



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 24, 2017 – 11:53 PM EDT

PDB ID : 3G71  
Title : Co-crystal structure of Bruceantin bound to the large ribosomal subunit  
Authors : Gurel, G.; Blaha, G.; Moore, P.B.; Steitz, T.A.  
Deposited on : unknown  
Resolution : 2.85 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030345  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030345

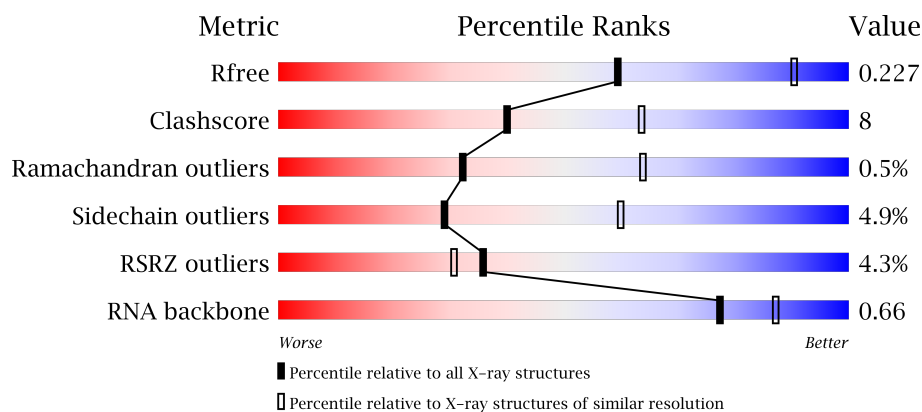
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.85 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	100719	2469 (2.90-2.82)
Clashscore	112137	2749 (2.90-2.82)
Ramachandran outliers	110173	2687 (2.90-2.82)
Sidechain outliers	110143	2690 (2.90-2.82)
RSRZ outliers	101464	2487 (2.90-2.82)
RNA backbone	2435	1033 (3.20-2.52)

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

Mol	Chain	Length	Quality of chain
1	0	2923	<div> <div>54%</div> <div>34%</div> <div>5%</div> <div>6%</div> </div>
2	A	237	<div> <div>6%</div> <div>84%</div> <div>14%</div> <div>.</div> </div>
3	B	337	<div> <div>85%</div> <div>14%</div> <div>.</div> </div>
4	C	246	<div> <div>84%</div> <div>13%</div> <div>.</div> </div>


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Mol	Chain	Length	Quality of chain
5	D	177	
6	E	172	
7	F	119	
8	G	348	
9	H	177	
10	I	70	
11	J	142	
12	K	132	
13	L	165	
14	M	194	
15	N	186	
16	O	115	
17	P	143	
18	Q	95	
19	R	150	
20	S	81	
21	T	119	
22	U	53	
23	V	65	
24	W	154	
25	X	82	
26	Y	142	
27	Z	73	
28	1	56	
29	2	50	

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Mol	Chain	Length	Quality of chain
30	3	92	
31	9	122	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
32	MG	0	8002	-	-	-	X
32	MG	0	8004	-	-	-	X
32	MG	0	8006	-	-	-	X
32	MG	0	8008	-	-	-	X
32	MG	0	8009	-	-	-	X
32	MG	0	8011	-	-	-	X
32	MG	0	8012	-	-	-	X
32	MG	0	8014	-	-	-	X
32	MG	0	8028	-	-	-	X
32	MG	0	8041	-	-	-	X
32	MG	0	8043	-	-	-	X
32	MG	0	8047	-	-	-	X
32	MG	0	8062	-	-	-	X
32	MG	0	8067	-	-	-	X
32	MG	0	8070	-	-	-	X
32	MG	0	8072	-	-	-	X
32	MG	9	8040	-	-	-	X
33	K	0	8402	-	-	-	X
34	NA	0	8504	-	-	-	X
34	NA	0	8511	-	-	-	X
34	NA	0	8519	-	-	-	X
34	NA	0	8521	-	-	-	X
34	NA	0	8522	-	-	-	X
34	NA	0	8523	-	-	-	X
34	NA	0	8527	-	-	-	X
34	NA	0	8528	-	-	-	X
34	NA	0	8530	-	-	-	X
34	NA	0	8534	-	-	-	X
34	NA	0	8535	-	-	-	X
34	NA	0	8537	-	-	-	X
34	NA	0	8542	-	-	-	X
34	NA	0	8547	-	-	-	X
34	NA	0	8553	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
34	NA	0	8555	-	-	-	X
34	NA	0	8556	-	-	-	X
34	NA	0	8558	-	-	-	X
34	NA	0	8559	-	-	-	X
34	NA	0	8560	-	-	-	X
34	NA	0	8562	-	-	-	X
34	NA	0	8563	-	-	-	X
34	NA	0	8564	-	-	-	X
34	NA	0	8565	-	-	-	X
34	NA	0	8568	-	-	-	X
34	NA	0	8575	-	-	-	X
34	NA	9	8572	-	-	-	X
34	NA	M	8539	-	-	-	X
35	CL	0	8815	-	-	-	X
35	CL	0	8816	-	-	-	X
36	SR	0	8902	-	-	-	X
36	SR	0	8903	-	-	-	X
36	SR	0	8904	-	-	-	X
36	SR	0	8908	-	-	-	X
36	SR	0	8949	-	-	-	X
36	SR	B	8987	-	-	-	X
37	WIN	0	9101	-	-	-	X

## 2 Entry composition

There are 39 unique types of molecules in this entry. The entry contains 99174 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	0	2754	Total	C	N	O	P	0	0	0
			59021	26349	10873	19054	2745			

- Molecule 2 is a protein called 50S ribosomal protein L2P.

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

- Molecule 3 is a protein called 50S ribosomal protein L3P.

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

- Molecule 4 is a protein called 50S ribosomal protein L4P.

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

- Molecule 5 is a protein called 50S ribosomal protein L5P.

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

- Molecule 6 is a protein called 50S ribosomal protein L6P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	E	172	Total	C	N	O	S	0	0	0
			1358	840	224	290	4			

- Molecule 7 is a protein called 50S ribosomal protein L7Ae.

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

- Molecule 8 is a protein called 50S ribosomal protein L10E.

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

- Molecule 9 is a protein called 50S ribosomal protein L10e.

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

- Molecule 10 is a protein called 50S ribosomal protein L11P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	I	70	Total	C	N	O	S	0	0	0
			520	323	81	115	1			

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	M	194	Total	C	N	O	S	0	0	0
			1559	943	333	282	1			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	P	143	Total	C	N	O		0	0	0
			1137	683	229	225				

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	R	150	Total	C	N	O	S	0	0	0
			1150	713	209	224	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	S	81	Total	C	N	O	S	0	0	0
			642	389	111	139	3			

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



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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	U	53	Total	C	N	O	S	0	0	0
			411	244	75	87	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	V	65	Total	C	N	O	S	0	0	0
			500	304	94	101	1			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	X	82	Total	C	N	O	S	0	0	0
			655	402	129	123	1			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
26	Y	142	Total	C	N	O	0	0	0
			1131	686	228	217			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	Z	73	Total	C	N	O	S	0	0	0
			574	343	113	113	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	1	56	Total	C	N	O	S	0	0	0
			431	258	86	83	4			

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

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

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

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

- Molecule 31 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	9	122	Total	C	N	O	P	0	0	0
			2599	1160	471	847	121			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
32	0	85	Total	Mg	0	0
			85	85		
32	9	2	Total	Mg	0	0
			2	2		
32	K	1	Total	Mg	0	0
			1	1		
32	B	1	Total	Mg	0	0
			1	1		
32	A	1	Total	Mg	0	0
			1	1		
32	T	1	Total	Mg	0	0
			1	1		
32	2	1	Total	Mg	0	0
			1	1		
32	Y	1	Total	Mg	0	0
			1	1		

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

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

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	0	66	Total Na 66 66	0	0
34	J	1	Total Na 1 1	0	0
34	Q	1	Total Na 1 1	0	0
34	H	1	Total Na 1 1	0	0
34	C	1	Total Na 1 1	0	0
34	R	1	Total Na 1 1	0	0
34	9	2	Total Na 2 2	0	0
34	S	1	Total Na 1 1	0	0
34	M	1	Total Na 1 1	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	0	9	Total Cl 9 9	0	0
35	J	3	Total Cl 3 3	0	0
35	K	1	Total Cl 1 1	0	0
35	B	1	Total Cl 1 1	0	0
35	A	1	Total Cl 1 1	0	0
35	N	1	Total Cl 1 1	0	0
35	O	1	Total Cl 1 1	0	0
35	R	1	Total Cl 1 1	0	0

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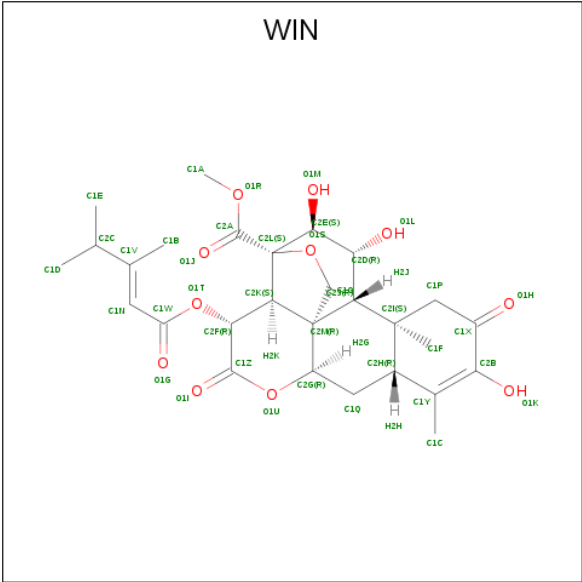
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	Y	1	Total 1	Cl 1	0	0
35	L	1	Total 1	Cl 1	0	0
35	3	1	Total 1	Cl 1	0	0
35	M	1	Total 1	Cl 1	0	0

- Molecule 36 is STRONTIUM ION (three-letter code: SR) (formula: Sr).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	0	95	Total 95	Sr 95	0	0
36	1	1	Total 1	Sr 1	0	0
36	B	2	Total 2	Sr 2	0	0
36	3	2	Total 2	Sr 2	0	0
36	A	2	Total 2	Sr 2	0	0
36	R	1	Total 1	Sr 1	0	0
36	9	3	Total 3	Sr 3	0	0
36	S	1	Total 1	Sr 1	0	0
36	F	1	Total 1	Sr 1	0	0

- Molecule 37 is methyl (5beta,7alpha,9beta,10alpha,11alpha,12alpha,13beta,15alpha)-15-{|(2 E)-3,4-dimethylpent-2-enoyl|oxy}-3,11,12-trihydroxy-2,16-dioxo-13,20-epoxypicras-3-en-21-oate (three-letter code: WIN) (formula: C<sub>28</sub>H<sub>36</sub>O<sub>11</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
37	0	1	Total	C	O	0	0
			39	28	11		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	O	1	Total	Cd	0	0
			1	1		
38	Z	1	Total	Cd	0	0
			1	1		
38	1	1	Total	Cd	0	0
			1	1		
38	3	1	Total	Cd	0	0
			1	1		
38	U	1	Total	Cd	0	0
			1	1		

- Molecule 39 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
39	0	5993	Total	O	0	0
			5993	5993		
39	A	107	Total	O	0	0
			107	107		
39	B	146	Total	O	0	0
			146	146		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
39	C	171	Total 171	O 171	0	0
39	D	45	Total 45	O 45	0	0
39	E	40	Total 40	O 40	0	0
39	F	25	Total 25	O 25	0	0
39	G	18	Total 18	O 18	0	0
39	H	62	Total 62	O 62	0	0
39	I	5	Total 5	O 5	0	0
39	J	52	Total 52	O 52	0	0
39	K	53	Total 53	O 53	0	0
39	L	79	Total 79	O 79	0	0
39	M	128	Total 128	O 128	0	0
39	N	62	Total 62	O 62	0	0
39	O	40	Total 40	O 40	0	0
39	P	65	Total 65	O 65	0	0
39	Q	43	Total 43	O 43	0	0
39	R	77	Total 77	O 77	0	0
39	S	28	Total 28	O 28	0	0
39	T	32	Total 32	O 32	0	0
39	U	27	Total 27	O 27	0	0
39	V	12	Total 12	O 12	0	0
39	W	65	Total 65	O 65	0	0

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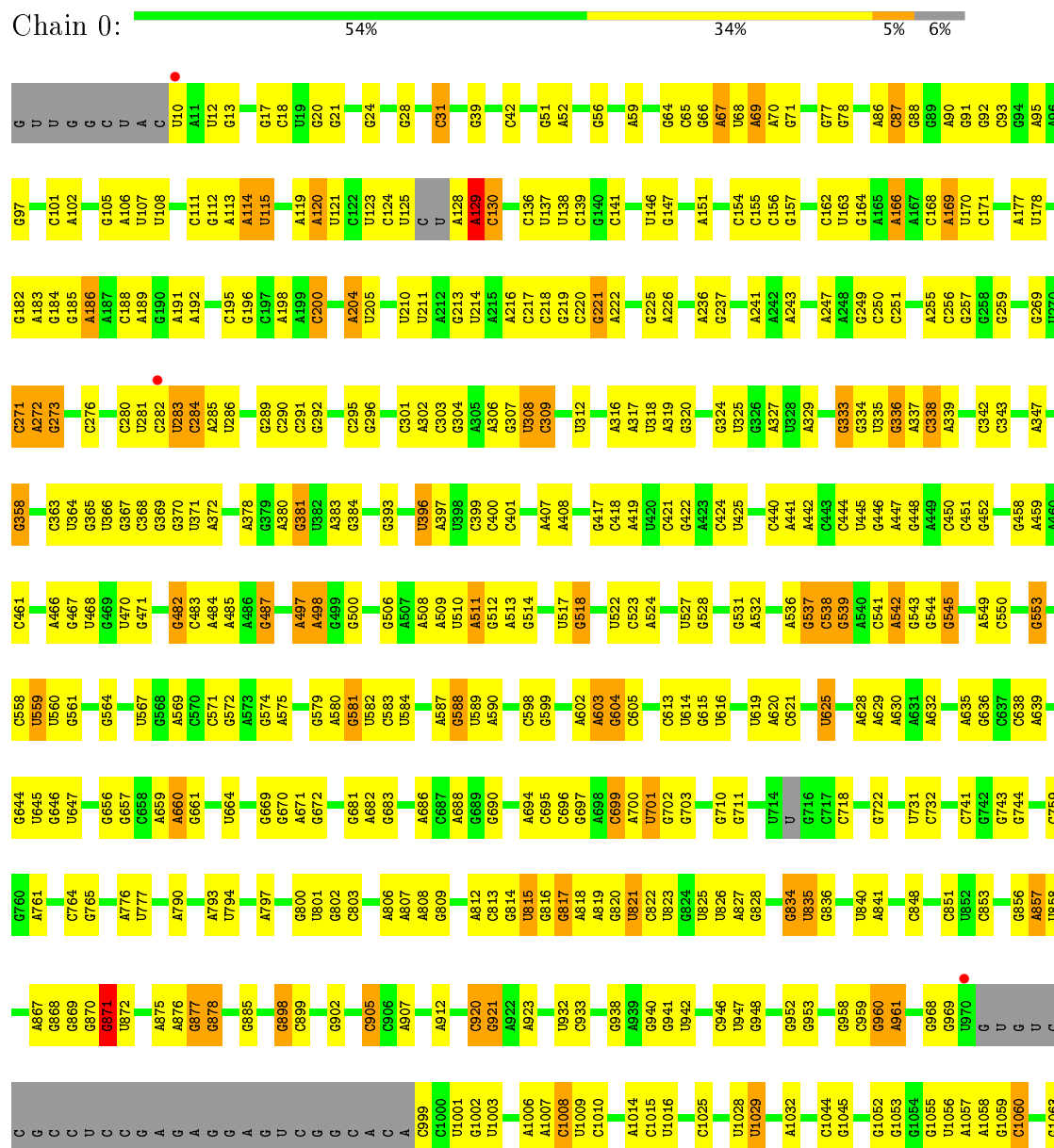
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
39	X	20	Total 20	O 20	0	0
39	Y	94	Total 94	O 94	0	0
39	Z	28	Total 28	O 28	0	0
39	1	52	Total 52	O 52	0	0
39	2	39	Total 39	O 39	0	0
39	3	66	Total 66	O 66	0	0
39	9	149	Total 149	O 149	0	0

### 3 Residue-property plots

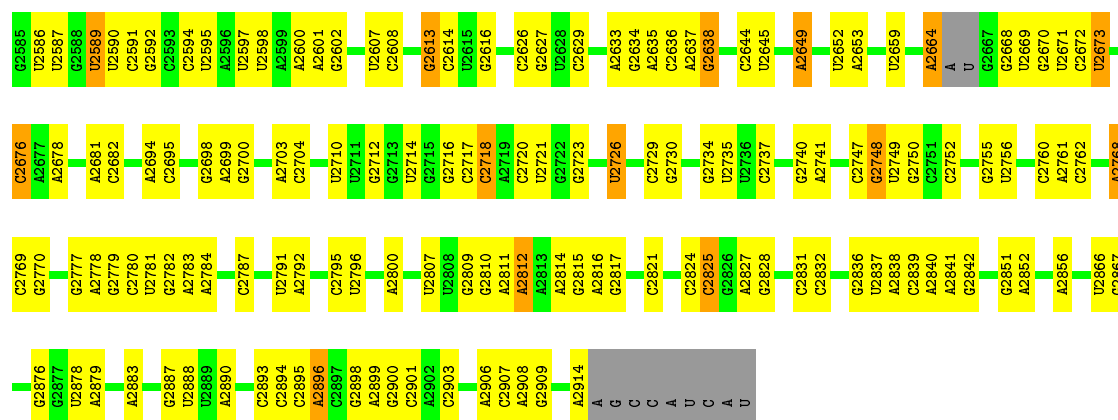
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

- Molecule 1: 23S ribosomal RNA

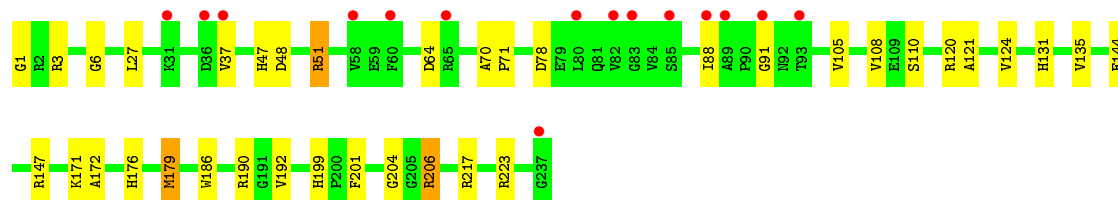
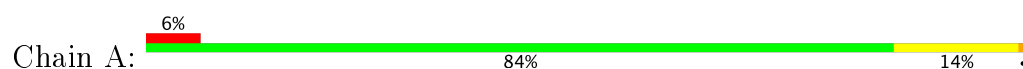




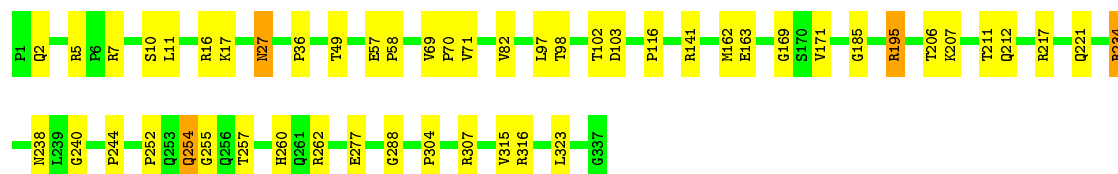
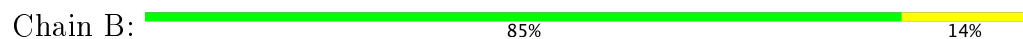
A2486	G2379	U2265	C	G1947	C1834	U1741	A1641	G1546	A1434	A1352	C1238	G1165	U1066
C2487	A2380	A2266	C	G1948	U1835	A1742	A1642	G1556	U1435	A1353	G1239	A1166	A1067
A2488	C2381	G2267	C	G1951	C	C	C1643	G1557	C	C1354	A1242	G1167	
G2489	A2382	C2268	C	U	U1838	U1749	C1644	C1558	U1439	A1357	C1243	U1169	G1071
A2490	G2270	C2269	C	A	A1839	C	U1645	A1559	U1440	C1360	U1244	U1170	G1072
G2491	G2271	C2270	C	C	A1840	G1752	C1652	U1561	G1441	C1361	C1245	A1171	A1073
C2492	U2277	C2046	A	U	C1844	A1755	A1653	C1562	A1442	C1362	A1246	G1172	G1074
G2493	U2287	C2047	C	U	U1845	G1756	U1654	U1561	G1443	C1363	U1249	A1173	G1075
C2498	C2388	G2050	C	A	U1846	C	U1655	C1566	G1444	G1364	G1250	G1174	G1076
U2499	U2389	A2054	A	G	A1847	A1759	A1656	G1567	U1445	G1365	C1251	G1175	G1077
	C2392	U2282	C	A	G1848	G1760	A1657	G1568	U1446	C1366	G1257	G1176	A1078
C2502	A2291	U2064	A	C	U1849	U1761	A1658	U1569	U1447		C1257	A1177	A1081
A2503	A2401	G2070	U	C	G1855	C1762		C1570	G1453	G1370	C1258	U1180	
G2504	A2402	C2071	C	C	C1763	C1763	A1664	C1571	U1454	U1371	A1259	A1181	C1084
A2505	A2300	G2072	G	U1964	C1856	U1766	G1665	A1572	C1455	A1372	G1260	C1182	
G2506	A2301	C2073	C	C1965	A1857	C1767	C1666	A1573	C1456	G1375	C1268	C1183	G1087
C2507	A2302	A2074	A	U1967	A1858	A1768	A1667	G1576	U1457	C1376	G1269	U1185	A1088
G2508	U2308	C2309	A	U1967	C1861	C1769	U1668	U1577		C1377		C1186	A1097
A2509	C2310	G2079	C	A1968	C1862	U1770	A1677	U1587	U1463	G1378	C1273	A1187	A1098
C2510	G2415	G2080	C	U1970	C1864	G1773	A1678	U1588	C1464	C1378		A1188	G1099
A2511	G2416	A2081	U	G1971	G1868		C1679	G1589	C1474	A1381	U1278	U1189	G1100
U2512	C2417	C2082	A	U1972	G1868	A1778	C1680		C1477	G1382	U1279	G1190	C1104
C2515	U2419	A2083	C	A1973	G1873	A1779	A1682	G1592	U1478	C1384	C1289	A1191	C1105
G2516	G2420	C2087	C	G1974	C1877	C1779	C1683	C1593	C1478	G1385	G1290	A1192	A1106
A2521	G2421	C2088	C	U1975	U1878	A1783	U1684	C1594	U1482	C1386	A1291	A1193	
G2524	U2422	G2089	G	U1980	U1879	U1784	A1685	C1595	C1483	G1387		U1197	U1109
C2525	G2426	C2091	C	A1981	C1880	C1787	C1686	U1596	G1484	C1391	U1294	A1198	G1110
G2526	U2435	G2092	G	U1992	C1881	U1788	C1687	A1597	A1485	A1392	G1295	A1199	U1115
C2533	A2436	C2093	C	C1993	U1882	G1789	C1692	A1603	C1495	C1393	G1299	C1201	U1116
G2534	G2437	G2094	A	U1994	U1883	C1790	C1692	G1604	A1496	C1394	G1300	A1202	A1117
C2535	C2438	A2095	C	G1995	C1886	U1791	C1692	G1605	G1497	C1395	G1306	G1203	A1118
G2536	A2439	U2096	U	U1996	A1886	G1795	U1702	A1606	U1500	C1397	U1307	C1204	G1119
C2537	C2443	A2100	C	U1996	U1903	A1796	U1706	A1607		G1398	A1308	U1205	U1120
A2538	U2444	A2101	C	C2002	A1904	A1797	G1706	A1607	U1503	A1399		U1206	G1121
G2539	C2347	G2102	G	U2003	C1903	C1798	G1707	C1613	A1504	A1406	G1311	C1207	U1130
U2540	G2446	A2103	C	U2004	A1909	G1799	G1707	G1614	U1505	A1407	G1312	C1208	G1131
G2541	C2462	C2104	G	G2005	A1910	G1800	A1710	A1615	U1506	U1408	G1313	G1210	A1132
C2542	U2465	C2105	G	C2006	A1919	C1803	C1714	A1616	A1515	G1409	G1314	C1212	A1133
U2546	A2466	G2110	A	U2007	C1920	A1804	C1715	C1617	U1516	G1410	G1315	G1213	G1137
C2547	G2467	G2111	C	U2008	A1921	G1805	A1716	G1622	U1524	A1413	G1316	G1214	
G2548	A2468	G2112	C	A2011	A1922	C1811	C1716	C1623	U1525	A1414	G1322	A1215	U1149
A2553	C2472	C2114	C	G2013	C1928	U1813	U1722	A1624	G1525	A1415	A1328	G1216	A1150
U2563	U2473	U2115	G	U2016	G1929	G1814	G1723	U1625	A1527	G1415		G1217	G1151
G2564	A2474	U2116	C	U2017	U1937	A1815	U1724	A1626	U1528	U1419	G1329	U1218	A1154
C2565	G2475	G2121	C	U2018	G1938	C1816	C1725	G1627	G1529	C1420	G1330	U1219	G1155
A2566	C2476	C2122	A	A2022	U1939	U1817	C1730	A1631	A1535	C1421	G1331	C1229	G1158
G2578	U2373	U2133	C	U2032	C1940	C1818	A1732	A1632	U1536	U1422	G1332	C1230	G1159
A2583	G2481	G2134	G	A1941	G1941	G1819	A1733	G1634	C1536	C1423	U1333	A1230	G1160
G2584	A2483	U2034	G	C1943	C1943	G1820	C1735	U1635	U1544	A1427	C1342	U1234	A1161
		U2034	G			A1829	A1736	A1637	C1545		C1343	U1237	U1164



