O	17:O:44:VAL:HG23	2.05	0.57
1:0:2587:U:H2'	1:0:2589:U:H5"	1.87	0.57
7:E:3:VAL:HG22	7:E:49:ILE:HB	1.86	0.57
4:B:258:GLY:H	4:B:260:HIS:HE1	1.53	0.57
1:0:613:C:H2'	1:0:614:U:H6	1.70	0.57
1:0:2637:A:C2'	31:4:74:C:H5"	2.21	0.57
1:0:506:G:H22	1:0:509:A:H5"	1.69	0.57
4:B:5:ARG:HD2	4:B:8:LYS:NZ	2.19	0.57
1:0:291:C:H2'	1:0:292:G:O4'	2.05	0.57
1:0:282:C:H1'	1:0:368:C:H42	1.69	0.57
15:M:154:LEU:HG	15:M:155:GLU:H	1.70	0.57
11:I:19:MET:HE2	11:I:79:PHE:HA	1.87	0.57
1:0:2816:A:H5"	1:0:2817:G:H5'	1.87	0.57
5:C:107:ARG:NH1	5:C:107:ARG:HB3	2.20	0.57
1:0:2721:U:H4'	12:J:87:ARG:HG3	1.86	0.57
3:A:128:LEU:HD21	3:A:131:HIS:HE1	1.69	0.57
4:B:314:ALA:HB3	4:B:317:PRO:HG3	1.87	0.57
4:B:85:ARG:NH1	40:B:9113:HOH:O	2.37	0.57
1:0:1130:U:H2'	1:0:1131:G:O4'	2.04	0.57
3:A:36:ASP:OD2	3:A:85:SER:HB2	2.05	0.57
3:A:192:VAL:HB	40:A:9066:HOH:O	2.04	0.57
7:E:81:GLU:HG2	7:E:134:SER:CB	2.35	0.57
4:B:307:ARG:HG3	4:B:307:ARG:HH11	1.69	0.57
19:Q:111:ILE:HG23	19:Q:145:LEU:HD11	1.87	0.57
5:C:115:LEU:O	5:C:118:THR:HB	2.05	0.56
4:B:212:GLN:OE1	4:B:216:LYS:HD3	2.05	0.56
1:0:2515:C:H2'	1:0:2516:G:O4'	2.05	0.56
1:0:1563:G:O2'	1:0:1564:C:OP2	2.19	0.56
4:B:268:ARG:NH2	4:B:325:PRO:HG3	2.19	0.56
12:J:109:LEU:HD13	12:J:113:ILE:HD11	1.87	0.56
1:0:1669:A:H2'	1:0:1670:G:C8	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1118:A:H62	1:0:1244:U:H3	1.52	0.56
26:X:187:VAL:CG2	26:X:192:ASP:HB2	2.35	0.56
22:T:14:GLU:O	22:T:17:THR:HB	2.05	0.56
7:E:69:ILE:HA	7:E:72:MET:CE	2.35	0.56
15:M:36:ALA:HB1	15:M:118:ILE:HD12	1.86	0.56
6:D:136:ARG:HD2	6:D:155:HIS:O	2.05	0.56
4:B:56:ASP:OD1	4:B:322:ARG:HB3	2.04	0.56
5:C:77:ALA:O	5:C:78:ARG:HG3	2.04	0.56
1:0:2812:A:C2	1:0:2814:A:N6	2.67	0.56
6:D:23:VAL:HG22	6:D:73:VAL:HB	1.87	0.56
15:M:69:TYR:HE2	15:M:183:ASP:OD2	1.89	0.56
10:H:63:GLU:HA	40:H:9029:HOH:O	2.04	0.56
6:D:50:VAL:O	6:D:71:ALA:HA	2.04	0.56
1:0:500:G:H21	19:Q:98:ASN:HD21	1.52	0.56
18:P:25:PRO:HB2	40:P:4350:HOH:O	2.05	0.56
17:O:115:SER:N	17:O:118:GLN:HE21	1.89	0.56
6:D:27:ILE:HG22	6:D:28:GLY:N	2.16	0.56
15:M:154:LEU:O	15:M:155:GLU:HB3	2.05	0.56
1:0:2251:G:H2'	1:0:2252:A:C8	2.40	0.56
15:M:184:ILE:HG22	15:M:185:GLU:N	2.19	0.56
14:L:107:ARG:NH1	14:L:107:ARG:CG	2.69	0.56
1:0:2506:A:O2'	1:0:2507:G:O5'	2.23	0.56
1:0:1666:C:C2'	1:0:1667:A:H5'	2.36	0.56
1:0:308:U:H5'	21:S:97:ARG:NH2	2.20	0.56
1:0:794:U:H3	1:0:819:A:H61	1.53	0.56
1:0:1641:A:C2'	1:0:1642:A:H5'	2.35	0.56
22:T:17:THR:CG2	22:T:18:GLY:N	2.69	0.56
4:B:265:LEU:CD2	4:B:316:ARG:HD3	2.35	0.56
1:0:1787:C:OP1	17:O:68:LYS:HE2	2.06	0.56
27:Y:21:VAL:HG12	40:Y:8711:HOH:O	2.06	0.56
1:0:482:G:H4'	1:0:508:A:N1	2.21	0.56
1:0:168:C:O2'	1:0:169:A:H5'	2.06	0.56
5:C:118:THR:O	5:C:136:VAL:HG13	2.06	0.56
15:M:71:TRP:HE3	15:M:175:LEU:HD22	1.70	0.56
1:0:2507:G:H2'	1:0:2510:C:H42	1.71	0.56
1:0:2698:G:H2'	1:0:2699:A:C8	2.41	0.56
1:0:2791:U:H1'	1:0:2792:A:H5"	1.88	0.56
25:W:76:ARG:HH11	25:W:76:ARG:HG3	1.68	0.56
13:K:125:PHE:CE1	13:K:140:VAL:HG13	2.41	0.56
3:A:94:LEU:HG	3:A:99:ILE:HD11	1.87	0.56
14:L:99:ARG:NH2	14:L:170:ASN:HD22	1.97	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:O:10:ALA:HA	17:O:13:VAL:CG1	2.34	0.56
4:B:175:LEU:O	4:B:175:LEU:HD23	2.05	0.56
8:F:48:VAL:HG12	8:F:97:ALA:HB2	1.88	0.56
15:M:12:ARG:HD3	15:M:18:THR:OG1	2.05	0.56
24:V:29:VAL:O	24:V:30:ASN:HB2	2.06	0.56
21:S:71:VAL:CG1	21:S:90:PRO:HB3	2.24	0.56
20:R:51:GLN:HE21	20:R:53:ASN:ND2	2.00	0.56
24:V:21:LEU:HB3	24:V:26:ILE:HG12	1.87	0.56
3:A:107:ASN:OD1	3:A:120:ARG:HD2	2.06	0.56
2:9:3041:C:O4'	6:D:50:VAL:HG23	2.06	0.56
1:0:88:G:N7	29:1:28:LYS:HD2	2.20	0.56
3:A:179:MET:HG2	3:A:186:TRP:CB	2.36	0.56
1:0:588:G:O6	24:V:154:ARG:NH1	2.39	0.55
8:F:60:VAL:HG12	8:F:60:VAL:O	2.06	0.55
11:I:75:PRO:HD3	11:I:136:SER:OG	2.06	0.55
4:B:74:ILE:HD13	4:B:309:VAL:HG21	1.87	0.55
6:D:37:ALA:O	6:D:40:ILE:HG12	2.06	0.55
15:M:87:LEU:CD1	15:M:186:LEU:HD21	2.34	0.55
1:0:1205:U:C2'	1:0:1206:U:H5"	2.36	0.55
11:I:75:PRO:HG2	11:I:105:LEU:CD2	2.35	0.55
10:H:99:LYS:HD3	10:H:119:LYS:HD3	1.88	0.55
1:0:2807:U:P	4:B:27:ASN:HD21	2.28	0.55
1:0:2106:C:H5'	1:0:2284:G:H21	1.70	0.55
5:C:1:MET:HG2	5:C:2:GLN:N	2.20	0.55
40:0:7890:HOH:O	30:2:60:LYS:HG3	2.07	0.55
1:0:380:A:OP2	14:L:9:ARG:HD2	2.05	0.55
25:W:15:ARG:NH1	25:W:15:ARG:HB3	2.19	0.55
6:D:94:ALA:HB3	6:D:174:VAL:HA	1.88	0.55
13:K:53:ARG:NH2	13:K:57:VAL:HG12	2.22	0.55
1:0:1150:A:C2	9:G:20:VAL:HG21	2.41	0.55
1:0:449:A:N7	5:C:43:LYS:HG2	2.22	0.55
1:0:1528:A:H2'	1:0:1529:G:O4'	2.07	0.55
1:0:1666:C:O2'	1:0:1667:A:H5"	2.06	0.55
14:L:71:SER:O	14:L:73:ARG:NH1	2.36	0.55
28:Z:25:LYS:CD	29:1:49:GLU:H	2.16	0.55
1:0:545:G:C8	1:0:545:G:H5'	2.39	0.55
1:0:1462:C:H2'	1:0:1463:A:H8	1.71	0.55
2:9:3041:C:C6	6:D:50:VAL:HG21	2.42	0.55
1:0:2320:U:H4'	1:0:2321:A:O4'	2.07	0.55
1:0:1132:A:N6	1:0:1229:C:H2'	2.22	0.55
1:0:1057:A:H2'	1:0:1058:A:C8	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:621:C:H5'	26:X:132:ASP:OD2	2.06	0.55
23:U:12:THR:CG2	23:U:15:GLU:HG3	2.26	0.55
24:V:4:LEU:O	24:V:32:CYS:HA	2.06	0.55
1:0:1667:A:H2'	1:0:1668:U:C6	2.41	0.55
4:B:312:ARG:HD3	4:B:315:VAL:HG13	1.88	0.55
1:0:968:G:H1'	10:H:32:LYS:HD2	1.89	0.55
15:M:170:GLU:O	15:M:174:GLU:HG3	2.07	0.55
1:0:1167:G:O2'	1:0:1168:C:H5'	2.06	0.55
24:V:6:GLN:CB	24:V:26:ILE:HD12	2.34	0.55
1:0:2769:C:O2'	1:0:2770:G:H5'	2.07	0.55
4:B:87:TYR:HD1	40:B:9055:HOH:O	1.90	0.55
19:Q:119:VAL:HG12	19:Q:119:VAL:O	2.05	0.55
3:A:211:LYS:HB3	3:A:212:PRO:CD	2.31	0.55
1:0:470:U:O2'	28:Z:16:HIS:CD2	2.60	0.55
7:E:31:ARG:NH1	7:E:68:HIS:CG	2.75	0.55
5:C:233:THR:HG22	5:C:234:VAL:H	1.71	0.55
1:0:1654:U:H2'	3:A:47:HIS:HD2	1.72	0.55
13:K:120:LEU:HD12	13:K:133:VAL:HG21	1.89	0.55
14:L:120:VAL:HG11	14:L:130:GLU:HG3	1.87	0.55
23:U:8:ILE:HG21	23:U:59:ILE:HG13	1.88	0.54
3:A:53:ALA:HB3	40:A:9078:HOH:O	2.05	0.54
8:F:48:VAL:HG23	8:F:74:PHE:CB	2.36	0.54
4:B:96:PRO:HG3	40:B:9113:HOH:O	2.06	0.54
1:0:1853:C:OP1	3:A:231:LYS:HG3	2.08	0.54
1:0:263:U:O4'	8:F:59:ILE:HD13	2.06	0.54
23:U:44:GLY:O	23:U:48:GLU:HG2	2.06	0.54
21:S:71:VAL:HG12	21:S:72:ILE:N	2.22	0.54
17:O:103:THR:O	17:O:107:GLU:HG3	2.07	0.54
5:C:129:HIS:CE1	5:C:231:ARG:HA	2.42	0.54
1:0:2291:A:C8	1:0:2309:C:H5'	2.41	0.54
1:0:1717:A:H5"	17:O:54:LYS:HB2	1.87	0.54
21:S:32:ARG:NH1	21:S:38:ARG:NH1	2.55	0.54
1:0:2073:G:OP2	1:0:2490:A:H5'	2.07	0.54
6:D:99:ASP:CB	6:D:103:ASN:HB2	2.37	0.54
6:D:23:VAL:HG23	6:D:23:VAL:O	2.07	0.54
1:0:1182:C:H1'	1:0:1192:A:C8	2.40	0.54
3:A:96:LEU:HD22	3:A:128:LEU:HD13	1.90	0.54
15:M:159:TYR:HB3	15:M:162:ASP:HB2	1.90	0.54
1:0:2314:G:C2'	1:0:2315:C:H5'	2.37	0.54
11:I:93:ARG:CB	11:I:93:ARG:HH11	2.17	0.54
8:F:91:VAL:CG1	8:F:92:GLY:H	2.17	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:S:26:THR:HA	21:S:39:ASN:HB3	1.89	0.54
1:0:625:U:H5"	1:0:1044:C:N4	2.23	0.54
40:0:9823:HOH:O	28:Z:1:THR:HA	2.08	0.54
1:0:553:G:P	26:X:204:ARG:HH22	2.31	0.54
1:0:1283:G:O2'	1:0:1284:G:H5'	2.06	0.54
1:0:2715:G:N2	4:B:264:GLU:OE1	2.40	0.54
4:B:79:MET:HE1	40:B:9104:HOH:O	2.07	0.54
1:0:1119:G:H22	1:0:1246:A:H2	1.47	0.54
40:0:5224:HOH:O	11:I:47:THR:HB	2.07	0.54
15:M:47:LEU:HD12	15:M:92:ALA:HB1	1.90	0.54
2:9:3044:A:O4'	6:D:76:ARG:NE	2.40	0.54
13:K:143:THR:CG2	13:K:144:ASP:N	2.70	0.54
7:E:7:ILE:HD11	7:E:11:VAL:C	2.28	0.54
9:G:16:LYS:O	9:G:20:VAL:HG23	2.07	0.54
1:0:2894:C:O2'	1:0:2895:C:H5'	2.07	0.54
1:0:2896:A:N3	1:0:2896:A:H2'	2.23	0.54
1:0:1687:C:O2	28:Z:9:GLY:HA2	2.08	0.54
1:0:2637:A:C8	31:4:74:C:H3'	2.43	0.54
1:0:2718:C:H6	1:0:2718:C:H5'	1.73	0.54
4:B:162:MET:CE	4:B:308:LEU:HD21	2.34	0.54
13:K:57:VAL:O	13:K:57:VAL:HG12	2.08	0.54
1:0:558:C:C2'	1:0:559:C:H5"	2.38	0.54
1:0:2432:C:O2'	1:0:2433:A:H5'	2.08	0.54
1:0:681:G:N3	1:0:681:G:H5'	2.23	0.54
3:A:94:LEU:HD12	3:A:98:GLU:HB2	1.89	0.54
4:B:162:MET:HE2	4:B:310:ARG:HD3	1.90	0.54
1:0:2102:G:H5"	1:0:2538:A:C2	2.43	0.54
1:0:420:U:H2'	1:0:421:C:C6	2.42	0.54
1:0:2563:U:H2'	1:0:2565:C:O5'	2.08	0.54
1:0:69:A:H5'	1:0:69:A:C8	2.43	0.54
24:V:122:ARG:CG	24:V:122:ARG:NH1	2.70	0.53
4:B:41:PHE:CD1	4:B:79:MET:HE2	2.43	0.53
4:B:17:LYS:O	4:B:260:HIS:HD2	1.91	0.53
1:0:1946:C:H2'	1:0:1971:G:C8	2.43	0.53
1:0:1053:G:OP1	10:H:12:PRO:HG3	2.07	0.53
1:0:2638:G:H5'	40:0:8342:HOH:O	2.09	0.53
1:0:21:G:H4'	19:Q:2:ILE:HG22	1.89	0.53
1:0:2717:C:H2'	1:0:2718:C:C5'	2.38	0.53
1:0:1118:A:C8	1:0:1119:G:H5"	2.42	0.53
11:I:130:VAL:HG12	11:I:131:THR:N	2.23	0.53
4:B:141:ARG:HD2	4:B:163:GLU:OE2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2456:A:H2'	1:0:2457:U:C6	2.43	0.53
2:9:3069:U:OP1	15:M:4:PRO:HG3	2.08	0.53
1:0:2487:C:H2'	1:0:2488:A:O4'	2.08	0.53
10:H:54:THR:O	10:H:55:VAL:HG13	2.07	0.53
14:L:98:GLN:O	14:L:102:GLU:HG3	2.07	0.53
1:0:1733:A:H4'	4:B:212:GLN:HA	1.88	0.53
1:0:65:C:O2'	1:0:66:G:H5'	2.08	0.53
2:9:3048:C:H4'	15:M:141:ARG:HH21	1.73	0.53
25:W:43:VAL:HG12	25:W:44:ASP:N	2.23	0.53
26:X:152:LYS:HB3	26:X:160:LYS:HG3	1.90	0.53
2:9:3092:G:H2'	2:9:3093:A:H8	1.72	0.53
1:0:281:U:O2'	1:0:282:C:H5'	2.08	0.53
15:M:11:ARG:HG3	15:M:14:ARG:NH1	2.23	0.53
1:0:136:C:H2'	1:0:137:U:O4'	2.08	0.53
8:F:13:GLU:OE2	8:F:78:GLU:HG2	2.09	0.53
24:V:19:ASP:O	24:V:23:MET:HG3	2.09	0.53
19:Q:96:VAL:HG13	19:Q:106:GLY:HA3	1.90	0.53
9:G:23:ILE:HD13	9:G:67:LEU:HD23	1.91	0.53
1:0:244:C:OP2	8:F:38:LYS:HE3	2.09	0.53
6:D:11:HIS:C	6:D:13:MET:H	2.11	0.53
16:N:14:LEU:CD2	16:N:102:ILE:HD11	2.39	0.53
1:0:558:C:H2'	1:0:559:C:C5'	2.39	0.53
1:0:60:A:O2'	1:0:61:G:H5'	2.09	0.53
25:W:31:ILE:O	25:W:35:GLU:HG3	2.08	0.53
1:0:2094:G:H4'	4:B:245:SER:HB3	1.91	0.53
20:R:57:THR:CG2	20:R:58:MET:N	2.72	0.53
1:0:560:C:H2'	1:0:561:G:H8	1.72	0.53
4:B:217:ARG:HG3	4:B:257:THR:HG22	1.89	0.53
4:B:139:ASP:CB	4:B:165:ARG:HE	2.21	0.53
1:0:920:C:H4'	1:0:921:G:C2	2.44	0.53
1:0:514:G:O5'	1:0:514:G:H8	1.92	0.53
24:V:139:GLY:O	24:V:141:HIS:HD2	1.91	0.53
1:0:1159:G:H21	1:0:1189:A:H8	1.57	0.53
6:D:11:HIS:O	6:D:12:GLU:HB3	2.09	0.53
1:0:316:A:H5'	21:S:54:ASP:OD2	2.08	0.53
8:F:99:THR:HG23	8:F:99:THR:O	2.08	0.53
1:0:256:C:H2'	1:0:257:G:O4'	2.09	0.53
1:0:299:U:H5'	40:0:7672:HOH:O	2.08	0.53
14:L:60:VAL:C	14:L:61:ILE:HD12	2.30	0.53
13:K:97:VAL:HG12	13:K:98:GLU:O	2.09	0.53
1:0:821:U:H2'	1:0:822:C:H6	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:U:20:LEU:HD11	23:U:53:ILE:HG23	1.91	0.53
1:0:2270:G:H4'	3:A:223:ARG:NH1	2.24	0.53
1:0:1684:A:H1'	29:1:43:ARG:HH22	1.74	0.53
1:0:2866:U:H4'	1:0:2867:G:H5'	1.90	0.53
22:T:9:CYS:HA	22:T:52:THR:HG23	1.91	0.53
15:M:182:GLY:O	15:M:183:ASP:O	2.27	0.53
2:9:3008:G:O6	15:M:11:ARG:NH1	2.42	0.53
24:V:149:LEU:HG	24:V:153:MET:HE2	1.91	0.53
1:0:2081:A:H4'	11:I:69:TYR:CE1	2.44	0.53
1:0:2363:G:O3'	18:P:11:ARG:NH1	2.42	0.53
6:D:99:ASP:HA	40:D:5675:HOH:O	2.09	0.52
23:U:49:LEU:O	23:U:53:ILE:HG13	2.09	0.52
1:0:1972:U:H2'	1:0:1973:A:H5'	1.90	0.52
26:X:165:GLU:HB3	40:X:8895:HOH:O	2.09	0.52
26:X:106:THR:HG23	26:X:107:PRO:HD2	1.89	0.52
1:0:2912:C:O2'	1:0:2913:A:H5'	2.09	0.52
24:V:38:THR:HG22	24:V:39:ASP:N	2.24	0.52
5:C:180:SER:HB2	40:C:8654:HOH:O	2.09	0.52
7:E:145:ALA:HB1	7:E:168:ILE:CD1	2.38	0.52
6:D:23:VAL:CG2	6:D:73:VAL:HB	2.39	0.52
1:0:288:A:H2'	1:0:289:G:C8	2.44	0.52
1:0:1477:C:H5'	1:0:1868:G:C5'	2.38	0.52
4:B:215:VAL:HB	4:B:234:ARG:HH12	1.73	0.52
1:0:2356:A:H2'	1:0:2357:G:O4'	2.09	0.52
5:C:132:ASP:HB3	40:C:8571:HOH:O	2.09	0.52
1:0:2569:A:H2'	1:0:2570:G:O5'	2.08	0.52
1:0:2499:U:H2'	1:0:2500:C:H6	1.74	0.52
1:0:1289:C:O2'	1:0:1290:G:H5'	2.09	0.52
2:9:3023:U:C6	2:9:3023:U:H5"	2.44	0.52
3:A:88:ILE:HG22	3:A:88:ILE:O	2.09	0.52
2:9:3091:C:H2'	2:9:3092:G:O4'	2.09	0.52
10:H:58:ARG:HG3	10:H:58:ARG:NH1	2.23	0.52
4:B:280:VAL:HG13	4:B:333:GLU:O	2.10	0.52
5:C:5:ILE:CD1	5:C:16:VAL:HG23	2.34	0.52
3:A:33:GLU:CD	3:A:33:GLU:H	2.10	0.52
1:0:1474:C:H5'	1:0:1474:C:C6	2.37	0.52
11:I:6:PHE:HB3	11:I:109:TYR:OH	2.10	0.52
4:B:138:GLY:O	4:B:139:ASP:O	2.26	0.52
1:0:1926:G:H2'	1:0:1927:A:H8	1.74	0.52
21:S:24:ARG:HH21	21:S:39:ASN:HD22	1.58	0.52
22:T:46:ALA:HB1	22:T:52:THR:HG21	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2361:A:H2'	1:0:2362:A:C8	2.44	0.52
1:0:2330:U:H4'	1:0:2331:C:OP1	2.10	0.52
1:0:702:G:O2'	1:0:703:G:H5'	2.10	0.52
1:0:876:A:H2'	1:0:876:A:N3	2.24	0.52
9:G:67:LEU:O	9:G:71:LEU:HG	2.09	0.52
10:H:76:GLU:C	10:H:77:LEU:HD23	2.29	0.52
1:0:812:A:H2'	1:0:813:C:C6	2.44	0.52
2:9:3107:C:H2'	2:9:3108:C:C6	2.44	0.52
1:0:2591:C:H2'	1:0:2592:G:O4'	2.10	0.52
1:0:2241:C:O2'	1:0:2242:U:H5'	2.09	0.52
1:0:1595:G:O2'	1:0:1596:U:H5'	2.09	0.52
1:0:2531:U:O2'	1:0:2532:A:H5'	2.08	0.52
19:Q:114:VAL:HA	19:Q:144:GLU:O	2.10	0.52
1:0:1838:U:O2'	1:0:2644:C:H5'	2.09	0.52
1:0:635:A:H2'	1:0:636:G:H5"	1.92	0.52
10:H:56:GLN:HE22	10:H:93:GLN:HG2	1.73	0.52
1:0:1298:U:H2'	1:0:1299:G:C8	2.44	0.52
25:W:76:ARG:O	25:W:77:PHE:HB3	2.10	0.52
1:0:1384:C:H5'	25:W:30:MET:HG2	1.91	0.52
4:B:125:GLU:O	4:B:129:ARG:HG3	2.09	0.52
1:0:1155:G:H2'	1:0:1156:C:C6	2.45	0.52
1:0:538:C:H5"	1:0:539:G:C8	2.45	0.52
1:0:1181:A:H2'	1:0:1182:C:O4'	2.09	0.52
15:M:164:ASP:OD2	15:M:167:ASP:HA	2.09	0.52
1:0:746:A:H4'	1:0:747:G:H5'	1.91	0.52
26:X:212:ARG:HD2	40:X:8902:HOH:O	2.09	0.52
30:2:42:ARG:HH11	30:2:42:ARG:HG3	1.74	0.52
1:0:1333:U:H2'	1:0:1334:C:H6	1.73	0.52
1:0:2265:U:H2'	1:0:2266:A:H8	1.74	0.52
1:0:1681:G:H5"	1:0:1682:A:H5'	1.92	0.52
27:Y:13:ARG:NH1	40:Y:8717:HOH:O	2.43	0.52
29:1:39:ARG:HG2	40:1:3143:HOH:O	2.10	0.52
3:A:210:GLY:HA3	40:A:9058:HOH:O	2.09	0.52
1:0:2781:U:C2'	1:0:2782:G:H5'	2.39	0.52
1:0:1098:A:H2'	1:0:1099:G:O4'	2.10	0.52
1:0:1164:U:H3	1:0:1192:A:H2	1.58	0.52
26:X:154:ARG:HH12	26:X:155:ARG:CG	2.22	0.52
1:0:2072:G:C6	1:0:2533:C:H1'	2.45	0.52
19:Q:39:THR:HB	19:Q:42:GLU:HG3	1.91	0.52
17:O:7:LYS:HD2	17:O:21:VAL:CG2	2.40	0.52
1:0:2795:C:O2'	1:0:2796:U:H5'	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:381:G:H5"	40:L:8869:HOH:O	2.09	0.52