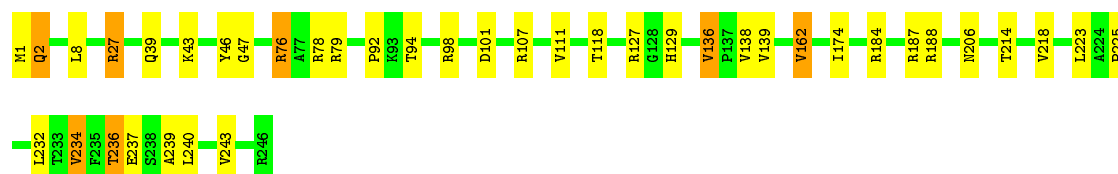
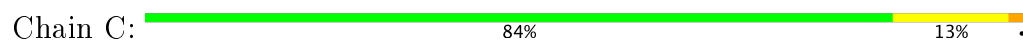
• Molecule 2: 50S ribosomal protein L2P



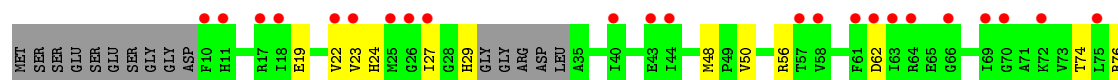
• Molecule 3: 50S ribosomal protein L3P

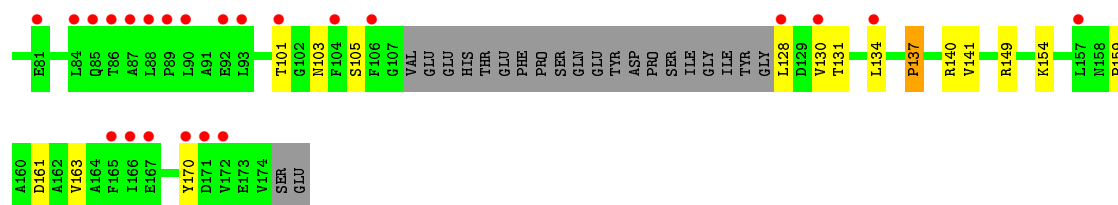


• Molecule 4: 50S ribosomal protein L4P

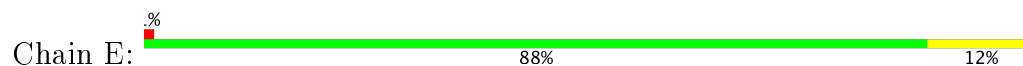


• Molecule 5: 50S ribosomal protein L5P





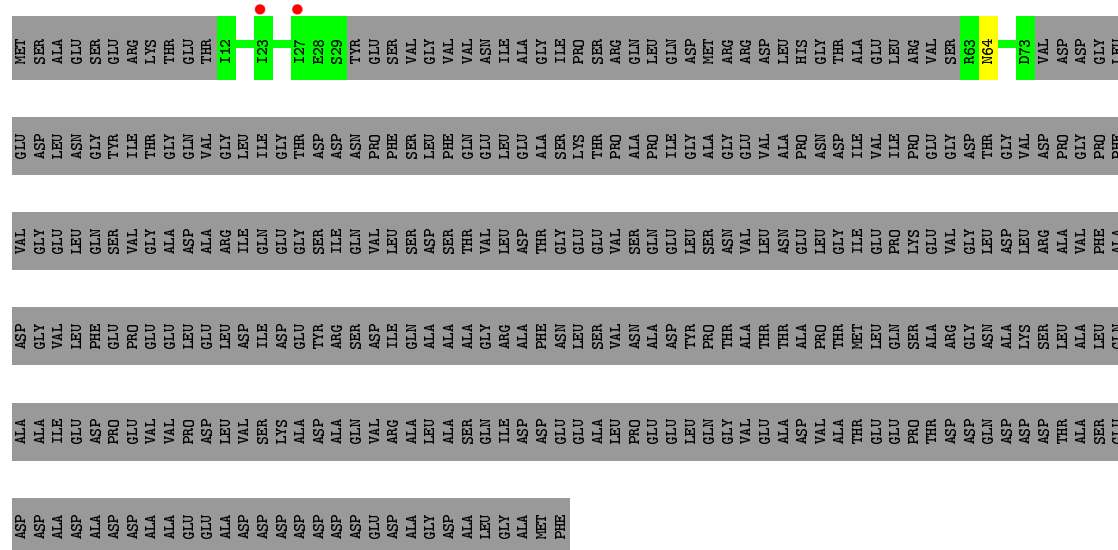
• Molecule 6: 50S ribosomal protein L6P



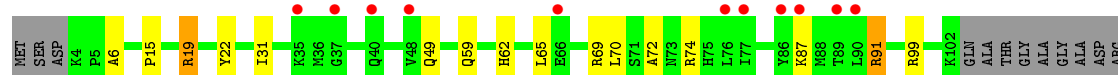
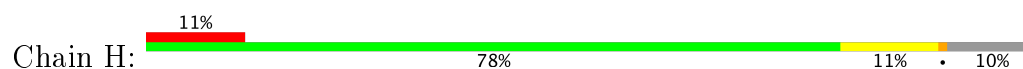
• Molecule 7: 50S ribosomal protein L7Ae

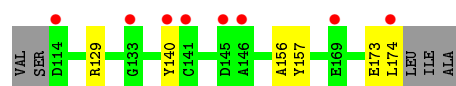


• Molecule 8: 50S ribosomal protein L10E

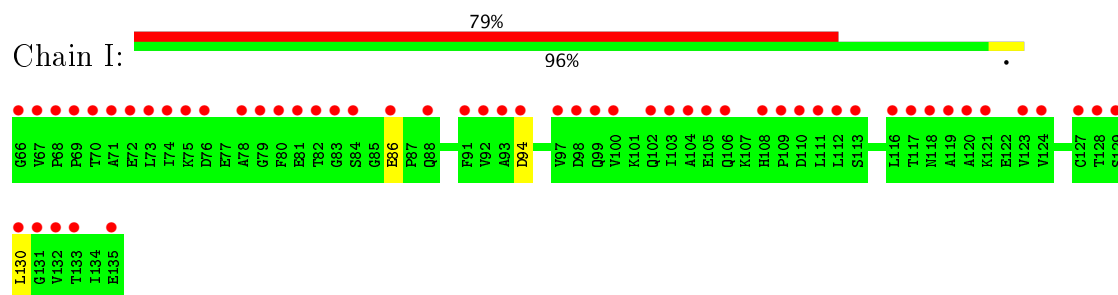


• Molecule 9: 50S ribosomal protein L10e

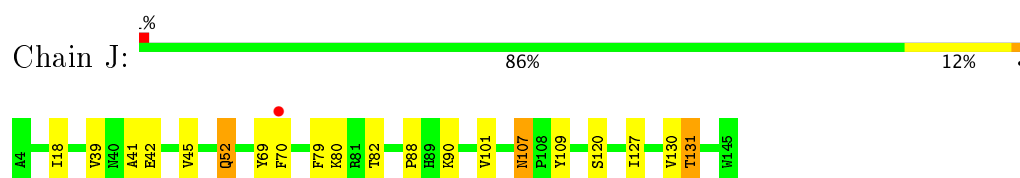




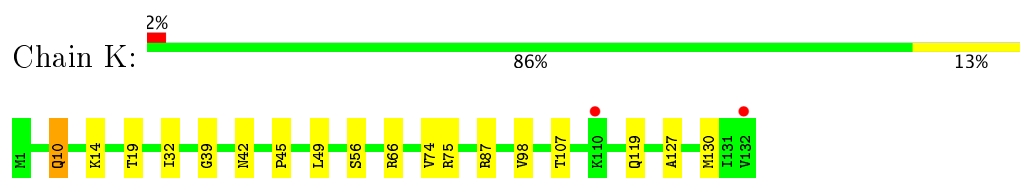
- Molecule 10: 50S ribosomal protein L11P



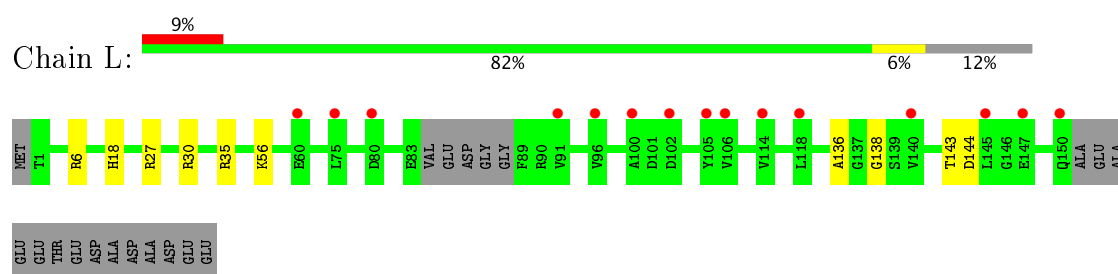
- Molecule 11: 50S ribosomal protein L13P



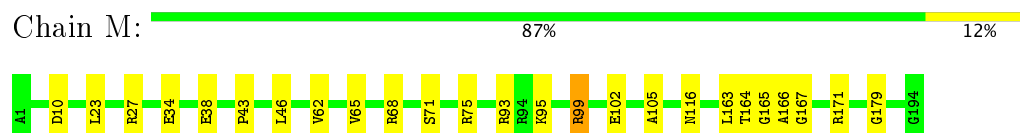
- Molecule 12: 50S ribosomal protein L14P



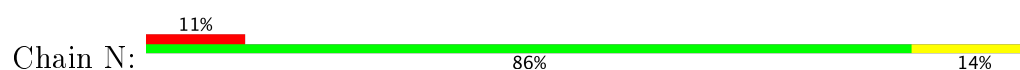
- Molecule 13: 50S ribosomal protein L15P

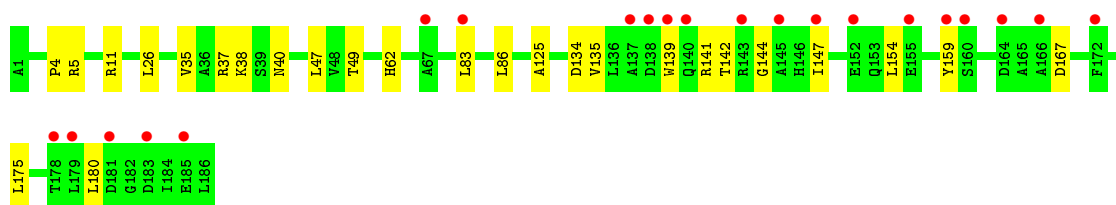


- Molecule 14: 50S ribosomal protein L15e



- Molecule 15: 50S ribosomal protein L18P





- Molecule 16: 50S ribosomal protein L18e

Chain O: 90% 9% .



- Molecule 17: 50S ribosomal protein L19e

Chain P: 87% 13% .



- Molecule 18: 50S ribosomal protein L21e

Chain Q: 87% 12% .



- Molecule 19: 50S ribosomal protein L22P

Chain R: 89% 9% .



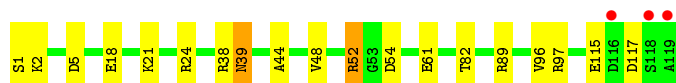
- Molecule 20: 50S ribosomal protein L23P

Chain S: 88% 12% .



- Molecule 21: 50S ribosomal protein L24P

Chain T: 84% 14% .




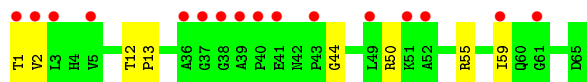
- Molecule 22: 50S ribosomal protein L24e

Chain U:  91% 9%




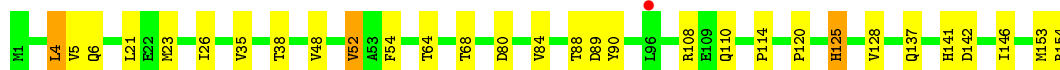
- Molecule 23: 50S ribosomal protein L29P

Chain V:  25% 88% 12%




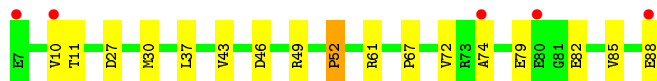
- Molecule 24: 50S ribosomal protein L30P

Chain W:  81% 18% .%



- Molecule 25: 50S ribosomal protein L31e

Chain X:  6% 79% 20% .




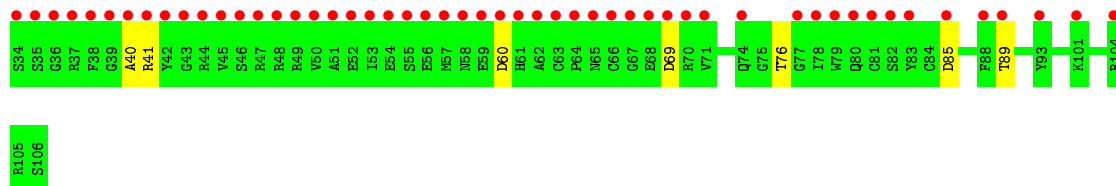
- Molecule 26: 50S ribosomal protein L32e

Chain Y:  89% 10% .%




- Molecule 27: 50S ribosomal protein L37Ae

Chain Z:  71% 90% 10%

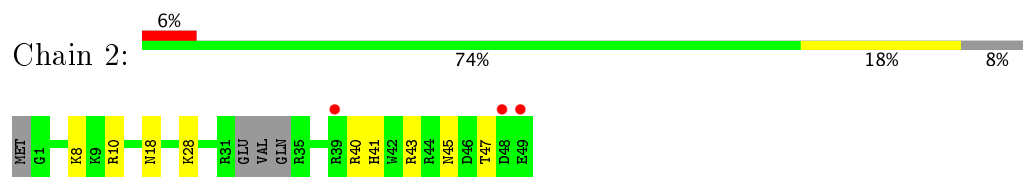


- Molecule 28: 50S ribosomal protein L37e

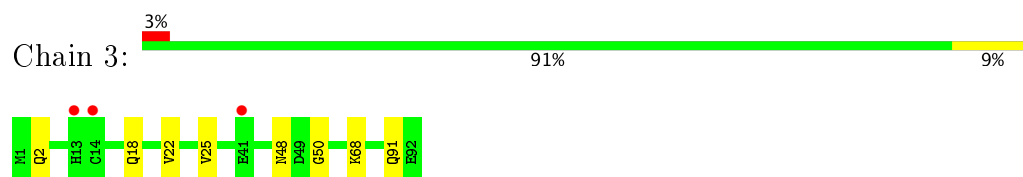
Chain 1:  80% 20%



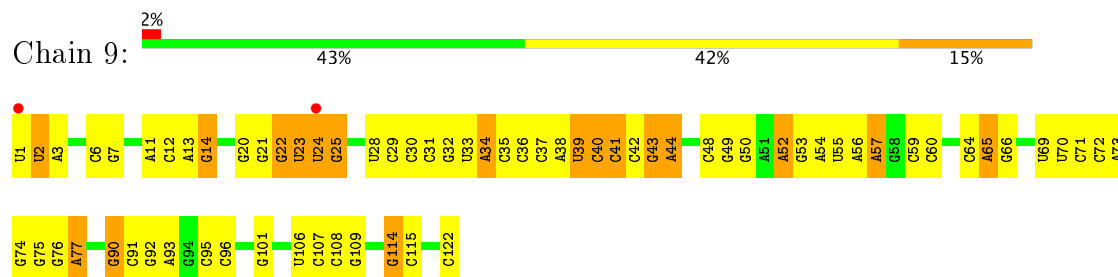
- Molecule 29: 50S ribosomal protein L39e



- Molecule 30: 50S ribosomal protein L44E



- Molecule 31: 5S ribosomal RNA



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	212.21Å 299.54Å 574.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.76 – 2.85 85.61 – 2.40	Depositor EDS
% Data completeness (in resolution range)	91.2 (49.76-2.85) 91.0 (85.61-2.40)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.00 (at 2.40Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.186 , 0.233 0.182 , 0.227	Depositor DCC
$R_{free}$ test set	3763 reflections (0.99%)	DCC
Wilson B-factor (Å <sup>2</sup> )	58.3	Xtriage
Anisotropy	0.215	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 80.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	99174	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.57% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, OMG, CL, SR, NA, K, UR3, CD, OMU, WIN, 1MA, PSU

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	0	0.39	0/65958	0.68	10/102869 (0.0%)
2	A	0.51	1/1787 (0.1%)	0.76	0/2408
3	B	0.53	0/2690	0.77	0/3652
4	C	0.56	0/1885	0.79	0/2552
5	D	0.63	0/1111	0.71	2/1498 (0.1%)
6	E	0.60	0/1383	0.68	0/1880
7	F	0.54	0/901	0.70	0/1224
8	G	0.50	0/241	0.66	0/324
9	H	0.61	0/1302	0.76	0/1743
10	I	0.58	0/527	0.63	0/716
11	J	0.62	0/1136	0.73	0/1530
12	K	0.49	0/1004	0.80	0/1351
13	L	0.52	0/1130	0.74	0/1509
14	M	0.51	0/1583	0.74	0/2116
15	N	0.55	0/1474	0.75	0/1999
16	O	0.50	0/874	0.72	1/1181 (0.1%)
17	P	0.53	0/1148	0.66	0/1528
18	Q	0.51	0/749	0.75	0/1005
19	R	0.57	0/1173	0.76	0/1578
20	S	0.54	0/649	0.65	0/875
21	T	0.47	0/958	0.76	1/1289 (0.1%)
22	U	0.58	0/418	0.68	0/562
23	V	0.43	0/503	0.68	0/675
24	W	0.52	0/1219	0.77	1/1655 (0.1%)
25	X	0.52	0/665	0.75	0/895
26	Y	0.51	0/1147	0.72	0/1536
27	Z	0.68	0/585	0.71	0/781
28	1	0.55	0/438	0.73	0/578
29	2	0.45	0/401	0.70	0/529
30	3	0.56	0/771	0.67	0/1024
31	9	0.33	0/2904	0.69	1/4526 (0.0%)
All	All	0.44	1/98714 (0.0%)	0.70	16/147588 (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	31
24	W	0	1
31	9	0	1
All	All	0	33

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	192	VAL	CB-CG1	-5.05	1.42	1.52

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	871	G	C5'-C4'-O4'	-7.01	100.69	109.10
1	0	2726	U	N1-C1'-C2'	5.93	121.71	114.00
1	0	1942	A	C5'-C4'-C3'	5.70	125.13	116.00
1	0	1504	A	C1'-O4'-C4'	-5.67	105.36	109.90
31	9	39	U	N1-C1'-C2'	5.64	121.34	114.00
1	0	1504	A	N9-C1'-C2'	5.62	121.30	114.00
21	T	52	ARG	N-CA-C	5.46	125.75	111.00
16	O	66	GLY	N-CA-C	5.40	126.60	113.10
1	0	2316	G	C5'-C4'-C3'	-5.27	107.57	116.00
1	0	129	A	C2'-C3'-O3'	5.25	122.11	113.70
1	0	1165	G	C5'-C4'-O4'	5.24	115.39	109.10
1	0	1120	U	C5'-C4'-C3'	-5.20	107.68	116.00
5	D	170	TYR	N-CA-C	5.11	124.81	111.00
24	W	4	LEU	CA-CB-CG	5.10	127.04	115.30
1	0	1819	G	C5'-C4'-C3'	5.07	124.12	116.00
5	D	137	PRO	N-CA-C	5.05	125.23	112.10

There are no chirality outliers.

All (33) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	1078	A	Sidechain
1	0	1260	G	Sidechain
1	0	1635	U	Sidechain

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Mol	Chain	Res	Type	Group
1	0	1749	U	Sidechain
1	0	1819	G	Sidechain
1	0	1829	A	Sidechain
1	0	1848	G	Sidechain
1	0	1877	G	Sidechain
1	0	1878	G	Sidechain
1	0	1972	U	Sidechain
1	0	221	G	Sidechain
1	0	2308	U	Sidechain
1	0	2465	A	Sidechain
1	0	2493	C	Sidechain
1	0	2503	A	Sidechain
1	0	2607	U	Sidechain
1	0	2673	U	Sidechain
1	0	2842	G	Sidechain
1	0	333	G	Sidechain
1	0	396	U	Sidechain
1	0	458	G	Sidechain
1	0	471	G	Sidechain
1	0	482	G	Sidechain
1	0	518	G	Sidechain
1	0	619	U	Sidechain
1	0	625	U	Sidechain
1	0	722	G	Sidechain
1	0	815	U	Sidechain
1	0	817	G	Sidechain
1	0	818	A	Sidechain
1	0	867	A	Sidechain
31	9	90	G	Sidechain
24	W	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	59021	0	29812	1012	0
2	A	1754	0	1766	26	0
3	B	2625	0	2533	33	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	1860	0	1813	23	0
5	D	1094	0	1085	14	0
6	E	1358	0	1266	10	0
7	F	890	0	843	2	0
8	G	240	0	231	1	0
9	H	1282	0	1292	14	0
10	I	520	0	500	2	0
11	J	1120	0	1098	16	0
12	K	994	0	1027	12	0
13	L	1118	0	1076	9	0
14	M	1559	0	1573	15	0
15	N	1445	0	1401	14	0
16	O	865	0	873	8	0
17	P	1137	0	1123	12	0
18	Q	735	0	729	7	0
19	R	1150	0	1122	11	0
20	S	642	0	605	6	0
21	T	950	0	924	9	0
22	U	411	0	364	3	0
23	V	500	0	511	6	0
24	W	1196	0	1137	20	0
25	X	655	0	653	7	0
26	Y	1131	0	1133	12	0
27	Z	574	0	534	6	0
28	1	431	0	426	10	0
29	2	396	0	413	8	0
30	3	755	0	729	5	0
31	9	2599	0	1325	77	0
32	0	85	0	0	0	0
32	2	1	0	0	0	0
32	9	2	0	0	0	0
32	A	1	0	0	0	0
32	B	1	0	0	0	0
32	K	1	0	0	0	0
32	T	1	0	0	0	0
32	Y	1	0	0	0	0
33	0	2	0	0	0	0
34	0	66	0	0	0	0
34	9	2	0	0	0	0
34	C	1	0	0	0	0
34	H	1	0	0	0	0
34	J	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	M	1	0	0	0	0
34	Q	1	0	0	0	0
34	R	1	0	0	0	0
34	S	1	0	0	0	0
35	0	9	0	0	0	0
35	3	1	0	0	0	0
35	A	1	0	0	0	0
35	B	1	0	0	0	0
35	J	3	0	0	1	0
35	K	1	0	0	1	0
35	L	1	0	0	0	0
35	M	1	0	0	0	0
35	N	1	0	0	0	0
35	O	1	0	0	0	0
35	R	1	0	0	0	0
35	Y	1	0	0	0	0
36	0	95	0	0	0	0
36	1	1	0	0	0	0
36	3	2	0	0	0	0
36	9	3	0	0	0	0
36	A	2	0	0	0	0
36	B	2	0	0	0	0
36	F	1	0	0	0	0
36	R	1	0	0	0	0
36	S	1	0	0	0	0
37	0	39	0	36	13	0
38	1	1	0	0	0	0
38	3	1	0	0	0	0
38	O	1	0	0	0	0
38	U	1	0	0	0	0
38	Z	1	0	0	0	0
39	0	5993	0	0	125	0
39	1	52	0	0	0	0
39	2	39	0	0	0	0
39	3	66	0	0	0	0
39	9	149	0	0	7	0
39	A	107	0	0	3	0
39	B	146	0	0	1	0
39	C	171	0	0	5	0
39	D	45	0	0	0	0
39	E	40	0	0	0	0
39	F	25	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
39	G	18	0	0	0	0
39	H	62	0	0	2	0
39	I	5	0	0	1	0
39	J	52	0	0	1	0
39	K	53	0	0	0	0
39	L	79	0	0	3	0
39	M	128	0	0	0	0
39	N	62	0	0	0	0
39	O	40	0	0	2	0
39	P	65	0	0	0	0
39	Q	43	0	0	0	0
39	R	77	0	0	1	0
39	S	28	0	0	0	0
39	T	32	0	0	0	0
39	U	27	0	0	0	0
39	V	12	0	0	0	0
39	W	65	0	0	1	0
39	X	20	0	0	0	0
39	Y	94	0	0	3	0
39	Z	28	0	0	1	0
All	All	99174	0	59953	1243	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 8.