15:M:180:LEU:O	15:M:181:ASP:HB3	2.10	0.52
1:0:894:A:C2	5:C:87:ARG:NH2	2.77	0.52
2:9:3049:G:O2'	2:9:3050:G:H5'	2.11	0.51
15:M:34:LEU:HA	15:M:47:LEU:HD23	1.93	0.51
3:A:51:ARG:HB2	40:A:9078:HOH:O	2.09	0.51
1:0:1151:G:OP1	9:G:63:ARG:NH1	2.42	0.51
1:0:138:U:H5"	1:0:139:C:OP2	2.11	0.51
1:0:328:U:O4'	5:C:202:THR:HG22	2.10	0.51
1:0:1423:C:O2'	1:0:1424:A:H5'	2.10	0.51
3:A:55:VAL:HG22	3:A:68:ILE:O	2.10	0.51
8:F:58:GLU:HG3	8:F:61:MET:HE1	1.91	0.51
3:A:36:ASP:HB2	3:A:85:SER:H	1.74	0.51
3:A:48:ASP:HB3	40:A:9078:HOH:O	2.08	0.51
16:N:14:LEU:HD23	16:N:102:ILE:HD11	1.93	0.51
1:0:241:A:C2	1:0:378:A:H4'	2.45	0.51
5:C:25:PRO:HG2	40:C:8525:HOH:O	2.10	0.51
29:1:48:ASP:O	29:1:49:GLU:HB2	2.11	0.51
1:0:1751:G:C2'	1:0:1752:G:H5"	2.40	0.51
25:W:78:GLU:HG2	25:W:79:GLU:N	2.23	0.51
16:N:96:VAL:HG13	16:N:100:GLN:HB2	1.93	0.51
21:S:41:ARG:NH1	21:S:41:ARG:HG2	2.25	0.51
6:D:10:PHE:CG	6:D:11:HIS:N	2.78	0.51
4:B:215:VAL:HB	4:B:234:ARG:NH1	2.25	0.51
1:0:2644:C:O2'	1:0:2645:U:H5'	2.10	0.51
4:B:71:VAL:HG11	4:B:296:LEU:HD22	1.93	0.51
1:0:2886:C:O2'	1:0:2887:G:H5'	2.10	0.51
2:9:3059:C:H2'	2:9:3060:C:C6	2.45	0.51
4:B:55:ASN:HB3	4:B:63:GLU:HA	1.91	0.51
1:0:1118:A:C8	1:0:1118:A:C3'	2.93	0.51
1:0:1158:G:O2'	1:0:1159:G:H5'	2.11	0.51
3:A:179:MET:HA	3:A:179:MET:CE	2.41	0.51
1:0:1406:A:H4'	1:0:1407:A:H5"	1.92	0.51
1:0:2667:G:H1'	1:0:2914:A:N3	2.25	0.51
1:0:1636:G:O2'	1:0:1637:A:H5'	2.10	0.51
15:M:78:MET:HB2	15:M:79:PRO:HD3	1.93	0.51
15:M:5:ARG:HG3	18:P:18:PRO:HB3	1.91	0.51
1:0:2721:U:OP1	22:T:17:THR:HG23	2.10	0.51
1:0:793:A:H5"	17:O:83:LYS:HG2	1.93	0.51
1:0:2820:A:H2'	1:0:2821:C:C6	2.44	0.51
23:U:11:MET:HB3	23:U:15:GLU:HB2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:V:54:PHE:CZ	24:V:140:LYS:HB2	2.46	0.51
10:H:76:GLU:O	10:H:77:LEU:HD23	2.11	0.51
1:0:138:U:OP2	1:0:139:C:H5	1.94	0.51
5:C:140:VAL:HB	40:C:8659:HOH:O	2.10	0.51
1:0:2735:U:H2'	1:0:2736:U:C6	2.46	0.51
1:0:2470:A:H5"	40:0:3679:HOH:O	2.10	0.51
17:O:16:VAL:HG13	17:O:20:ARG:CZ	2.41	0.51
2:9:3039:U:H3'	2:9:3040:C:H5"	1.93	0.51
1:0:1730:G:C5'	1:0:1731:C:C6	2.94	0.51
4:B:307:ARG:HG3	4:B:307:ARG:NH1	2.26	0.51
1:0:2443:C:O3'	13:K:56:LYS:HE3	2.11	0.51
26:X:177:LYS:HE3	26:X:183:GLU:OE2	2.11	0.51
24:V:126:ASP:HB3	24:V:135:GLY:O	2.11	0.51
15:M:115:VAL:HG22	40:M:8860:HOH:O	2.11	0.51
1:0:1881:A:OP1	3:A:199:HIS:HE1	1.94	0.51
5:C:218:VAL:N	40:C:8631:HOH:O	2.43	0.51
18:P:53:HIS:CE1	18:P:55:ARG:HB2	2.46	0.51
1:0:830:G:H2'	1:0:831:U:C6	2.46	0.51
30:2:14:CYS:HB3	30:2:16:GLU:HG2	1.93	0.51
14:L:114:VAL:HG23	36:L:8818:CL:CL	2.48	0.51
24:V:119:HIS:HD2	24:V:120:PRO:O	1.94	0.51
10:H:59:HIS:HA	10:H:62:LEU:HD23	1.92	0.51
20:R:10:VAL:HG11	23:U:36:ALA:CA	2.41	0.51
1:0:603:A:H4'	1:0:604:G:O5'	2.11	0.51
1:0:1921:A:O2'	1:0:1922:A:H5'	2.12	0.51
1:0:1947:G:H2'	1:0:1948:G:H8	1.76	0.51
6:D:91:ALA:HB2	6:D:106:PHE:CD2	2.45	0.51
1:0:352:A:H2'	1:0:353:G:C8	2.46	0.51
6:D:67:ASP:O	6:D:69:ILE:HG13	2.11	0.50
11:I:131:THR:HG22	11:I:133:GLY:N	2.27	0.50
30:2:65:THR:CG2	30:2:67:LEU:HG	2.42	0.50
7:E:11:VAL:HG11	7:E:22:VAL:HG13	1.92	0.50
15:M:73:ALA:HB2	15:M:163:PHE:CZ	2.46	0.50
1:0:1730:G:H5'	1:0:1731:C:C6	2.46	0.50
1:0:2900:G:H2'	1:0:2901:C:O4'	2.11	0.50
18:P:86:VAL:HG11	18:P:91:LEU:HD21	1.92	0.50
2:9:3002:U:OP2	2:9:3002:U:H4'	2.11	0.50
1:0:262:A:OP2	8:F:91:VAL:HG11	2.11	0.50
15:M:67:ALA:HA	15:M:71:TRP:HB3	1.93	0.50
30:2:48:ASN:ND2	30:2:50:GLY:H	2.10	0.50
3:A:123:GLY:HA3	3:A:162:GLY:HA2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2413:A:N7	15:M:109:PRO:HB3	2.27	0.50
1:0:1942:A:H5'	3:A:233:THR:HB	1.94	0.50
5:C:118:THR:CG2	5:C:137:PRO:HB3	2.41	0.50
25:W:15:ARG:HH11	25:W:15:ARG:CB	2.21	0.50
6:D:57:THR:HG23	6:D:63:ILE:CB	2.42	0.50
27:Y:26:VAL:O	27:Y:30:GLU:HG3	2.10	0.50
25:W:21:PRO:HG2	25:W:24:LYS:HD3	1.92	0.50
1:0:2720:C:O2	12:J:87:ARG:NH2	2.44	0.50
7:E:31:ARG:HH12	7:E:68:HIS:CG	2.28	0.50
15:M:184:ILE:HG22	15:M:185:GLU:HG3	1.93	0.50
29:1:36:ASN:HB3	29:1:39:ARG:HG3	1.93	0.50
1:0:1894:C:N4	1:0:1939:U:H2'	2.27	0.50
1:0:391:U:OP2	14:L:84:LYS:NZ	2.41	0.50
1:0:2334:C:O2'	1:0:2335:C:H5'	2.12	0.50
6:D:58:VAL:HG12	6:D:59:GLY:N	2.27	0.50
1:0:2611:G:H5'	1:0:2613:G:C8	2.46	0.50
5:C:93:LYS:O	5:C:98:ARG:NH2	2.41	0.50
12:J:34:VAL:HB	40:J:7169:HOH:O	2.11	0.50
7:E:15:GLN:NE2	7:E:40:VAL:O	2.43	0.50
15:M:159:TYR:HE2	15:M:163:PHE:HE2	1.59	0.50
24:V:149:LEU:HG	24:V:153:MET:HE1	1.92	0.50
8:F:48:VAL:HG23	8:F:74:PHE:HB3	1.93	0.50
2:9:3013:A:O2'	2:9:3014:G:H5"	2.11	0.50
1:0:1768:C:H2'	1:0:1769:C:O4'	2.12	0.50
1:0:2089:A:O2'	1:0:2090:G:H5'	2.11	0.50
20:R:57:THR:HG22	20:R:58:MET:N	2.26	0.50
1:0:2780:C:H1'	7:E:143:GLN:NE2	2.24	0.50
10:H:20:ILE:HG23	10:H:120:ILE:CD1	2.41	0.50
4:B:24:PRO:HG2	4:B:204:GLY:HA2	1.92	0.50
1:0:1730:G:C5'	1:0:1731:C:H6	2.24	0.50
23:U:64:GLY:O	23:U:65:ASP:CB	2.59	0.50
1:0:1741:U:O2'	1:0:2723:G:H4'	2.10	0.50
8:F:39:SER:HB3	8:F:45:ALA:HB2	1.93	0.50
1:0:101:C:H2'	1:0:102:A:H8	1.76	0.50
12:J:45:PRO:HB2	40:J:7169:HOH:O	2.11	0.50
6:D:154:LYS:HD2	6:D:154:LYS:N	2.17	0.50
26:X:189:ASN:C	26:X:189:ASN:HD22	2.14	0.50
2:9:3028:U:H2'	2:9:3029:C:C6	2.47	0.50
3:A:109:GLU:HG2	3:A:116:GLY:H	1.76	0.50
4:B:205:VAL:O	4:B:307:ARG:NE	2.45	0.50
4:B:125:GLU:OE2	4:B:129:ARG:NH1	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:204:A:C2'	1:0:205:U:H5'	2.41	0.50
19:Q:34:GLU:HG2	19:Q:46:TYR:OH	2.12	0.50
1:0:1501:A:OP2	17:O:37:ARG:HD2	2.12	0.50
40:0:5897:HOH:O	4:B:298:LYS:HD3	2.11	0.50
23:U:12:THR:HG23	23:U:14:ALA:H	1.77	0.50
1:0:289:G:O2'	1:0:290:C:H5'	2.12	0.50
25:W:78:GLU:CG	25:W:79:GLU:H	2.24	0.50
1:0:945:U:H2'	1:0:946:C:H6	1.76	0.50
8:F:21:GLU:O	8:F:24:ARG:HG3	2.11	0.50
1:0:2364:A:H5"	18:P:15:LYS:HD3	1.92	0.50
1:0:1250:C:O2'	1:0:1251:C:H5'	2.11	0.50
24:V:90:TYR:N	24:V:90:TYR:CD1	2.79	0.50
7:E:69:ILE:HA	7:E:72:MET:HE3	1.94	0.50
17:O:13:VAL:HG21	17:O:41:ARG:HG2	1.94	0.50
19:Q:39:THR:HG22	19:Q:42:GLU:H	1.77	0.50
1:0:1269:G:H2'	1:0:1270:U:C6	2.47	0.50
1:0:960:G:H4'	40:0:7764:HOH:O	2.11	0.50
1:0:1419:U:H2'	1:0:1685:A:C2	2.47	0.50
1:0:12:U:H2'	1:0:13:G:H5'	1.93	0.50
1:0:2672:C:O2'	1:0:2673:U:H5'	2.12	0.50
19:Q:104:PHE:HB2	19:Q:109:MET:HE1	1.94	0.49
1:0:1165:G:OP1	1:0:1165:G:H3'	2.12	0.49
1:0:1701:A:H5'	40:0:6649:HOH:O	2.11	0.49
10:H:40:ALA:HB1	10:H:137:TYR:CE2	2.47	0.49
12:J:58:THR:HG22	12:J:59:LYS:HG3	1.93	0.49
1:0:316:A:N3	1:0:336:G:O2'	2.40	0.49
12:J:62:PRO:HG3	12:J:65:ARG:HH21	1.76	0.49
1:0:412:C:O2'	1:0:413:G:H5'	2.12	0.49
13:K:10:SER:O	13:K:11:ARG:HB3	2.12	0.49
1:0:1535:G:H2'	1:0:1536:C:C6	2.47	0.49
1:0:447:A:O2'	1:0:448:G:H5'	2.12	0.49
1:0:951:A:C2'	1:0:952:G:H5'	2.42	0.49
6:D:99:ASP:CB	6:D:103:ASN:H	2.24	0.49
6:D:75:LEU:HD22	6:D:79:MET:HB3	1.94	0.49
21:S:9:LYS:NZ	21:S:13:ARG:NH1	2.60	0.49
15:M:151:ASP:O	15:M:154:LEU:HB2	2.11	0.49
8:F:48:VAL:CG2	8:F:74:PHE:HB3	2.42	0.49
2:9:3003:A:N6	2:9:3022:G:H1'	2.27	0.49
1:0:105:G:O2'	1:0:106:A:H5'	2.12	0.49
12:J:75:ARG:HE	12:J:94:ALA:HB3	1.77	0.49
5:C:168:ARG:NH2	5:C:190:ALA:O	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:K:143:THR:CG2	13:K:144:ASP:H	2.25	0.49
10:H:3:ALA:HA	10:H:58:ARG:NH1	2.27	0.49
20:R:11:THR:H	20:R:14:ALA:HB3	1.77	0.49
1:0:2540:G:O2'	1:0:2541:U:H5"	2.12	0.49
1:0:629:A:H2'	1:0:630:A:O4'	2.13	0.49
15:M:64:SER:C	15:M:66:LEU:H	2.16	0.49
19:Q:106:GLY:HA2	19:Q:109:MET:CE	2.40	0.49
6:D:41:LEU:HA	6:D:44:ILE:CG2	2.41	0.49
1:0:1342:C:C2'	1:0:1343:C:H5'	2.42	0.49
9:G:20:VAL:O	9:G:24:VAL:HG23	2.12	0.49
1:0:2090:G:H2'	1:0:2091:G:C8	2.47	0.49
1:0:1211:G:O2'	1:0:1212:C:H5'	2.13	0.49
1:0:1218:U:H2'	1:0:1219:U:C6	2.47	0.49
1:0:2635:A:O2'	1:0:2636:C:H5'	2.12	0.49
1:0:709:G:O2'	16:N:25:VAL:HG12	2.12	0.49
1:0:2520:G:O2'	1:0:2521:A:H5'	2.12	0.49
1:0:1778:A:H2'	1:0:1779:A:H5'	1.93	0.49
1:0:2570:G:H5"	40:0:5298:HOH:O	2.13	0.49
7:E:92:PRO:HB2	40:E:4917:HOH:O	2.12	0.49
14:L:24:GLN:O	14:L:28:GLN:HG3	2.12	0.49
40:9:9094:HOH:O	15:M:23:ARG:HD3	2.12	0.49
13:K:121:ILE:HG12	13:K:141:GLU:HB2	1.94	0.49
5:C:1:MET:HG2	5:C:2:GLN:NE2	2.27	0.49
1:0:861:A:H4'	1:0:1697:G:H4'	1.94	0.49
10:H:16:ARG:HH21	10:H:18:GLU:CD	2.16	0.49
27:Y:57:CYS:SG	27:Y:59:TYR:HB3	2.52	0.49
12:J:30:LYS:O	12:J:55:VAL:HG13	2.13	0.49
1:0:2499:U:H2'	1:0:2500:C:C6	2.47	0.49
2:9:3106:C:O2'	2:9:3107:C:H5'	2.13	0.49
1:0:945:U:H2'	1:0:946:C:C6	2.46	0.49
20:R:33:SER:O	20:R:37:VAL:HG23	2.13	0.49
27:Y:39:CYS:O	27:Y:42:CYS:O	2.31	0.49
1:0:441:A:H1'	1:0:442:A:N7	2.28	0.49
4:B:84:LEU:HD13	4:B:84:LEU:O	2.12	0.49
1:0:1181:A:O2'	1:0:1182:C:H5'	2.13	0.49
6:D:173:GLU:HG3	6:D:174:VAL:N	2.27	0.49
27:Y:30:GLU:HA	27:Y:33:MET:HE3	1.94	0.49
2:9:3052:A:O2'	2:9:3053:G:H5'	2.13	0.49
14:L:30:GLU:O	14:L:34:GLU:HG3	2.12	0.49
1:0:1044:C:H5"	40:0:9518:HOH:O	2.12	0.49
1:0:1482:A:O2'	1:0:1483:C:H5'	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1007:A:H2'	10:H:19:TYR:CZ	2.48	0.49
40:0:6650:HOH:O	26:X:158:LYS:HD3	2.12	0.49
1:0:1205:U:H2'	1:0:1206:U:H5"	1.94	0.49
1:0:1268:C:O2'	1:0:1269:G:H5'	2.12	0.49
1:0:1268:C:H2'	1:0:1269:G:H8	1.78	0.49
9:G:63:ARG:O	9:G:67:LEU:HG	2.12	0.49
1:0:1527:A:H1'	1:0:1528:A:C8	2.47	0.49
1:0:887:G:H2'	1:0:888:U:C6	2.47	0.49
7:E:100:ASP:HB2	40:E:2789:HOH:O	2.13	0.49
1:0:344:C:H2'	1:0:345:G:O4'	2.13	0.49
14:L:164:THR:HG22	14:L:166:ALA:H	1.78	0.49
1:0:2815:G:N7	11:I:80:LYS:NZ	2.58	0.49
2:9:3018:U:H2'	2:9:3019:G:H8	1.78	0.49
6:D:154:LYS:H	6:D:154:LYS:CD	2.14	0.48
1:0:596:C:H2'	1:0:597:A:C8	2.47	0.48
7:E:49:ILE:HD11	7:E:69:ILE:HD12	1.94	0.48
1:0:1654:U:H2'	3:A:47:HIS:CD2	2.47	0.48
13:K:118:LEU:HB2	40:K:8878:HOH:O	2.13	0.48
1:0:101:C:H2'	1:0:102:A:C8	2.48	0.48
16:N:80:ASP:OD1	16:N:81:PHE:N	2.46	0.48
1:0:2101:A:H2'	5:C:63:SER:OG	2.13	0.48
1:0:1913:C:H2'	1:0:1914:C:H6	1.78	0.48
26:X:186:ARG:HG2	26:X:186:ARG:HH11	1.78	0.48
6:D:25:MET:CE	6:D:41:LEU:HG	2.37	0.48
1:0:558:C:C2'	1:0:559:C:C5'	2.92	0.48
5:C:194:PHE:CD2	5:C:234:VAL:HG11	2.47	0.48
1:0:2781:U:H2'	1:0:2782:G:H5'	1.95	0.48
10:H:38:LYS:HE2	10:H:42:ASP:HB2	1.95	0.48
40:0:9995:HOH:O	17:O:81:LYS:HG2	2.12	0.48
4:B:14:GLY:HA2	4:B:15:PRO:C	2.33	0.48
1:0:1086:A:C6	24:V:11:VAL:HG11	2.48	0.48
15:M:116:PHE:N	40:M:8860:HOH:O	2.46	0.48
1:0:1187:U:O2'	1:0:1189:A:H2	1.96	0.48
7:E:11:VAL:HG12	7:E:12:ASP:H	1.77	0.48
6:D:81:GLU:O	6:D:85:GLN:HG3	2.13	0.48
1:0:185:G:H4'	1:0:186:A:H4'	1.94	0.48
1:0:2895:C:H4'	40:W:4132:HOH:O	2.13	0.48
1:0:1913:C:H2'	1:0:1914:C:C6	2.48	0.48
1:0:95:A:H5"	1:0:97:G:O4'	2.14	0.48
1:0:1252:A:H2'	1:0:1253:C:O4'	2.12	0.48
1:0:249:G:O2'	1:0:250:C:H5'	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:366:U:H2'	1:0:367:G:O4'	2.12	0.48
26:X:235:GLU:CD	26:X:235:GLU:H	2.17	0.48
10:H:46:GLN:NE2	10:H:137:TYR:HE2	2.09	0.48
5:C:246:ARG:NE	40:C:8631:HOH:O	2.38	0.48
15:M:164:ASP:OD1	15:M:167:ASP:HA	2.13	0.48
8:F:48:VAL:HG12	8:F:97:ALA:CB	2.43	0.48
1:0:2699:A:H2'	1:0:2700:G:O4'	2.12	0.48
11:I:47:THR:HG22	11:I:48:GLY:N	2.29	0.48
1:0:2781:U:H1'	7:E:139:GLU:OE2	2.13	0.48
18:P:64:GLU:HG3	18:P:74:ASP:OD2	2.13	0.48
10:H:17:ARG:HD3	10:H:23:ILE:HD12	1.96	0.48
1:0:2427:C:OP2	30:2:84:ARG:HD2	2.12	0.48
26:X:112:GLU:OE1	26:X:112:GLU:HA	2.13	0.48
1:0:2712:G:H5'	40:J:4183:HOH:O	2.14	0.48
14:L:164:THR:HG23	14:L:165:GLY:N	2.28	0.48
16:N:47:ARG:NH1	16:N:47:ARG:HG3	2.16	0.48
1:0:290:C:O2'	1:0:291:C:H5'	2.13	0.48
5:C:194:PHE:HA	5:C:234:VAL:HG13	1.95	0.48
1:0:858:U:H2'	1:0:859:C:C6	2.48	0.48
1:0:236:A:H4'	1:0:237:G:H5'	1.96	0.48
17:O:97:ARG:HD2	40:O:163:HOH:O	2.13	0.48
16:N:105:ASN:HD21	16:N:109:SER:H	1.62	0.48
18:P:30:VAL:O	18:P:30:VAL:HG12	2.13	0.48
1:0:189:A:OP1	14:L:171:ARG:NH2	2.46	0.48
1:0:1173:A:H4'	1:0:1174:A:C8	2.49	0.48
26:X:189:ASN:ND2	26:X:192:ASP:H	2.12	0.48
4:B:212:GLN:HB2	4:B:257:THR:CG2	2.38	0.48
1:0:1500:U:P	17:O:41:ARG:HH22	2.37	0.48
8:F:32:GLY:N	40:F:3111:HOH:O	2.46	0.48
9:G:19:GLU:O	9:G:23:ILE:HG13	2.14	0.48
2:9:3060:C:O2'	2:9:3061:C:H5'	2.13	0.48
6:D:55:LYS:O	6:D:56:ARG:HB2	2.13	0.48
5:C:214:THR:HG21	40:C:8610:HOH:O	2.13	0.48
1:0:2271:G:H5'	40:A:9045:HOH:O	2.14	0.48
1:0:776:A:OP1	28:Z:28:HIS:HE1	1.97	0.48
1:0:1096:U:O2'	1:0:1097:A:H5'	2.13	0.48
1:0:1835:U:C5	1:0:1840:A:N7	2.69	0.48
4:B:320:GLN:HE21	4:B:321:PRO:HD2	1.79	0.48
1:0:960:G:N3	1:0:960:G:C2'	2.77	0.48
2:9:3107:C:H2'	2:9:3108:C:H6	1.76	0.48
10:H:73:LEU:HD21	10:H:146:VAL:HA	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1335:C:H2'	1:0:1336:U:C6	2.48	0.48
5:C:242:GLU:HG3	40:C:8589:HOH:O	2.14	0.48
1:0:2401:A:H2'	1:0:2402:A:C8	2.48	0.48
21:S:71:VAL:CG1	21:S:72:ILE:N	2.76	0.48
6:D:103:ASN:ND2	6:D:134:LEU:H	2.12	0.48
6:D:23:VAL:HG21	6:D:45:THR:CG2	2.44	0.48
10:H:29:ALA:C	10:H:30:GLN:HG3	2.34	0.48
15:M:154:LEU:O	15:M:155:GLU:CB	2.62	0.48
5:C:162:VAL:CG1	5:C:192:ILE:HD11	2.43	0.48
1:0:2837:U:H1'	4:B:307:ARG:HH12	1.78	0.48
3:A:70:ALA:HA	3:A:71:PRO:HD3	1.78	0.48
24:V:115:THR:HG23	40:V:5420:HOH:O	2.13	0.48
1:0:541:C:O2'	1:0:542:A:H5"	2.14	0.48
8:F:60:VAL:O	8:F:60:VAL:CG1	2.61	0.48
1:0:1819:G:H2'	1:0:1820:G:C4'	2.40	0.48
1:0:2503:A:P	10:H:151:ARG:HH22	2.37	0.48
1:0:1298:U:H2'	1:0:1299:G:H8	1.79	0.48
1:0:1236:A:C8	11:I:63:ILE:HD11	2.49	0.48
13:K:129:ALA:O	13:K:133:VAL:HG23	2.14	0.48
1:0:2595:U:H2'	1:0:2596:A:C8	2.48	0.48
16:N:99:GLU:HG3	40:N:6044:HOH:O	2.13	0.48
1:0:415:A:O2'	1:0:416:G:H5'	2.14	0.48
28:Z:56:GLU:OXT	28:Z:56:GLU:HG2	2.14	0.48
9:G:12:ILE:HG13	40:G:6833:HOH:O	2.13	0.47
11:I:131:THR:HG22	11:I:134:GLU:H	1.78	0.47
4:B:7:ARG:HD3	4:B:9:GLY:O	2.14	0.47
1:0:1878:G:O2'	1:0:1879:U:OP2	2.32	0.47
1:0:894:A:N1	5:C:87:ARG:NH2	2.61	0.47
1:0:1021:G:O2'	1:0:1022:A:H5'	2.14	0.47
20:R:38:ALA:O	20:R:42:GLU:HG3	2.14	0.47
15:M:86:LEU:HD12	15:M:125:ALA:HB2	1.96	0.47
19:Q:84:ALA:O	19:Q:88:PHE:HD1	1.97	0.47
18:P:32:GLU:HA	18:P:71:TYR:OH	2.14	0.47
1:0:542:A:H2'	1:0:543:G:O4'	2.14	0.47
11:I:76:ASP:HA	40:I:5907:HOH:O	2.13	0.47
6:D:57:THR:HG23	6:D:63:ILE:CG2	2.42	0.47
1:0:2569:A:C2'	1:0:2570:G:O5'	2.62	0.47
1:0:2498:C:O2'	1:0:2499:U:H5'	2.14	0.47
6:D:59:GLY:O	6:D:61:PHE:N	2.39	0.47
1:0:2349:G:O2'	1:0:2350:G:H5'	2.13	0.47
1:0:1066:U:H2'	1:0:1067:A:C8	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:217:ARG:CG	3:A:217:ARG:HH11	2.27	0.47
1:0:1362:U:H2'	1:0:1363:G:C8	2.50	0.47
13:K:149:ARG:O	13:K:150:GLN:HB2	2.14	0.47
23:U:58:THR:O	23:U:62:GLU:HG3	2.14	0.47
30:2:11:CYS:HB2	30:2:20:HIS:CE1	2.48	0.47
5:C:142:ASP:OD1	5:C:236:THR:HG23	2.13	0.47
4:B:190:MET:HE2	4:B:194:PHE:HD1	1.76	0.47
30:2:17:HIS:O	30:2:18:GLN:HG3	2.14	0.47
13:K:134:GLU:HG3	40:K:8861:HOH:O	2.13	0.47
1:0:946:C:H2'	1:0:947:U:C6	2.49	0.47
1:0:1042:U:O2'	1:0:1043:C:H5'	2.14	0.47
1:0:2379:G:N3	1:0:2418:G:H2'	2.28	0.47
10:H:2:PRO:HD2	10:H:5:MET:SD	2.54	0.47
10:H:30:GLN:H	10:H:66:ARG:HH11	1.61	0.47
19:Q:119:VAL:O	19:Q:119:VAL:CG1	2.61	0.47
1:0:222:A:H2'	1:0:223:G:O4'	2.13	0.47
1:0:1871:U:O4'	1:0:1873:G:C8	2.67	0.47
13:K:101:ASP:C	13:K:103:ALA:H	2.17	0.47
1:0:622:G:O2'	1:0:623:U:H5'	2.14	0.47
1:0:200:U:H2'	40:0:3874:HOH:O	2.15	0.47
1:0:1789:G:O6	17:O:73:HIS:HE1	1.97	0.47
1:0:1592:G:O2'	1:0:1593:C:O4'	2.31	0.47
14:L:72:ALA:HB2	14:L:93:ARG:HG2	1.97	0.47
2:9:3049:G:H2'	2:9:3050:G:O4'	2.14	0.47
1:0:1189:A:H1'	1:0:1209:C:H1'	1.94	0.47
1:0:286:U:H2'	1:0:287:C:C6	2.50	0.47
21:S:96:VAL:HG13	21:S:97:ARG:N	2.30	0.47
19:Q:25:PHE:CE2	19:Q:29:LYS:CE	2.97	0.47
1:0:1328:A:C8	26:X:169:ARG:HD3	2.48	0.47
1:0:1131:G:C6	1:0:1230:A:C4	3.03	0.47
1:0:1249:U:H2'	1:0:1250:C:C6	2.49	0.47
40:0:7221:HOH:O	14:L:178:LYS:HB2	2.15	0.47
16:N:44:ASN:CG	16:N:67:SER:HB2	2.34	0.47
10:H:158:THR:HB	10:H:159:PRO:HD3	1.97	0.47
1:0:889:C:H2'	1:0:890:C:C6	2.50	0.47
7:E:108:LEU:HD11	7:E:164:ASP:HB2	1.97	0.47
24:V:3:ALA:O	24:V:54:PHE:HA	2.14	0.47
3:A:105:VAL:HG11	3:A:154:ALA:HB1	1.96	0.47
1:0:962:C:H5'	40:0:7312:HOH:O	2.15	0.47
11:I:45:VAL:HG22	11:I:46:ILE:N	2.29	0.47
23:U:39:ALA:O	23:U:41:GLU:N	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:V:65:VAL:HG12	24:V:116:LEU:HD13	1.95	0.47
1:0:2252:A:H2'	1:0:2253:G:O4'	2.14	0.47
1:0:653:C:H2'	1:0:654:A:C8	2.49	0.47
1:0:1515:A:H2'	1:0:1516:C:C6	2.50	0.47
1:0:1574:C:H2'	1:0:1575:C:C6	2.50	0.47
1:0:856:G:H2'	40:0:5807:HOH:O	2.13	0.47
1:0:1562:C:H42	1:0:2738:G:H1	1.62	0.47
1:0:2257:G:H4'	1:0:2259:C:C2	2.50	0.47
3:A:94:LEU:N	3:A:94:LEU:HD23	2.29	0.47
15:M:71:TRP:N	40:M:8840:HOH:O	2.48	0.47
4:B:53:LEU:CD1	4:B:327:VAL:HG22	2.43	0.47
1:0:1500:U:OP2	17:O:41:ARG:NH2	2.48	0.47
15:M:61:ALA:CB	15:M:88:ALA:HB2	2.43	0.47
6:D:94:ALA:HB3	6:D:174:VAL:CA	2.45	0.47
12:J:28:GLU:OE2	12:J:58:THR:HG21	2.14	0.47
14:L:120:VAL:CG1	14:L:130:GLU:HG3	2.43	0.47
1:0:947:U:H2'	1:0:948:G:C8	2.50	0.47
24:V:144:GLU:O	24:V:148:ASP:OD2	2.33	0.47
17:O:31:ILE:HG12	17:O:43:LEU:HD13	1.96	0.47
1:0:907:A:H2'	1:0:908:A:C8	2.50	0.47
1:0:69:A:H5'	1:0:69:A:H8	1.80	0.47
19:Q:114:VAL:HG13	19:Q:114:VAL:O	2.15	0.47
1:0:1753:C:O2	4:B:229:ARG:NH2	2.46	0.47
40:0:9568:HOH:O	4:B:214:PRO:HD2	2.15	0.47
1:0:1309:U:O2'	1:0:1310:U:H5'	2.15	0.47
1:0:2626:C:H2'	1:0:2627:G:C8	2.50	0.47
5:C:13:ASP:OD1	5:C:13:ASP:O	2.32	0.47
19:Q:132:ARG:HG2	19:Q:133:ALA:N	2.29	0.47
15:M:49:THR:CG2	15:M:58:LEU:HD11	2.45	0.47
6:D:95:THR:C	6:D:97:GLN:N	2.68	0.47
27:Y:30:GLU:HG2	27:Y:33:MET:HE3	1.97	0.47
2:9:3014:G:C8	2:9:3014:G:H5'	2.50	0.47
16:N:98:LEU:O	16:N:102:ILE:HG13	2.14	0.47
16:N:96:VAL:CG1	16:N:100:GLN:HB2	2.44	0.47
11:I:99:GLU:HA	40:I:7377:HOH:O	2.15	0.47
1:0:1361:C:H2'	1:0:1362:U:C6	2.50	0.47
1:0:1659:A:H2'	1:0:1660:G:O4'	2.15	0.47
1:0:1001:U:O2'	1:0:1002:G:H5'	2.15	0.47
2:9:3006:C:H4'	15:M:35:VAL:HG11	1.97	0.46
5:C:16:VAL:HG12	5:C:17:ASP:H	1.78	0.46
29:1:25:VAL:O	29:1:29:THR:HG23	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:S:18:GLU:O	21:S:21:LYS:HG2	2.14	0.46
1:0:407:A:O2'	1:0:408:A:H5'	2.14	0.46
1:0:2300:A:H4'	1:0:2301:A:O5'	2.15	0.46
15:M:37:ARG:NE	40:M:8835:HOH:O	2.48	0.46
1:0:1942:A:O2'	1:0:1943:C:H5'	2.15	0.46
1:0:31:C:H4'	40:S:7242:HOH:O	2.14	0.46
1:0:1189:A:O2'	1:0:1208:C:H2'	2.14	0.46
1:0:907:A:H2'	1:0:908:A:H8	1.79	0.46
1:0:2697:A:H2'	1:0:2698:G:O4'	2.15	0.46
25:W:30:MET:HE1	25:W:58:ALA:HB3	1.98	0.46
1:0:1741:U:H5'	1:0:1742:A:OP1	2.14	0.46
26:X:234:VAL:HG12	26:X:235:GLU:N	2.30	0.46
28:Z:28:HIS:CD2	28:Z:31:LYS:HG3	2.50	0.46
28:Z:28:HIS:CE1	28:Z:31:LYS:HE2	2.49	0.46
1:0:666:A:H2'	1:0:667:C:O4'	2.15	0.46
1:0:220:C:C2	13:K:48:LYS:HE2	2.50	0.46
1:0:2906:A:H5'	1:0:2907:C:O4'	2.16	0.46
1:0:2388:C:O2'	1:0:2389:U:H5'	2.15	0.46
1:0:2087:C:O2'	1:0:2088:C:H5'	2.15	0.46
1:0:1826:C:O2'	1:0:1827:G:H5'	2.15	0.46
24:V:48:VAL:HG12	24:V:48:VAL:O	2.15	0.46
1:0:2419:U:H5"	1:0:2420:G:H5'	1.96	0.46
25:W:9:VAL:HG13	25:W:88:GLU:OE1	2.15	0.46
14:L:9:ARG:HG3	40:L:8846:HOH:O	2.15	0.46
1:0:1168:C:H2'	1:0:1169:U:O4'	2.16	0.46
1:0:1421:C:O2'	1:0:1422:U:H5'	2.15	0.46
12:J:62:PRO:HG3	12:J:65:ARG:NH2	2.30	0.46
20:R:33:SER:OG	20:R:36:GLU:HG3	2.14	0.46
26:X:112:GLU:CD	26:X:115:ARG:NH1	2.69	0.46
10:H:79:GLU:C	10:H:80:GLU:HG3	2.35	0.46
1:0:162:C:H2'	1:0:163:U:H5'	1.97	0.46
21:S:19:ARG:HD3	21:S:67:LEU:O	2.14	0.46
5:C:236:THR:O	5:C:237:GLU:C	2.53	0.46
21:S:9:LYS:HB2	40:S:7242:HOH:O	2.15	0.46
17:O:10:ALA:CA	17:O:13:VAL:HG12	2.43	0.46
7:E:81:GLU:HA	7:E:133:VAL:O	2.15	0.46
4:B:5:ARG:HD2	4:B:8:LYS:HZ3	1.81	0.46
1:0:907:A:H4'	1:0:1328:A:C2	2.51	0.46
1:0:1477:C:C5'	1:0:1868:G:H5"	2.45	0.46
26:X:107:PRO:HB3	26:X:182:PHE:CD2	2.51	0.46
10:H:116:ALA:O	10:H:117:PHE:C	2.54	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2689:A:H2'	1:0:2690:U:H5'	1.98	0.46
1:0:1304:U:H2'	1:0:1305:C:C6	2.51	0.46
19:Q:50:VAL:HA	19:Q:55:GLN:O	2.16	0.46
1:0:1819:G:H2'	1:0:1820:G:C5'	2.45	0.46
10:H:56:GLN:NE2	10:H:93:GLN:HG2	2.30	0.46
19:Q:25:PHE:CZ	19:Q:29:LYS:HE2	2.50	0.46
1:0:1925:G:O2'	1:0:1926:G:H5'	2.15	0.46
1:0:2826:G:C6	1:0:2913:A:N6	2.84	0.46
30:2:91:GLN:O	30:2:92:GLU:HB2	2.15	0.46
26:X:141:THR:HG23	40:X:8889:HOH:O	2.15	0.46
2:9:3023:U:C3'	2:9:3024:U:C5'	2.84	0.46
15:M:37:ARG:HH11	15:M:37:ARG:HG3	1.80	0.46
1:0:1840:A:H4'	1:0:1841:C:O5'	2.15	0.46
6:D:136:ARG:HB2	6:D:137:PRO:HD2	1.96	0.46
40:0:5085:HOH:O	27:Y:13:ARG:HD3	2.16	0.46
7:E:137:ASP:OD1	7:E:139:GLU:HB2	2.16	0.46
28:Z:28:HIS:CD2	28:Z:30:LYS:HB2	2.50	0.46
28:Z:28:HIS:HD2	28:Z:31:LYS:H	1.63	0.46
16:N:44:ASN:OD1	16:N:67:SER:HB2	2.16	0.46
24:V:73:LEU:O	24:V:74:GLU:HG3	2.16	0.46
1:0:2112:A:H2'	1:0:2113:G:C8	2.50	0.46
1:0:1739:G:O2'	1:0:1740:U:H5'	2.15	0.46
24:V:21:LEU:HB3	24:V:26:ILE:CG1	2.46	0.46
3:A:36:ASP:CA	3:A:83:GLY:HA3	2.44	0.46
1:0:2830:U:O2'	1:0:2831:C:H5'	2.15	0.46
1:0:396:U:O2'	1:0:397:A:P	2.73	0.46
1:0:171:C:OP2	14:L:84:LYS:HG3	2.16	0.46
1:0:343:C:O2'	1:0:344:C:H5'	2.16	0.46
1:0:2256:G:O2'	1:0:2257:G:H5'	2.16	0.46
12:J:125:ALA:C	12:J:127:ALA:H	2.19	0.46
1:0:602:A:O2'	1:0:605:C:H4'	2.16	0.46
11:I:15:ARG:NH1	11:I:43:ARG:NH1	2.63	0.46
1:0:2847:G:O2'	1:0:2848:G:H5'	2.15	0.46
16:N:42:GLU:HB2	40:N:2176:HOH:O	2.16	0.46
20:R:81:ILE:HG22	23:U:29:ASN:OD1	2.16	0.46
1:0:1909:A:H2'	1:0:1910:A:C8	2.51	0.46
2:9:3102:G:O2'	2:9:3103:A:H5'	2.15	0.46
19:Q:29:LYS:NZ	40:Q:8945:HOH:O	2.49	0.46
4:B:175:LEU:C	4:B:175:LEU:HD23	2.36	0.46
13:K:73:VAL:HG23	13:K:74:THR:N	2.29	0.46
1:0:2251:G:H2'	1:0:2252:A:H8	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:W:43:VAL:CG1	25:W:44:ASP:N	2.78	0.46
1:0:820:G:H5'	1:0:821:U:H5'	1.97	0.46
1:0:2044:G:OP1	25:W:23:HIS:HE1	1.99	0.46
1:0:2815:G:OP2	11:I:99:GLU:HG2	2.15	0.46
3:A:217:ARG:HG3	40:A:9008:HOH:O	2.15	0.46
1:0:622:G:P	26:X:148:GLY:HA3	2.56	0.46
14:L:66:SER:HB3	14:L:128:TRP:CD1	2.51	0.46
1:0:1087:G:H4'	1:0:1088:A:OP1	2.16	0.46
11:I:103:VAL:HG12	40:I:5907:HOH:O	2.16	0.46
7:E:154:ILE:HG13	7:E:156:ASP:OD1	2.16	0.46
7:E:7:ILE:HG22	7:E:45:ASP:O	2.16	0.46
15:M:73:ALA:HB1	15:M:74:PRO:CD	2.46	0.46
1:0:613:C:H2'	1:0:614:U:C6	2.51	0.46
1:0:1056:U:H2'	1:0:1057:A:O4'	2.15	0.46
6:D:10:PHE:CD1	6:D:11:HIS:N	2.84	0.46
1:0:2692:G:HO2'	1:0:2693:U:P	2.39	0.46
11:I:56:LYS:HE2	11:I:60:ARG:NH2	2.31	0.46
1:0:1783:A:O2'	1:0:1784:U:H5'	2.16	0.46
1:0:526:U:H2'	1:0:527:U:C6	2.51	0.46
1:0:39:G:N2	1:0:444:C:C2	2.84	0.46
1:0:2842:G:C2'	1:0:2843:A:H5'	2.46	0.46
1:0:1544:U:H2'	1:0:1545:C:H6	1.81	0.46
6:D:27:ILE:HB	40:D:5858:HOH:O	2.16	0.46
8:F:58:GLU:HA	8:F:61:MET:CE	2.39	0.46
3:A:36:ASP:CB	3:A:85:SER:H	2.29	0.46
40:9:9090:HOH:O	24:V:13:MET:HA	2.14	0.46
23:U:8:ILE:CG2	23:U:59:ILE:HG13	2.46	0.46
13:K:133:VAL:HG13	40:K:8878:HOH:O	2.16	0.46
29:1:20:ARG:HG3	29:1:39:ARG:HH21	1.81	0.46
27:Y:42:CYS:SG	27:Y:44:GLU:HB2	2.56	0.46
2:9:3104:A:O2'	2:9:3105:A:H5'	2.16	0.46
1:0:834:G:H3'	1:0:835:U:H4'	1.97	0.46
12:J:101:ASN:O	12:J:102:GLU:HB2	2.16	0.46
23:U:5:VAL:HG11	23:U:9:ARG:NH1	2.31	0.46
21:S:111:ARG:HB3	21:S:119:ALA:HB2	1.98	0.46
1:0:2115:U:H2'	1:0:2116:U:C6	2.50	0.46
12:J:55:VAL:CG1	12:J:56:SER:N	2.78	0.45
4:B:36:PRO:CA	4:B:168:GLY:HA3	2.43	0.45
22:T:14:GLU:OE1	22:T:15:PRO:HD2	2.16	0.45
22:T:52:THR:HG22	22:T:54:THR:N	2.31	0.45
1:0:2362:A:H2'	1:0:2363:G:C8	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:876:A:C2'	1:0:876:A:N3	2.80	0.45
1:0:958:G:O2'	1:0:959:C:H5'	2.15	0.45
14:L:184:ARG:HG3	14:L:185:PRO:HA	1.98	0.45
6:D:27:ILE:HD11	6:D:37:ALA:CB	2.46	0.45
1:0:1942:A:H5'	3:A:233:THR:CB	2.46	0.45
1:0:559:C:H2'	1:0:560:C:O4'	2.17	0.45
1:0:1115:U:O2'	1:0:1116:U:H5'	2.16	0.45
1:0:283:U:H5"	1:0:284:C:P	2.56	0.45
6:D:38:GLU:OE2	6:D:51:ARG:CZ	2.64	0.45
8:F:117:GLU:C	8:F:119:ARG:N	2.69	0.45
29:1:36:ASN:O	29:1:39:ARG:HG3	2.16	0.45
1:0:1780:G:O2'	1:0:1781:G:H5'	2.16	0.45
15:M:22:GLN:HG2	15:M:26:LEU:HD22	1.97	0.45
19:Q:17:MET:CE	19:Q:19:ARG:NH2	2.79	0.45
16:N:26:TRP:CE3	16:N:26:TRP:HA	2.51	0.45
1:0:2385:G:H2'	1:0:2386:U:C6	2.51	0.45
1:0:2296:C:H2'	1:0:2297:U:H6	1.81	0.45
15:M:33:ARG:NH1	15:M:103:ASP:OD2	2.47	0.45
15:M:47:LEU:CD1	15:M:97:VAL:HG11	2.45	0.45
7:E:80:TRP:O	7:E:134:SER:HA	2.16	0.45
15:M:161:GLY:O	15:M:162:ASP:C	2.54	0.45
1:0:1406:A:H4'	1:0:1407:A:C5'	2.46	0.45
15:M:132:ASN:O	15:M:135:VAL:HG12	2.16	0.45
1:0:695:C:H2'	1:0:696:C:C6	2.51	0.45
24:V:55:GLY:CA	24:V:146:ILE:HG13	2.46	0.45
3:A:95:PRO:HA	3:A:153:ARG:HA	1.98	0.45
3:A:88:ILE:CD1	3:A:100:PRO:HD3	2.40	0.45
5:C:27:ARG:O	5:C:31:ILE:HG13	2.17	0.45
7:E:69:ILE:HA	7:E:72:MET:HE2	1.97	0.45
1:0:1080:C:O5'	1:0:1080:C:H6	1.99	0.45
1:0:512:G:O3'	1:0:513:A:C8	2.68	0.45
11:I:54:VAL:O	11:I:58:GLU:HG3	2.15	0.45
24:V:108:ARG:HE	24:V:114:PRO:HG3	1.82	0.45
1:0:326:G:O2'	1:0:327:A:H5'	2.16	0.45
1:0:1525:G:H5'	1:0:1526:A:OP2	2.16	0.45
10:H:83:TYR:C	10:H:83:TYR:CD1	2.90	0.45
15:M:37:ARG:HD3	15:M:37:ARG:HA	1.78	0.45
3:A:94:LEU:HG	3:A:99:ILE:CD1	2.47	0.45
1:0:2717:C:OP1	4:B:207:LYS:HG3	2.15	0.45
1:0:1377:C:H5'	1:0:1377:C:C6	2.47	0.45
19:Q:111:ILE:HG23	19:Q:145:LEU:CD1	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:L:66:SER:HB3	14:L:128:TRP:NE1	2.31	0.45
1:0:1799:G:H21	17:O:88:GLN:HE22	1.65	0.45
1:0:2578:G:H5'	1:0:2578:G:H8	1.81	0.45
4:B:264:GLU:HG2	4:B:267:LYS:CE	2.28	0.45
26:X:189:ASN:HD22	26:X:192:ASP:H	1.64	0.45
26:X:203:VAL:CG1	26:X:228:VAL:HG22	2.46	0.45
1:0:2769:C:C2'	1:0:2770:G:H5'	2.45	0.45
1:0:120:A:N3	1:0:120:A:H2'	2.32	0.45
7:E:101:GLU:OE2	7:E:115:ARG:HD3	2.16	0.45
3:A:186:TRP:CG	3:A:187:PRO:HA	2.52	0.45
1:0:920:C:H5"	1:0:921:G:O5'	2.17	0.45
8:F:28:ALA:HB3	8:F:99:THR:O	2.17	0.45
5:C:140:VAL:HG12	5:C:141:SER:N	2.31	0.45
1:0:710:G:O2'	1:0:711:G:H5'	2.15	0.45
1:0:1398:G:O4'	17:O:25:PRO:HG3	2.17	0.45
1:0:2032:U:H2'	1:0:2033:G:H5'	1.98	0.45
1:0:1314:U:H2'	40:0:6245:HOH:O	2.17	0.45
1:0:2809:G:H2'	1:0:2810:G:O4'	2.17	0.45
1:0:899:C:H5'	40:0:3638:HOH:O	2.17	0.45
1:0:1706:G:OP1	17:O:65:ARG:HD2	2.16	0.45
1:0:1902:G:H2'	1:0:1903:U:O4'	2.16	0.45
3:A:39:ALA:O	3:A:61:GLU:HG3	2.16	0.45
1:0:2121:G:O2'	1:0:2122:C:H5'	2.17	0.45
7:E:16:ASP:O	7:E:17:HIS:HB2	2.16	0.45
10:H:66:ARG:HD3	40:H:9029:HOH:O	2.17	0.45
1:0:2521:A:OP2	10:H:3:ALA:HB3	2.17	0.45
1:0:2415:A:H2'	1:0:2416:G:H5'	1.98	0.45
18:P:86:VAL:HG13	18:P:91:LEU:HD11	1.97	0.45
1:0:1679:C:O2'	1:0:1685:A:N1	2.46	0.45
1:0:708:A:H2'	1:0:709:G:O4'	2.17	0.45
1:0:2065:C:O2'	1:0:2066:C:H5'	2.17	0.45
1:0:128:A:O2'	1:0:129:A:H5'	2.17	0.45
21:S:53:GLY:HA3	40:S:6384:HOH:O	2.17	0.45
14:L:115:LEU:HD13	14:L:116:ASN:HB2	1.99	0.45
1:0:2011:A:H4'	1:0:2012:U:O5'	2.17	0.45
26:X:99:ALA:HB2	26:X:233:TYR:CZ	2.52	0.45
24:V:21:LEU:CD2	24:V:48:VAL:HG11	2.39	0.45
1:0:1119:G:N2	1:0:1246:A:N1	2.64	0.45
1:0:1641:A:H2'	1:0:1642:A:C5'	2.44	0.45
25:W:9:VAL:HG13	25:W:88:GLU:CD	2.37	0.45
6:D:10:PHE:CE1	6:D:11:HIS:HB3	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:H:136:ALA:HB3	10:H:146:VAL:HG21	1.97	0.45
16:N:26:TRP:HE3	16:N:26:TRP:HA	1.81	0.45
1:0:696:C:O2'	1:0:697:G:H5'	2.16	0.45
1:0:750:A:H2'	1:0:751:U:C6	2.51	0.45
1:0:1850:U:H2'	1:0:1851:G:H8	1.81	0.45
4:B:145:HIS:HD2	4:B:146:THR:O	1.99	0.45
1:0:333:G:O2'	1:0:334:G:H5'	2.17	0.45
25:W:75:ALA:O	25:W:83:ALA:HA	2.17	0.45
7:E:126:ILE:HB	7:E:131:LEU:HD23	1.99	0.45
24:V:48:VAL:CG1	24:V:48:VAL:O	2.65	0.45
1:0:2839:C:H2'	1:0:2840:A:H5"	1.99	0.45
2:9:3014:G:O2'	2:9:3015:C:H5'	2.16	0.45
4:B:314:ALA:CB	4:B:317:PRO:HG3	2.47	0.45
4:B:268:ARG:HH21	4:B:325:PRO:HG3	1.82	0.45
1:0:790:A:H2'	1:0:791:A:O4'	2.17	0.45
15:M:4:PRO:HD2	40:M:8859:HOH:O	2.16	0.45
40:0:6495:HOH:O	29:1:20:ARG:HB3	2.17	0.45
1:0:485:A:N3	1:0:487:G:H5"	2.31	0.45
4:B:75:GLU:C	4:B:77:PRO:HD3	2.36	0.45
13:K:24:ALA:HB2	13:K:30:ARG:HD2	1.99	0.45
6:D:41:LEU:CA	6:D:44:ILE:HG22	2.45	0.45
1:0:1192:A:O2'	1:0:1193:A:OP1	2.35	0.45
3:A:34:ASP:OD1	3:A:35:GLY:N	2.49	0.45
2:9:3028:U:H5"	15:M:40:ASN:ND2	2.32	0.45