All (1243) 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)
1:0:871:G:H8	1:0:871:G:H5'	1.10	1.15
1:0:1160:G:H5'	1:0:1161:A:H5'	1.26	1.12
1:0:871:G:C8	1:0:871:G:H5'	1.88	1.08
31:9:76:G:H3'	31:9:77:A:H5''	1.36	1.05
31:9:56:A:H2'	31:9:57:A:H5''	1.37	1.04
1:0:156:C:H5''	14:M:171:ARG:HD3	1.43	0.99
1:0:1701:A:H4'	1:0:1702:U:H5''	1.49	0.94
1:0:656:G:H5'	16:O:3:THR:HG22	1.48	0.94
1:0:542:A:H5'	1:0:542:A:H8	1.33	0.93
1:0:1242:A:H5'	11:J:82:THR:HG23	1.47	0.93
1:0:545:G:H8	1:0:545:G:H5'	1.31	0.93
1:0:2540:G:H4'	37:0:9101:WIN:H1O	1.50	0.91
1:0:870:G:H2'	1:0:871:G:H5''	1.53	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2717:C:C2'	1:0:2718:C:H5''	2.02	0.90
1:0:1666:C:C2'	1:0:1667:A:H5''	2.02	0.90
15:N:37:ARG:NH1	31:9:6:C:H5''	1.87	0.90
1:0:2506:A:HO2'	1:0:2507:G:H8	0.94	0.89
1:0:381:G:H5''	39:0:2945:HOH:O	1.74	0.86
12:K:10:GLN:H	12:K:10:GLN:HE21	1.18	0.86
1:0:1603:A:H5'	1:0:1605:G:O4'	1.74	0.86
17:P:115:SER:H	17:P:118:GLN:HE21	1.22	0.86
1:0:1474:C:H6	1:0:1474:C:H5'	1.40	0.85
1:0:2586:U:H3	1:0:2592:G:H22	1.22	0.85
1:0:1119:G:H2'	11:J:52:GLN:NE2	1.92	0.85
1:0:1160:G:C5'	1:0:1161:A:H5'	2.06	0.84
1:0:2812:A:H2	1:0:2814:A:H62	1.26	0.84
1:0:1160:G:H5'	1:0:1161:A:C5'	2.06	0.84
1:0:1372:A:H3'	39:0:6923:HOH:O	1.76	0.84
1:0:2717:C:H2'	1:0:2718:C:H5''	1.57	0.84
1:0:541:C:H2'	1:0:542:A:H5''	1.59	0.83
1:0:877:G:H5'	1:0:878:G:OP1	1.79	0.83
1:0:1205:U:H2'	1:0:1206:U:H5''	1.59	0.82
1:0:1593:C:H5'	17:P:116:SER:O	1.79	0.82
1:0:823:U:H3'	39:0:3123:HOH:O	1.78	0.82
1:0:2487:C:C2	37:0:9101:WIN:H1F	2.15	0.82
1:0:1666:C:H2'	1:0:1667:A:H5''	1.61	0.82
31:9:29:C:H2'	31:9:30:C:H5'	1.62	0.81
1:0:657:G:OP1	4:C:27:ARG:NH2	2.14	0.81
1:0:506:G:H22	1:0:509:A:C5'	1.94	0.81
31:9:56:A:C2'	31:9:57:A:H5''	2.11	0.81
1:0:506:G:H22	1:0:509:A:H5''	1.46	0.79
1:0:1118:A:H3'	1:0:1118:A:H8	1.47	0.79
1:0:500:G:H21	19:R:98:ASN:HD21	1.26	0.79
1:0:1205:U:H2'	1:0:1206:U:C5'	2.12	0.78
1:0:541:C:C2'	1:0:542:A:H5''	2.13	0.78
1:0:1835:U:H5	1:0:1840:A:N7	1.81	0.78
1:0:1118:A:H62	1:0:1244:U:H3	1.29	0.78
1:0:1118:A:H3'	1:0:1118:A:C8	2.19	0.77
1:0:2637:A:H5'	39:0:3948:HOH:O	1.84	0.77
1:0:157:G:H4'	14:M:95:LYS:HE2	1.66	0.77
1:0:1666:C:O2'	1:0:1667:A:H5''	1.83	0.77
1:0:871:G:H8	1:0:871:G:C5'	1.96	0.77
1:0:1300:G:H1'	39:0:3448:HOH:O	1.83	0.77
1:0:2756:U:H3	1:0:2896:A:H2	1.33	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1474:C:C6	1:0:1474:C:H5'	2.20	0.76
1:0:1684:A:H1'	29:2:43:ARG:HH22	1.49	0.76
1:0:2533:C:H5'	1:0:2533:C:H6	1.50	0.76
1:0:1116:U:HO2'	1:0:1118:A:H2	1.31	0.75
1:0:870:G:C2'	1:0:871:G:H5''	2.16	0.75
31:9:24:U:H3'	31:9:25:G:H5'	1.67	0.75
1:0:545:G:C8	1:0:545:G:H5'	2.17	0.75
1:0:681:G:N3	1:0:681:G:H5'	2.01	0.75
1:0:2506:A:O2'	1:0:2507:G:H8	1.70	0.75
1:0:1667:A:H8	1:0:1667:A:H5'	1.52	0.75
1:0:1701:A:H5'	39:0:5659:HOH:O	1.86	0.74
1:0:1116:U:H3	1:0:1246:A:H62	1.31	0.74
19:R:8:ALA:HB1	19:R:13:THR:HG21	1.70	0.74
31:9:73:A:H61	31:9:108:C:H42	1.33	0.74
31:9:92:G:H2'	31:9:93:A:C8	2.22	0.73
21:T:24:ARG:HH21	21:T:39:ASN:HD22	1.35	0.73
1:0:1666:C:H2'	1:0:1667:A:C5'	2.18	0.73
1:0:2005:G:H3'	1:0:2005:G:OP2	1.89	0.73
1:0:1206:U:H6	1:0:1206:U:H5'	1.54	0.73
1:0:2420:G:O2'	1:0:2421:G:H5'	1.89	0.73
1:0:281:U:H2'	1:0:282:C:O4'	1.89	0.72
1:0:2717:C:O2'	1:0:2718:C:H5''	1.89	0.72
1:0:182:G:H5'	39:0:4102:HOH:O	1.90	0.72
1:0:559:U:H5'	1:0:559:U:H6	1.55	0.71
1:0:2291:A:C8	1:0:2309:C:H5'	2.25	0.71
1:0:2578:G:H5'	1:0:2578:G:H8	1.55	0.71
1:0:544:G:H2'	1:0:545:G:H5''	1.73	0.71
31:9:14:G:H5'	31:9:14:G:H8	1.56	0.70
1:0:12:U:H2'	1:0:13:G:H5'	1.74	0.70
1:0:1116:U:O2'	1:0:1118:A:H2	1.74	0.69
1:0:1278:A:H4'	1:0:1279:U:C4	2.28	0.69
1:0:1701:A:H4'	1:0:1702:U:C5'	2.21	0.69
1:0:541:C:H2'	1:0:542:A:C5'	2.22	0.69
1:0:2635:A:O2'	1:0:2636:C:H5'	1.93	0.69
1:0:450:C:OP1	4:C:184:ARG:NH2	2.24	0.69
1:0:542:A:H5'	1:0:542:A:C8	2.22	0.69
1:0:853:C:H3'	39:0:3276:HOH:O	1.91	0.69
1:0:1834:C:H2'	1:0:1840:A:N6	2.07	0.68
1:0:93:C:H5''	23:V:1:THR:HB	1.74	0.68
1:0:2769:C:C2'	1:0:2770:G:H5'	2.24	0.68
1:0:603:A:H5''	1:0:604:G:OP1	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2502:C:H2'	1:0:2503:A:H5'	1.76	0.68
1:0:2768:A:H2'	1:0:2769:C:O4'	1.93	0.67
1:0:1189:A:H1'	1:0:1209:C:O4'	1.94	0.67
1:0:2716:G:H5''	3:B:206:THR:HG21	1.74	0.67
1:0:1119:G:H2'	11:J:52:GLN:HE22	1.58	0.67
1:0:1632:A:H2'	1:0:1633:C:H5'	1.76	0.67
3:B:238:ASN:HD22	3:B:240:GLY:H	1.43	0.67
1:0:2502:C:C2'	1:0:2503:A:H5'	2.25	0.67
3:B:221:GLN:HE22	12:K:42:ASN:HD22	1.41	0.67
1:0:1119:G:N2	1:0:1246:A:C2	2.60	0.67
1:0:1625:U:H4'	39:0:3427:HOH:O	1.94	0.66
1:0:20:G:H21	19:R:117:HIS:HD2	1.41	0.66
1:0:1189:A:H1'	1:0:1209:C:C1'	2.24	0.66
1:0:188:C:H5''	14:M:163:LEU:HD21	1.77	0.66
1:0:1377:C:H6	1:0:1377:C:H5'	1.61	0.66
1:0:2908:A:H2'	1:0:2909:G:O4'	1.96	0.66
39:0:4058:HOH:O	35:K:8812:CL:CL	2.50	0.65
1:0:2468:A:H61	30:3:48:ASN:HD21	1.44	0.65
1:0:2443:C:H1'	13:L:56:LYS:HE3	1.76	0.65
1:0:2320:U:H4'	1:0:2321:A:O4'	1.97	0.65
15:N:141:ARG:HH21	31:9:48:C:H4'	1.59	0.65
1:0:2710:U:H1'	39:0:7520:HOH:O	1.96	0.65
1:0:671:A:O2'	1:0:672:G:H2'	1.97	0.65
1:0:1973:A:H2'	1:0:1974:G:O4'	1.96	0.65
31:9:49:G:O2'	31:9:50:G:H5'	1.97	0.65
25:X:37:LEU:HD13	25:X:85:VAL:HG21	1.79	0.65
1:0:308:U:H5'	1:0:309:C:OP1	1.96	0.65
1:0:821:U:H2'	1:0:822:C:H6	1.61	0.65
1:0:544:G:C2'	1:0:545:G:H5''	2.27	0.64
31:9:39:U:H1'	31:9:44:A:H61	1.61	0.64
24:W:137:GLN:HE21	24:W:141:HIS:HE1	1.45	0.64
1:0:136:C:H2'	1:0:137:U:O4'	1.97	0.64
1:0:871:G:C8	1:0:871:G:C5'	2.74	0.64
1:0:1181:A:H2'	1:0:1182:C:H5'	1.78	0.64
1:0:1184:C:H1'	39:0:7308:HOH:O	1.98	0.64
31:9:75:G:H1	31:9:106:U:H3	1.45	0.64
1:0:1947:G:H2'	1:0:1948:G:H8	1.63	0.64
31:9:3:A:N6	31:9:22:G:H1'	2.13	0.64
1:0:1183:C:N4	1:0:1184:C:H41	1.94	0.64
1:0:2787:C:H5	39:0:3383:HOH:O	1.81	0.64
1:0:2827:A:H2'	1:0:2828:G:O4'	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:3:2:GLN:HE21	30:3:91:GLN:HE21	1.45	0.63
1:0:371:U:H2'	1:0:372:A:H8	1.63	0.63
1:0:1641:A:H2'	1:0:1642:A:H5'	1.80	0.63
1:0:2491:G:H1'	39:0:6473:HOH:O	1.97	0.63
1:0:1166:A:H1'	1:0:1192:A:C2	2.33	0.63
1:0:1165:G:H4'	1:0:1174:A:O2'	1.99	0.63
31:9:7:G:H5'	39:9:5071:HOH:O	1.98	0.63
1:0:2896:A:H5''	39:0:5399:HOH:O	1.99	0.62
14:M:164:THR:HG22	14:M:166:ALA:H	1.63	0.62
1:0:2533:C:C6	1:0:2533:C:H5'	2.33	0.62
39:0:4183:HOH:O	12:K:39:GLY:HA2	1.99	0.62
1:0:482:G:H4'	1:0:508:A:N1	2.15	0.62
1:0:272:A:H5'	1:0:273:G:OP2	1.99	0.62
1:0:2419:U:H5''	1:0:2420:G:H5'	1.81	0.62
1:0:1835:U:C5	1:0:1840:A:N7	2.67	0.62
1:0:1886:A:H4'	39:Z:395:HOH:O	1.99	0.62
1:0:1762:C:H2'	1:0:1763:C:H6	1.64	0.62
1:0:2486:A:H3'	39:0:3735:HOH:O	1.99	0.62
1:0:2748:G:H2'	39:0:7410:HOH:O	2.00	0.62
15:N:141:ARG:NH2	31:9:48:C:H4'	2.15	0.62
31:9:1:U:H4'	31:9:3:A:OP1	1.99	0.61
1:0:1800:G:H1'	17:P:88:GLN:NE2	2.15	0.61
1:0:1819:G:H5'	39:0:3491:HOH:O	1.99	0.61
1:0:2401:A:H2'	1:0:2402:A:C8	2.35	0.61
1:0:285:A:H2'	1:0:286:U:O4'	2.00	0.61
24:W:4:LEU:HD23	24:W:54:PHE:HB3	1.81	0.61
1:0:440:C:H2'	1:0:441:A:C8	2.36	0.61
1:0:1741:U:H5'	1:0:1742:A:OP1	2.00	0.61
1:0:56:G:H5''	23:V:50:ARG:NH1	2.15	0.61
16:O:32:ARG:HE	16:O:35:LYS:HD2	1.66	0.61
1:0:282:C:H1'	1:0:368:C:N4	2.15	0.61
1:0:820:G:H3'	39:0:6936:HOH:O	2.01	0.61
31:9:76:G:H3'	31:9:77:A:C5'	2.22	0.61
1:0:1201:C:H5''	39:0:5584:HOH:O	1.99	0.60
1:0:1528:A:H2'	1:0:1529:G:O4'	2.00	0.60
1:0:553:G:P	26:Y:204:ARG:HH22	2.24	0.60
1:0:656:G:H1'	39:C:7042:HOH:O	2.00	0.60
24:W:88:THR:HG23	24:W:110:GLN:HB3	1.83	0.60
1:0:1015:C:H2'	1:0:1016:U:H6	1.66	0.60
1:0:1097:A:H5''	24:W:125:HIS:NE2	2.16	0.60
1:0:558:C:C2'	1:0:559:U:H5''	2.32	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1187:U:O2'	1:0:1189:A:H2	1.83	0.60
1:0:1213:C:O2'	1:0:1214:G:H5'	2.02	0.60
1:0:2054:A:N3	19:R:128:ARG:NH2	2.49	0.60
1:0:1189:A:H3'	39:0:7609:HOH:O	2.02	0.60
1:0:1209:C:H2'	1:0:1210:G:H8	1.65	0.60
1:0:2472:C:O2'	1:0:2634:G:H4'	2.01	0.60
31:9:12:C:H5'	31:9:70:U:O4'	2.00	0.60
1:0:814:G:H4'	39:0:7240:HOH:O	2.01	0.60
31:9:24:U:H3'	31:9:25:G:C5'	2.31	0.60
15:N:11:ARG:HD3	31:9:114:G:O6	2.02	0.59
1:0:2426:G:H1'	39:0:5391:HOH:O	2.01	0.59
1:0:1166:A:H61	1:0:1180:U:H3	1.50	0.59
1:0:1972:U:H2'	1:0:1973:A:H5'	1.85	0.59
1:0:2563:U:H2'	1:0:2565:C:O5'	2.02	0.59
1:0:1120:U:H5''	1:0:1120:U:C6	2.38	0.59
1:0:282:C:O2'	1:0:283:U:H5'	2.02	0.59
1:0:338:C:H4'	4:C:174:ILE:CD1	2.32	0.59
1:0:399:C:H5'	14:M:179:GLY:O	2.03	0.59
4:C:127:ARG:NH2	4:C:225:PRO:HG2	2.18	0.59
7:F:91:VAL:HG12	7:F:92:GLY:H	1.68	0.59
1:0:2712:G:H5'	39:0:4183:HOH:O	2.02	0.59
1:0:2851:G:O2'	1:0:2852:A:H5'	2.03	0.59
1:0:2616:G:H1'	39:0:8327:HOH:O	2.03	0.58
1:0:2781:U:H1'	6:E:139:GLU:OE2	2.03	0.58
31:9:13:A:O2'	31:9:14:G:H5''	2.02	0.58
1:0:2252:A:C5	1:0:2253:G:H1'	2.38	0.58
1:0:56:G:H5''	23:V:50:ARG:HH12	1.67	0.58
31:9:39:U:H3'	31:9:40:C:H5''	1.85	0.58
1:0:1446:U:H2'	20:S:55:GLN:NE2	2.17	0.58
1:0:1189:A:H1'	1:0:1209:C:H1'	1.84	0.58
1:0:2241:C:H2'	1:0:2242:U:C6	2.38	0.58
1:0:2270:G:H4'	2:A:223:ARG:NH1	2.18	0.58
1:0:2721:U:H4'	12:K:87:ARG:HG3	1.83	0.58
1:0:558:C:O2'	1:0:559:U:H5''	2.03	0.58
1:0:1363:G:P	4:C:76:ARG:HH22	2.26	0.58
1:0:1328:A:OP1	26:Y:169:ARG:HD2	2.03	0.58
1:0:821:U:H2'	1:0:822:C:C6	2.39	0.58
1:0:902:G:N7	13:L:18:HIS:HD2	2.02	0.58
1:0:1165:G:H1'	1:0:1174:A:H1'	1.85	0.58
1:0:1441:G:O2'	1:0:1442:A:H5'	2.04	0.58
1:0:1790:C:H2'	1:0:1791:U:H6	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:67:A:H5''	1:0:69:A:C8	2.39	0.58
1:0:960:G:H4'	39:0:7253:HOH:O	2.04	0.58
1:0:1679:C:H5'	39:0:4173:HOH:O	2.04	0.58
1:0:2524:G:H21	1:0:2526:C:N4	2.02	0.58
1:0:2783:A:H3'	39:0:4201:HOH:O	2.03	0.58
29:2:40:ARG:HD2	29:2:47:THR:HG22	1.84	0.58
24:W:137:GLN:HE21	24:W:141:HIS:CE1	2.21	0.58
1:0:1973:A:H5'	1:0:1973:A:H8	1.68	0.57
1:0:2894:C:O2'	1:0:2895:C:H5'	2.04	0.57
1:0:952:G:N3	1:0:2302:A:H2'	2.19	0.57
3:B:36:PRO:HG3	3:B:169:GLY:H	1.68	0.57
22:U:39:ASN:ND2	22:U:44:ARG:HH11	2.02	0.57
1:0:1118:A:C8	1:0:1118:A:C3'	2.83	0.57
1:0:1733:A:H4'	3:B:212:GLN:HA	1.85	0.57
1:0:2670:G:O2'	1:0:2671:U:H5'	2.03	0.57
1:0:1419:U:H2'	1:0:1685:A:C2	2.39	0.57
1:0:2769:C:H2'	1:0:2770:G:O4'	2.04	0.57
1:0:2769:C:H2'	1:0:2770:G:H5'	1.85	0.57
1:0:407:A:H5'	39:0:5296:HOH:O	2.04	0.57
1:0:1441:G:H1'	39:0:7717:HOH:O	2.03	0.57
1:0:2769:C:O2'	1:0:2770:G:H5'	2.04	0.57
31:9:14:G:H5'	31:9:14:G:C8	2.38	0.57
5:D:154:LYS:HD2	5:D:154:LYS:H	1.69	0.57
1:0:1994:A:P	12:K:66:ARG:HH22	2.28	0.57
5:D:140:ARG:HB3	31:9:29:C:H5''	1.86	0.57
1:0:1015:C:H2'	1:0:1016:U:C6	2.40	0.57
1:0:1838:U:O2'	1:0:2644:C:H5'	2.05	0.57
31:9:55:U:H4'	31:9:56:A:C8	2.39	0.57
1:0:2780:C:H1'	6:E:143:GLN:HE21	1.69	0.57
1:0:1166:A:P	1:0:1174:A:H4'	2.44	0.57
1:0:1819:G:H2'	1:0:1820:G:H4'	1.86	0.57
1:0:68:U:O2'	1:0:69:A:H5''	2.05	0.57
1:0:2365:G:H4'	18:Q:45:PRO:O	2.05	0.57
1:0:1008:C:H5''	9:H:19:ARG:HH12	1.68	0.57
1:0:1667:A:C8	1:0:1667:A:H5'	2.37	0.57
1:0:2781:U:O2'	1:0:2782:G:H5'	2.04	0.57
1:0:2900:G:H2'	1:0:2901:C:O4'	2.05	0.56
17:P:115:SER:H	17:P:118:GLN:NE2	1.99	0.56
1:0:1132:A:N6	1:0:1229:C:H2'	2.20	0.56
1:0:625:U:H3'	39:0:7631:HOH:O	2.04	0.56
1:0:969:G:H1	1:0:999:C:H42	1.53	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2534:C:H1'	39:0:8179:HOH:O	2.04	0.56
1:0:119:A:H2'	1:0:120:A:H5''	1.86	0.56
1:0:65:C:O2'	1:0:66:G:H5'	2.04	0.56
1:0:794:U:H3	1:0:819:A:H61	1.54	0.56
1:0:560:U:H2'	1:0:561:G:H8	1.69	0.56
1:0:95:A:H5''	1:0:97:G:O4'	2.05	0.56
31:9:38:A:H2'	31:9:39:U:C6	2.41	0.56
1:0:2755:G:H1'	39:0:3447:HOH:O	2.06	0.56
1:0:69:A:H5'	1:0:69:A:H8	1.69	0.56
1:0:797:A:N6	1:0:816:G:H1'	2.20	0.56
25:X:61:ARG:HH12	25:X:67:PRO:HD3	1.70	0.56
1:0:1279:U:O2	1:0:1279:U:H2'	2.05	0.56
1:0:2032:U:H5'	39:0:3222:HOH:O	2.04	0.56
1:0:2760:C:H5''	39:0:4329:HOH:O	2.06	0.56
5:D:103:ASN:HD22	5:D:134:LEU:H	1.54	0.56
1:0:1634:G:H3'	39:0:8650:HOH:O	2.06	0.56
1:0:2756:U:N3	1:0:2896:A:H2	2.02	0.56
15:N:144:GLY:O	15:N:147:ILE:HG22	2.05	0.56
1:0:162:C:H2'	1:0:163:U:H5'	1.88	0.55
1:0:441:A:H1'	1:0:442:A:N7	2.21	0.55
1:0:731:U:H2'	1:0:732:C:C6	2.41	0.55
1:0:1845:A:OP2	2:A:190:ARG:NH1	2.39	0.55
1:0:1205:U:C2'	1:0:1206:U:H5''	2.34	0.55
1:0:1330:A:H5''	39:Y:7277:HOH:O	2.06	0.55
1:0:196:G:H2'	39:0:6170:HOH:O	2.05	0.55
1:0:613:C:H2'	1:0:614:U:H6	1.71	0.55
4:C:139:VAL:HG13	39:C:6251:HOH:O	2.06	0.55
1:0:2597:U:H1'	39:0:4058:HOH:O	2.05	0.55
1:0:2769:C:H2'	1:0:2770:G:C5'	2.36	0.55
1:0:1422:U:H2'	1:0:1423:C:C6	2.41	0.55
1:0:1497:G:H4'	1:0:1627:G:O2'	2.07	0.55
1:0:1654:U:H2'	2:A:47:HIS:HD2	1.71	0.55
31:9:29:C:C2'	31:9:30:C:H5'	2.33	0.55
31:9:55:U:H4'	31:9:56:A:H8	1.71	0.55
1:0:1701:A:H5''	1:0:1702:U:H3'	1.88	0.55
1:0:776:A:OP1	28:1:28:HIS:HE1	1.89	0.55
31:9:95:C:O2'	31:9:96:C:H5'	2.06	0.55
5:D:76:ARG:NH2	31:9:44:A:H1'	2.21	0.55
1:0:317:A:OP1	21:T:52:ARG:O	2.24	0.55
1:0:31:C:H2'	39:0:7619:HOH:O	2.05	0.55
1:0:306:A:P	21:T:38:ARG:HH21	2.30	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1182:C:H1'	1:0:1192:A:H8	1.71	0.55
1:0:371:U:H2'	1:0:372:A:C8	2.42	0.55
1:0:468:U:H3'	39:0:7448:HOH:O	2.05	0.55
1:0:559:U:H5'	1:0:559:U:C6	2.40	0.55
9:H:72:ALA:HB2	9:H:156:ALA:HB2	1.87	0.55
1:0:1364:G:H1'	39:0:3619:HOH:O	2.06	0.55
1:0:2509:A:H2'	1:0:2510:C:O4'	2.07	0.55
1:0:2613:G:O2'	1:0:2614:C:H5'	2.07	0.55
4:C:162:VAL:HG22	4:C:232:LEU:HD21	1.89	0.55
9:H:59:GLN:HE21	9:H:129:ARG:HE	1.55	0.55
1:0:1118:A:H8	1:0:1119:G:H5''	1.71	0.55
1:0:1173:A:H4'	1:0:1174:A:C8	2.41	0.55
1:0:1632:A:C2'	1:0:1633:C:H5'	2.37	0.55
1:0:588:G:O6	24:W:154:ARG:NH1	2.40	0.55
1:0:625:U:H5''	1:0:1044:C:N4	2.22	0.55
1:0:2050:G:H5''	19:R:80:TYR:O	2.06	0.55
1:0:1527:A:H1'	1:0:1528:A:C8	2.42	0.54