5:C:162:VAL:HG13	5:C:232:LEU:HD21	2.00	0.45
2:9:3114:G:H2'	2:9:3115:C:C6	2.52	0.45
6:D:94:ALA:O	6:D:95:THR:O	2.34	0.45
1:0:396:U:H1'	40:0:7960:HOH:O	2.17	0.45
1:0:1836:A:H1'	28:Z:1:THR:O	2.17	0.45
1:0:2825:C:H4'	1:0:2826:G:O5'	2.17	0.45
1:0:407:A:H2'	1:0:408:A:C8	2.51	0.45
5:C:8:LEU:HD13	5:C:147:LEU:HD21	1.98	0.45
1:0:400:C:O2'	1:0:401:C:H5'	2.16	0.45
24:V:72:PRO:HG2	24:V:77:ALA:HB3	1.98	0.45
1:0:912:A:C4	1:0:1294:A:C2	3.04	0.45
5:C:51:TYR:CE2	28:Z:53:LYS:HB3	2.52	0.45
21:S:73:HIS:CD2	21:S:88:PRO:HG3	2.52	0.45
2:9:3049:G:H5"	40:M:8847:HOH:O	2.16	0.44
6:D:170:TYR:CD1	6:D:170:TYR:N	2.85	0.44
1:0:2416:G:O2'	15:M:25:ARG:HG2	2.17	0.44
15:M:42:HIS:CG	15:M:62:HIS:HE1	2.35	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:499:G:O2'	1:0:500:G:H5'	2.17	0.44
1:0:2314:G:H2'	1:0:2315:C:H5'	1.99	0.44
1:0:2776:A:H2'	1:0:2777:G:O4'	2.16	0.44
1:0:764:C:C2'	1:0:765:G:H5'	2.46	0.44
25:W:34:ARG:NH1	25:W:48:VAL:O	2.47	0.44
1:0:1803:C:H2'	1:0:1804:A:C8	2.52	0.44
1:0:1759:A:N3	1:0:1818:C:H2'	2.31	0.44
1:0:278:A:H2'	1:0:279:C:O4'	2.17	0.44
24:V:21:LEU:HD22	24:V:26:ILE:HD13	1.96	0.44
4:B:140:LEU:HD13	4:B:175:LEU:HA	1.98	0.44
25:W:41:PHE:O	25:W:43:VAL:HG23	2.17	0.44
17:O:16:VAL:HG12	17:O:17:GLY:N	2.32	0.44
1:0:661:G:C5	1:0:686:A:C2	3.06	0.44
30:2:3:MET:O	30:2:90:PHE:HA	2.16	0.44
19:Q:4:TYR:CZ	19:Q:15:LYS:HB3	2.52	0.44
3:A:17:ARG:HD2	40:A:9018:HOH:O	2.17	0.44
1:0:737:A:H2'	1:0:738:G:O4'	2.17	0.44
1:0:1372:A:H3'	40:0:7526:HOH:O	2.18	0.44
24:V:110:GLN:NE2	24:V:110:GLN:HA	2.32	0.44
6:D:104:PHE:CE2	6:D:166:ILE:CD1	3.00	0.44
10:H:46:GLN:HB3	10:H:167:ARG:H	1.83	0.44
6:D:19:GLU:O	6:D:133:ASN:HB3	2.18	0.44
15:M:48:VAL:HG11	15:M:55:ASP:HB3	1.98	0.44
24:V:64:THR:O	24:V:68:THR:HG22	2.17	0.44
1:0:2828:G:O2'	1:0:2829:G:H5'	2.17	0.44
4:B:258:GLY:N	4:B:260:HIS:CE1	2.81	0.44
10:H:28:ILE:HA	10:H:63:GLU:OE1	2.18	0.44
40:0:5354:HOH:O	10:H:58:ARG:HG3	2.17	0.44
1:0:137:U:OP1	1:0:259:G:O2'	2.34	0.44
1:0:447:A:OP1	21:S:2:LYS:HG2	2.17	0.44
24:V:35:VAL:HG23	24:V:41:TYR:CD2	2.52	0.44
1:0:2274:A:O2'	1:0:2275:G:H5'	2.17	0.44
8:F:84:GLY:O	8:F:89:LEU:HB2	2.17	0.44
1:0:541:C:H2'	1:0:542:A:H5'	1.99	0.44
1:0:2524:G:H21	1:0:2526:C:N4	2.15	0.44
7:E:101:GLU:HB2	7:E:116:THR:O	2.17	0.44
1:0:2883:A:H2'	1:0:2884:G:O4'	2.18	0.44
26:X:107:PRO:HB3	26:X:182:PHE:CE2	2.53	0.44
5:C:79:ARG:O	5:C:87:ARG:HG2	2.16	0.44
1:0:932:U:H2'	1:0:933:C:C6	2.53	0.44
1:0:758:A:H2'	1:0:759:C:O4'	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1213:C:O2'	1:0:1214:G:H5'	2.18	0.44
1:0:1657:A:H2'	1:0:1658:A:C8	2.53	0.44
1:0:1790:C:H2'	1:0:1791:U:H6	1.82	0.44
1:0:1994:A:P	12:J:66:ARG:HH22	2.41	0.44
5:C:21:VAL:HG13	40:C:8603:HOH:O	2.17	0.44
10:H:154:TYR:C	10:H:154:TYR:CD1	2.90	0.44
7:E:108:LEU:HB3	40:E:1306:HOH:O	2.16	0.44
1:0:1544:U:H2'	1:0:1545:C:C6	2.53	0.44
25:W:12:ILE:HD12	25:W:36:HIS:ND1	2.32	0.44
1:0:1321:A:H2'	1:0:1322:G:C8	2.53	0.44
1:0:1616:A:H2'	1:0:1618:G:C8	2.53	0.44
10:H:43:TYR:HA	10:H:44:PRO:HD3	1.80	0.44
13:K:145:LEU:HD23	13:K:145:LEU:O	2.18	0.44
1:0:1192:A:H3'	1:0:1193:A:H5'	1.99	0.44
24:V:26:ILE:HG13	24:V:26:ILE:O	2.18	0.44
1:0:523:C:H2'	1:0:524:A:C8	2.53	0.44
21:S:32:ARG:HH12	21:S:38:ARG:HH12	1.63	0.44
26:X:126:PRO:HG2	26:X:128:PHE:CZ	2.51	0.44
30:2:35:TRP:HA	30:2:38:ARG:NH1	2.32	0.44
19:Q:113:HIS:HE1	19:Q:144:GLU:CD	2.21	0.44
1:0:1422:U:H2'	1:0:1423:C:C6	2.53	0.44
1:0:952:G:N3	1:0:2302:A:H2'	2.32	0.44
11:I:13:ASP:OD1	11:I:15:ARG:HB3	2.17	0.44
1:0:2842:G:H2'	1:0:2843:A:H5'	2.00	0.44
1:0:1849:G:H1'	1:0:2011:A:N1	2.33	0.44
15:M:140:GLN:HA	15:M:143:ARG:HD3	1.99	0.44
8:F:49:PHE:HE1	8:F:98:VAL:HG23	1.83	0.44
1:0:1139:U:H2'	1:0:1140:C:C6	2.52	0.44
1:0:883:U:H5"	40:0:3248:HOH:O	2.17	0.44
1:0:2100:A:H5'	40:0:7723:HOH:O	2.17	0.44
3:A:72:GLU:HG3	27:Y:66:GLY:HA2	1.99	0.44
1:0:2857:C:H2'	1:0:2858:U:C6	2.53	0.44
10:H:28:ILE:HG23	40:H:9029:HOH:O	2.17	0.44
1:0:1476:A:O2'	1:0:1477:C:H5'	2.17	0.44
1:0:1284:G:O2'	1:0:1285:U:H5'	2.17	0.44
1:0:538:C:OP2	26:X:134:HIS:HE1	2.01	0.44
7:E:126:ILE:HB	7:E:131:LEU:CD2	2.48	0.44
14:L:64:ARG:HD2	40:L:8886:HOH:O	2.17	0.44
22:T:31:PHE:CG	22:T:37:GLU:HG2	2.52	0.44
21:S:71:VAL:HG13	21:S:91:LEU:O	2.18	0.44
3:A:93:THR:C	3:A:94:LEU:HD23	2.38	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:M:91:ARG:HG3	15:M:186:LEU:HD23	2.00	0.44
1:0:1667:A:H2'	1:0:1668:U:H6	1.82	0.44
1:0:926:A:O2'	13:K:41:HIS:HD2	2.00	0.44
1:0:204:A:H2'	1:0:205:U:H5'	2.00	0.44
1:0:605:C:H2'	1:0:606:C:C6	2.53	0.44
2:9:3103:A:O2'	2:9:3104:A:H5'	2.18	0.44
11:I:90:LYS:HB2	36:I:8802:CL:CL	2.55	0.44
1:0:2730:G:O2'	1:0:2731:G:H5'	2.18	0.44
6:D:159:PRO:O	6:D:163:VAL:HG23	2.17	0.44
1:0:1278:A:H4'	1:0:1279:U:C4	2.53	0.44
5:C:237:GLU:HB2	40:C:8637:HOH:O	2.18	0.44
2:9:3023:U:H6	2:9:3023:U:C5'	2.30	0.44
5:C:127:ARG:HG2	5:C:127:ARG:HH11	1.83	0.44
14:L:24:GLN:HE21	14:L:27:ARG:HH11	1.64	0.44
1:0:2462:G:O6	30:2:61:PRO:HG3	2.18	0.44
23:U:42:ASN:HB3	40:U:7247:HOH:O	2.18	0.44
1:0:821:U:H2'	1:0:822:C:C6	2.53	0.44
15:M:77:ASN:OD1	15:M:79:PRO:HD2	2.18	0.44
24:V:76:ASP:O	24:V:77:ALA:C	2.56	0.44
5:C:7:ASP:OD1	5:C:11:ASN:N	2.48	0.44
1:0:1199:A:H2'	1:0:1200:A:C8	2.52	0.44
1:0:1855:G:H4'	1:0:1856:C:O5'	2.18	0.44
4:B:232:TRP:CD1	4:B:235:ARG:HD2	2.52	0.44
2:9:3057:A:C8	6:D:141:VAL:HG21	2.53	0.43
15:M:154:LEU:HG	15:M:155:GLU:N	2.32	0.43
8:F:57:GLU:HB2	14:L:23:LEU:HD11	2.00	0.43
1:0:2443:C:H5'	13:K:57:VAL:HG21	1.99	0.43
20:R:42:GLU:HG2	20:R:49:VAL:HG23	1.99	0.43
1:0:1380:U:H5'	40:0:9699:HOH:O	2.17	0.43
1:0:295:C:O2'	1:0:296:G:H5'	2.17	0.43
1:0:2372:A:H2'	1:0:2373:U:C6	2.53	0.43
5:C:78:ARG:CG	5:C:78:ARG:NH1	2.72	0.43
1:0:1180:U:H2'	1:0:1181:A:O4'	2.18	0.43
1:0:1943:C:O4'	3:A:212:PRO:HA	2.18	0.43
3:A:36:ASP:O	3:A:38:ILE:N	2.51	0.43
4:B:305:ASP:O	4:B:306:LYS:CB	2.64	0.43
1:0:949:U:H4'	18:P:95:GLU:HA	2.00	0.43
4:B:266:ASN:OD1	4:B:317:PRO:HA	2.17	0.43
1:0:1044:C:H3'	1:0:1045:G:H5"	2.00	0.43
4:B:129:ARG:NH2	4:B:176:ASP:OD1	2.50	0.43
1:0:2032:U:H2'	1:0:2033:G:C5'	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2254:G:O2'	1:0:2255:A:H5'	2.18	0.43
1:0:2353:A:H4'	1:0:2354:A:O5'	2.17	0.43
6:D:104:PHE:CE2	6:D:166:ILE:HD13	2.52	0.43
19:Q:128:ARG:HB2	19:Q:132:ARG:O	2.19	0.43
12:J:81:ARG:HD3	12:J:87:ARG:NH1	2.32	0.43
3:A:132:ASP:OD1	3:A:133:ARG:N	2.49	0.43
6:D:173:GLU:O	6:D:174:VAL:C	2.56	0.43
1:0:709:G:O2'	16:N:25:VAL:CG1	2.66	0.43
4:B:232:TRP:HD1	4:B:235:ARG:HD2	1.82	0.43
1:0:1609:C:H2'	1:0:1610:G:C8	2.54	0.43
4:B:102:THR:HG21	4:B:182:VAL:O	2.17	0.43
3:A:110:SER:N	3:A:114:ASP:OD2	2.49	0.43
11:I:74:ARG:HH12	11:I:76:ASP:HB2	1.79	0.43
1:0:1119:G:N2	1:0:1246:A:H2	2.09	0.43
11:I:46:ILE:HD11	11:I:53:ILE:HG23	2.00	0.43
13:K:144:ASP:O	13:K:147:GLU:HB2	2.19	0.43
15:M:166:ALA:O	15:M:167:ASP:O	2.35	0.43
1:0:1682:A:H2'	40:0:3244:HOH:O	2.19	0.43
24:V:11:VAL:O	24:V:12:ASN:HB2	2.17	0.43
1:0:848:C:H2'	1:0:849:C:C6	2.53	0.43
1:0:848:C:H5'	40:0:7610:HOH:O	2.19	0.43
1:0:2610:U:H4'	40:0:4172:HOH:O	2.18	0.43
1:0:2004:U:H4'	40:0:5688:HOH:O	2.17	0.43
4:B:60:SER:HA	4:B:61:PRO:HD3	1.87	0.43
1:0:2133:U:H4'	1:0:2134:G:H5'	1.99	0.43
24:V:122:ARG:NH2	40:V:4276:HOH:O	2.48	0.43
40:0:4762:HOH:O	3:A:212:PRO:HB2	2.19	0.43
28:Z:25:LYS:O	28:Z:25:LYS:HG2	2.19	0.43
26:X:187:VAL:HG12	26:X:205:ILE:HA	2.01	0.43
2:9:3007:G:H4'	15:M:55:ASP:OD2	2.18	0.43
2:9:3007:G:H5'	40:9:9094:HOH:O	2.18	0.43
1:0:1268:C:O2'	26:X:169:ARG:HB2	2.18	0.43
20:R:29:ASP:OD1	20:R:31:ARG:HG3	2.19	0.43
1:0:830:G:O2'	1:0:831:U:H5'	2.18	0.43
1:0:202:U:O2'	1:0:203:G:H5'	2.18	0.43
2:9:3034:A:H1'	15:M:153:GLN:HE22	1.84	0.43
1:0:90:A:H2'	1:0:91:G:O4'	2.18	0.43
1:0:2656:G:O2'	1:0:2657:G:H5'	2.18	0.43
27:Y:75:GLY:O	27:Y:78:THR:HB	2.18	0.43
40:0:6722:HOH:O	3:A:205:GLY:HA3	2.19	0.43
10:H:51:VAL:HG21	10:H:127:VAL:HG11	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:0:4589:HOH:O	5:C:76:ARG:HD3	2.18	0.43
1:0:1183:C:N4	1:0:1184:C:N4	2.64	0.43
1:0:1669:A:H2'	1:0:1670:G:H8	1.82	0.43
1:0:747:G:H2'	1:0:748:C:C6	2.54	0.43
1:0:1850:U:H2'	1:0:1851:G:C8	2.52	0.43
1:0:1677:U:OP2	29:1:8:LYS:NZ	2.49	0.43
18:P:66:LYS:HB2	18:P:70:ALA:O	2.19	0.43
1:0:1444:G:O2'	1:0:1502:A:N1	2.45	0.43
1:0:569:A:H5"	1:0:587:A:N1	2.34	0.43
12:J:118:ALA:C	12:J:120:ARG:H	2.22	0.43
1:0:712:C:O2'	1:0:713:U:H2'	2.19	0.43
1:0:1816:C:H2'	1:0:1817:U:O4'	2.19	0.43
1:0:816:G:C6	1:0:817:G:N1	2.87	0.43
29:1:48:ASP:O	29:1:49:GLU:CB	2.66	0.43
15:M:5:ARG:HG3	18:P:18:PRO:CB	2.48	0.43
30:2:73:GLU:HB2	40:2:8957:HOH:O	2.18	0.43
1:0:2515:C:O2'	1:0:2516:G:H5'	2.19	0.43
1:0:2896:A:H5"	40:0:6464:HOH:O	2.18	0.43
1:0:1470:A:OP1	14:L:93:ARG:HD2	2.18	0.43
1:0:2597:U:H2'	1:0:2598:U:H5'	1.99	0.43
1:0:2727:A:H2'	1:0:2728:C:H5'	2.00	0.43
1:0:24:G:N2	1:0:518:G:H1'	2.33	0.43
5:C:49:ASP:HB3	5:C:52:ALA:HB2	2.01	0.43
1:0:451:C:O2'	1:0:452:G:H5'	2.18	0.43
3:A:26:ASP:O	3:A:26:ASP:OD1	2.36	0.43
40:0:7789:HOH:O	4:B:211:THR:HG21	2.18	0.43
3:A:103:VAL:O	3:A:105:VAL:HG23	2.18	0.43
4:B:7:ARG:CG	4:B:7:ARG:NH1	2.82	0.43
30:2:65:THR:HB	30:2:83:TRP:H	1.84	0.43
1:0:1945:G:O2'	1:0:1946:C:H5'	2.19	0.43
22:T:52:THR:CG2	22:T:54:THR:HB	2.49	0.43
1:0:858:U:H2'	1:0:859:C:H6	1.84	0.43
1:0:2385:G:H2'	1:0:2386:U:H6	1.83	0.43
1:0:2786:G:H2'	40:0:7524:HOH:O	2.17	0.43
1:0:2326:U:H4'	1:0:2412:G:H4'	2.00	0.43
22:T:13:ILE:HG12	22:T:32:CYS:HB3	2.00	0.43
1:0:806:A:H2'	1:0:807:A:O4'	2.19	0.43
1:0:2505:G:HO2'	1:0:2506:A:H5'	1.83	0.43
28:Z:25:LYS:HD2	29:1:48:ASP:HA	2.01	0.43
1:0:1834:C:H2'	1:0:1840:A:N6	2.34	0.43
4:B:258:GLY:HA2	40:B:9029:HOH:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:307:ARG:CG	4:B:307:ARG:NH1	2.80	0.43
1:0:539:G:H2'	1:0:540:A:C8	2.54	0.43
6:D:58:VAL:CG1	6:D:59:GLY:N	2.82	0.43
1:0:1362:U:H2'	1:0:1363:G:H8	1.83	0.43
4:B:115:VAL:HA	4:B:116:PRO:HD3	1.78	0.43
1:0:125:U:H2'	40:0:4182:HOH:O	2.18	0.43
1:0:1142:C:O2'	1:0:1143:G:H5'	2.19	0.43
16:N:29:VAL:O	16:N:33:LEU:HG	2.19	0.43
1:0:177:A:H2'	1:0:178:U:O4'	2.18	0.43
11:I:93:ARG:HB3	11:I:93:ARG:NH1	2.20	0.43
4:B:41:PHE:HB3	4:B:190:MET:HE1	2.01	0.43
1:0:283:U:H5"	1:0:284:C:OP2	2.19	0.43
6:D:49:PRO:HG3	40:D:5828:HOH:O	2.17	0.43
7:E:101:GLU:CB	7:E:117:THR:HA	2.49	0.43
30:2:74:CYS:N	40:2:8990:HOH:O	2.52	0.43
1:0:553:G:H5'	40:0:3929:HOH:O	2.19	0.43
4:B:215:VAL:HA	4:B:220:VAL:HG22	2.01	0.43
1:0:1609:C:H2'	1:0:1610:G:H8	1.84	0.43
3:A:80:LEU:HD22	3:A:91:GLY:O	2.19	0.43
1:0:1503:U:H2'	1:0:1504:A:O4'	2.18	0.43
7:E:86:VAL:CG1	7:E:129:GLU:HA	2.48	0.43
1:0:2015:A:H2'	1:0:2016:U:O4'	2.19	0.43
1:0:1829:A:C2'	1:0:1830:C:H5'	2.48	0.43
1:0:1280:A:H3'	1:0:1280:A:OP1	2.18	0.43
1:0:2507:G:H2'	1:0:2510:C:N4	2.33	0.42
7:E:20:ILE:CD1	7:E:33:LEU:HD12	2.49	0.42
15:M:152:GLU:C	15:M:154:LEU:N	2.71	0.42
7:E:11:VAL:HG13	7:E:23:GLU:O	2.19	0.42
4:B:154:VAL:HA	4:B:155:PRO:HD3	1.87	0.42
13:K:133:VAL:HB	40:K:8861:HOH:O	2.18	0.42
8:F:33:THR:HG21	8:F:59:ILE:O	2.19	0.42
15:M:141:ARG:HB3	40:M:8868:HOH:O	2.19	0.42
1:0:2781:U:O2'	1:0:2782:G:H5'	2.19	0.42
1:0:1947:G:H2'	1:0:1948:G:C8	2.53	0.42
1:0:947:U:H2'	1:0:948:G:H8	1.83	0.42
16:N:26:TRP:HB2	40:N:3062:HOH:O	2.19	0.42
3:A:39:ALA:HB3	3:A:61:GLU:OE2	2.19	0.42
28:Z:53:LYS:HA	28:Z:53:LYS:HD3	1.85	0.42
1:0:491:C:O2'	1:0:492:C:H5'	2.19	0.42
18:P:3:SER:HB3	40:P:5998:HOH:O	2.19	0.42
1:0:1512:G:O2'	1:0:1513:C:H5'	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:36:ASP:CB	3:A:83:GLY:HA3	2.49	0.42
11:I:131:THR:HB	11:I:134:GLU:HG3	2.01	0.42
15:M:25:ARG:HA	15:M:28:LYS:HG3	2.00	0.42
1:0:1234:U:C4	4:B:244:PRO:HB3	2.54	0.42
7:E:11:VAL:CG1	7:E:22:VAL:HG13	2.49	0.42
7:E:7:ILE:HA	7:E:8:PRO:HD3	1.92	0.42
15:M:163:PHE:O	15:M:164:ASP:O	2.37	0.42
1:0:1419:U:H5'	1:0:1420:C:OP2	2.19	0.42
1:0:1679:C:H5'	40:0:9791:HOH:O	2.19	0.42
10:H:38:LYS:HE2	10:H:42:ASP:CB	2.50	0.42
1:0:1909:A:N1	1:0:2128:G:H1'	2.34	0.42
1:0:1399:A:H2'	1:0:1400:C:C6	2.55	0.42
19:Q:82:GLU:O	19:Q:86:LYS:HG3	2.19	0.42
1:0:2382:A:O2'	1:0:2383:G:H5'	2.20	0.42
19:Q:12:THR:HG22	19:Q:149:GLU:OE1	2.19	0.42
2:9:3025:G:C2'	2:9:3026:C:H5'	2.49	0.42
24:V:88:THR:CG2	24:V:90:TYR:HD1	2.31	0.42
1:0:541:C:C2'	1:0:542:A:C5'	2.85	0.42
3:A:192:VAL:HG13	40:A:9032:HOH:O	2.19	0.42
26:X:151:SER:HB3	26:X:154:ARG:HB3	2.02	0.42
4:B:62:ARG:CA	4:B:65:MET:HE3	2.49	0.42
15:M:86:LEU:O	15:M:90:LEU:HG	2.20	0.42
1:0:694:A:H2'	1:0:695:C:H5'	2.00	0.42
1:0:2004:U:H2'	1:0:2004:U:O2	2.18	0.42
1:0:789:C:H1'	1:0:827:A:C2	2.53	0.42
1:0:414:C:H5'	40:0:3106:HOH:O	2.19	0.42
24:V:82:GLU:O	24:V:86:GLU:HG3	2.20	0.42
1:0:2784:A:H1'	7:E:60:SER:OG	2.18	0.42
3:A:9:ARG:HG2	3:A:16:PHE:CD2	2.55	0.42
1:0:2716:G:C5'	4:B:206:THR:HG21	2.45	0.42
1:0:1819:G:H5'	40:0:6189:HOH:O	2.18	0.42
30:2:18:GLN:OE1	30:2:73:GLU:HB3	2.20	0.42
4:B:27:ASN:H	4:B:27:ASN:HD22	1.66	0.42
1:0:255:A:H2'	1:0:256:C:C6	2.54	0.42
1:0:703:G:O2'	1:0:704:C:H5'	2.19	0.42
26:X:99:ALA:HB2	26:X:233:TYR:CE2	2.54	0.42
22:T:34:SER:HA	22:T:37:GLU:OE1	2.20	0.42
1:0:757:C:OP1	13:K:27:ARG:HD2	2.19	0.42
1:0:669:G:O2'	1:0:670:G:H5'	2.20	0.42
1:0:494:C:H2'	1:0:496:G:OP2	2.19	0.42
1:0:872:U:O2'	1:0:873:G:H5'	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:383:A:H4'	40:0:5709:HOH:O	2.19	0.42
3:A:173:GLY:O	3:A:176:HIS:HB3	2.19	0.42
16:N:15:LYS:HD3	16:N:19:ARG:NH2	2.34	0.42
22:T:20:MET:CG	22:T:28:THR:HG23	2.49	0.42
6:D:18:ILE:HD13	6:D:84:LEU:HD12	2.02	0.42
25:W:70:ILE:O	25:W:70:ILE:HG23	2.19	0.42
23:U:12:THR:OG1	23:U:13:PRO:HD2	2.19	0.42
6:D:99:ASP:HB3	6:D:103:ASN:H	1.83	0.42
3:A:130:THR:HG22	3:A:131:HIS:O	2.19	0.42
7:E:11:VAL:CG1	7:E:12:ASP:N	2.82	0.42
15:M:184:ILE:HG22	15:M:185:GLU:H	1.84	0.42
1:0:631:A:C6	1:0:2074:A:H5'	2.55	0.42
4:B:279:THR:CG2	4:B:280:VAL:N	2.83	0.42
2:9:3002:U:OP2	2:9:3003:A:H5'	2.20	0.42
15:M:108:SER:HA	15:M:109:PRO:HD3	1.75	0.42
10:H:38:LYS:O	10:H:84:LYS:HE2	2.20	0.42
1:0:191:A:C4	1:0:237:G:N7	2.88	0.42
1:0:1565:C:H2'	1:0:1566:C:H6	1.83	0.42
13:K:34:GLY:HA3	13:K:38:HIS:CE1	2.55	0.42
1:0:1039:G:H2'	1:0:1040:A:O4'	2.20	0.42
7:E:9:GLU:HA	40:E:5240:HOH:O	2.19	0.42
1:0:1257:C:O2'	1:0:1258:G:H5'	2.20	0.42
1:0:2758:G:H2'	1:0:2759:C:C6	2.55	0.42
6:D:167:GLU:C	6:D:169:THR:H	2.23	0.42
7:E:20:ILE:HD12	7:E:33:LEU:HD12	2.01	0.42
2:9:3093:A:C5	2:9:3094:G:H1'	2.55	0.42
1:0:1730:G:H5"	1:0:1731:C:H6	1.85	0.42
3:A:27:LEU:HD21	3:A:55:VAL:HG21	2.01	0.42
13:K:145:LEU:O	13:K:148:GLU:HG3	2.20	0.42
5:C:7:ASP:OD2	5:C:9:ASP:HB2	2.19	0.42
8:F:56:PRO:HG2	14:L:43:PRO:O	2.19	0.42
1:0:347:A:O2'	1:0:348:C:H5'	2.19	0.42
1:0:1537:C:H1'	40:0:6946:HOH:O	2.19	0.42
1:0:317:A:H5"	21:S:52:ARG:HD2	2.02	0.42
4:B:294:TYR:HE2	40:B:9129:HOH:O	2.03	0.42
1:0:100:C:O2	21:S:17:HIS:HB3	2.19	0.42
40:9:9105:HOH:O	15:M:115:VAL:HG13	2.18	0.42
1:0:560:C:H2'	1:0:561:G:C8	2.54	0.42
1:0:272:A:H3'	40:0:7862:HOH:O	2.19	0.42
16:N:81:PHE:N	16:N:81:PHE:CD1	2.87	0.42
24:V:108:ARG:HE	24:V:114:PRO:CG	2.32	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:682:A:H2'	1:0:683:G:O4'	2.19	0.42
40:0:7810:HOH:O	14:L:55:LYS:HE2	2.19	0.42
20:R:30:ASP:HA	20:R:62:LYS:HE3	2.01	0.42
1:0:1644:C:O2'	1:0:1645:U:H5'	2.20	0.42
1:0:1552:G:H2'	1:0:1553:C:C6	2.55	0.42
1:0:646:G:H2'	1:0:647:U:C6	2.55	0.42
7:E:132:THR:O	7:E:132:THR:HG23	2.19	0.42
10:H:167:ARG:CG	40:H:8990:HOH:O	2.67	0.42
11:I:42:GLU:O	11:I:131:THR:HG23	2.19	0.42
24:V:65:VAL:CG1	24:V:116:LEU:HD13	2.49	0.42
1:0:1666:C:C2'	1:0:1667:A:C5'	2.97	0.42
1:0:308:U:H5'	21:S:97:ARG:HH21	1.83	0.42
25:W:14:LEU:HD12	25:W:67:PRO:O	2.19	0.42
1:0:1205:U:H2'	1:0:1206:U:C5'	2.50	0.42
1:0:2433:A:H2'	1:0:2434:A:C8	2.54	0.42
1:0:514:G:H5'	40:0:7435:HOH:O	2.20	0.42
1:0:1516:C:H2'	1:0:1517:U:C6	2.55	0.42
12:J:99:ASP:OD1	12:J:101:ASN:N	2.52	0.42
13:K:148:GLU:HA	40:K:8877:HOH:O	2.19	0.42
1:0:683:G:O2'	1:0:684:G:H5'	2.20	0.42
1:0:1979:G:H2'	40:0:3730:HOH:O	2.20	0.42
16:N:21:SER:HB2	16:N:106:PRO:O	2.20	0.42
6:D:92:GLU:O	6:D:93:LEU:O	2.37	0.42
1:0:1555:G:H4'	1:0:1630:A:H2	1.84	0.42
5:C:127:ARG:HG2	5:C:127:ARG:NH1	2.34	0.42
24:V:52:VAL:HG13	24:V:53:ALA:N	2.34	0.42
6:D:35:ALA:C	6:D:37:ALA:N	2.73	0.42
8:F:61:MET:HB3	14:L:19:GLN:OE1	2.19	0.42
1:0:1244:U:H4'	1:0:1246:A:O4'	2.20	0.42
1:0:86:A:C2	29:1:25:VAL:HG13	2.55	0.42
1:0:259:G:O2'	1:0:260:C:H5'	2.20	0.42
14:L:61:ILE:N	14:L:61:ILE:HD12	2.35	0.42
29:1:36:ASN:HB3	29:1:39:ARG:NE	2.34	0.42
1:0:710:G:H5'	16:N:25:VAL:HG13	2.02	0.42
22:T:37:GLU:HB3	40:T:408:HOH:O	2.19	0.42
12:J:118:ALA:O	12:J:120:ARG:N	2.53	0.42
1:0:1847:A:OP1	3:A:175:LYS:HG3	2.19	0.42
1:0:74:A:H2'	1:0:75:U:C6	2.54	0.42
10:H:88:ARG:NH1	10:H:135:THR:OG1	2.51	0.42
13:K:79:ASP:HB3	40:K:8862:HOH:O	2.20	0.42
1:0:922:A:N7	1:0:2281:C:H5'	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:X:116:LEU:HD12	26:X:173:ALA:HB3	2.01	0.42
4:B:185:GLY:HA2	40:B:9112:HOH:O	2.19	0.42
26:X:144:ARG:NE	40:X:8914:HOH:O	2.53	0.42
15:M:58:LEU:HD12	15:M:58:LEU:N	2.35	0.42
1:0:1845:A:O2'	1:0:1846:U:H5'	2.19	0.42
1:0:815:U:O2'	1:0:1598:A:H4'	2.19	0.42
24:V:119:HIS:CD2	24:V:120:PRO:HD2	2.55	0.42
1:0:696:C:HO2'	1:0:697:G:H5'	1.84	0.42
1:0:764:C:O2'	1:0:765:G:H5'	2.19	0.42
1:0:660:A:H4'	1:0:661:G:O5'	2.20	0.42
1:0:1829:A:H5"	40:0:3517:HOH:O	2.19	0.42
1:0:329:A:OP2	5:C:206:ASN:HB2	2.19	0.42
24:V:128:VAL:O	24:V:138:LEU:HD11	2.20	0.42
18:P:75:ILE:CD1	18:P:84:ILE:HD11	2.50	0.42
1:0:2464:C:H5"	1:0:2465:A:OP1	2.19	0.42
1:0:1724:U:H5"	40:0:4151:HOH:O	2.19	0.42
1:0:1171:A:H2'	1:0:1172:G:H5'	2.02	0.41
1:0:2064:U:H5'	1:0:2652:U:O3'	2.20	0.41
1:0:677:C:H4'	5:C:246:ARG:NH2	2.35	0.41
1:0:1299:G:N2	40:0:5073:HOH:O	2.52	0.41
4:B:254:GLN:HG2	4:B:255:GLY:H	1.85	0.41
1:0:314:G:N2	1:0:316:A:H3'	2.34	0.41
1:0:1400:C:O2'	1:0:1401:G:H5'	2.20	0.41
1:0:2281:C:C2'	1:0:2282:U:H5'	2.49	0.41
1:0:752:G:H2'	1:0:753:U:O4'	2.20	0.41
8:F:26:THR:HG21	8:F:103:GLU:HG3	2.01	0.41
12:J:22:ASP:O	12:J:110:LYS:HE3	2.20	0.41
4:B:158:LYS:HB2	40:B:9036:HOH:O	2.19	0.41
24:V:85:ALA:HB2	24:V:91:ASP:O	2.19	0.41
1:0:2661:U:H3	1:0:2812:A:H62	1.68	0.41
30:2:70:ARG:NH1	30:2:70:ARG:HG2	2.35	0.41
4:B:217:ARG:HG3	4:B:257:THR:CG2	2.51	0.41
1:0:2890:A:C4	22:T:56:ARG:CZ	3.03	0.41
15:M:73:ALA:HB1	15:M:74:PRO:HD2	2.01	0.41
26:X:106:THR:CG2	26:X:107:PRO:HD2	2.51	0.41
7:E:84:MET:HG2	7:E:168:ILE:HA	2.01	0.41
1:0:1407:A:O2'	1:0:1408:U:H3'	2.20	0.41
1:0:764:C:H2'	1:0:765:G:O4'	2.20	0.41
1:0:1393:A:H2'	1:0:1394:C:C6	2.55	0.41
1:0:941:G:C5	1:0:942:U:C4	3.09	0.41
19:Q:47:LEU:O	19:Q:51:ILE:HG13	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2453:G:H4'	13:K:50:GLY:C	2.40	0.41
1:0:566:A:H2'	1:0:567:U:O4'	2.20	0.41
14:L:46:LEU:HD22	14:L:50:ARG:HG3	2.02	0.41
1:0:47:G:N3	1:0:114:A:C2	2.89	0.41
23:U:43:PRO:O	23:U:46:ILE:HG22	2.19	0.41
24:V:139:GLY:O	24:V:141:HIS:CD2	2.71	0.41
14:L:164:THR:HB	40:L:8819:HOH:O	2.20	0.41
24:V:65:VAL:HA	24:V:68:THR:CG2	2.49	0.41
17:O:80:ARG:HG2	17:O:87:ARG:NH2	2.34	0.41
3:A:128:LEU:HG	40:A:9046:HOH:O	2.19	0.41
1:0:1171:A:C2'	1:0:1172:G:H5'	2.51	0.41
1:0:1184:C:H1'	40:0:7798:HOH:O	2.19	0.41
7:E:23:GLU:HG2	7:E:28:SER:CB	2.49	0.41
25:W:30:MET:CE	25:W:58:ALA:HB3	2.50	0.41
27:Y:46:ARG:HD2	27:Y:59:TYR:HB2	2.03	0.41
23:U:29:ASN:O	23:U:33:VAL:HG23	2.20	0.41
14:L:159:VAL:HG13	14:L:160:PHE:N	2.35	0.41
1:0:1311:G:C2	1:0:1312:G:C8	3.09	0.41
2:9:3098:C:O2'	2:9:3099:U:H5'	2.20	0.41
1:0:638:C:H2'	1:0:639:A:C8	2.55	0.41
1:0:1367:A:H2'	1:0:1368:U:O4'	2.20	0.41
12:J:14:LYS:HG3	12:J:32:ILE:O	2.20	0.41
1:0:1173:A:H2'	40:0:4746:HOH:O	2.20	0.41
1:0:559:C:N4	1:0:598:C:H42	2.19	0.41
3:A:103:VAL:HA	3:A:104:PRO:HD3	1.94	0.41
1:0:1845:A:OP2	3:A:190:ARG:NH1	2.54	0.41
14:L:69:LYS:O	14:L:73:ARG:NH2	2.42	0.41
10:H:54:THR:O	10:H:55:VAL:CG1	2.67	0.41
22:T:52:THR:HG22	22:T:54:THR:HB	2.02	0.41
1:0:170:U:H2'	1:0:171:C:H5'	2.01	0.41
1:0:1565:C:O4'	1:0:2738:G:H1'	2.20	0.41
40:0:4960:HOH:O	5:C:50:GLU:HG2	2.19	0.41
1:0:1966:U:H2'	1:0:1967:U:C6	2.54	0.41
9:G:14:GLU:HB3	40:G:4173:HOH:O	2.20	0.41
13:K:117:GLU:HA	40:K:8855:HOH:O	2.20	0.41
1:0:1245:C:O5'	1:0:1245:C:H6	2.03	0.41
40:0:7365:HOH:O	3:A:211:LYS:HG2	2.20	0.41
15:M:91:ARG:HG3	15:M:186:LEU:CD2	2.50	0.41
40:0:7890:HOH:O	30:2:61:PRO:HG2	2.21	0.41
1:0:2266:A:H2'	1:0:2267:G:C8	2.56	0.41
17:O:16:VAL:HG12	17:O:20:ARG:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2335:C:H2'	1:0:2336:G:H8	1.85	0.41
1:0:2032:U:O2'	1:0:2033:G:H5"	2.20	0.41
1:0:755:G:O2'	1:0:756:A:H5'	2.21	0.41
1:0:1051:C:H2'	1:0:1052:G:O4'	2.21	0.41
1:0:297:U:H2'	1:0:298:C:C6	2.56	0.41
1:0:1520:G:H2'	1:0:1521:C:C6	2.55	0.41
20:R:73:ASP:OD1	20:R:76:GLU:HG3	2.20	0.41
1:0:1453:G:H2'	1:0:1454:U:O4'	2.20	0.41
1:0:1119:G:H2'	11:I:52:GLN:HE22	1.83	0.41
21:S:49:GLU:HB3	21:S:59:GLU:CG	2.50	0.41
3:A:48:ASP:HA	3:A:49:PRO:HD3	1.91	0.41
1:0:2819:C:O4'	4:B:96:PRO:HB2	2.20	0.41
1:0:88:G:N3	29:1:24:TRP:HB2	2.36	0.41
8:F:59:ILE:HD11	40:L:8924:HOH:O	2.21	0.41
1:0:631:A:N3	1:0:2073:G:O2'	2.49	0.41
1:0:2103:A:N7	1:0:2538:A:N6	2.68	0.41
10:H:9:ILE:HD12	10:H:54:THR:HG22	2.03	0.41
1:0:1335:C:H2'	1:0:1336:U:H6	1.84	0.41
1:0:2689:A:C2'	1:0:2690:U:H5'	2.50	0.41
1:0:1705:C:H2'	1:0:1706:G:O4'	2.20	0.41
1:0:1804:A:H2'	1:0:1805:G:C8	2.55	0.41
30:2:3:MET:HG3	30:2:4:PRO:HD2	2.03	0.41
22:T:33:SER:O	22:T:37:GLU:HG3	2.20	0.41
1:0:2729:C:O2'	1:0:2730:G:H5'	2.20	0.41
6:D:93:LEU:HG	40:D:3862:HOH:O	2.20	0.41
1:0:1588:G:C6	1:0:1589:G:N1	2.88	0.41
5:C:84:VAL:O	5:C:85:LYS:HB2	2.21	0.41
1:0:324:G:O2'	1:0:325:U:H5'	2.21	0.41
1:0:2406:U:O2'	1:0:2407:G:H5'	2.20	0.41
1:0:2765:C:H2'	1:0:2766:A:C8	2.56	0.41
1:0:1119:G:H8	11:I:52:GLN:NE2	2.18	0.41
1:0:2502:C:O3'	10:H:151:ARG:NH2	2.54	0.41
1:0:2842:G:H2'	1:0:2843:A:C5'	2.50	0.41
1:0:1138:G:H2'	1:0:1139:U:O4'	2.21	0.41
1:0:1279:U:H2'	1:0:1279:U:O2	2.19	0.41
1:0:2783:A:H2'	1:0:2784:A:C8	2.55	0.41
1:0:73:C:O2'	1:0:74:A:H5'	2.21	0.41
1:0:671:A:O2'	1:0:672:G:H2'	2.21	0.41
7:E:102:VAL:HG11	7:E:148:ILE:HD11	2.03	0.41
23:U:45:ARG:C	23:U:47:LYS:N	2.71	0.41
23:U:1:THR:CG2	23:U:2:VAL:N	2.82	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:L:59:GLY:HA3	14:L:141:ILE:HD12	2.02	0.41
1:0:2502:C:H2'	1:0:2503:A:C5'	2.49	0.41
1:0:2502:C:O2'	1:0:2503:A:H5'	2.21	0.41
2:9:3020:G:H3'	40:9:9055:HOH:O	2.20	0.41
1:0:2837:U:H2'	40:0:7186:HOH:O	2.20	0.41
1:0:396:U:OP2	30:2:38:ARG:NH1	2.54	0.41
1:0:2756:U:O2	1:0:2896:A:H2	2.03	0.41
25:W:43:VAL:CG1	25:W:47:ALA:HB3	2.51	0.41
17:O:16:VAL:HG13	17:O:20:ARG:NH1	2.35	0.41
5:C:21:VAL:HG23	5:C:22:PHE:CD1	2.56	0.41
2:9:3031:C:O2'	2:9:3032:G:H5'	2.20	0.41
40:0:4806:HOH:O	3:A:11:ARG:NE	2.53	0.41
1:0:2741:A:H2'	1:0:2742:G:O4'	2.21	0.41
1:0:1557:G:O2'	1:0:1558:C:H5'	2.21	0.41
1:0:1165:G:O2'	1:0:1166:A:OP1	2.36	0.41
29:1:10:ARG:HH11	29:1:49:GLU:CD	2.24	0.41
1:0:1246:A:O2'	1:0:1247:A:H3'	2.21	0.41
11:I:45:VAL:CG2	11:I:129:PHE:HD1	2.33	0.41
13:K:121:ILE:HA	13:K:141:GLU:O	2.21	0.41
17:O:59:ARG:HH22	17:O:66:GLN:NE2	2.15	0.41
11:I:107:ASN:ND2	11:I:107:ASN:C	2.74	0.41
4:B:62:ARG:HA	4:B:65:MET:HE2	1.98	0.41
4:B:243:ASN:HA	4:B:244:PRO:C	2.40	0.41
1:0:1477:C:H2'	1:0:1478:U:C6	2.56	0.41
1:0:1787:C:H4'	1:0:2883:A:O4'	2.21	0.41
23:U:42:ASN:O	23:U:44:GLY:N	2.54	0.41
15:M:79:PRO:HG3	15:M:142:THR:O	2.21	0.41
1:0:1634:G:H2'	1:0:1635:U:C6	2.56	0.41
1:0:161:A:H2'	1:0:162:C:C6	2.55	0.41
11:I:54:VAL:HG11	11:I:138:THR:HG21	2.03	0.41
13:K:148:GLU:HB2	40:K:8894:HOH:O	2.20	0.41
1:0:1856:C:H5'	1:0:1858:A:O4'	2.21	0.41
40:0:7341:HOH:O	18:P:9:GLY:HA2	2.21	0.41
1:0:1123:A:C2	1:0:1129:C:H4'	2.56	0.41
1:0:2471:G:N3	1:0:2633:A:H2	2.18	0.41
1:0:1110:G:O2'	1:0:1111:U:H5'	2.20	0.41
1:0:862:U:H5'	40:0:7614:HOH:O	2.21	0.41
1:0:2055:A:H5'	19:Q:134:SER:HB2	2.03	0.41
28:Z:8:GLN:HE22	28:Z:11:LYS:NZ	2.18	0.41
15:M:38:LYS:HE3	15:M:38:LYS:HB2	1.78	0.41
1:0:1666:C:O2'	1:0:1667:A:C5'	2.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:53:LEU:HD21	4:B:270:ILE:HD12	2.03	0.41
40:0:5005:HOH:O	16:N:39:THR:HB	2.20	0.41
1:0:1730:G:H5'	1:0:1731:C:H5	1.85	0.41
1:0:1596:U:H2'	1:0:1598:A:OP2	2.21	0.41
28:Z:28:HIS:CD2	28:Z:31:LYS:H	2.39	0.41
1:0:855:U:H4'	1:0:856:G:O4'	2.20	0.41
23:U:5:VAL:CG1	23:U:9:ARG:NH1	2.84	0.41
40:0:4806:HOH:O	3:A:11:ARG:CZ	2.68	0.41
1:0:2724:U:H2'	1:0:2725:G:O4'	2.21	0.41
13:K:72:ASN:HB2	40:K:8886:HOH:O	2.20	0.41
40:0:3338:HOH:O	11:I:46:ILE:HA	2.22	0.40
13:K:66:VAL:HG23	13:K:67:ARG:N	2.36	0.40
21:S:41:ARG:NH1	21:S:42:VAL:O	2.53	0.40
1:0:1267:C:O2'	1:0:1268:C:H5'	2.21	0.40
1:0:926:A:O2'	13:K:41:HIS:CD2	2.75	0.40
11:I:63:ILE:HG22	11:I:64:GLY:N	2.36	0.40
1:0:921:G:H4'	1:0:924:G:N1	2.36	0.40
13:K:124:ASP:OD1	13:K:149:ARG:NH2	2.54	0.40
1:0:1592:G:H2'	1:0:1593:C:C6	2.55	0.40
1:0:1513:C:O2'	1:0:1514:C:H5'	2.21	0.40
11:I:88:PRO:O	11:I:94:GLY:HA3	2.21	0.40
1:0:2710:U:H2'	1:0:2711:U:C6	2.56	0.40
3:A:20:SER:C	3:A:22:ARG:H	2.24	0.40
21:S:43:ASN:C	21:S:45:GLY:H	2.24	0.40
1:0:1823:G:O2'	1:0:1824:C:H5'	2.21	0.40
17:O:115:SER:HG	17:O:118:GLN:HG3	1.81	0.40
6:D:104:PHE:CE2	6:D:132:VAL:HB	2.55	0.40
15:M:67:ALA:C	15:M:69:TYR:H	2.23	0.40
1:0:289:G:N1	1:0:363:A:C2	2.86	0.40
1:0:524:A:H5"	19:Q:29:LYS:HD3	2.04	0.40
10:H:3:ALA:HB2	10:H:58:ARG:HH12	1.87	0.40
1:0:2791:U:H4'	1:0:2792:A:OP1	2.19	0.40
1:0:88:G:H2'	1:0:89:G:C8	2.56	0.40
22:T:9:CYS:CA	22:T:52:THR:HG23	2.51	0.40
1:0:2335:C:H2'	1:0:2336:G:C8	2.57	0.40
7:E:108:LEU:CD1	7:E:164:ASP:HB2	2.51	0.40
24:V:73:LEU:HA	24:V:73:LEU:HD12	1.95	0.40
1:0:164:G:O3'	13:K:30:ARG:HB2	2.20	0.40
5:C:21:VAL:C	5:C:23:GLU:H	2.24	0.40
1:0:2325:C:H2'	1:0:2326:U:C6	2.57	0.40
1:0:1041:U:H4'	1:0:1295:G:H5'	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:150:THR:HA	5:C:203:ALA:O	2.21	0.40
8:F:111:ILE:O	8:F:115:VAL:HG23	2.21	0.40
8:F:70:LYS:C	8:F:72:VAL:H	2.25	0.40
1:0:731:U:H2'	1:0:732:C:C6	2.56	0.40
1:0:732:C:O2'	1:0:733:U:H5'	2.21	0.40
15:M:147:ILE:HD12	40:M:8847:HOH:O	2.21	0.40
14:L:133:LEU:O	14:L:134:ILE:HD13	2.22	0.40
3:A:36:ASP:HB2	3:A:83:GLY:HA3	2.04	0.40
10:H:20:ILE:CG2	10:H:120:ILE:CD1	2.99	0.40
4:B:7:ARG:CG	4:B:7:ARG:HH11	2.24	0.40
1:0:2526:C:H5'	1:0:2526:C:C6	2.56	0.40
20:R:10:VAL:CG1	23:U:36:ALA:HA	2.48	0.40
1:0:2284:G:H1'	40:0:3028:HOH:O	2.21	0.40
25:W:23:HIS:CD2	25:W:24:LYS:HG3	2.56	0.40
1:0:204:A:O2'	1:0:205:U:H5'	2.22	0.40
1:0:2088:C:H1'	1:0:2841:A:N1	2.36	0.40
2:9:3078:G:N2	2:9:3102:G:H2'	2.36	0.40
1:0:668:C:H2'	1:0:669:G:H8	1.86	0.40
30:2:55:VAL:HB	30:2:56:PRO:HD2	2.02	0.40
12:J:117:VAL:HG12	12:J:117:VAL:O	2.22	0.40
1:0:2549:C:H2'	1:0:2550:U:O4'	2.22	0.40
1:0:1800:G:H2'	1:0:1801:A:H8	1.86	0.40
5:C:12:THR:HB	40:C:8650:HOH:O	2.22	0.40
1:0:892:G:H5"	28:Z:54:ALA:HB2	2.04	0.40
1:0:1287:A:O4'	24:V:117:ARG:HD3	2.22	0.40
14:L:134:ILE:O	14:L:136:PRO:HD3	2.21	0.40
15:M:168:LEU:HA	15:M:169:PRO:HD3	1.88	0.40
2:9:3053:G:O2'	2:9:3054:A:H5'	2.21	0.40
1:0:1154:A:H2'	1:0:1155:G:C8	2.56	0.40
12:J:101:ASN:O	12:J:102:GLU:CB	2.70	0.40
1:0:1415:G:H5'	28:Z:12:ASN:O	2.21	0.40
19:Q:126:LYS:HA	19:Q:127:PRO:HD3	1.93	0.40
1:0:2748:G:H1'	40:0:8331:HOH:O	2.19	0.40
1:0:2398:A:H2'	1:0:2399:G:O4'	2.21	0.40
12:J:14:LYS:CB	12:J:45:PRO:HG2	2.46	0.40
24:V:88:THR:HG22	24:V:90:TYR:HD1	1.86	0.40
26:X:187:VAL:HB	26:X:203:VAL:CG2	2.51	0.40
3:A:35:GLY:O	3:A:36:ASP:CB	2.63	0.40
6:D:54:ALA:HB3	6:D:69:ILE:HD12	2.01	0.40
1:0:920:C:H4'	1:0:921:G:N2	2.36	0.40
1:0:1920:C:O2'	1:0:1921:A:H5'	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2613:G:O2'	1:0:2614:C:H5'	2.22	0.40
1:0:1218:U:H2'	1:0:1219:U:H6	1.87	0.40
12:J:66:ARG:HG2	12:J:66:ARG:HH11	1.86	0.40
1:0:2783:A:H3'	40:0:5613:HOH:O	2.21	0.40
12:J:114:ALA:HB3	12:J:117:VAL:HG23	2.03	0.40
24:V:1:MET:HB2	24:V:103:GLU:HG2	2.03	0.40
1:0:1614:G:H2'	40:0:5017:HOH:O	2.20	0.40