1:0:1741:U:O2'	1:0:2723:G:H4'	2.07	0.54
1:0:1979:G:H2'	39:0:3969:HOH:O	2.07	0.54
1:0:2064:U:H5'	1:0:2652:U:H4'	1.89	0.54
11:J:41:ALA:HB3	39:J:5907:HOH:O	2.06	0.54
16:O:38:ARG:NH1	39:O:7674:HOH:O	2.40	0.54
1:0:1677:U:OP2	29:2:8:LYS:NZ	2.39	0.54
1:0:69:A:H5'	1:0:69:A:C8	2.43	0.54
2:A:48:ASP:HB3	39:A:5706:HOH:O	2.07	0.54
1:0:121:U:OP2	29:2:10:ARG:NH2	2.38	0.54
1:0:841:A:H5''	39:0:6534:HOH:O	2.07	0.54
24:W:21:LEU:HD21	24:W:48:VAL:HG11	1.89	0.54
1:0:1191:A:H2	1:0:1206:U:H3	1.56	0.54
1:0:128:A:O2'	1:0:129:A:H5'	2.07	0.54
1:0:1790:C:H2'	1:0:1791:U:C6	2.42	0.54
1:0:1855:G:H4'	1:0:1856:C:O5'	2.07	0.54
1:0:2435:U:H1'	39:0:4462:HOH:O	2.07	0.54
1:0:2524:G:H21	1:0:2526:C:H41	1.56	0.54
1:0:2672:C:H1'	39:0:6210:HOH:O	2.07	0.54
1:0:1787:C:H4'	1:0:2883:A:O4'	2.07	0.54
1:0:836:G:H5''	39:0:3971:HOH:O	2.07	0.54
31:9:92:G:H2'	31:9:93:A:H8	1.70	0.54
1:0:1053:G:OP1	9:H:15:PRO:HG3	2.08	0.54
1:0:1762:C:H2'	1:0:1763:C:C6	2.43	0.54
1:0:1594:C:O2'	1:0:1607:A:H4'	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2414:A:H2'	1:0:2415:A:C8	2.42	0.54
1:0:2505:G:O2'	1:0:2506:A:H5'	2.08	0.54
1:0:2779:G:H21	6:E:143:GLN:NE2	2.06	0.54
1:0:2878:U:H2'	1:0:2879:A:O4'	2.08	0.54
1:0:10:U:O4	1:0:532:A:OP2	2.25	0.54
1:0:90:A:H2'	1:0:91:G:O4'	2.08	0.54
1:0:1921:A:O2'	1:0:1922:A:H5'	2.07	0.53
1:0:506:G:H22	1:0:509:A:H5'	1.69	0.53
37:0:9101:WIN:H1FB	37:0:9101:WIN:H1OA	1.89	0.53
29:2:41:HIS:H	29:2:45:ASN:HD22	1.56	0.53
1:0:1206:U:H2'	1:0:1207:A:O4'	2.08	0.53
1:0:1972:U:H2'	1:0:1973:A:C5'	2.39	0.53
1:0:2700:G:H3'	39:0:8266:HOH:O	2.08	0.53
1:0:694:A:H2'	1:0:695:C:H5'	1.90	0.53
2:A:121:ALA:O	2:A:124:VAL:HG22	2.08	0.53
6:E:95:VAL:HG11	6:E:131:LEU:HD11	1.90	0.53
1:0:1119:G:H8	11:J:52:GLN:HE22	1.55	0.53
1:0:445:U:H2'	1:0:446:G:H8	1.72	0.53
1:0:2487:C:C6	37:0:9101:WIN:O1K	2.61	0.53
31:9:64:C:H2'	31:9:65:A:H5'	1.91	0.53
20:S:33:SER:O	20:S:37:VAL:HG23	2.07	0.53
1:0:1119:G:H22	1:0:1246:A:H2	1.51	0.53
1:0:1477:C:H5'	1:0:1868:G:C5'	2.38	0.53
1:0:558:C:H2'	1:0:559:U:C5'	2.38	0.53
1:0:87:C:H2'	29:2:28:LYS:O	2.08	0.53
31:9:23:U:O2'	31:9:24:U:H4'	2.09	0.53
5:D:103:ASN:ND2	5:D:134:LEU:H	2.07	0.53
1:0:2445:U:H2'	1:0:2446:G:C8	2.43	0.53
1:0:316:A:N3	1:0:336:G:O2'	2.38	0.53
2:A:179:MET:HG2	2:A:186:TRP:HB2	1.91	0.53
1:0:1947:G:H2'	1:0:1948:G:C8	2.43	0.53
1:0:2111:G:H1'	39:0:3082:HOH:O	2.07	0.53
1:0:2344:G:N3	1:0:2344:G:H2'	2.23	0.53
1:0:1299:G:O6	13:L:6:ARG:HD3	2.08	0.53
1:0:1878:G:O2'	1:0:1879:U:OP2	2.27	0.53
1:0:447:A:O2'	1:0:448:G:H5'	2.09	0.53
1:0:635:A:H2'	1:0:636:G:H5'	1.90	0.53
1:0:848:C:H5'	39:0:7034:HOH:O	2.09	0.53
31:9:2:U:OP2	31:9:3:A:H5'	2.08	0.53
1:0:2795:C:O2'	1:0:2796:U:H5'	2.09	0.53
1:0:947:U:O2'	1:0:948:G:H5'	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:9:71:C:H2'	31:9:72:C:H6	1.74	0.53
1:0:407:A:H2'	1:0:408:A:C8	2.44	0.53
1:0:1803:C:H2'	1:0:1804:A:C8	2.44	0.52
1:0:195:C:H2'	1:0:196:G:H5'	1.90	0.52
1:0:450:C:H4'	4:C:46:TYR:CE1	2.43	0.52
13:L:136:ALA:HB3	39:L:6166:HOH:O	2.07	0.52
1:0:1181:A:C2'	1:0:1182:C:H5'	2.39	0.52
1:0:1375:A:C2'	1:0:1376:G:H5'	2.39	0.52
1:0:1603:A:H5''	1:0:1605:G:H5'	1.91	0.52
1:0:2387:U:H2'	1:0:2388:C:C6	2.44	0.52
6:E:137:ASP:O	6:E:141:VAL:HG23	2.10	0.52
1:0:2364:A:H5''	18:Q:15:LYS:HD3	1.91	0.52
1:0:1180:U:H4'	10:I:86:GLU:HG2	1.91	0.52
1:0:1268:C:H2'	1:0:1269:G:H8	1.74	0.52
1:0:2103:A:H2'	1:0:2104:C:H5'	1.90	0.52
39:0:6217:HOH:O	21:T:38:ARG:NH1	2.42	0.52
1:0:1427:A:H61	1:0:1440:U:H1'	1.73	0.52
1:0:2039:A:OP2	3:B:234:ARG:NH2	2.43	0.52
1:0:790:A:H1'	1:0:1710:A:H2'	1.91	0.52
1:0:1333:U:H2'	1:0:1334:C:C6	2.44	0.52
1:0:247:A:H2'	39:0:8680:HOH:O	2.09	0.52
31:9:34:A:H2'	31:9:35:C:O4'	2.10	0.52
1:0:10:U:O4	1:0:531:G:H2'	2.10	0.52
1:0:522:U:O2'	1:0:1366:C:H5'	2.09	0.52
37:0:9101:WIN:H1A	37:0:9101:WIN:H1BA	1.92	0.52
30:3:25:VAL:HG22	30:3:68:LYS:HG3	1.91	0.52
11:J:127:ILE:HG22	35:J:8801:CL:CL	2.46	0.52
28:1:8:GLN:HE22	28:1:11:LYS:NZ	2.08	0.52
3:B:217:ARG:HG3	3:B:257:THR:HG22	1.92	0.52
1:0:1596:U:H2'	1:0:1598:A:OP2	2.10	0.52
1:0:2542:C:H1'	39:0:6378:HOH:O	2.08	0.52
1:0:303:C:H2'	1:0:304:G:O4'	2.10	0.52
1:0:1060:C:H6	1:0:1060:C:H5'	1.75	0.52
1:0:1167:G:H2'	1:0:1168:C:C6	2.45	0.52
1:0:2248:C:H3'	39:0:4476:HOH:O	2.10	0.52
1:0:2256:G:O2'	1:0:2257:G:H5'	2.10	0.52
1:0:2717:C:H2'	1:0:2718:C:C5'	2.34	0.52
1:0:821:U:H3'	39:0:8455:HOH:O	2.10	0.52
1:0:249:G:O2'	1:0:250:C:H5'	2.10	0.52
30:3:2:GLN:HE21	30:3:91:GLN:NE2	2.07	0.52
3:B:221:GLN:HE22	12:K:42:ASN:ND2	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1928:C:H2'	1:0:1929:G:O4'	2.10	0.51
1:0:2584:G:H4'	39:0:6824:HOH:O	2.09	0.51
1:0:564:G:H1'	39:0:5694:HOH:O	2.10	0.51
5:D:141:VAL:HG21	31:9:57:A:H8	1.75	0.51
1:0:1175:G:H1'	1:0:1193:A:H2'	1.92	0.51
1:0:1940:C:H4'	39:0:7130:HOH:O	2.10	0.51
4:C:118:THR:O	4:C:136:VAL:HG13	2.09	0.51
13:L:143:THR:HG22	13:L:144:ASP:H	1.75	0.51
1:0:497:A:H2'	1:0:498:A:C5'	2.40	0.51
1:0:1444:G:H5''	20:S:11:THR:HG22	1.92	0.51
1:0:1313:A:H5'	26:Y:208:LYS:O	2.10	0.51
1:0:105:G:O2'	1:0:106:A:H5'	2.11	0.51
1:0:1205:U:H2'	1:0:1206:U:H5'	1.91	0.51
1:0:154:C:H2'	1:0:155:C:H6	1.76	0.51
1:0:2271:G:N3	1:0:2271:G:H2'	2.24	0.51
1:0:2271:G:H5'	39:A:3548:HOH:O	2.09	0.51
1:0:905:C:H3'	39:0:4139:HOH:O	2.10	0.51
1:0:1183:C:H41	1:0:1192:A:P	2.34	0.51
1:0:200:C:H2'	39:0:8130:HOH:O	2.11	0.51
1:0:2597:U:H2'	1:0:2598:U:H5'	1.91	0.51
1:0:1010:C:H4'	15:N:4:PRO:HB2	1.93	0.51
1:0:1856:C:H5'	1:0:1858:A:O4'	2.11	0.51
1:0:2088:C:H1'	1:0:2841:A:N1	2.26	0.51
1:0:1299:G:N7	13:L:6:ARG:NH1	2.59	0.51
1:0:1029:U:O2'	1:0:1273:C:OP1	2.26	0.51
1:0:1566:C:H2'	1:0:1567:G:C8	2.46	0.51
1:0:2353:A:H4'	1:0:2354:A:O5'	2.10	0.51
1:0:958:G:H2'	1:0:959:C:C6	2.45	0.51
14:M:99:ARG:HD2	14:M:167:GLY:HA2	1.93	0.51
27:Z:60:ASP:HB3	27:Z:69:ASP:HB3	1.93	0.51
1:0:1391:G:H2'	1:0:1392:A:H5'	1.93	0.51
1:0:1634:G:H2'	1:0:1635:U:C6	2.46	0.51
1:0:2510:C:H42	1:0:2564:G:H22	1.58	0.51
24:W:64:THR:O	24:W:68:THR:HG22	2.11	0.51
1:0:364:U:H2'	1:0:365:G:O4'	2.11	0.51
1:0:527:U:H2'	1:0:528:G:C8	2.46	0.51
1:0:1636:G:O2'	1:0:1637:A:H5'	2.10	0.50
1:0:1234:U:N3	3:B:244:PRO:HB3	2.25	0.50
1:0:1603:A:C5'	1:0:1605:G:H5'	2.41	0.50
1:0:1755:A:H2'	1:0:1756:G:O4'	2.11	0.50
31:9:90:G:H3'	39:9:2357:HOH:O	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1130:U:H4'	39:0:5437:HOH:O	2.11	0.50
2:A:199:HIS:HD2	2:A:201:PHE:H	1.59	0.50
20:S:17:ASP:HB3	20:S:23:LYS:HB2	1.93	0.50
1:0:1118:A:C8	1:0:1119:G:H5''	2.45	0.50
1:0:1525:G:H5'	1:0:1526:A:OP2	2.11	0.50
1:0:2002:C:H2'	1:0:2003:U:H5'	1.94	0.50
7:F:2:VAL:HG22	7:F:57:GLU:OE1	2.11	0.50
1:0:1864:C:C5	14:M:75:ARG:NH1	2.79	0.50
1:0:10:U:H6	1:0:10:U:H3'	1.76	0.50
1:0:1980:U:O2	1:0:2008:U:H4'	2.10	0.50
1:0:280:C:H2'	1:0:281:U:O4'	2.11	0.50
1:0:1189:A:O2'	1:0:1208:C:H2'	2.12	0.50
1:0:1413:A:H2'	1:0:1414:A:O4'	2.12	0.50
1:0:324:G:O2'	1:0:325:U:H5'	2.12	0.50
1:0:899:C:H5'	39:0:7471:HOH:O	2.11	0.50
1:0:1406:A:H4'	1:0:1407:A:H5''	1.92	0.50
1:0:1566:C:H2'	1:0:1567:G:H8	1.76	0.50
1:0:2467:A:O2'	1:0:2468:A:H2'	2.11	0.50
1:0:441:A:H8	1:0:441:A:O5'	1.95	0.50
1:0:485:A:N3	1:0:487:G:H5''	2.27	0.50
1:0:656:G:H5'	16:O:3:THR:CG2	2.33	0.50
1:0:338:C:H4'	4:C:174:ILE:HD11	1.94	0.50
1:0:2081:A:H4'	11:J:69:TYR:CE1	2.47	0.50
1:0:1066:U:H2'	1:0:1067:A:C8	2.47	0.50
1:0:1116:U:O2'	1:0:1118:A:C2	2.50	0.50
1:0:2659:U:H5''	39:0:8896:HOH:O	2.11	0.50
1:0:380:A:H2'	39:0:6974:HOH:O	2.11	0.50
1:0:1377:C:H5'	1:0:1377:C:C6	2.45	0.50
1:0:2135:A:O2'	1:0:2136:G:H5'	2.12	0.50
1:0:2511:A:H2'	1:0:2512:U:O4'	2.12	0.50
1:0:2898:G:H4'	3:B:288:GLY:HA2	1.94	0.50
1:0:1864:C:H5	14:M:75:ARG:NH1	2.10	0.49
1:0:1878:G:H1'	39:0:5431:HOH:O	2.12	0.49
1:0:2703:A:H2'	1:0:2704:C:H6	1.77	0.49
1:0:536:A:H3'	39:0:3958:HOH:O	2.11	0.49
1:0:969:G:H1	1:0:999:C:N4	2.10	0.49
1:0:1589:G:H22	1:0:1605:G:H1'	1.77	0.49
1:0:1644:C:H2'	1:0:1645:U:H6	1.77	0.49
1:0:170:U:H2'	1:0:171:C:H5'	1.94	0.49
1:0:21:G:H4'	19:R:2:ILE:HG22	1.93	0.49
1:0:2345:A:H3'	1:0:2346:C:C6	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2415:A:H2'	1:0:2416:G:H5'	1.93	0.49
1:0:319:A:H4'	1:0:338:C:C5	2.47	0.49
1:0:711:G:H1'	39:0:6793:HOH:O	2.11	0.49
1:0:920:C:H4'	1:0:921:G:C2	2.47	0.49
1:0:1307:A:H2'	1:0:1308:A:C8	2.47	0.49
1:0:2521:A:OP2	9:H:6:ALA:HB3	2.11	0.49
1:0:459:A:H4'	39:0:4687:HOH:O	2.12	0.49
1:0:941:G:C5	1:0:942:U:C4	3.00	0.49
31:9:114:G:H2'	31:9:115:C:C6	2.48	0.49
1:0:857:A:H4'	2:A:176:HIS:CD2	2.46	0.49
13:L:138:GLY:HA3	39:L:4360:HOH:O	2.11	0.49
1:0:451:C:O2'	1:0:452:G:H5'	2.12	0.49
1:0:500:G:H21	19:R:98:ASN:ND2	2.05	0.49
1:0:797:A:H61	1:0:816:G:H1'	1.77	0.49
1:0:2720:C:O2	12:K:87:ARG:NH2	2.45	0.49
1:0:2578:G:C8	1:0:2578:G:H5'	2.43	0.49
1:0:2781:U:C2'	1:0:2782:G:H5'	2.42	0.49
1:0:2103:A:N6	37:0:9101:WIN:O1G	2.41	0.49
1:0:2538:A:H1'	37:0:9101:WIN:O1M	2.12	0.49
1:0:1115:U:O2'	1:0:1116:U:H5'	2.11	0.49
1:0:1172:G:H5''	39:0:7015:HOH:O	2.12	0.49
1:0:660:A:H4'	1:0:661:G:O5'	2.13	0.49
1:0:932:U:H2'	1:0:933:C:C6	2.48	0.49
1:0:2807:U:P	3:B:27:ASN:HD21	2.34	0.49
1:0:1181:A:H2'	1:0:1182:C:C5'	2.42	0.49
1:0:1398:G:O2'	1:0:1399:A:H5'	2.13	0.49
1:0:2072:G:H3'	1:0:2073:G:C5'	2.43	0.49
31:9:64:C:C2'	31:9:65:A:H5'	2.43	0.49
14:M:23:LEU:HD13	14:M:27:ARG:HH21	1.78	0.49
1:0:1244:U:OP1	11:J:18:ILE:HD13	2.13	0.49
1:0:1453:G:H2'	1:0:1454:U:O4'	2.13	0.49
1:0:2325:U:O2'	1:0:2411:C:H1'	2.13	0.49
1:0:2498:C:O2'	1:0:2499:U:H5'	2.12	0.49
1:0:281:U:O2'	1:0:282:C:H5'	2.13	0.49
1:0:2821:C:H4'	3:B:116:PRO:HG3	1.95	0.49
1:0:941:G:O2'	1:0:942:U:H5'	2.12	0.49
1:0:2032:U:H2'	1:0:2033:G:C5'	2.43	0.49
1:0:2510:C:H5'	1:0:2511:A:OP2	2.13	0.49
1:0:2524:G:N2	1:0:2526:C:H41	2.11	0.49
1:0:2729:C:O2'	1:0:2730:G:H5'	2.12	0.49
1:0:28:G:H1'	39:0:3446:HOH:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:9:73:A:H61	31:9:108:C:N4	2.06	0.49
1:0:1423:C:O2'	1:0:1424:A:H5'	2.13	0.49
1:0:1589:G:N2	1:0:1605:G:H1'	2.27	0.49
1:0:250:C:O2'	1:0:251:C:H5'	2.13	0.49
1:0:669:G:O2'	1:0:670:G:H5'	2.12	0.49
1:0:946:C:H2'	1:0:947:U:C6	2.47	0.49
4:C:127:ARG:HD3	4:C:129:HIS:HE1	1.77	0.49
1:0:1333:U:H2'	1:0:1334:C:H6	1.78	0.48
1:0:12:U:C2'	1:0:13:G:H5'	2.42	0.48
1:0:1603:A:H5'	1:0:1605:G:C4'	2.43	0.48
1:0:2887:G:H2'	1:0:2888:U:C6	2.47	0.48
1:0:589:U:H2'	1:0:590:A:H8	1.78	0.48
1:0:1735:C:OP2	3:B:234:ARG:HG3	2.13	0.48
8:G:64:ASN:N	8:G:64:ASN:HD22	2.10	0.48
1:0:1980:U:O2'	1:0:1981:A:H5'	2.13	0.48
39:0:7291:HOH:O	3:B:211:THR:HG21	2.12	0.48
1:0:130:C:H2'	39:0:7324:HOH:O	2.13	0.48
1:0:1495:C:H1'	1:0:1573:A:H1'	1.94	0.48
1:0:2269:C:H2'	1:0:2270:G:H5'	1.95	0.48
1:0:2375:A:H2'	1:0:2376:C:C6	2.47	0.48
1:0:271:C:H41	1:0:378:A:H2	1.61	0.48
1:0:64:G:H2'	1:0:65:C:O4'	2.13	0.48
14:M:102:GLU:OE1	14:M:164:THR:HG21	2.13	0.48
15:N:40:ASN:ND2	31:9:28:U:H5''	2.28	0.48
1:0:1120:U:H5'	1:0:1121:G:OP2	2.12	0.48
1:0:583:C:H2'	1:0:584:U:H6	1.78	0.48
31:9:107:C:H5	39:9:3167:HOH:O	1.96	0.48
31:9:73:A:N6	31:9:108:C:H42	2.06	0.48
1:0:1058:A:H2'	1:0:1060:C:H5''	1.95	0.48
1:0:1797:A:H4'	1:0:1798:C:C5	2.49	0.48
37:0:9101:WIN:O1L	37:0:9101:WIN:H1FA	2.14	0.48
31:9:107:C:O2'	31:9:108:C:H5'	2.14	0.48
24:W:108:ARG:HH21	24:W:114:PRO:HG2	1.79	0.48
1:0:120:A:H2'	1:0:120:A:N3	2.28	0.48
1:0:1250:C:O2'	1:0:1251:C:H5'	2.13	0.48
1:0:137:U:H2'	1:0:139:C:C5	2.49	0.48
1:0:210:U:H2'	1:0:211:U:C6	2.48	0.48
1:0:24:G:N2	1:0:518:G:H1'	2.29	0.48
1:0:2563:U:O2'	1:0:2564:G:H3'	2.13	0.48
1:0:2768:A:O2'	1:0:2769:C:H5'	2.12	0.48
1:0:659:A:H5''	39:0:6799:HOH:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:M:34:GLU:HB3	14:M:38:GLU:HG3	1.95	0.48
1:0:1714:C:O2'	1:0:1715:C:H5'	2.13	0.48
1:0:2893:C:O2'	1:0:2894:C:H5'	2.13	0.48
1:0:816:G:H5'	1:0:1598:A:H4'	1.95	0.48
1:0:961:A:H4'	39:0:6342:HOH:O	2.13	0.48
19:R:40:ALA:O	19:R:44:VAL:HG23	2.14	0.48
1:0:107:U:H2'	1:0:108:U:H5'	1.96	0.48
1:0:1183:C:H42	1:0:1184:C:H41	1.62	0.48
1:0:1209:C:H2'	1:0:1210:G:C8	2.49	0.48
1:0:1268:C:H2'	1:0:1269:G:C8	2.48	0.48
1:0:2269:C:C2'	1:0:2270:G:H5'	2.44	0.48
1:0:2507:G:H2'	1:0:2510:C:H42	1.78	0.48
1:0:2072:G:C6	1:0:2533:C:H1'	2.49	0.48
1:0:2839:C:H2'	1:0:2840:A:H5''	1.94	0.48
1:0:368:C:H2'	1:0:369:G:H5'	1.96	0.48
1:0:2717:C:OP1	3:B:207:LYS:HG3	2.13	0.48
1:0:1104:C:H4'	11:J:88:PRO:HD3	1.96	0.48
1:0:1603:A:H5''	1:0:1604:G:H3'	1.95	0.48
1:0:2379:G:H5'	1:0:2381:C:O4'	2.14	0.48
1:0:2540:G:H4'	37:0:9101:WIN:C1O	2.35	0.48
1:0:2718:C:H6	1:0:2718:C:H5'	1.79	0.48
1:0:292:G:H2'	1:0:358:G:N2	2.28	0.48
1:0:301:C:H2'	1:0:302:A:H8	1.79	0.48
1:0:877:G:C5'	1:0:878:G:OP1	2.58	0.48
3:B:212:GLN:HB2	3:B:257:THR:HG21	1.96	0.48
5:D:159:PRO:O	5:D:163:VAL:HG23	2.14	0.48
1:0:1641:A:C2'	1:0:1642:A:H5'	2.44	0.48
1:0:2073:G:H5''	39:0:8581:HOH:O	2.14	0.48
1:0:214:U:H5'	39:0:5454:HOH:O	2.14	0.48
1:0:710:G:H1'	39:O:1484:HOH:O	2.14	0.48
1:0:812:A:H2'	1:0:813:C:C6	2.48	0.48
1:0:2270:G:H4'	2:A:223:ARG:HH12	1.79	0.48
1:0:1289:C:O2'	1:0:1290:G:H5'	2.14	0.47
1:0:1845:A:P	2:A:190:ARG:HH11	2.37	0.47
1:0:621:C:H5'	26:Y:132:ASP:OD2	2.14	0.47
1:0:1185:U:H2'	1:0:1186:C:C6	2.49	0.47
1:0:123:U:H2'	1:0:124:C:C6	2.49	0.47
1:0:2487:C:O2	37:0:9101:WIN:H1F	2.13	0.47
1:0:1477:C:O2'	1:0:1478:U:H5'	2.14	0.47
1:0:1559:A:H4'	39:0:5067:HOH:O	2.14	0.47
1:0:1568:G:O2'	1:0:1569:U:H5'	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1903:U:O2'	1:0:1904:A:N7	2.46	0.47
1:0:2090:G:H2'	1:0:2091:G:C8	2.49	0.47
1:0:226:A:H1'	1:0:393:G:C5	2.49	0.47
31:9:42:C:H5'	31:9:43:G:OP2	2.14	0.47
14:M:43:PRO:HG3	14:M:62:VAL:HG21	1.96	0.47
19:R:39:THR:HG23	19:R:107:GLU:O	2.14	0.47
1:0:1014:A:H2'	1:0:1015:C:H5'	1.94	0.47
1:0:1370:G:H5''	39:R:4608:HOH:O	2.14	0.47