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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
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
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

All (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
6	D	173	GLU
8	F	101	ALA
13	K	80	ASP
15	M	154	LEU
15	M	164	ASP
15	M	183	ASP
27	Y	81	ARG
30	2	56	PRO
3	A	34	ASP
4	B	34	GLY
4	B	169	GLY
6	D	20	LYS
6	D	171	ASP

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Mol	Chain	Res	Type
11	I	143	LYS
15	M	162	ASP
15	M	167	ASP
23	U	43	PRO
24	V	77	ALA
3	A	132	ASP
4	B	185	GLY
11	I	7	ASP
12	J	119	GLN
15	M	65	ASP
15	M	181	ASP
21	S	44	ALA
21	S	53	GLY
25	W	77	PHE
27	Y	20	ARG
30	2	57	GLY
6	D	16	PRO
6	D	61	PHE
11	I	5	GLU
20	R	30	ASP
27	Y	41	ASN
3	A	37	VAL
4	B	2	GLN
4	B	107	SER
6	D	60	GLU
11	I	65	ASN
14	L	83	SER
18	P	78	GLY
18	P	18	PRO
24	V	49	ASN
3	A	112	PRO
6	D	27	ILE
23	U	40	PRO
8	F	64	PRO
8	F	71	GLY
10	H	55	VAL
3	A	211	LYS