1:0:1419:U:H5'	1:0:1420:C:OP2	2.15	0.47
1:0:1484:G:H3'	39:0:7776:HOH:O	2.15	0.47
1:0:1681:G:H5''	1:0:1682:A:H5'	1.96	0.47
1:0:1815:A:H2'	1:0:1816:C:O4'	2.14	0.47
1:0:2100:A:H5'	39:C:7192:HOH:O	2.14	0.47
1:0:816:G:C6	1:0:817:G:N1	2.82	0.47
1:0:834:G:H3'	1:0:835:U:H4'	1.97	0.47
12:K:32:ILE:HD11	12:K:56:SER:HB3	1.96	0.47
1:0:189:A:OP1	14:M:171:ARG:NH2	2.46	0.47
26:Y:177:LYS:HD3	26:Y:181:GLY:O	2.15	0.47
1:0:1028:U:H1'	39:0:8330:HOH:O	2.14	0.47
1:0:1861:C:H4'	2:A:6:GLY:O	2.15	0.47
1:0:2437:A:H2'	1:0:2438:G:C8	2.50	0.47
1:0:960:G:H3'	1:0:960:G:N3	2.28	0.47
1:0:1415:G:H5'	28:1:12:ASN:O	2.14	0.47
11:J:107:ASN:HD22	11:J:109:TYR:H	1.61	0.47
23:V:55:ARG:O	23:V:59:ILE:HG12	2.15	0.47
1:0:1071:G:H4'	26:Y:154:ARG:NH2	2.30	0.47
1:0:2134:G:N2	1:0:2242:U:C2	2.82	0.47
1:0:2598:U:O2	1:0:2600:A:H8	1.98	0.47
1:0:571:C:H6	1:0:571:C:O5'	1.96	0.47
1:0:1056:U:H2'	1:0:1057:A:O4'	2.14	0.47
1:0:2509:A:OP2	1:0:2510:C:H5	1.98	0.47
1:0:2587:OMU:H2'	1:0:2589:U:H5''	1.97	0.47
1:0:960:G:N3	1:0:960:G:C2'	2.77	0.47
1:0:2372:A:H2'	1:0:2373:U:C6	2.50	0.47
1:0:307:G:H3'	39:0:6217:HOH:O	2.14	0.47
1:0:396:U:H1'	39:0:7529:HOH:O	2.14	0.47
1:0:2389:U:H4'	18:Q:53:HIS:CD2	2.48	0.47
1:0:1120:U:H6	1:0:1120:U:H5''	1.78	0.47
1:0:1496:A:H5'	1:0:1572:A:H1'	1.96	0.47
1:0:2338:G:H1'	5:D:105:SER:OG	2.15	0.47
1:0:2737:C:OP2	17:P:61:ARG:NH2	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:366:U:H2'	1:0:367:G:O4'	2.14	0.47
1:0:1503:U:H2'	1:0:1504:A:O4'	2.14	0.47
1:0:1666:C:C2'	1:0:1667:A:C5'	2.80	0.47
1:0:421:C:H2'	1:0:422:G:H8	1.80	0.47
1:0:470:U:O2'	28:1:16:HIS:HD2	1.98	0.47
1:0:1342:C:C2'	1:0:1343:C:H5'	2.45	0.47
1:0:1409:G:C2	1:0:1410:G:C8	3.03	0.47
1:0:2281:C:C2'	1:0:2282:U:H5'	2.44	0.47
39:0:5919:HOH:O	6:E:31:ARG:NH1	2.43	0.47
1:0:1130:U:H5'	39:0:7596:HOH:O	2.14	0.46
1:0:2005:G:O2'	1:0:2008:U:OP2	2.33	0.46
1:0:2241:C:O2'	1:0:2242:U:H5'	2.16	0.46
1:0:2445:U:H2'	1:0:2446:G:H8	1.78	0.46
1:0:396:U:O2'	1:0:418:C:H4'	2.14	0.46
1:0:506:G:N2	1:0:509:A:H5''	2.24	0.46
1:0:690:G:H4'	1:0:741:C:O2	2.15	0.46
1:0:821:U:H4'	27:Z:41:ARG:HH12	1.80	0.46
1:0:1427:A:H61	1:0:1440:U:C1'	2.28	0.46
1:0:1735:C:O2'	1:0:1736:A:H5'	2.15	0.46
1:0:2541:U:H4'	39:0:4427:HOH:O	2.15	0.46
1:0:2598:U:O2	1:0:2600:A:C8	2.69	0.46
1:0:558:C:H2'	1:0:559:U:H5''	1.96	0.46
1:0:946:C:H2'	1:0:947:U:H6	1.81	0.46
31:9:20:G:O2'	31:9:21:G:H5'	2.15	0.46
31:9:39:U:H3	31:9:42:C:H5''	1.81	0.46
6:E:116:THR:HG22	6:E:151:LEU:HD22	1.96	0.46
1:0:1363:G:OP1	4:C:76:ARG:NH2	2.48	0.46
1:0:1942:A:O2'	1:0:1943:C:H5'	2.15	0.46
1:0:213:G:N2	1:0:225:G:H2'	2.31	0.46
1:0:2382:A:H5'	39:0:3538:HOH:O	2.14	0.46
1:0:1052:G:H2'	1:0:1052:G:N3	2.30	0.46
1:0:1773:G:C8	27:Z:40:ALA:HA	2.50	0.46
1:0:2668:G:H2'	1:0:2669:U:C6	2.50	0.46
1:0:1201:C:H2'	1:0:1202:A:H5'	1.97	0.46
1:0:1545:C:H2'	1:0:1546:G:O4'	2.16	0.46
1:0:2326:C:H4'	1:0:2412:G:H4'	1.98	0.46
1:0:2348:C:H5'	5:D:22:VAL:HG11	1.97	0.46
1:0:2594:C:O2'	1:0:2595:U:H5'	2.15	0.46
1:0:2866:U:H4'	1:0:2867:G:H5'	1.96	0.46
1:0:1025:C:H5'	24:W:23:MET:O	2.15	0.46
1:0:1063:G:H5''	39:0:6221:HOH:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1158:G:O2'	1:0:1159:G:H5'	2.16	0.46
1:0:1422:U:H2'	1:0:1423:C:H6	1.78	0.46
1:0:146:U:O2'	1:0:147:G:H5'	2.16	0.46
1:0:164:G:H3'	39:0:8328:HOH:O	2.16	0.46
1:0:216:A:O2'	1:0:217:C:H5'	2.15	0.46
1:0:2392:C:H4'	39:0:9136:HOH:O	2.15	0.46
1:0:256:C:H2'	1:0:257:G:O4'	2.16	0.46
1:0:512:G:O3'	1:0:513:A:H8	1.99	0.46
1:0:700:A:H5''	1:0:701:U:H5'	1.97	0.46
1:0:2100:A:C2	37:0:9101:WIN:H1DB	2.51	0.46
1:0:1384:C:H5'	25:X:30:MET:HG2	1.96	0.46
1:0:255:A:H2'	1:0:256:C:C6	2.49	0.46
1:0:2638:G:H5'	39:0:3790:HOH:O	2.15	0.46
1:0:2851:G:C2'	1:0:2852:A:H5'	2.45	0.46
1:0:517:U:H2'	1:0:518:G:H5'	1.97	0.46
15:N:159:TYR:HE1	31:9:50:G:H5''	1.80	0.46
1:0:2629:C:H41	2:A:206:ARG:HH21	1.64	0.46
4:C:1:MET:HG2	4:C:2:GLN:H	1.81	0.46
9:H:49:GLN:HE21	9:H:140:TYR:HE2	1.63	0.46
24:W:4:LEU:HD22	24:W:52:VAL:HG21	1.97	0.46
1:0:1919:A:H4'	39:0:3679:HOH:O	2.16	0.46
1:0:236:A:H8	1:0:236:A:OP1	1.99	0.46
1:0:2896:A:N3	1:0:2896:A:H2'	2.31	0.46
1:0:2899:A:O2'	1:0:2900:G:H5'	2.16	0.46
1:0:682:A:H2'	1:0:683:G:O4'	2.15	0.46
3:B:17:LYS:O	3:B:260:HIS:HD2	1.99	0.46
1:0:2548:C:H5'	3:B:252:PRO:HD2	1.98	0.46
1:0:1667:A:H2'	1:0:1668:U:C6	2.50	0.46
1:0:183:A:O2'	1:0:184:G:H5'	2.16	0.46
1:0:602:A:O2'	1:0:605:C:H4'	2.15	0.46
1:0:800:G:H2'	1:0:801:U:C6	2.50	0.46
31:9:29:C:H2'	31:9:30:C:C5'	2.40	0.46
2:A:199:HIS:CD2	2:A:201:PHE:H	2.33	0.46
20:S:11:THR:H	20:S:14:ALA:HB3	1.79	0.46
1:0:101:C:H2'	1:0:102:A:C8	2.51	0.46
1:0:1716:A:H4'	17:P:55:LYS:HD3	1.97	0.46
1:0:1769:C:O2'	1:0:1770:U:H5'	2.15	0.46
1:0:523:C:H2'	1:0:524:A:C8	2.51	0.46
1:0:1314:U:H5''	1:0:1316:G:O4'	2.16	0.45
1:0:168:C:H6	1:0:168:C:O5'	1.98	0.45
1:0:1731:C:H1'	39:0:5883:HOH:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1834:C:H2'	1:0:1840:A:H62	1.80	0.45
1:0:466:A:H2'	1:0:467:G:O4'	2.16	0.45
1:0:960:G:H2'	1:0:960:G:N3	2.31	0.45
31:9:108:C:O2'	31:9:109:G:H5'	2.17	0.45
17:P:105:LEU:HD21	17:P:137:LEU:HD11	1.98	0.45
1:0:1160:G:H5'	1:0:1161:A:C4'	2.46	0.45
1:0:1204:C:H2'	1:0:1205:U:O4'	2.16	0.45
1:0:1562:C:O2	1:0:1562:C:H2'	2.16	0.45
1:0:2300:A:H4'	1:0:2301:A:O5'	2.16	0.45
1:0:2505:G:C2'	1:0:2506:A:H5'	2.46	0.45
1:0:364:U:H2'	1:0:365:G:C8	2.51	0.45
1:0:702:G:O2'	1:0:703:G:H5'	2.17	0.45
4:C:47:GLY:HA2	4:C:92:PRO:HB2	1.97	0.45
1:0:1007:A:H2'	9:H:22:TYR:CZ	2.52	0.45
1:0:1500:U:P	17:P:41:ARG:HH22	2.39	0.45
1:0:204:A:H2'	1:0:205:U:H5'	1.98	0.45
1:0:2348:C:H1'	5:D:131:THR:HG21	1.96	0.45
1:0:2064:U:H4'	1:0:2653:A:OP1	2.16	0.45
1:0:834:G:H4'	1:0:835:U:OP2	2.15	0.45
31:9:31:C:H2'	31:9:32:G:O4'	2.17	0.45
1:0:1362:U:H5'	39:0:7682:HOH:O	2.16	0.45
1:0:1593:C:OP1	17:P:117:SER:HB3	2.16	0.45
1:0:2256:G:C2'	1:0:2257:G:H5'	2.47	0.45
1:0:820:G:C5	2:A:171:LYS:HB2	2.51	0.45
25:X:61:ARG:NH1	25:X:67:PRO:HD3	2.31	0.45
1:0:1131:G:C6	1:0:1230:A:C4	3.04	0.45
1:0:2269:C:H2'	1:0:2270:G:C5'	2.46	0.45
1:0:2694:A:H4'	6:E:91:PHE:CE1	2.51	0.45
1:0:657:G:P	4:C:27:ARG:HH22	2.40	0.45
12:K:74:VAL:HG12	12:K:75:ARG:HG3	1.97	0.45
1:0:1375:A:H2'	1:0:1376:G:H5'	1.99	0.45
1:0:1706:G:C6	1:0:1707:G:C6	3.05	0.45
1:0:2740:G:H2'	1:0:2741:A:O4'	2.16	0.45
1:0:51:G:O2'	1:0:52:A:H5'	2.17	0.45
1:0:1687:C:O2	28:1:9:GLY:HA2	2.17	0.45
3:B:238:ASN:HD22	3:B:240:GLY:N	2.12	0.45
3:B:315:VAL:HG23	3:B:316:ARG:HG2	1.99	0.45
1:0:1220:U:H4'	9:H:174:LEU:HD21	1.98	0.45
13:L:30:ARG:NH1	39:L:165:HOH:O	2.48	0.45
1:0:569:A:H5''	1:0:587:A:N1	2.32	0.45
1:0:59:A:H5'	39:0:2959:HOH:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:Y:144:ARG:NH1	39:Y:4909:HOH:O	2.49	0.45
1:0:1202:A:H2'	1:0:1203:G:H5'	1.98	0.45
1:0:221:G:H2'	1:0:222:A:C8	2.51	0.45
1:0:243:A:H61	1:0:269:G:C1'	2.30	0.45
1:0:527:U:H2'	1:0:528:G:H8	1.81	0.45
1:0:558:C:H2'	1:0:559:U:H5'	1.99	0.45
24:W:6:GLN:HB2	24:W:26:ILE:HD11	1.99	0.45
1:0:1616:A:H5''	1:0:1617:C:OP1	2.17	0.45
1:0:334:G:H2'	1:0:335:U:O4'	2.16	0.45
1:0:363:C:O2'	1:0:364:U:H5'	2.17	0.45
31:9:22:G:H5'	31:9:23:U:OP1	2.17	0.45
4:C:188:ARG:HD3	39:C:2507:HOH:O	2.15	0.45
1:0:1149:U:H5''	1:0:1151:G:O4'	2.17	0.45
1:0:1375:A:O2'	1:0:1376:G:H5'	2.17	0.45
1:0:1937:U:O2'	1:0:1938:G:H5'	2.17	0.45
1:0:1849:G:H1'	1:0:2011:A:N1	2.32	0.45
1:0:664:U:O4	1:0:681:G:H5''	2.16	0.45
1:0:820:G:OP1	27:Z:41:ARG:NH2	2.50	0.45
1:0:1439:C:H5''	29:2:41:HIS:HE1	1.82	0.45
31:9:36:C:C5	31:9:37:C:C5	3.05	0.45
1:0:2083:A:N6	11:J:90:LYS:HE3	2.32	0.45
1:0:1783:A:O2'	1:0:1784:U:H5'	2.17	0.44
1:0:2291:A:N9	1:0:2309:C:H5'	2.32	0.44
1:0:424:C:H2'	1:0:425:U:C6	2.51	0.44
1:0:558:C:C2'	1:0:559:U:C5'	2.95	0.44
1:0:646:G:H2'	1:0:647:U:C6	2.51	0.44
20:S:51:GLN:HE21	20:S:53:ASN:HD21	1.64	0.44
1:0:1249:U:H2'	1:0:1250:C:C6	2.52	0.44
1:0:1398:G:H2'	1:0:1399:A:C8	2.52	0.44
1:0:1447:U:H3'	1:0:1506:U:O2	2.16	0.44
1:0:1506:U:H6	1:0:1506:U:H5'	1.82	0.44
1:0:2121:G:O2'	1:0:2122:C:H5'	2.16	0.44
1:0:2241:C:H2'	1:0:2242:U:H6	1.79	0.44
1:0:319:A:H4'	1:0:338:C:C4	2.52	0.44
1:0:629:A:H2'	1:0:630:A:O4'	2.17	0.44
1:0:711:G:C2	1:0:718:C:C2	3.06	0.44
1:0:807:A:O2'	1:0:808:A:H5'	2.18	0.44
5:D:141:VAL:HG21	31:9:57:A:C8	2.52	0.44
15:N:37:ARG:NH1	31:9:6:C:OP1	2.45	0.44
1:0:538:C:OP2	26:Y:134:HIS:HE1	2.00	0.44
1:0:1098:A:H2'	1:0:1099:G:O4'	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1768:C:H2'	1:0:1769:C:O4'	2.18	0.44
1:0:2004:U:H4'	39:0:4302:HOH:O	2.18	0.44
1:0:2510:C:H42	1:0:2564:G:N2	2.16	0.44
1:0:2678:A:H4'	39:0:6889:HOH:O	2.18	0.44
1:0:383:A:H2'	1:0:384:G:O4'	2.18	0.44
1:0:483:C:C4	1:0:484:A:C6	3.06	0.44
1:0:583:C:H2'	1:0:584:U:C6	2.53	0.44
1:0:968:G:O2'	1:0:969:G:H5'	2.17	0.44
1:0:793:A:H5''	17:P:83:LYS:HG2	1.99	0.44
19:R:39:THR:HG22	19:R:42:GLU:H	1.83	0.44
1:0:1626:A:H2'	1:0:1627:G:C5'	2.48	0.44
1:0:1634:G:H2'	1:0:1635:U:H6	1.82	0.44
1:0:2256:G:H2'	1:0:2257:G:C5'	2.48	0.44
1:0:2831:C:C2'	1:0:2832:C:H5'	2.48	0.44
1:0:645:U:O2	1:0:761:A:H2	2.01	0.44
1:0:802:G:O2'	1:0:803:C:H5'	2.17	0.44
31:9:3:A:OP2	31:9:25:G:N2	2.51	0.44
5:D:22:VAL:HG22	5:D:74:THR:HG22	2.00	0.44
24:W:80:ASP:O	24:W:84:VAL:HG23	2.18	0.44
1:0:1445:G:N2	1:0:1678:A:H1'	2.33	0.44
1:0:1622:G:H2'	1:0:1623:C:H5'	1.98	0.44
1:0:177:A:H2'	1:0:178:U:O4'	2.17	0.44
1:0:2105:C:H2'	1:0:2106:C:C6	2.52	0.44
1:0:282:C:HO2'	1:0:368:C:N4	2.15	0.44
28:1:8:GLN:HE22	28:1:11:LYS:HZ2	1.65	0.44
31:9:52:A:H2'	31:9:53:G:O4'	2.18	0.44
3:B:254:GLN:HG2	3:B:255:GLY:N	2.32	0.44
12:K:14:LYS:HB2	12:K:45:PRO:HG2	1.99	0.44
1:0:1197:G:H1'	1:0:1203:G:N2	2.33	0.44
1:0:1535:G:H2'	1:0:1536:C:C6	2.53	0.44
1:0:815:U:O2'	1:0:1598:A:H4'	2.17	0.44
1:0:628:1MA:H4'	39:0:7268:HOH:O	2.18	0.44
31:9:2:U:OP2	31:9:2:U:H4'	2.18	0.44
1:0:2838:A:OP1	3:B:307:ARG:NH2	2.50	0.44
23:V:1:THR:HG23	23:V:2:VAL:HG23	2.00	0.44
24:W:48:VAL:HG12	24:W:52:VAL:HB	1.98	0.44
1:0:1311:G:C2	1:0:1312:G:C8	3.06	0.44
1:0:1439:C:O5'	1:0:1439:C:H6	2.00	0.44
1:0:1664:A:H8	1:0:1664:A:OP1	2.01	0.44
1:0:1994:A:OP1	12:K:66:ARG:NH2	2.51	0.44
1:0:517:U:C2'	1:0:518:G:H5'	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:920:C:H5''	1:0:921:G:O5'	2.18	0.44
13:L:27:ARG:HH21	13:L:30:ARG:HG2	1.82	0.44
1:0:1330:A:C5'	39:Y:7277:HOH:O	2.65	0.44
1:0:1515:A:H2'	1:0:1516:U:C6	2.53	0.44
1:0:1666:C:H2'	1:0:1667:A:H5'	1.97	0.44
1:0:2041:G:O2'	1:0:2042:U:H5'	2.17	0.44
1:0:2094:G:O6	1:0:2649:A:H2	2.00	0.44
1:0:2626:C:H2'	1:0:2627:G:C8	2.53	0.44
1:0:271:C:H4'	1:0:272:A:OP1	2.17	0.44
1:0:2824:C:H5''	1:0:2825:C:H5'	1.99	0.44
1:0:333:G:O2'	1:0:334:G:H5'	2.18	0.44
31:9:59:C:H2'	31:9:60:C:C6	2.52	0.44
2:A:51:ARG:NH1	2:A:120:ARG:O	2.51	0.44
2:A:70:ALA:HB1	27:Z:89:THR:HG21	2.00	0.44
1:0:1170:U:H2'	1:0:1172:G:OP2	2.18	0.44
1:0:1088:A:C6	1:0:1291:A:H1'	2.53	0.44
1:0:1587:U:H2'	1:0:1588:G:O4'	2.17	0.44
1:0:1844:C:O5'	1:0:1844:C:H6	2.01	0.44
1:0:2281:C:H2'	1:0:2282:U:H5'	2.00	0.44
1:0:2809:G:H2'	1:0:2810:G:O4'	2.18	0.44
1:0:39:G:N2	1:0:444:C:C2	2.86	0.44
1:0:445:U:H2'	1:0:446:G:C8	2.52	0.44
39:0:2979:HOH:O	28:1:10:LYS:HG3	2.18	0.44
1:0:1592:G:O2'	1:0:1593:C:O5'	2.36	0.43
1:0:2502:C:H2'	1:0:2503:A:C5'	2.47	0.43
1:0:2634:G:OP2	2:A:204:GLY:N	2.48	0.43
1:0:2856:A:H4'	25:X:11:THR:HB	1.99	0.43
1:0:638:C:H2'	1:0:639:A:C8	2.53	0.43
1:0:764:C:H2'	1:0:765:G:O4'	2.18	0.43
1:0:851:C:O2	1:0:2022:A:H2	2.01	0.43
1:0:1119:G:H8	11:J:52:GLN:NE2	2.16	0.43
1:0:1321:A:H2'	1:0:1322:G:C8	2.53	0.43
1:0:1361:C:H2'	1:0:1362:U:C6	2.53	0.43
1:0:1544:U:H2'	1:0:1545:C:C6	2.54	0.43
1:0:169:A:H5''	39:0:5578:HOH:O	2.18	0.43
1:0:241:A:C2	1:0:378:A:H4'	2.53	0.43
1:0:635:A:H2	39:0:3734:HOH:O	2.00	0.43
3:B:141:ARG:HD2	3:B:163:GLU:OE2	2.18	0.43
24:W:125:HIS:HE1	39:W:3071:HOH:O	2.01	0.43
1:0:1003:U:H4'	9:H:91:ARG:O	2.18	0.43
1:0:101:C:H2'	1:0:102:A:H8	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1654:U:H2'	2:A:47:HIS:CD2	2.51	0.43
1:0:1759:A:N3	1:0:1818:C:H2'	2.33	0.43
1:0:2831:C:H2'	1:0:2832:C:H5'	2.00	0.43
1:0:329:A:OP2	4:C:206:ASN:HB2	2.17	0.43
1:0:111:C:O2'	1:0:112:G:H5'	2.18	0.43
1:0:1406:A:H4'	1:0:1407:A:C5'	2.48	0.43
1:0:1595:G:O2'	1:0:1596:U:H5'	2.19	0.43
1:0:2438:G:H2'	1:0:2439:C:O4'	2.18	0.43
1:0:2649:A:H5'	1:0:2649:A:H8	1.83	0.43
1:0:694:A:C2'	1:0:695:C:H5'	2.48	0.43
28:1:21:ARG:HD2	28:1:37:CYS:SG	2.57	0.43
6:E:112:ALA:HA	6:E:113:PRO:HD3	1.90	0.43
15:N:83:LEU:HD13	15:N:175:LEU:HD23	2.00	0.43
1:0:106:A:H2'	1:0:107:U:O4'	2.19	0.43
1:0:1881:A:OP1	2:A:199:HIS:HE1	2.02	0.43
1:0:1883:U:H5'	1:0:2012:U:OP2	2.19	0.43
1:0:2698:G:H2'	1:0:2699:A:C8	2.54	0.43
1:0:2783:A:H2'	1:0:2784:A:C8	2.53	0.43
1:0:289:G:O2'	1:0:290:C:H5'	2.19	0.43
1:0:419:A:H1'	1:0:1921:A:C2	2.53	0.43
1:0:1734:C:OP1	3:B:234:ARG:HD3	2.19	0.43
1:0:1427:A:N6	1:0:1440:U:H1'	2.33	0.43
1:0:1504:A:H4'	1:0:1506:U:C5	2.53	0.43
1:0:1626:A:H2'	1:0:1627:G:H5'	2.00	0.43
1:0:2488:A:H1'	39:0:3241:HOH:O	2.19	0.43
1:0:2633:A:H5'	39:0:5222:HOH:O	2.18	0.43
1:0:271:C:C2	1:0:273:G:O4'	2.72	0.43
1:0:312:U:C2	1:0:320:G:N2	2.87	0.43
1:0:820:G:H5'	1:0:821:U:H5'	1.99	0.43
1:0:92:G:H4'	23:V:44:GLY:HA3	1.99	0.43
31:9:49:G:H5''	39:9:4707:HOH:O	2.19	0.43
1:0:2676:C:H4'	11:J:70:PHE:CE1	2.54	0.43
25:X:74:ALA:HB2	25:X:85:VAL:HG13	2.01	0.43
1:0:111:C:H2'	1:0:112:G:O4'	2.18	0.43
1:0:1211:G:H2'	1:0:1212:C:C6	2.53	0.43
1:0:1622:G:C2'	1:0:1623:C:H5'	2.48	0.43
1:0:2114:C:OP1	2:A:1:GLY:HA2	2.19	0.43
1:0:2507:G:H2'	1:0:2510:C:N4	2.33	0.43
1:0:2591:C:H2'	1:0:2592:G:O4'	2.19	0.43
1:0:1439:C:H5''	29:2:41:HIS:CE1	2.52	0.43
31:9:3:A:H2	31:9:21:G:N3	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1184:C:O2'	1:0:1185:U:OP2	2.30	0.43