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
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

All (133) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	3	ARG
3	A	33	GLU
3	A	36	ASP
3	A	55	VAL
3	A	68	ILE
3	A	69	LEU
3	A	78	ASP
3	A	94	LEU
3	A	131	HIS
3	A	153	ARG
3	A	179	MET
3	A	217	ARG
4	B	7	ARG
4	B	11	LEU
4	B	27	ASN
4	B	33	ASP
4	B	63	GLU
4	B	97	LEU
4	B	98	THR
4	B	103	ASP
4	B	162	MET
4	B	251	VAL
4	B	254	GLN
4	B	264	GLU
4	B	307	ARG
4	B	312	ARG
5	C	2	GLN
5	C	27	ARG
5	C	67	GLN
5	C	91	PRO
5	C	94	THR
5	C	101	ASP
5	C	115	LEU
5	C	136	VAL
5	C	187	ARG
5	C	214	THR
5	C	222	ASP
5	C	223	LEU
5	C	234	VAL
5	C	236	THR
5	C	240	LEU
6	D	24	HIS

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Mol	Chain	Res	Type
6	D	61	PHE
6	D	99	ASP
6	D	100	ASP
6	D	131	THR
6	D	133	ASN
6	D	136	ARG
6	D	137	PRO
6	D	149	ARG
6	D	170	TYR
7	E	7	ILE
7	E	102	VAL
7	E	164	ASP
8	F	12	LEU
8	F	78	GLU
10	H	18	GLU
10	H	68	SER
10	H	84	LYS
10	H	111	ASP
10	H	154	TYR
10	H	159	PRO
10	H	171	LEU
11	I	46	ILE
11	I	52	GLN
11	I	74	ARG
11	I	76	ASP
11	I	79	PHE
11	I	107	ASN
11	I	112	ASP
11	I	120	SER
11	I	125	SER
11	I	127	ILE
12	J	4	LEU
12	J	7	ASP
12	J	10	GLN
12	J	98	VAL
13	K	30	ARG
13	K	35	ARG
13	K	80	ASP
13	K	83	GLU
13	K	117	GLU
14	L	46	LEU
14	L	68	ARG

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Mol	Chain	Res	Type
14	L	93	ARG
14	L	99	ARG
14	L	116	ASN
14	L	164	THR
15	M	26	LEU
15	M	128	ASP
15	M	139	TRP
15	M	152	GLU
15	M	163	PHE
16	N	3	THR
17	O	91	LYS
17	O	98	ILE
18	P	11	ARG
18	P	16	ASN
18	P	18	PRO
18	P	95	GLU
19	Q	13	THR
19	Q	39	THR
19	Q	82	GLU
19	Q	132	ARG
21	S	39	ASN
21	S	73	HIS
21	S	96	VAL
23	U	43	PRO
23	U	65	ASP
24	V	35	VAL
24	V	52	VAL
24	V	73	LEU
24	V	76	ASP
24	V	122	ARG
24	V	142	ASP
24	V	146	ILE
24	V	154	ARG
25	W	15	ARG
25	W	27	ASP
25	W	44	ASP
25	W	72	VAL
26	X	115	ARG
26	X	141	THR
26	X	154	ARG
26	X	163	THR
26	X	172	THR

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Mol	Chain	Res	Type
26	X	189	ASN
26	X	200	THR
26	X	203	VAL
26	X	231	PRO
27	Y	44	GLU
29	1	18	ASN
30	2	56	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (77) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	5	GLN
3	A	92	ASN
3	A	199	HIS
4	B	27	ASN
4	B	145	HIS
4	B	191	ASN
4	B	221	GLN
4	B	238	ASN
4	B	256	GLN
4	B	260	HIS
4	B	320	GLN
4	B	332	ASN
5	C	2	GLN
5	C	39	GLN
5	C	129	HIS
6	D	47	GLN
6	D	103	ASN
6	D	133	ASN
7	E	106	ASN
7	E	143	GLN
9	G	64	ASN
10	H	56	GLN
10	H	59	HIS
10	H	70	ASN
11	I	107	ASN
11	I	126	ASN
12	J	10	GLN
13	K	18	HIS
13	K	41	HIS
13	K	42	ASN
13	K	116	HIS

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Mol	Chain	Res	Type
14	L	24	GLN
14	L	26	GLN
14	L	58	GLN
14	L	77	HIS
14	L	143	ASN
14	L	170	ASN
15	M	107	ASN
15	M	153	GLN
17	O	50	GLN
17	O	66	GLN
17	O	73	HIS
17	O	88	GLN
17	O	118	GLN
18	P	16	ASN
18	P	40	HIS
19	Q	61	GLN
19	Q	94	ASN
19	Q	98	ASN
19	Q	113	HIS
19	Q	117	HIS
20	R	9	HIS
20	R	51	GLN
21	S	39	ASN
21	S	73	HIS
22	T	39	ASN
22	T	48	ASN
23	U	60	GLN
24	V	12	ASN
24	V	110	GLN
24	V	119	HIS
24	V	125	HIS
24	V	141	HIS
25	W	23	HIS
26	X	134	HIS
26	X	149	GLN
26	X	189	ASN
28	Z	8	GLN
28	Z	16	HIS
28	Z	28	HIS
29	1	16	ASN
29	1	18	ASN
29	1	41	HIS

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Mol	Chain	Res	Type
29	1	45	ASN
30	2	15	ASN
30	2	30	GLN
30	2	48	ASN

5.3.3 RNA

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%)

All (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
1	0	70	A
1	0	71	G
1	0	87	C
1	0	88	G
1	0	114	A
1	0	115	U
1	0	130	C
1	0	141	C
1	0	151	A
1	0	166	A
1	0	169	A
1	0	186	A
1	0	191	A
1	0	192	A
1	0	200	U
1	0	219	G
1	0	237	G
1	0	271	C
1	0	272	A
1	0	273	G

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Mol	Chain	Res	Type
1	0	283	U
1	0	284	C
1	0	285	A
1	0	308	U
1	0	309	C
1	0	318	C
1	0	336	G
1	0	337	A
1	0	345	G
1	0	358	G
1	0	381	G
1	0	397	A
1	0	417	G
1	0	457	U
1	0	461	C
1	0	487	G
1	0	498	A
1	0	510	U
1	0	511	A
1	0	514	G
1	0	516	A
1	0	537	G
1	0	538	C
1	0	539	G
1	0	542	A
1	0	545	G
1	0	553	G
1	0	559	C
1	0	581	G
1	0	588	G
1	0	604	G
1	0	605	C
1	0	620	A
1	0	632	A
1	0	644	G
1	0	660	A
1	0	688	A
1	0	701	U
1	0	717	C
1	0	759	C
1	0	777	U
1	0	809	G

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Mol	Chain	Res	Type
1	0	821	U
1	0	835	U
1	0	840	U
1	0	857	A
1	0	868	G
1	0	869	G
1	0	871	G
1	0	872	U
1	0	875	A
1	0	877	G
1	0	878	G
1	0	882	A
1	0	898	G
1	0	905	C
1	0	920	C
1	0	921	G
1	0	923	A
1	0	953	G
1	0	960	G
1	0	961	A
1	0	1006	A
1	0	1008	C
1	0	1029	U
1	0	1045	G
1	0	1059	G
1	0	1060	C
1	0	1072	G
1	0	1081	A
1	0	1088	A
1	0	1109	U
1	0	1110	G
1	0	1119	G
1	0	1129	C
1	0	1130	U
1	0	1161	A
1	0	1162	G
1	0	1164	U
1	0	1165	G
1	0	1166	A
1	0	1171	A
1	0	1174	A
1	0	1175	G

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Mol	Chain	Res	Type
1	0	1185	U
1	0	1192	A
1	0	1193	A
1	0	1206	U
1	0	1208	C
1	0	1216	G
1	0	1238	C
1	0	1239	G
1	0	1279	U
1	0	1287	A
1	0	1289	C
1	0	1342	C
1	0	1353	C
1	0	1360	C
1	0	1377	C
1	0	1407	A
1	0	1409	G
1	0	1451	C
1	0	1474	C
1	0	1505	U
1	0	1506	U
1	0	1524	U
1	0	1525	G
1	0	1526	A
1	0	1528	A
1	0	1563	G
1	0	1564	C
1	0	1580	A
1	0	1592	G
1	0	1625	U
1	0	1626	A
1	0	1633	C
1	0	1634	G
1	0	1656	A
1	0	1667	A
1	0	1682	A
1	0	1684	A
1	0	1685	A
1	0	1692	C
1	0	1701	A
1	0	1722	U
1	0	1723	G