1:0:1294:A:H2'	1:0:1295:G:O4'	2.18	0.43
1:0:138:U:OP2	1:0:139:C:H5	2.01	0.43
1:0:1571:G:H1'	1:0:1627:G:N2	2.34	0.43
1:0:1846:U:O2'	2:A:172:ALA:HB2	2.17	0.43
1:0:2073:G:OP2	1:0:2490:A:H5'	2.19	0.43
1:0:2115:U:H2'	1:0:2116:U:C6	2.53	0.43
1:0:42:C:H1'	39:0:3438:HOH:O	2.18	0.43
15:N:4:PRO:HG3	31:9:69:U:OP1	2.19	0.43
1:0:2716:G:H5'	3:B:262:ARG:HG3	2.00	0.43
1:0:447:A:P	21:T:1:SER:HB2	2.59	0.43
1:0:1001:U:O2'	1:0:1002:G:H5'	2.19	0.43
1:0:1200:A:H3'	39:0:4912:HOH:O	2.18	0.43
1:0:1202:A:C2'	1:0:1203:G:H5'	2.49	0.43
1:0:2837:U:H2'	39:0:6433:HOH:O	2.17	0.43
1:0:571:C:H2'	1:0:572:G:O4'	2.18	0.43
1:0:661:G:C5	1:0:686:A:C2	3.07	0.43
1:0:1482:A:O2'	1:0:1483:C:H5'	2.18	0.43
1:0:1592:G:H2'	1:0:1593:C:C6	2.54	0.43
1:0:2070:G:H2'	1:0:2072:G:OP1	2.18	0.43
1:0:2266:A:H2'	1:0:2267:G:C8	2.54	0.43
1:0:2781:U:H2'	1:0:2782:G:C5'	2.48	0.43
1:0:836:G:H1'	39:0:7509:HOH:O	2.18	0.43
1:0:1845:A:O2'	1:0:1846:U:H5'	2.19	0.42
1:0:1966:U:H2'	1:0:1967:U:C6	2.54	0.42
1:0:2438:G:H5'	39:0:5494:HOH:O	2.18	0.42
1:0:255:A:H2'	1:0:256:C:H6	1.84	0.42
1:0:2566:A:H2	1:0:2695:C:O2	2.02	0.42
1:0:369:G:H2'	1:0:370:G:H8	1.84	0.42
1:0:696:C:H2'	1:0:697:G:O4'	2.19	0.42
1:0:699:C:C2	1:0:743:G:N2	2.87	0.42
11:J:42:GLU:O	11:J:131:THR:HG23	2.19	0.42
1:0:1119:G:N2	1:0:1246:A:N1	2.67	0.42
1:0:1205:U:C2'	1:0:1206:U:C5'	2.89	0.42
1:0:1245:C:O5'	1:0:1245:C:H6	2.02	0.42
1:0:1381:A:N3	1:0:1382:G:H1'	2.34	0.42
1:0:1386:G:O2'	1:0:1387:G:H5'	2.19	0.42
1:0:1421:C:O2'	1:0:1422:U:H5'	2.19	0.42
1:0:1434:A:H2'	1:0:1436:C:C5	2.54	0.42
1:0:1562:C:N4	39:0:5067:HOH:O	2.52	0.42
1:0:1613:C:H2'	1:0:1614:G:O4'	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1795:G:H2'	1:0:1796:A:O4'	2.19	0.42
1:0:1803:C:H2'	1:0:1804:A:H8	1.83	0.42
1:0:2045:G:H2'	1:0:2046:G:O4'	2.19	0.42
1:0:2102:G:C2	1:0:2104:C:C4	3.08	0.42
1:0:2816:A:H5''	1:0:2817:G:H5'	2.01	0.42
1:0:538:C:H5''	1:0:539:G:C8	2.53	0.42
1:0:912:A:C4	1:0:1294:A:C2	3.07	0.42
31:9:1:U:O2'	31:9:3:A:H5''	2.19	0.42
1:0:1407:A:O2'	1:0:1408:U:H3'	2.19	0.42
1:0:615:G:H2'	1:0:616:U:C6	2.54	0.42
1:0:166:A:O2'	1:0:898:G:O6	2.36	0.42
31:9:91:C:H2'	31:9:92:G:O4'	2.19	0.42
1:0:1010:C:OP1	15:N:5:ARG:NH1	2.53	0.42
1:0:1130:U:H2'	1:0:1131:G:O4'	2.18	0.42
1:0:1393:A:H2'	1:0:1394:C:C6	2.54	0.42
1:0:1968:A:H2'	1:0:1969:A:C8	2.55	0.42
1:0:2079:G:H2'	1:0:2080:G:O4'	2.19	0.42
1:0:2239:C:H2'	1:0:2240:U:C6	2.54	0.42
1:0:2252:A:H2'	1:0:2253:G:O4'	2.19	0.42
1:0:2487:C:H2'	1:0:2488:A:O4'	2.18	0.42
1:0:2546:U:H4'	39:B:3923:HOH:O	2.20	0.42
1:0:276:C:O5'	1:0:276:C:H6	2.03	0.42
4:C:218:VAL:HG12	39:C:5065:HOH:O	2.19	0.42
18:Q:19:ARG:HH21	31:9:11:A:P	2.42	0.42
1:0:1396:C:H1'	17:P:1:THR:O	2.19	0.42
1:0:1761:U:H5'	17:P:81:LYS:O	2.20	0.42
1:0:1992:U:H2'	1:0:1994:A:OP2	2.19	0.42
1:0:2345:A:H3'	1:0:2346:C:H6	1.83	0.42
1:0:2039:A:H4'	1:0:2760:C:O2'	2.20	0.42
1:0:295:C:H2'	1:0:296:G:O4'	2.20	0.42
1:0:308:U:C4	1:0:342:C:H1'	2.54	0.42
1:0:524:A:H5''	19:R:29:LYS:HD3	2.00	0.42
16:O:32:ARG:HH21	16:O:35:LYS:NZ	2.17	0.42
26:Y:187:VAL:HG23	26:Y:192:ASP:HB2	2.00	0.42
1:0:2589:U:H2'	1:0:2590:U:C6	2.54	0.42
1:0:272:A:H3'	39:0:7395:HOH:O	2.19	0.42
1:0:2777:G:O2'	1:0:2778:A:H5'	2.20	0.42
1:0:470:U:O2'	28:1:16:HIS:CD2	2.72	0.42
1:0:542:A:H2'	1:0:543:G:O4'	2.19	0.42
1:0:567:U:O5'	1:0:567:U:H6	2.02	0.42
1:0:670:G:H2'	1:0:671:A:C8	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:699:C:C2	1:0:744:G:C2	3.07	0.42
1:0:812:A:H2'	1:0:813:C:O4'	2.19	0.42
1:0:876:A:N3	1:0:876:A:H2'	2.34	0.42
30:3:48:ASN:ND2	30:3:50:GLY:H	2.17	0.42
14:M:164:THR:HG22	14:M:165:GLY:N	2.34	0.42
1:0:1181:A:N1	1:0:1192:A:O2'	2.42	0.42
1:0:1211:G:H2'	1:0:1212:C:H6	1.83	0.42
1:0:1218:U:H2'	1:0:1219:U:C6	2.54	0.42
1:0:1463:U:H2'	1:0:1464:C:C6	2.55	0.42
1:0:1788:U:C2	1:0:1805:G:N2	2.88	0.42
1:0:2649:A:H5'	1:0:2649:A:C8	2.55	0.42
1:0:342:C:H2'	1:0:343:C:H6	1.84	0.42
1:0:574:G:O2'	1:0:575:A:H5'	2.20	0.42
1:0:958:G:H2'	1:0:959:C:H6	1.84	0.42
9:H:69:ARG:HD3	39:H:6314:HOH:O	2.20	0.42
1:0:1055:G:OP2	9:H:99:ARG:NH1	2.53	0.42
15:N:35:VAL:HG11	31:9:6:C:H4'	2.01	0.42
21:T:18:GLU:O	21:T:21:LYS:HG2	2.20	0.42
1:0:113:A:H2'	1:0:115:U:O4	2.20	0.42
1:0:1576:G:H2'	1:0:1577:U:C6	2.55	0.42
1:0:204:A:C2'	1:0:205:U:H5'	2.49	0.42
1:0:825:U:H5''	1:0:826:U:OP1	2.19	0.42
2:A:70:ALA:HA	2:A:71:PRO:HD3	1.88	0.42
11:J:80:LYS:HE3	11:J:101:VAL:O	2.20	0.42
1:0:447:A:OP1	21:T:2:LYS:HG2	2.20	0.42
1:0:1074:G:H4'	1:0:1260:G:C6	2.54	0.42
1:0:1099:G:H2'	1:0:1100:G:O4'	2.20	0.42
1:0:1154:A:H2'	1:0:1155:G:C8	2.55	0.42
1:0:1202:A:H2'	1:0:1203:G:C5'	2.50	0.42
1:0:1819:G:H2'	1:0:1820:G:C5'	2.50	0.42
1:0:210:U:H2'	1:0:211:U:H6	1.84	0.42
1:0:2419:U:H5''	1:0:2420:G:C5'	2.50	0.42
1:0:482:G:O4'	1:0:511:A:C2	2.72	0.42
1:0:907:A:H4'	1:0:1328:A:C2	2.55	0.42
2:A:71:PRO:HG2	2:A:91:GLY:HA2	2.02	0.42
1:0:138:U:OP1	1:0:259:G:H5'	2.20	0.42
1:0:1556:G:O2'	1:0:1557:G:H5'	2.19	0.42
1:0:1682:A:H5''	39:0:4695:HOH:O	2.20	0.42
1:0:1706:G:C5	1:0:1707:G:C6	3.08	0.42
1:0:1789:G:H2'	1:0:1790:C:O5'	2.20	0.42
1:0:1873:G:H3'	39:0:4169:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1878:G:O2'	1:0:1879:U:P	2.78	0.42
1:0:2416:G:H2'	1:0:2417:C:C6	2.55	0.42
1:0:812:A:H1'	39:0:8714:HOH:O	2.19	0.42
1:0:185:G:H4'	1:0:186:A:H4'	2.02	0.41
1:0:17:G:H2'	1:0:18:C:C6	2.56	0.41
1:0:1942:A:H4'	39:A:241:HOH:O	2.19	0.41
1:0:2039:A:H2'	1:0:2040:C:C6	2.54	0.41
1:0:218:C:C5	1:0:220:C:C4	3.07	0.41
1:0:581:G:O2'	1:0:582:U:H5'	2.20	0.41
31:9:56:A:C3'	31:9:57:A:H5''	2.50	0.41
16:O:73:ASP:HA	16:O:92:VAL:O	2.20	0.41
1:0:1819:G:H2'	1:0:1820:G:C4'	2.50	0.41
1:0:2533:C:H6	1:0:2533:C:C5'	2.27	0.41
1:0:2564:G:OP2	1:0:2565:C:H5''	2.20	0.41
1:0:2583:A:H5'	39:0:6007:HOH:O	2.21	0.41
1:0:1855:G:H8	2:A:144:GLU:OE2	2.04	0.41
9:H:59:GLN:NE2	9:H:129:ARG:HE	2.15	0.41
1:0:107:U:C2'	1:0:108:U:H5'	2.51	0.41
1:0:1166:A:OP1	1:0:1174:A:H4'	2.19	0.41
1:0:1268:C:O2'	1:0:1269:G:H5'	2.20	0.41
1:0:1909:A:H2'	1:0:1910:A:C8	2.56	0.41
1:0:283:U:H5	1:0:284:C:C4	2.37	0.41
1:0:2540:G:O2'	37:0:9101:WIN:H2G	2.20	0.41
4:C:107:ARG:O	4:C:111:VAL:HG23	2.20	0.41
9:H:31:ILE:HG23	39:H:6314:HOH:O	2.19	0.41
18:Q:25:PRO:HA	18:Q:26:PRO:HD3	1.87	0.41
1:0:1098:A:OP1	24:W:128:VAL:HG22	2.20	0.41
1:0:168:C:H5'	1:0:2277:U:OP1	2.21	0.41
1:0:1766:U:O2	1:0:1778:A:H5'	2.21	0.41
1:0:2016:U:H2'	1:0:2017:U:O4'	2.20	0.41
1:0:1741:U:C4	1:0:2033:G:C8	3.08	0.41
1:0:2251:G:H2'	1:0:2252:A:C8	2.54	0.41
1:0:2354:A:C2	1:0:2367:A:C8	3.09	0.41
1:0:1014:A:H5''	31:9:101:G:O2'	2.20	0.41
31:9:39:U:H3'	31:9:40:C:C5'	2.49	0.41
1:0:710:G:OP1	16:O:24:ALA:HB3	2.21	0.41
16:O:70:LEU:O	16:O:92:VAL:HG21	2.21	0.41
22:U:14:GLU:O	22:U:17:THR:HB	2.20	0.41
1:0:1706:G:C6	1:0:1707:G:N1	2.88	0.41
1:0:2087:C:O2'	1:0:2088:C:H5'	2.20	0.41
1:0:2103:A:H2'	1:0:2104:C:C5'	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2473:U:O3'	1:0:2474:A:H3'	2.20	0.41
1:0:2538:A:O2'	37:0:9101:WIN:H1AB	2.21	0.41
1:0:2815:G:N7	11:J:80:LYS:NZ	2.69	0.41
1:0:317:A:H4'	39:0:8457:HOH:O	2.19	0.41
1:0:2714:U:H4'	3:B:10:SER:HB2	2.02	0.41
4:C:138:VAL:O	4:C:234:VAL:HA	2.21	0.41
4:C:39:GLN:O	4:C:43:LYS:HD3	2.20	0.41
12:K:130:MET:SD	22:U:25:ASP:O	2.78	0.41
1:0:125:U:H2'	39:0:8451:HOH:O	2.21	0.41
1:0:1684:A:O2'	1:0:1685:A:H5''	2.20	0.41
1:0:2265:U:H2'	1:0:2266:A:C8	2.55	0.41
1:0:2092:G:H2'	1:0:2613:G:OP1	2.21	0.41
1:0:2906:A:H5'	1:0:2907:C:O4'	2.20	0.41
31:9:28:U:H2'	31:9:29:C:C6	2.55	0.41
18:Q:25:PRO:HB2	39:9:4350:HOH:O	2.19	0.41
24:W:137:GLN:NE2	24:W:141:HIS:HE1	2.14	0.41
24:W:48:VAL:HG12	24:W:48:VAL:O	2.20	0.41
1:0:1306:U:H5''	4:C:184:ARG:HD2	2.03	0.41
1:0:1456:C:H2'	1:0:1457:U:C6	2.55	0.41
1:0:2515:C:H2'	1:0:2516:G:O4'	2.21	0.41
1:0:2664:A:OP1	1:0:2664:A:H8	2.03	0.41
1:0:2734:G:O2'	1:0:2735:U:H5'	2.21	0.41
1:0:318:U:H5'	1:0:339:A:N3	2.36	0.41
1:0:579:G:H2'	1:0:580:A:C8	2.56	0.41
1:0:1688:G:O2'	28:1:5:THR:HG23	2.20	0.41
3:B:304:PRO:HD2	3:B:307:ARG:NE	2.36	0.41
4:C:236:THR:HG22	4:C:239:ALA:H	1.86	0.41
9:H:70:LEU:O	9:H:74:ARG:HB2	2.20	0.41
1:0:1076:G:C2	1:0:1084:C:C2	3.09	0.41
1:0:1290:G:H3'	39:0:4115:HOH:O	2.20	0.41
1:0:1624:A:H5'	1:0:1626:A:O4'	2.21	0.41
1:0:1736:A:H1'	39:0:7468:HOH:O	2.20	0.41
1:0:185:G:H4'	1:0:186:A:OP1	2.21	0.41
1:0:1973:A:H5'	1:0:1973:A:C8	2.53	0.41
1:0:2326:C:H4'	1:0:2412:G:C4'	2.51	0.41
1:0:400:C:O2'	1:0:401:C:H5'	2.21	0.41
1:0:549:A:O2'	1:0:550:C:H5'	2.21	0.41
1:0:559:U:H2'	1:0:560:U:O4'	2.20	0.41
1:0:806:A:H2'	1:0:807:A:O4'	2.21	0.41
14:M:65:VAL:HG21	14:M:105:ALA:HB2	2.03	0.41
1:0:1167:G:H4'	10:I:130:LEU:HD21	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1165:G:O3'	1:0:1174:A:H4'	2.20	0.41
1:0:1185:U:H5'	39:0:7308:HOH:O	2.21	0.41
1:0:282:C:H1'	1:0:368:C:H41	1.83	0.41
1:0:327:A:H4'	1:0:329:A:C8	2.56	0.41
3:B:102:THR:HB	3:B:103:ASP:H	1.71	0.41
1:0:10:U:H3'	1:0:10:U:C6	2.56	0.41
1:0:1631:A:H2'	1:0:1632:A:C8	2.56	0.41
1:0:1762:C:O2'	1:0:1763:C:H5'	2.20	0.41
1:0:2089:A:O2'	1:0:2090:G:H5'	2.21	0.41
1:0:2812:A:C2	1:0:2814:A:N6	2.75	0.41
1:0:291:C:H2'	1:0:292:G:O4'	2.21	0.41
1:0:318:U:H5'	1:0:339:A:C4	2.56	0.41
31:9:35:C:H5''	39:9:4078:HOH:O	2.20	0.41
5:D:23:VAL:HG12	5:D:130:VAL:HG22	2.02	0.41
1:0:1383:U:H5'	25:X:27:ASP:OD1	2.21	0.41
1:0:940:G:O2'	1:0:1032:A:N1	2.52	0.41
1:0:1652:C:H4'	27:Z:76:THR:HG21	2.03	0.41
1:0:1811:A:C2	1:0:2752:C:H1'	2.56	0.41
1:0:2047:C:H5'	39:0:6092:HOH:O	2.21	0.41
1:0:2074:A:H1'	39:0:6299:HOH:O	2.21	0.41
1:0:2385:G:H2'	1:0:2386:U:C6	2.56	0.41
1:0:2481:G:H5''	39:0:3267:HOH:O	2.20	0.41
1:0:2908:A:O5'	1:0:2908:A:H8	2.04	0.41
3:B:10:SER:O	3:B:16:ARG:NH1	2.53	0.41
3:B:69:VAL:HA	3:B:70:PRO:HD3	1.92	0.41
24:W:88:THR:HG22	24:W:89:ASP:H	1.86	0.41
1:0:1159:G:H21	1:0:1189:A:H8	1.69	0.40
1:0:1778:A:H2'	1:0:1779:A:H5'	2.03	0.40
1:0:2121:G:H1'	39:0:3302:HOH:O	2.20	0.40
1:0:2672:C:H2'	1:0:2673:U:H6	1.85	0.40
1:0:856:G:H2'	39:0:4459:HOH:O	2.22	0.40
3:B:195:ARG:HG2	3:B:323:LEU:HD22	2.02	0.40
1:0:2548:C:OP2	3:B:5:ARG:NH2	2.54	0.40
1:0:1342:C:O2'	1:0:1343:C:H5'	2.21	0.40
1:0:1972:U:C2'	1:0:1973:A:C5'	3.00	0.40
1:0:2002:C:C2'	1:0:2003:U:H5'	2.51	0.40
1:0:2114:C:O2'	1:0:2115:U:H5'	2.21	0.40
1:0:283:U:H5	1:0:284:C:N3	2.18	0.40
1:0:327:A:H4'	1:0:329:A:N7	2.37	0.40
1:0:304:G:H1'	1:0:347:A:N6	2.36	0.40
1:0:383:A:H4'	39:0:4330:HOH:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:9:54:A:O2'	31:9:55:U:H5'	2.21	0.40
31:9:73:A:H2'	31:9:74:G:O4'	2.20	0.40
2:A:135:VAL:HG11	2:A:147:ARG:NH2	2.36	0.40
18:Q:47:VAL:HA	18:Q:48:PRO:HD3	1.94	0.40
24:W:5:VAL:HG11	24:W:153:MET:CE	2.52	0.40
26:Y:134:HIS:H	26:Y:134:HIS:CD2	2.39	0.40
1:0:1072:G:OP2	26:Y:154:ARG:NH2	2.55	0.40
1:0:1183:C:H5	1:0:1192:A:OP1	2.03	0.40
1:0:1804:A:H2'	1:0:1805:G:C8	2.56	0.40
1:0:10:U:C4	1:0:532:A:C8	3.10	0.40
3:B:57:GLU:HA	3:B:58:PRO:HD2	1.98	0.40
15:N:86:LEU:HD12	15:N:125:ALA:HB2	2.03	0.40
1:0:1008:C:O2'	1:0:1009:U:H5'	2.21	0.40
1:0:1016:U:H1'	39:0:8342:HOH:O	2.20	0.40
1:0:1132:A:H2'	1:0:1133:A:C8	2.57	0.40
1:0:1361:C:H2'	1:0:1362:U:H6	1.86	0.40
1:0:137:U:OP1	1:0:259:G:O2'	2.40	0.40
1:0:1788:U:O2'	1:0:1789:G:H5'	2.22	0.40
1:0:1812:G:H4'	1:0:1814:G:O4'	2.22	0.40
1:0:282:C:O2'	1:0:283:U:C5'	2.70	0.40
1:0:537:G:O4'	1:0:538:C:C5	2.75	0.40
1:0:598:C:H2'	1:0:599:G:H8	1.86	0.40
6:E:49:ILE:HD11	6:E:69:ILE:HD12	2.02	0.40
1:0:308:U:H5'	21:T:97:ARG:NH2	2.36	0.40
1:0:113:A:OP2	1:0:114:A:H2'	2.21	0.40
1:0:1167:G:H1'	39:I:6825:HOH:O	2.21	0.40
1:0:1175:G:H1'	1:0:1193:A:C2'	2.51	0.40
1:0:1211:G:O2'	1:0:1212:C:H5'	2.22	0.40
1:0:1257:C:O2'	1:0:1258:G:H5'	2.22	0.40
1:0:1331:G:OP2	26:Y:142:SER:OG	2.33	0.40
1:0:1537:C:H1'	39:0:6076:HOH:O	2.22	0.40
1:0:1594:C:O2'	1:0:1595:G:H5'	2.22	0.40
1:0:1657:A:H2'	1:0:1658:A:C8	2.56	0.40
1:0:2245:C:H6	1:0:2245:C:O5'	2.04	0.40
1:0:2401:A:H2'	1:0:2402:A:H8	1.82	0.40
1:0:77:G:C2'	1:0:78:G:H5'	2.51	0.40
1:0:827:A:H2'	1:0:828:G:O4'	2.22	0.40
31:9:33:U:H2'	39:9:3797:HOH:O	2.20	0.40
1:0:2629:C:N4	2:A:206:ARG:HH21	2.18	0.40
5:D:48:MET:HB3	31:9:41:C:H4'	2.04	0.40
1:0:316:A:H5'	21:T:54:ASP:OD2	2.22	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	
2	A	235/237 (99%)	218 (93%)	14 (6%)	3 (1%)	14	39
3	B	335/337 (99%)	307 (92%)	26 (8%)	2 (1%)	28	60
4	C	244/246 (99%)	224 (92%)	18 (7%)	2 (1%)	22	52
5	D	134/177 (76%)	121 (90%)	10 (8%)	3 (2%)	8	25
6	E	170/172 (99%)	161 (95%)	9 (5%)	0	100	100
7	F	117/119 (98%)	109 (93%)	7 (6%)	1 (1%)	20	49
8	G	25/348 (7%)	25 (100%)	0	0	100	100
9	H	156/177 (88%)	150 (96%)	5 (3%)	1 (1%)	28	60
10	I	68/70 (97%)	58 (85%)	10 (15%)	0	100	100
11	J	140/142 (99%)	134 (96%)	6 (4%)	0	100	100
12	K	130/132 (98%)	125 (96%)	4 (3%)	1 (1%)	22	52
13	L	141/165 (86%)	127 (90%)	14 (10%)	0	100	100
14	M	192/194 (99%)	187 (97%)	4 (2%)	1 (0%)	32	64
15	N	184/186 (99%)	173 (94%)	8 (4%)	3 (2%)	11	33
16	O	113/115 (98%)	111 (98%)	2 (2%)	0	100	100
17	P	141/143 (99%)	139 (99%)	2 (1%)	0	100	100
18	Q	93/95 (98%)	88 (95%)	4 (4%)	1 (1%)	17	44
19	R	148/150 (99%)	142 (96%)	6 (4%)	0	100	100
20	S	79/81 (98%)	75 (95%)	4 (5%)	0	100	100
21	T	117/119 (98%)	111 (95%)	5 (4%)	1 (1%)	20	49
22	U	51/53 (96%)	47 (92%)	4 (8%)	0	100	100
23	V	63/65 (97%)	61 (97%)	2 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
24	W	152/154 (99%)	148 (97%)	4 (3%)	0	100	100
25	X	80/82 (98%)	77 (96%)	2 (2%)	1 (1%)	14	39
26	Y	140/142 (99%)	139 (99%)	1 (1%)	0	100	100
27	Z	71/73 (97%)	65 (92%)	6 (8%)	0	100	100
28	1	54/56 (96%)	52 (96%)	2 (4%)	0	100	100
29	2	42/50 (84%)	41 (98%)	1 (2%)	0	100	100
30	3	90/92 (98%)	88 (98%)	2 (2%)	0	100	100
All	All	3705/4172 (89%)	3503 (94%)	182 (5%)	20 (0%)	32	64

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	37	VAL
5	D	137	PRO
15	N	154	LEU
15	N	139	TRP
3	B	2	GLN
5	D	56	ARG
12	K	127	ALA
15	N	167	ASP
2	A	27	LEU
3	B	185	GLY
4	C	8	LEU
7	F	100	ASP
14	M	71	SER
9	H	19	ARG
21	T	44	ALA
4	C	79	ARG
5	D	27	ILE
18	Q	18	PRO
2	A	88	ILE
25	X	52	PRO

### 5.3.2 Protein sidechains ⓘ

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	A	179/179 (100%)	168 (94%)	11 (6%)	22	49
3	B	282/282 (100%)	268 (95%)	14 (5%)	28	59
4	C	193/193 (100%)	176 (91%)	17 (9%)	12	31
5	D	117/148 (79%)	108 (92%)	9 (8%)	15	37
6	E	152/152 (100%)	146 (96%)	6 (4%)	37	69
7	F	93/93 (100%)	90 (97%)	3 (3%)	44	76
8	G	27/282 (10%)	27 (100%)	0	100	100
9	H	134/145 (92%)	128 (96%)	6 (4%)	32	63
10	I	58/58 (100%)	57 (98%)	1 (2%)	66	88
11	J	118/118 (100%)	110 (93%)	8 (7%)	18	43
12	K	106/106 (100%)	100 (94%)	6 (6%)	24	53
13	L	113/127 (89%)	112 (99%)	1 (1%)	82	94
14	M	158/158 (100%)	152 (96%)	6 (4%)	38	70
15	N	149/149 (100%)	140 (94%)	9 (6%)	22	50
16	O	93/93 (100%)	90 (97%)	3 (3%)	44	76
17	P	113/113 (100%)	108 (96%)	5 (4%)	33	64
18	Q	79/79 (100%)	75 (95%)	4 (5%)	28	58
19	R	117/117 (100%)	112 (96%)	5 (4%)	33	65
20	S	71/71 (100%)	70 (99%)	1 (1%)	71	90
21	T	105/105 (100%)	96 (91%)	9 (9%)	12	32
22	U	44/44 (100%)	44 (100%)	0	100	100
23	V	51/51 (100%)	49 (96%)	2 (4%)	37	69
24	W	130/130 (100%)	123 (95%)	7 (5%)	26	55
25	X	66/66 (100%)	57 (86%)	9 (14%)	4	11
26	Y	120/120 (100%)	116 (97%)	4 (3%)	43	74
27	Z	60/60 (100%)	59 (98%)	1 (2%)	66	88
28	1	46/46 (100%)	45 (98%)	1 (2%)	57	84
29	2	42/46 (91%)	41 (98%)	1 (2%)	54	82
30	3	79/79 (100%)	77 (98%)	2 (2%)	53	81
All	All	3095/3410 (91%)	2944 (95%)	151 (5%)	29	60

All (151) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	3	ARG
2	A	51	ARG
2	A	64	ASP
2	A	78	ASP
2	A	105	VAL
2	A	108	VAL
2	A	110	SER
2	A	131	HIS
2	A	179	MET
2	A	206	ARG
2	A	217	ARG
3	B	7	ARG
3	B	11	LEU
3	B	27	ASN
3	B	49	THR
3	B	71	VAL
3	B	82	VAL
3	B	97	LEU
3	B	98	THR
3	B	162	MET
3	B	171	VAL
3	B	195	ARG
3	B	234	ARG
3	B	254	GLN
3	B	277	GLU
4	C	2	GLN
4	C	27	ARG
4	C	76	ARG
4	C	78	ARG
4	C	94	THR
4	C	98	ARG
4	C	101	ASP
4	C	136	VAL
4	C	162	VAL
4	C	187	ARG
4	C	214	THR
4	C	223	LEU
4	C	234	VAL
4	C	236	THR
4	C	237	GLU
4	C	240	LEU
4	C	243	VAL

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Mol	Chain	Res	Type
5	D	19	GLU
5	D	24	HIS
5	D	29	HIS
5	D	50	VAL
5	D	62	ASP
5	D	101	THR
5	D	128	LEU
5	D	149	ARG
5	D	161	ASP
6	E	16	ASP
6	E	36	PRO
6	E	61	THR
6	E	102	VAL
6	E	156	ASP
6	E	164	ASP
7	F	12	LEU
7	F	50	VAL
7	F	60	VAL
9	H	62	HIS
9	H	65	LEU
9	H	87	LYS
9	H	91	ARG
9	H	157	TYR
9	H	173	GLU
10	I	94	ASP
11	J	39	VAL
11	J	45	VAL
11	J	52	GLN
11	J	79	PHE
11	J	107	ASN
11	J	120	SER
11	J	130	VAL
11	J	131	THR
12	K	10	GLN
12	K	19	THR
12	K	49	LEU
12	K	98	VAL
12	K	107	THR
12	K	119	GLN
13	L	35	ARG
14	M	10	ASP
14	M	46	LEU

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Mol	Chain	Res	Type
14	M	68	ARG
14	M	93	ARG
14	M	99	ARG
14	M	116	ASN
15	N	26	LEU
15	N	38	LYS
15	N	47	LEU
15	N	49	THR
15	N	62	HIS
15	N	134	ASP
15	N	135	VAL
15	N	142	THR
15	N	180	LEU
16	O	3	THR
16	O	25	VAL
16	O	80	ASP
17	P	13	VAL
17	P	21	VAL
17	P	52	LYS
17	P	91	LYS
17	P	98	ILE
18	Q	11	ARG
18	Q	16	ASN
18	Q	18	PRO
18	Q	57	ASP
19	R	13	THR
19	R	39	THR
19	R	119	VAL
19	R	125	ARG
19	R	132	ARG
20	S	81	ILE
21	T	5	ASP
21	T	39	ASN
21	T	48	VAL
21	T	61	GLU
21	T	82	THR
21	T	89	ARG
21	T	96	VAL
21	T	115	GLU
21	T	117	ASP
23	V	12	THR
23	V	13	PRO

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Mol	Chain	Res	Type
24	W	35	VAL
24	W	38	THR
24	W	52	VAL
24	W	120	PRO
24	W	125	HIS
24	W	142	ASP
24	W	146	ILE
25	X	10	VAL
25	X	43	VAL
25	X	46	ASP
25	X	49	ARG
25	X	52	PRO
25	X	72	VAL
25	X	79	GLU
25	X	82	GLU
25	X	88	GLU
26	Y	154	ARG
26	Y	174	VAL
26	Y	189	ASN
26	Y	203	VAL
27	Z	85	ASP
28	1	14	THR
29	2	18	ASN
30	3	18	GLN
30	3	22	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (66) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	47	HIS
2	A	176	HIS
2	A	199	HIS
3	B	27	ASN
3	B	145	HIS
3	B	238	ASN
3	B	260	HIS
3	B	320	GLN
3	B	332	ASN
4	C	2	GLN
4	C	67	GLN
4	C	73	GLN
4	C	129	HIS

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Mol	Chain	Res	Type
5	D	103	ASN
6	E	143	GLN
8	G	64	ASN
9	H	49	GLN
9	H	59	GLN
10	I	102	GLN
11	J	52	GLN
11	J	107	ASN
12	K	10	GLN
12	K	42	ASN
13	L	18	HIS
13	L	41	HIS
14	M	24	GLN
14	M	58	GLN
14	M	137	ASN
14	M	170	ASN
15	N	40	ASN
15	N	107	ASN
17	P	50	GLN
17	P	66	GLN
17	P	88	GLN
17	P	89	ASN
17	P	118	GLN
18	Q	40	HIS
19	R	94	ASN
19	R	98	ASN
19	R	117	HIS
19	R	123	GLN
20	S	51	GLN
20	S	55	GLN
21	T	39	ASN
22	U	39	ASN
22	U	48	ASN
23	V	60	GLN
24	W	110	GLN
24	W	119	HIS
24	W	125	HIS
24	W	141	HIS
25	X	23	HIS
26	Y	119	GLN
26	Y	129	ASN
26	Y	134	HIS

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Mol	Chain	Res	Type
26	Y	189	ASN
28	1	8	GLN
28	1	16	HIS
28	1	28	HIS
29	2	16	ASN
29	2	18	ASN
29	2	41	HIS
29	2	45	ASN
30	3	2	GLN
30	3	30	GLN
30	3	48	ASN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2745/2923 (93%)	238 (8%)	26 (0%)
31	9	121/122 (99%)	17 (14%)	1 (0%)
All	All	2866/3045 (94%)	255 (8%)	27 (0%)

All (255) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	0	31	C
1	0	67	A
1	0	69	A
1	0	70	A
1	0	71	G
1	0	86	A
1	0	87	C
1	0	88	G
1	0	114	A
1	0	115	U
1	0	120	A
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

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Mol	Chain	Res	Type
1	0	198	A
1	0	200	C
1	0	204	A
1	0	219	G
1	0	237	G
1	0	271	C
1	0	272	A
1	0	273	G
1	0	283	U
1	0	284	C
1	0	308	U
1	0	309	C
1	0	336	G
1	0	337	A
1	0	358	G
1	0	381	G
1	0	397	A
1	0	417	G
1	0	461	C
1	0	487	G
1	0	497	A
1	0	498	A
1	0	510	U
1	0	511	A
1	0	514	G
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	U
1	0	581	G
1	0	588	G
1	0	604	G
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	759	C

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Mol	Chain	Res	Type
1	0	777	U
1	0	809	G
1	0	821	U
1	0	835	U
1	0	840	U
1	0	857	A
1	0	858	U
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	885	G
1	0	898	G
1	0	905	C
1	0	920	C
1	0	921	G
1	0	923	A
1	0	938	G
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	1087	G
1	0	1088	A
1	0	1106	A
1	0	1109	U
1	0	1110	G
1	0	1119	G
1	0	1130	U
1	0	1137	G
1	0	1151	G
1	0	1164	U

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Mol	Chain	Res	Type
1	0	1165	G
1	0	1166	A
1	0	1174	A
1	0	1175	G
1	0	1185	U
1	0	1193	A
1	0	1205	U
1	0	1206	U
1	0	1216	G
1	0	1237	U
1	0	1238	C
1	0	1239	G
1	0	1279	U
1	0	1289	C
1	0	1331	G
1	0	1342	C
1	0	1353	C
1	0	1357	A
1	0	1360	C
1	0	1377	C
1	0	1378	G
1	0	1407	A
1	0	1409	G
1	0	1474	C
1	0	1485	A
1	0	1505	U
1	0	1506	U
1	0	1524	U
1	0	1525	G
1	0	1526	A
1	0	1535	G
1	0	1592	G
1	0	1617	C
1	0	1625	U
1	0	1626	A
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

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Mol	Chain	Res	Type
1	0	1701	A
1	0	1722	U
1	0	1723	G
1	0	1725	C
1	0	1730	G
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	1965	C
1	0	1971	G
1	0	1973	A
1	0	1978	A
1	0	1980	U
1	0	1996	U
1	0	2006	C
1	0	2008	U
1	0	2011	A
1	0	2012	U
1	0	2013	G
1	0	2033	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	2110	G
1	0	2133	U
1	0	2243	C
1	0	2258	A
1	0	2271	G
1	0	2291	A

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Mol	Chain	Res	Type
1	0	2317	C
1	0	2320	U
1	0	2321	A
1	0	2345	A
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	2480	G
1	0	2483	A
1	0	2507	G
1	0	2509	A
1	0	2511	A
1	0	2533	C
1	0	2537	G
1	0	2541	U
1	0	2553	A
1	0	2564	G
1	0	2589	U
1	0	2601	A
1	0	2602	G
1	0	2608	C
1	0	2613	G
1	0	2638	G
1	0	2645	U
1	0	2649	A
1	0	2664	A
1	0	2676	C
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	2792	A
1	0	2800	A

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Mol	Chain	Res	Type
1	0	2811	A
1	0	2812	A
1	0	2825	C
1	0	2836	G
1	0	2876	G
1	0	2890	A
1	0	2896	A
1	0	2903	C
1	0	2914	A
31	9	2	U
31	9	14	G
31	9	22	G
31	9	23	U
31	9	24	U
31	9	25	G
31	9	34	A
31	9	40	C
31	9	41	C
31	9	43	G
31	9	44	A
31	9	52	A
31	9	57	A
31	9	66	G
31	9	77	A
31	9	114	G
31	9	122	C

All (27) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	129	A
1	0	338	C
1	0	603	A
1	0	644	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	1165	G
1	0	1237	U

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Mol	Chain	Res	Type
1	0	1246	A
1	0	1352	A
1	0	1377	C
1	0	1474	C
1	0	1667	A
1	0	1684	A
1	0	1979	G
1	0	2467	A
1	0	2526	C
1	0	2536	C
1	0	2649	A
1	0	2718	C
1	0	2761	A
1	0	2791	U
31	9	65	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
1	OMU	0	2587	1,34	14,22,23	1.00	1 (7%)	18,31,34	3.70	2 (11%)
1	OMG	0	2588	1	18,26,27	1.01	2 (11%)	22,38,41	2.47	5 (22%)
1	UR3	0	2619	1	14,22,23	0.78	0	16,32,35	0.69	0
1	PSU	0	2621	1	16,21,22	1.68	3 (18%)	20,30,33	6.14	5 (25%)
1	1MA	0	628	1,34	16,25,26	1.12	1 (6%)	13,37,40	1.24	1 (7%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMU	0	2587	1,34	-	0/5/27/28	0/2/2/2
1	OMG	0	2588	1	-	0/5/27/28	0/3/3/3
1	UR3	0	2619	1	-	0/3/25/26	0/2/2/2
1	PSU	0	2621	1	-	0/7/25/26	0/2/2/2
1	1MA	0	628	1,34	-	0/3/25/26	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	0	2621	PSU	C5-C1'	-5.16	1.47	1.52
1	0	2588	OMG	C8-N7	-2.02	1.30	1.34
1	0	2587	OMU	C4-N3	2.37	1.37	1.33
1	0	2621	PSU	C4-N3	2.60	1.37	1.33
1	0	2621	PSU	C2-N1	2.65	1.43	1.38
1	0	628	1MA	C6-N6	2.90	1.34	1.27
1	0	2588	OMG	C6-N1	3.26	1.39	1.33

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	2621	PSU	N1-C2-N3	-19.38	114.46	128.40
1	0	2621	PSU	C5-C4-N3	-12.70	115.01	125.43
1	0	2588	OMG	C5-C6-N1	-8.31	111.66	123.48
1	0	628	1MA	C2-N3-C4	-3.70	110.73	116.41
1	0	2587	OMU	C5-C4-N3	-3.49	114.79	123.12
1	0	2588	OMG	C2-N3-C4	-2.78	111.92	115.16
1	0	2588	OMG	N3-C2-N1	-2.43	123.91	127.46
1	0	2621	PSU	C5-C1'-C2'	-2.21	111.74	115.55
1	0	2588	OMG	C6-C5-C4	-2.18	118.68	120.84
1	0	2621	PSU	C6-N1-C2	2.75	119.76	115.36
1	0	2588	OMG	C6-N1-C2	6.33	125.17	116.06
1	0	2621	PSU	C4-N3-C2	13.83	127.25	115.16
1	0	2587	OMU	C4-N3-C2	15.19	127.17	114.13

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	0	2587	OMU	1	0
1	0	628	1MA	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 306 ligands modelled in this entry, 305 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
37	WIN	0	9101	-	38,43,43	1.88	8 (21%)	48,71,71	3.65	25 (52%)

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
37	WIN	0	9101	-	-	0/20/110/110	0/3/5/5

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	0	9101	WIN	C2B-C1X	-3.96	1.40	1.46
37	0	9101	WIN	C1N-C1W	-2.84	1.39	1.46
37	0	9101	WIN	C1B-C1V	2.11	1.54	1.50
37	0	9101	WIN	O1U-C2G	2.30	1.49	1.46
37	0	9101	WIN	O1U-C1Z	2.33	1.38	1.34
37	0	9101	WIN	C1C-C1Y	3.46	1.56	1.50
37	0	9101	WIN	C1N-C1V	5.23	1.41	1.33
37	0	9101	WIN	C2M-C2G	5.33	1.61	1.53