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Mol	Chain	Res	Type
1	0	1725	C
1	0	1731	C
1	0	1752	G
1	0	1778	A
1	0	1798	C
1	0	1819	G
1	0	1820	G
1	0	1829	A
1	0	1856	C
1	0	1879	U
1	0	1919	A
1	0	1942	A
1	0	1971	G
1	0	1973	A
1	0	1974	G
1	0	1978	A
1	0	1979	G
1	0	1980	U
1	0	1996	U
1	0	2004	U
1	0	2006	C
1	0	2008	U
1	0	2011	A
1	0	2012	U
1	0	2013	G
1	0	2034	U
1	0	2064	U
1	0	2072	G
1	0	2073	G
1	0	2074	A
1	0	2096	A
1	0	2101	A
1	0	2102	G
1	0	2103	A
1	0	2110	G
1	0	2238	A
1	0	2258	A
1	0	2271	G
1	0	2272	G
1	0	2291	A
1	0	2317	C
1	0	2321	A

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Mol	Chain	Res	Type
1	0	2354	A
1	0	2361	A
1	0	2369	A
1	0	2379	G
1	0	2422	U
1	0	2462	G
1	0	2476	C
1	0	2483	A
1	0	2507	G
1	0	2511	A
1	0	2533	C
1	0	2537	G
1	0	2540	G
1	0	2541	U
1	0	2553	A
1	0	2564	G
1	0	2578	G
1	0	2589	U
1	0	2601	A
1	0	2602	G
1	0	2608	C
1	0	2613	G
1	0	2634	G
1	0	2638	G
1	0	2649	A
1	0	2664	A
1	0	2681	A
1	0	2682	C
1	0	2726	U
1	0	2747	C
1	0	2748	G
1	0	2749	U
1	0	2750	G
1	0	2762	C
1	0	2768	A
1	0	2786	G
1	0	2792	A
1	0	2800	A
1	0	2811	A
1	0	2825	C
1	0	2850	C
1	0	2876	G

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Mol	Chain	Res	Type
1	0	2890	A
1	0	2896	A
1	0	2903	C
1	0	2914	A
2	9	3002	U
2	9	3014	G
2	9	3022	G
2	9	3023	U
2	9	3024	U
2	9	3025	G
2	9	3026	C
2	9	3040	C
2	9	3041	C
2	9	3043	G
2	9	3044	A
2	9	3052	A
2	9	3057	A
2	9	3066	G
2	9	3077	A
2	9	3114	G
2	9	3122	C
31	4	76	A

All (31) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	10	U
1	0	69	A
1	0	129	A
1	0	284	C
1	0	338	C
1	0	603	A
1	0	604	G
1	0	699	C
1	0	834	G
1	0	857	A
1	0	871	G
1	0	877	G
1	0	898	G
1	0	1080	C
1	0	1164	U
1	0	1232	A

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Mol	Chain	Res	Type
1	0	1237	U
1	0	1352	A
1	0	1450	C
1	0	1563	G
1	0	1684	A
1	0	1856	C
1	0	1979	G
1	0	2011	A
1	0	2467	A
1	0	2526	C
1	0	2718	C
1	0	2726	U
1	0	2791	U
2	9	3024	U
2	9	3065	A

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

All (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
32	0	9500	ZLD	C9-C8	2.62	1.55	1.51
32	0	9500	ZLD	C20-C21	2.69	1.61	1.50
32	0	9500	ZLD	C5-C16	3.71	1.44	1.37
32	0	9500	ZLD	C24-C23	4.50	1.68	1.50
32	0	9500	ZLD	C20-N19	4.92	1.54	1.46
32	0	9500	ZLD	C1-C2	5.10	1.49	1.39
32	0	9500	ZLD	C17-C16	5.33	1.51	1.40
32	0	9500	ZLD	C3-C17	5.97	1.50	1.39
32	0	9500	ZLD	C3-C1	6.14	1.49	1.38

All (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
32	0	9500	ZLD	C1-C3-C17	2.27	124.27	119.29
32	0	9500	ZLD	C16-C17-N19	2.68	123.58	120.48
32	0	9500	ZLD	C8-C6-N4	2.78	104.52	101.88
32	0	9500	ZLD	C5-C16-C17	3.16	125.96	123.39
32	0	9500	ZLD	F18-C16-C17	3.26	121.53	118.45
32	0	9500	ZLD	O22-C21-C20	3.33	119.47	111.84
32	0	9500	ZLD	C23-C24-N19	4.45	117.86	110.02
32	0	9500	ZLD	O10-C7-N4	6.45	114.16	109.97
32	0	9500	ZLD	C2-N4-C7	6.78	133.92	125.80

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

All (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
1	0	1199	A	9.3
6	D	63	ILE	9.0
23	U	40	PRO	8.6
1	0	735	C	8.4
6	D	57	THR	8.3
15	M	184	ILE	7.9
15	M	166	ALA	7.7
10	H	171	LEU	7.4
6	D	26	GLY	7.3
1	0	1177	A	7.2
13	K	81	VAL	7.2
1	0	1169	U	7.1
1	0	10	U	6.8
2	9	3002	U	6.7
1	0	1170	U	6.6
1	0	736	A	6.5
23	U	38	GLY	6.5
1	0	497	A	6.4
1	0	1181	A	6.4
3	A	237	GLY	6.4
1	0	1172	G	6.3
21	S	118	SER	6.3
6	D	62	ASP	6.3

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Mol	Chain	Res	Type	RSRZ
23	U	43	PRO	6.3
1	0	970	U	6.2
1	0	1195	G	6.2
6	D	69	ILE	6.1
1	0	1190	G	6.0
21	S	116	ASP	6.0
9	G	26	MET	6.0
6	D	10	PHE	6.0
1	0	1200	A	6.0
1	0	1175	G	5.9
6	D	90	LEU	5.9
1	0	1161	A	5.8
1	0	1206	U	5.8
1	0	1194	A	5.8
3	A	37	VAL	5.8
1	0	272	A	5.7
1	0	1966	U	5.7
1	0	1951	G	5.7
1	0	1180	U	5.7
1	0	1191	A	5.7
1	0	1196	C	5.6
1	0	999	C	5.6
1	0	2637	A	5.5
9	G	23	ILE	5.5
1	0	1192	A	5.4
1	0	1162	G	5.4
15	M	2	THR	5.4
21	S	117	ASP	5.3
23	U	41	GLU	5.2
2	9	3024	U	5.1
1	0	1198	U	5.1
6	D	11	HIS	5.1
15	M	95	ALA	5.1
1	0	514	G	5.0
13	K	80	ASP	5.0
1	0	1965	C	5.0
1	0	1202	A	5.0
15	M	165	ALA	4.9
27	Y	11	SER	4.9
31	4	77	PHE	4.9
1	0	1000	C	4.9
1	0	1163	G	4.9

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Mol	Chain	Res	Type	RSRZ
7	E	45	ASP	4.8
2	9	3025	G	4.8
1	0	1178	G	4.7
1	0	1171	A	4.7
1	0	1967	U	4.6
10	H	83	TYR	4.6
1	0	2511	A	4.6
1	0	1164	U	4.6
6	D	27	ILE	4.5
1	0	1173	A	4.5
1	0	1176	C	4.5
1	0	2237	G	4.5
1	0	1948	G	4.5
22	T	47	ARG	4.5
1	0	1193	A	4.4
1	0	1207	A	4.4
8	F	28	ALA	4.4
1	0	1203	G	4.4
1	0	969	G	4.4
15	M	68	GLU	4.4
25	W	88	GLU	4.3
9	G	22	ALA	4.3
1	0	1208	C	4.3
10	H	138	CYS	4.3
6	D	66	GLY	4.2
1	0	2769	C	4.2
1	0	1947	G	4.2
1	0	1964	U	4.2
2	9	3023	U	4.2
29	1	27	LEU	4.2
25	W	65	ASN	4.2
6	D	61	PHE	4.1
9	G	25	GLU	4.1
29	1	39	ARG	4.1
25	W	80	GLU	4.1
1	0	1168	C	4.1
26	X	235	GLU	4.1
4	B	1	PRO	4.1
15	M	39	SER	4.1
1	0	1197	G	4.0
1	0	1525	G	4.0
1	0	1182	C	4.0

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Mol	Chain	Res	Type	RSRZ
1	0	1205	U	4.0
1	0	737	A	4.0
29	1	35	ARG	4.0
23	U	37	GLY	4.0
1	0	960	G	4.0
1	0	282	C	4.0
18	P	18	PRO	3.9
6	D	170	TYR	3.9
6	D	92	GLU	3.9
1	0	1179	C	3.9
1	0	1950	G	3.9
6	D	56	ARG	3.9
8	F	119	ARG	3.9
1	0	138	U	3.9
29	1	28	LYS	3.8
25	W	77	PHE	3.8
3	A	236	GLY	3.8
9	G	69	ARG	3.8
9	G	21	ASP	3.8
10	H	37	GLN	3.8
26	X	95	THR	3.7
10	H	143	ALA	3.7
1	0	2911	C	3.7
23	U	10	ASP	3.7
23	U	36	ALA	3.7
4	B	117	GLU	3.7
13	K	60	GLU	3.6
1	0	280	C	3.6
15	M	153	GLN	3.6
27	Y	37	HIS	3.6
1	0	2512	U	3.6
1	0	1184	C	3.6
1	0	2344	G	3.6
1	0	2748	G	3.6
2	9	3072	C	3.6
8	F	106	ALA	3.6
6	D	58	VAL	3.6
10	H	39	ASP	3.6
6	D	64	ARG	3.5
25	W	85	VAL	3.5
3	A	133	ARG	3.5
8	F	90	GLU	3.5

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Mol	Chain	Res	Type	RSRZ
15	M	162	ASP	3.5
8	F	16	ALA	3.5
1	0	1174	A	3.5
2	9	3122	C	3.4
7	E	42	VAL	3.4
4	B	57	GLU	3.4
9	G	73	ASP	3.4
10	H	139	ASN	3.4
15	M	158	LEU	3.4
15	M	1	ALA	3.4
16	N	23	GLY	3.4
1	0	1201	C	3.3
1	0	2345	A	3.3
15	M	97	VAL	3.3
25	W	7	GLU	3.3
31	4	76	A	3.3
1	0	1185	U	3.3
15	M	152	GLU	3.2
10	H	140	VAL	3.2
27	Y	34	ASN	3.2
16	N	1	SER	3.2
9	G	72	ASP	3.2
10	H	24	PRO	3.2
6	D	51	ARG	3.2
25	W	82	GLU	3.2
18	P	76	VAL	3.2
13	K	99	GLU	3.2
20	R	81	ILE	3.2
10	H	82	ASP	3.2
1	0	1204	C	3.2
1	0	2508	C	3.2
9	G	65	THR	3.2
10	H	115	ALA	3.2
29	1	49	GLU	3.2
1	0	2914	A	3.1
25	W	74	ALA	3.1
1	0	1165	G	3.1
2	9	3065	A	3.1
10	H	142	ASP	3.1
17	O	122	LEU	3.1
10	H	141	GLU	3.1
13	K	150	GLN	3.1

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Mol	Chain	Res	Type	RSRZ
2	9	3073	G	3.1
15	M	179	LEU	3.1
21	S	115	GLU	3.1
6	D	44	ILE	3.1
21	S	107	LYS	3.1
23	U	2	VAL	3.1
1	0	1167	G	3.1
10	H	21	THR	3.1
15	M	178	THR	3.1
1	0	2004	U	3.1
9	G	66	LEU	3.1
15	M	76	GLY	3.1
1	0	2910	A	3.1
8	F	44	SER	3.1
25	W	71	ARG	3.1
9	G	68	GLU	3.1
15	M	160	SER	3.0
6	D	70	GLY	3.0
6	D	12	GLU	3.0
24	V	86	GLU	3.0
1	0	1625	U	3.0
27	Y	45	ASP	3.0
1	0	2909	G	3.0
7	E	6	GLU	3.0
1	0	2335	C	3.0
1	0	2913	A	3.0
15	M	149	GLU	3.0
27	Y	44	GLU	3.0
1	0	2510	C	3.0
15	M	138	ASP	3.0
15	M	155	GLU	3.0
10	H	78	GLY	3.0
31	4	74	C	2.9
15	M	167	ASP	2.9
9	G	24	VAL	2.9
10	H	169	GLU	2.9
15	M	67	ALA	2.9
1	0	2507	G	2.9
13	K	102	ASP	2.9
1	0	2238	A	2.9
9	G	29	SER	2.9
10	H	146	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
8	F	114	LYS	2.9
20	R	77	VAL	2.8
1	0	2825	C	2.8
9	G	12	ILE	2.8
12	J	132	VAL	2.8
30	2	56	PRO	2.8
27	Y	59	TYR	2.8
9	G	18	GLU	2.8
27	Y	36	ASP	2.8
25	W	75	ALA	2.8
8	F	21	GLU	2.8
6	D	40	ILE	2.8
23	U	46	ILE	2.8
10	H	22	GLY	2.8
1	0	809	G	2.8
26	X	236	VAL	2.8
1	0	2912	C	2.8
10	H	73	LEU	2.7
1	0	1166	A	2.7
7	E	43	ASP	2.7
10	H	25	GLY	2.7
6	D	52	THR	2.7
1	0	281	U	2.7
10	H	79	GLU	2.7
6	D	87	ALA	2.7
13	K	79	ASP	2.7
21	S	35	TYR	2.7
27	Y	35	GLU	2.7
2	9	3074	G	2.7
18	P	95	GLU	2.7
1	0	1279	U	2.7
13	K	77	ALA	2.7
27	Y	31	SER	2.7
29	1	24	TRP	2.7
8	F	22	VAL	2.7
9	G	14	GLU	2.7
10	H	76	GLU	2.7
14	L	22	GLU	2.7
8	F	17	LEU	2.6
10	H	167	ARG	2.6
24	V	91	ASP	2.6
15	M	185	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
23	U	14	ALA	2.6
25	W	10	VAL	2.6
8	F	105	ASP	2.6
10	H	23	ILE	2.6
10	H	116	ALA	2.6
27	Y	25	ARG	2.6
29	1	26	MET	2.6
1	0	358	G	2.6
23	U	8	ILE	2.6
1	0	808	A	2.6
29	1	44	ARG	2.6
27	Y	22	SER	2.6
1	0	2826	G	2.6
17	O	108	LEU	2.6
7	E	89	SER	2.6
15	M	183	ASP	2.6
1	0	1183	C	2.6
13	K	104	ASP	2.5
30	2	8	ASN	2.5
10	H	145	HIS	2.5
1	0	1929	G	2.5
6	D	107	GLY	2.5
8	F	107	ASP	2.5
1	0	716	G	2.5
2	9	3109	G	2.5
10	H	34	GLY	2.5
13	K	82	ALA	2.5
2	9	3108	C	2.5
13	K	148	GLU	2.5
20	R	78	ALA	2.5
6	D	28	GLY	2.5
27	Y	21	VAL	2.5
10	H	166	GLU	2.5
11	I	5	GLU	2.5
18	P	81	GLU	2.5
1	0	351	G	2.5
7	E	100	ASP	2.5
8	F	118	LEU	2.5
1	0	284	C	2.5
12	J	119	GLN	2.5
8	F	15	ASP	2.5
10	H	44	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
7	E	111	LYS	2.4
8	F	19	ALA	2.4
26	X	234	VAL	2.4
2	9	3066	G	2.4
27	Y	24	ARG	2.4
30	2	29	ARG	2.4
3	A	35	GLY	2.4
9	G	17	GLN	2.4
10	H	111	ASP	2.4
6	D	18	ILE	2.4
2	9	3107	C	2.4
21	S	83	ASP	2.4
1	0	2645	U	2.4
6	D	50	VAL	2.4
30	2	57	GLY	2.4
8	F	117	GLU	2.4
14	L	25	TRP	2.4
1	0	734	U	2.4
1	0	2509	A	2.4
6	D	53	LYS	2.4
8	F	25	ASP	2.4
6	D	22	VAL	2.4
8	F	103	GLU	2.4
10	H	42	ASP	2.4
1	0	1160	G	2.4
1	0	293	A	2.4
15	M	175	LEU	2.4
7	E	88	TYR	2.4
15	M	164	ASP	2.4
3	A	145	MET	2.3
1	0	288	A	2.3
7	E	10	ASP	2.3
20	R	16	ASN	2.3
31	4	75	C	2.3
10	H	35	ARG	2.3
4	B	319	ASP	2.3
6	D	42	GLY	2.3
8	F	26	THR	2.3
5	C	135	GLU	2.3
25	W	76	ARG	2.3
27	Y	20	ARG	2.3
1	0	1186	C	2.3

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Mol	Chain	Res	Type	RSRZ
10	H	45	VAL	2.3
6	D	104	PHE	2.3
10	H	38	LYS	2.3
1	0	1913	C	2.3
14	L	75	ARG	2.3
29	1	20	ARG	2.3
5	C	143	ASP	2.3
1	0	1488	U	2.3
1	0	354	A	2.2
1	0	1919	A	2.2
1	0	298	C	2.2
5	C	63	SER	2.2
23	U	32	ALA	2.2
3	A	31	LYS	2.2
6	D	65	GLU	2.2
4	B	105	PHE	2.2
8	F	110	ASP	2.2
1	0	128	A	2.2
1	0	2569	A	2.2
3	A	97	ALA	2.2
6	D	85	GLN	2.2
20	R	70	GLU	2.2
21	S	82	THR	2.2
9	G	71	LEU	2.2
23	U	49	LEU	2.2
24	V	76	ASP	2.2
13	K	83	GLU	2.2
13	K	91	VAL	2.2
30	2	55	VAL	2.2
18	P	84	ILE	2.2
13	K	75	LEU	2.2
15	M	159	TYR	2.2
1	0	1189	A	2.2
25	W	41	PHE	2.2
7	E	170	ARG	2.2
6	D	86	THR	2.2
13	K	76	LEU	2.2
1	0	1159	G	2.2
27	Y	32	GLU	2.2
29	1	31	ARG	2.2
30	2	1	MET	2.2
15	M	147	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
8	F	70	LYS	2.2
1	0	362	G	2.2
1	0	2506	A	2.2
9	G	70	ALA	2.2
15	M	92	ALA	2.2
9	G	27	ILE	2.1
12	J	100	GLU	2.1
21	S	106	GLU	2.1
1	0	295	C	2.1
3	A	38	ILE	2.1
13	K	105	TYR	2.1
6	D	93	LEU	2.1
1	0	365	G	2.1
6	D	89	PRO	2.1
9	G	63	ARG	2.1
3	A	96	LEU	2.1
1	0	283	U	2.1
1	0	2419	U	2.1
10	H	86	THR	2.1
1	0	805	G	2.1
1	0	1970	G	2.1
11	I	70	PHE	2.1
27	Y	43	GLY	2.1
20	R	20	PHE	2.1
6	D	129	ASP	2.1
18	P	17	LYS	2.1
18	P	21	ARG	2.1
27	Y	80	ARG	2.1
1	0	2850	C	2.1
6	D	13	MET	2.1
8	F	24	ARG	2.1
1	0	1213	C	2.0
12	J	101	ASN	2.0
15	M	40	ASN	2.0
17	O	18	LYS	2.0
4	B	118	ASP	2.0
11	I	110	ASP	2.0
1	0	2908	A	2.0
15	M	6	TYR	2.0
30	2	2	GLN	2.0
6	D	73	VAL	2.0
5	C	61	PHE	2.0

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Mol	Chain	Res	Type	RSRZ
15	M	163	PHE	2.0
23	U	59	ILE	2.0
3	A	203	GLY	2.0
15	M	7	LYS	2.0
7	E	98	GLU	2.0
10	H	162	ARG	2.0
11	I	111	GLU	2.0
10	H	36	LYS	2.0
16	N	20	SER	2.0
1	0	371	U	2.0
21	S	33	GLU	2.0
15	M	134	ASP	2.0
1	0	1981	A	2.0

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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
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

There are no such residues in this entry.