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	0	9101	WIN	C2F-O1T-C1W	-9.20	104.94	116.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	0	9101	WIN	O1J-C2A-C2L	-6.25	111.90	123.63
37	0	9101	WIN	O1H-C1X-C1P	-5.26	111.59	120.52
37	0	9101	WIN	O1U-C1Z-C2F	-5.22	106.04	118.07
37	0	9101	WIN	O1U-C2G-C1Q	-5.02	96.58	104.75
37	0	9101	WIN	C1O-C2M-C2K	-4.86	92.00	101.01
37	0	9101	WIN	O1T-C1W-O1G	-4.44	115.53	123.32
37	0	9101	WIN	C2H-C1Q-C2G	-3.33	102.67	111.46
37	0	9101	WIN	O1L-C2D-C2J	-3.15	101.83	111.92
37	0	9101	WIN	O1T-C2F-C2K	-2.99	102.92	109.72
37	0	9101	WIN	C1F-C2I-C2J	-2.92	106.07	113.13
37	0	9101	WIN	O1S-C1O-C2M	-2.43	103.02	105.79
37	0	9101	WIN	O1I-C1Z-C2F	-2.04	118.54	122.19
37	0	9101	WIN	O1K-C2B-C1X	2.25	120.02	115.76
37	0	9101	WIN	C2I-C2J-C2D	2.40	120.98	115.18
37	0	9101	WIN	C1F-C2I-C2H	2.85	114.87	109.89
37	0	9101	WIN	C2M-C2J-C2D	2.98	116.06	110.02
37	0	9101	WIN	C1A-O1R-C2A	3.40	121.87	115.97
37	0	9101	WIN	C1Q-C2G-C2M	4.00	121.06	113.72
37	0	9101	WIN	C1C-C1Y-C2H	5.24	130.28	116.40
37	0	9101	WIN	C1V-C1N-C1W	5.51	142.36	126.97
37	0	9101	WIN	O1U-C1Z-O1I	5.97	127.45	118.51
37	0	9101	WIN	C2I-C2H-C1Y	6.10	120.23	112.23
37	0	9101	WIN	C1O-C2M-C2G	6.35	123.74	112.77
37	0	9101	WIN	O1R-C2A-C2L	9.10	125.14	111.56

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
37	0	9101	WIN	13	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	0	2749/2923 (94%)	-0.68	10 (0%) 92 92	24, 56, 105, 182	0
2	A	237/237 (100%)	0.07	15 (6%) 21 16	35, 71, 114, 133	0
3	B	337/337 (100%)	-0.43	0 100 100	34, 65, 95, 108	0
4	C	246/246 (100%)	-0.42	0 100 100	31, 56, 80, 91	0
5	D	140/177 (79%)	1.44	46 (32%) 0 0	80, 120, 142, 152	0
6	E	172/172 (100%)	-0.15	2 (1%) 79 77	55, 81, 105, 112	0
7	F	119/119 (100%)	0.64	11 (9%) 10 6	64, 90, 122, 137	0
8	G	29/348 (8%)	0.83	2 (6%) 18 13	89, 109, 116, 119	0
9	H	160/177 (90%)	0.64	19 (11%) 5 3	57, 84, 120, 128	0
10	I	70/70 (100%)	3.82	55 (78%) 0 0	142, 164, 183, 184	0
11	J	142/142 (100%)	-0.43	1 (0%) 87 86	47, 60, 82, 104	0
12	K	132/132 (100%)	-0.42	2 (1%) 74 72	44, 61, 86, 91	0
13	L	145/165 (87%)	0.42	15 (10%) 7 5	35, 87, 131, 142	0
14	M	194/194 (100%)	-0.43	0 100 100	38, 55, 75, 82	0
15	N	186/186 (100%)	0.38	21 (11%) 6 4	55, 83, 139, 146	0
16	O	115/115 (100%)	-0.41	0 100 100	43, 66, 84, 88	0
17	P	143/143 (100%)	-0.26	1 (0%) 87 86	50, 70, 86, 94	0
18	Q	95/95 (100%)	-0.50	0 100 100	49, 60, 76, 89	0
19	R	150/150 (100%)	-0.57	0 100 100	38, 56, 78, 84	0
20	S	81/81 (100%)	-0.00	2 (2%) 58 54	56, 76, 100, 108	0
21	T	119/119 (100%)	-0.06	3 (2%) 58 54	48, 71, 100, 127	0
22	U	53/53 (100%)	-0.28	0 100 100	56, 72, 95, 102	0
23	V	65/65 (100%)	1.51	16 (24%) 1 0	66, 94, 137, 144	0
24	W	154/154 (100%)	-0.46	1 (0%) 89 88	44, 60, 79, 90	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
25	X	82/82 (100%)	-0.08	5 (6%) 22 17	55, 71, 97, 111	0
26	Y	142/142 (100%)	-0.58	1 (0%) 87 86	31, 53, 80, 102	0
27	Z	73/73 (100%)	4.54	52 (71%) 0 0	99, 132, 149, 150	0
28	1	56/56 (100%)	-0.48	0 100 100	33, 41, 52, 62	0
29	2	46/50 (92%)	0.04	3 (6%) 20 15	48, 79, 112, 122	0
30	3	92/92 (100%)	0.29	3 (3%) 47 40	58, 85, 99, 109	0
31	9	122/122 (100%)	-0.82	2 (1%) 72 70	46, 78, 108, 156	0
All	All	6646/7217 (92%)	-0.24	288 (4%) 36 31	24, 64, 122, 184	0

All (288) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
27	Z	46	SER	18.1
27	Z	58	ASN	18.0
27	Z	35	SER	16.8
23	V	1	THR	14.1
27	Z	50	VAL	13.9
10	I	74	ILE	13.8
27	Z	43	GLY	11.2
23	V	39	ALA	10.7
27	Z	55	SER	10.5
27	Z	53	ILE	10.0
27	Z	47	ARG	9.9
10	I	128	THR	9.6
27	Z	45	VAL	9.5
27	Z	42	TYR	9.1
5	D	63	ILE	8.8
27	Z	44	ARG	8.7
27	Z	69	ASP	8.3
27	Z	59	GLU	7.9
10	I	70	THR	7.8
27	Z	38	PHE	7.6
23	V	40	PRO	7.6
27	Z	49	ARG	7.6
10	I	72	GLU	7.2
27	Z	34	SER	7.0
10	I	104	ALA	6.9
10	I	83	GLY	6.7
15	N	166	ALA	6.6
10	I	71	ALA	6.6

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Mol	Chain	Res	Type	RSRZ
10	I	97	VAL	6.6
27	Z	48	ARG	6.5
27	Z	54	GLU	6.5
27	Z	57	MET	6.2
10	I	102	GLN	6.1
10	I	132	VAL	5.9
10	I	66	GLY	5.8
27	Z	51	ALA	5.7
10	I	106	GLN	5.7
5	D	88	LEU	5.6
10	I	93	ALA	5.6
10	I	91	PHE	5.5
10	I	100	VAL	5.4
27	Z	68	GLU	5.3
23	V	43	PRO	5.3
5	D	69	ILE	5.3
2	A	85	SER	5.2
10	I	79	GLY	5.2
7	F	106	ALA	5.1
10	I	111	LEU	5.1
10	I	105	GLU	5.1
10	I	108	HIS	5.1
2	A	37	VAL	5.0
10	I	99	GLN	5.0
5	D	57	THR	5.0
27	Z	82	SER	4.9
5	D	90	LEU	4.9
10	I	73	LEU	4.8
5	D	27	ILE	4.7
31	9	1	U	4.7
5	D	172	VAL	4.6
20	S	81	ILE	4.6
27	Z	62	ALA	4.6
5	D	10	PHE	4.6
27	Z	81	CYS	4.6
10	I	112	LEU	4.5
10	I	80	PHE	4.5
5	D	18	ILE	4.5
27	Z	40	ALA	4.5
5	D	89	PRO	4.4
5	D	44	ILE	4.4
5	D	87	ALA	4.4

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Mol	Chain	Res	Type	RSRZ
10	I	127	CYS	4.4
27	Z	52	GLU	4.3
5	D	25	MET	4.3
5	D	26	GLY	4.3
21	T	119	ALA	4.3
9	H	141	CYS	4.3
27	Z	37	ARG	4.3
13	L	60	GLU	4.2
27	Z	56	GLU	4.2
10	I	92	VAL	4.2
27	Z	39	GLY	4.2
27	Z	36	GLY	4.2
27	Z	78	ILE	4.2
10	I	116	LEU	4.1
27	Z	70	ARG	4.1
23	V	38	GLY	4.1
27	Z	60	ASP	4.0
10	I	113	SER	4.0
10	I	110	ASP	4.0
13	L	80	ASP	4.0
10	I	88	GLN	4.0
15	N	145	ALA	3.9
7	F	49	PHE	3.9
10	I	69	PRO	3.9
5	D	85	GLN	3.9
10	I	130	LEU	3.9
27	Z	77	GLY	3.8
2	A	237	GLY	3.8
5	D	40	ILE	3.8
27	Z	83	TYR	3.8
5	D	61	PHE	3.8
13	L	106	VAL	3.7
10	I	78	ALA	3.7
10	I	94	ASP	3.7
10	I	98	ASP	3.7
27	Z	63	CYS	3.7
10	I	109	PRO	3.7
27	Z	67	GLY	3.7
10	I	75	LYS	3.7
5	D	130	VAL	3.6
5	D	134	LEU	3.6
2	A	80	LEU	3.5

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Mol	Chain	Res	Type	RSRZ
10	I	103	ILE	3.5
10	I	117	THR	3.5
2	A	82	VAL	3.5
8	G	23	ILE	3.5
10	I	124	VAL	3.5
7	F	99	THR	3.5
9	H	40	GLN	3.5
15	N	185	GLU	3.5
15	N	179	LEU	3.5
7	F	75	ILE	3.5
10	I	81	GLU	3.5
9	H	77	ILE	3.5
27	Z	41	ARG	3.5
10	I	84	SER	3.4
27	Z	64	PRO	3.4
15	N	178	THR	3.4
9	H	146	ALA	3.4
2	A	31	LYS	3.4
13	L	91	VAL	3.4
27	Z	79	TRP	3.4
15	N	147	ILE	3.4
10	I	121	LYS	3.3
5	D	128	LEU	3.3
5	D	64	ARG	3.3
9	H	90	LEU	3.3
9	H	133	GLY	3.3
10	I	76	ASP	3.3
9	H	86	TYR	3.3
31	9	24	U	3.3
27	Z	61	HIS	3.3
5	D	92	GLU	3.2
7	F	119	ARG	3.2
27	Z	93	TYR	3.2
29	2	49	GLU	3.2
27	Z	66	CYS	3.2
5	D	104	PHE	3.2
27	Z	80	GLN	3.2
29	2	39	ARG	3.2
1	0	1198	U	3.1
2	A	83	GLY	3.1
26	Y	235	GLU	3.1
7	F	15	ASP	3.1

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Mol	Chain	Res	Type	RSRZ
5	D	170	TYR	3.1
27	Z	89	THR	3.1
5	D	106	PHE	3.1
1	0	1172	G	3.1
10	I	120	ALA	3.0
5	D	58	VAL	3.0
5	D	84	LEU	3.0
23	V	2	VAL	3.0
5	D	22	VAL	2.9
2	A	65	ARG	2.9
5	D	86	THR	2.9
2	A	88	ILE	2.9
29	2	48	ASP	2.9
13	L	96	VAL	2.9
10	I	86	GLU	2.9
13	L	147	GLU	2.9
2	A	60	PHE	2.9
7	F	44	SER	2.8
9	H	76	LEU	2.8
8	G	27	ILE	2.8
9	H	174	LEU	2.8
15	N	155	GLU	2.8
23	V	59	ILE	2.8
25	X	80	GLU	2.8
23	V	52	ALA	2.8
5	D	166	ILE	2.8
5	D	62	ASP	2.8
9	H	35	LYS	2.8
5	D	81	GLU	2.8
15	N	138	ASP	2.8
25	X	88	GLU	2.8
23	V	51	LYS	2.7
9	H	48	VAL	2.7
13	L	75	LEU	2.7
23	V	41	GLU	2.7
1	0	282	C	2.7
27	Z	104	ARG	2.7
5	D	75	LEU	2.7
9	H	114	ASP	2.7
15	N	160	SER	2.7
13	L	102	ASP	2.7
10	I	67	VAL	2.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
13	L	114	VAL	2.6
13	L	100	ALA	2.6
15	N	172	PHE	2.6
21	T	116	ASP	2.6
23	V	37	GLY	2.6
21	T	118	SER	2.6
24	W	96	LEU	2.6
2	A	58	VAL	2.6
11	J	70	PHE	2.6
25	X	10	VAL	2.6
10	I	135	GLU	2.6
7	F	17	LEU	2.6
9	H	37	GLY	2.6
2	A	91	GLY	2.5
9	H	145	ASP	2.5
12	K	132	VAL	2.5
5	D	66	GLY	2.5
10	I	82	THR	2.5
5	D	23	VAL	2.5
30	3	14	CYS	2.5
27	Z	85	ASP	2.4
13	L	118	LEU	2.4
10	I	131	GLY	2.4
5	D	43	GLU	2.4
10	I	68	PRO	2.4
10	I	123	VAL	2.4
5	D	70	GLY	2.4
1	0	1169	U	2.4
1	0	1199	A	2.4
6	E	10	ASP	2.4
10	I	118	ASN	2.4
15	N	137	ALA	2.4
27	Z	88	PHE	2.3
15	N	140	GLN	2.3
7	F	97	ALA	2.3
13	L	140	VAL	2.3
27	Z	71	VAL	2.3
5	D	11	HIS	2.3
1	0	1171	A	2.3
27	Z	101	LYS	2.3
12	K	110	LYS	2.3
1	0	970	U	2.2

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Mol	Chain	Res	Type	RSRZ
9	H	169	GLU	2.2
9	H	89	THR	2.2
15	N	181	ASP	2.2
5	D	157	LEU	2.2
15	N	83	LEU	2.2
23	V	3	LEU	2.2
15	N	183	ASP	2.2
13	L	150	GLN	2.2
7	F	117	GLU	2.2
2	A	36	ASP	2.2
9	H	87	LYS	2.2
25	X	7	GLU	2.1
15	N	139	TRP	2.1
13	L	105	TYR	2.1
5	D	93	LEU	2.1
1	0	10	U	2.1
5	D	17	ARG	2.1
27	Z	74	GLN	2.1
2	A	89	ALA	2.1
10	I	119	ALA	2.1
15	N	152	GLU	2.1
23	V	36	ALA	2.1
10	I	129	SER	2.1
15	N	143	ARG	2.1
1	0	1948	G	2.1
30	3	41	GLU	2.1
5	D	171	ASP	2.1
15	N	164	ASP	2.1
25	X	74	ALA	2.1
6	E	170	ARG	2.1
2	A	93	THR	2.1
15	N	159	TYR	2.1
17	P	71	TYR	2.1
9	H	66	GLU	2.1
5	D	72	LYS	2.1
27	Z	65	ASN	2.1
15	N	67	ALA	2.0
23	V	5	VAL	2.0
7	F	63	ILE	2.0
9	H	140	TYR	2.0
5	D	167	GLU	2.0
20	S	76	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
23	V	61	GLY	2.0
1	0	1177	A	2.0
30	3	13	HIS	2.0
5	D	101	THR	2.0
10	I	133	THR	2.0
5	D	165	PHE	2.0
13	L	145	LEU	2.0
23	V	49	LEU	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
1	1MA	0	628	23/24	0.98	0.15	-	34,36,38,39	0
1	OMG	0	2588	24/25	0.99	0.12	-	42,44,46,48	0
1	OMU	0	2587	21/22	0.99	0.10	-	43,44,46,48	0
1	UR3	0	2619	21/22	0.98	0.14	-	45,48,51,54	0
1	PSU	0	2621	20/21	0.98	0.12	-	30,35,50,51	0

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
34	NA	0	8565	1/1	0.81	1.92	146.34	100,100,100,100	0
34	NA	0	8547	1/1	0.95	0.88	54.24	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
34	NA	0	8542	1/1	0.80	0.70	51.61	62,62,62,62	0
34	NA	0	8556	1/1	0.50	1.47	51.44	68,68,68,68	0
34	NA	0	8564	1/1	0.98	0.66	49.96	95,95,95,95	0
34	NA	0	8562	1/1	0.89	0.62	31.79	82,82,82,82	0
34	NA	0	8519	1/1	0.96	0.33	27.51	50,50,50,50	0
34	NA	0	8527	1/1	0.68	0.56	26.32	86,86,86,86	0
34	NA	0	8535	1/1	0.85	0.38	25.04	63,63,63,63	0
34	NA	9	8572	1/1	0.49	0.50	24.43	117,117,117,117	0
32	MG	9	8040	1/1	0.70	0.36	23.68	97,97,97,97	0
34	NA	0	8555	1/1	0.81	0.58	20.53	53,53,53,53	0
34	NA	0	8558	1/1	0.87	0.50	18.32	63,63,63,63	0
32	MG	0	8072	1/1	0.70	0.31	17.80	82,82,82,82	0
33	K	0	8402	1/1	0.89	0.46	15.10	90,90,90,90	0
36	SR	0	8903	1/1	1.00	0.21	14.91	66,66,66,66	0
34	NA	0	8553	1/1	0.87	0.42	13.88	69,69,69,69	0
34	NA	0	8559	1/1	0.73	0.25	12.73	95,95,95,95	0
36	SR	0	8949	1/1	0.66	0.20	11.90	146,146,146,146	0
32	MG	0	8009	1/1	0.99	0.35	11.25	42,42,42,42	0
32	MG	0	8047	1/1	0.89	0.39	10.97	71,71,71,71	0
34	NA	0	8504	1/1	0.68	0.34	10.50	46,46,46,46	0
32	MG	0	8070	1/1	0.98	0.28	10.27	64,64,64,64	0
34	NA	0	8560	1/1	0.67	0.54	10.15	97,97,97,97	0
34	NA	0	8575	1/1	0.95	0.27	9.71	87,87,87,87	0
34	NA	0	8511	1/1	0.87	0.22	8.93	67,67,67,67	0
36	SR	B	8987	1/1	0.76	0.54	8.91	200,200,200,200	0
34	NA	0	8530	1/1	0.90	0.30	8.26	60,60,60,60	0
36	SR	0	8908	1/1	0.81	0.29	8.10	175,175,175,175	0
37	WIN	0	9101	39/39	0.83	0.33	7.92	125,127,128,129	0
32	MG	0	8041	1/1	0.95	0.23	7.56	32,32,32,32	0
32	MG	0	8028	1/1	0.99	0.25	7.51	30,30,30,30	0
34	NA	0	8563	1/1	0.71	0.24	6.64	82,82,82,82	0
32	MG	0	8014	1/1	0.97	0.20	6.51	33,33,33,33	0
34	NA	0	8534	1/1	0.95	0.26	6.37	47,47,47,47	0
34	NA	0	8537	1/1	0.87	0.21	6.34	50,50,50,50	0
34	NA	M	8539	1/1	0.97	0.29	6.16	53,53,53,53	0
32	MG	0	8067	1/1	0.98	0.26	5.95	34,34,34,34	0
32	MG	0	8062	1/1	0.82	0.28	5.78	61,61,61,61	0
35	CL	0	8815	1/1	0.89	0.14	5.33	83,83,83,83	0
34	NA	0	8521	1/1	0.94	0.26	4.88	71,71,71,71	0
34	NA	0	8522	1/1	0.56	0.14	4.48	108,108,108,108	0
36	SR	0	8904	1/1	0.97	0.20	4.45	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	0	8006	1/1	0.81	0.17	3.60	33,33,33,33	0
32	MG	0	8012	1/1	0.98	0.20	3.59	26,26,26,26	0
32	MG	0	8011	1/1	0.98	0.24	3.39	30,30,30,30	0
35	CL	0	8816	1/1	0.98	0.22	3.07	75,75,75,75	0
32	MG	0	8008	1/1	0.98	0.16	3.05	32,32,32,32	0
36	SR	0	8902	1/1	0.89	0.17	2.86	70,70,70,70	0
34	NA	0	8568	1/1	0.87	0.22	2.75	57,57,57,57	0
34	NA	0	8523	1/1	0.77	0.16	2.60	65,65,65,65	0
32	MG	0	8004	1/1	0.99	0.17	2.50	29,29,29,29	0
34	NA	0	8528	1/1	0.93	0.17	2.41	60,60,60,60	0
32	MG	0	8043	1/1	0.92	0.16	2.33	58,58,58,58	0
32	MG	0	8002	1/1	0.89	0.18	2.08	26,26,26,26	0
34	NA	0	8533	1/1	0.89	0.15	1.87	72,72,72,72	0
32	MG	0	8050	1/1	0.71	0.19	1.75	74,74,74,74	0
36	SR	0	8962	1/1	0.88	0.18	1.65	180,180,180,180	0
32	MG	0	8055	1/1	0.99	0.20	1.36	49,49,49,49	0
32	MG	0	8084	1/1	0.88	0.14	1.29	36,36,36,36	0
32	MG	A	8051	1/1	0.88	0.29	1.21	98,98,98,98	0
32	MG	0	8088	1/1	0.98	0.18	1.13	46,46,46,46	0
36	SR	A	8930	1/1	0.82	0.26	0.98	169,169,169,169	0
34	NA	C	8503	1/1	0.54	0.25	0.85	46,46,46,46	0
38	CD	1	8702	1/1	0.99	0.14	0.79	72,72,72,72	0
32	MG	0	8075	1/1	0.72	0.11	0.65	58,58,58,58	0
32	MG	0	8001	1/1	0.94	0.15	0.61	26,26,26,26	0
32	MG	0	8003	1/1	0.98	0.15	0.60	35,35,35,35	0
35	CL	O	8808	1/1	0.97	0.20	0.28	79,79,79,79	0
34	NA	0	8569	1/1	0.98	0.16	0.23	61,61,61,61	0
32	MG	B	8042	1/1	0.98	0.13	0.18	62,62,62,62	0
34	NA	J	8538	1/1	0.85	0.21	0.04	67,67,67,67	0
36	SR	0	8943	1/1	0.84	0.10	-0.03	95,95,95,95	0
34	NA	Q	8540	1/1	0.87	0.13	-0.28	58,58,58,58	0
34	NA	0	8520	1/1	0.90	0.10	-0.36	55,55,55,55	0
34	NA	0	8515	1/1	0.82	0.15	-0.37	50,50,50,50	0
38	CD	U	8701	1/1	1.00	0.12	-0.37	71,71,71,71	0
36	SR	0	8972	1/1	0.68	0.14	-0.45	164,164,164,164	0
35	CL	K	8812	1/1	0.98	0.11	-0.69	57,57,57,57	0
35	CL	0	8805	1/1	0.97	0.10	-0.78	76,76,76,76	0
32	MG	0	8021	1/1	0.98	0.10	-0.80	43,43,43,43	0
36	SR	0	8910	1/1	0.71	0.11	-0.95	106,106,106,106	0
36	SR	A	8929	1/1	0.89	0.09	-0.98	142,142,142,142	0
36	SR	0	8969	1/1	0.84	0.14	-0.99	173,173,173,173	0
32	MG	0	8034	1/1	0.93	0.14	-1.05	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
36	SR	0	8975	1/1	0.90	0.07	-1.10	154,154,154,154	0
35	CL	L	8810	1/1	0.94	0.09	-1.11	69,69,69,69	0
36	SR	0	8935	1/1	0.98	0.09	-1.23	93,93,93,93	0
32	MG	0	8045	1/1	0.95	0.08	-1.26	30,30,30,30	0
35	CL	J	8821	1/1	0.96	0.09	-1.36	78,78,78,78	0
32	MG	0	8058	1/1	0.97	0.07	-1.46	23,23,23,23	0
36	SR	0	8992	1/1	0.94	0.11	-1.80	137,137,137,137	0
34	NA	0	8545	1/1	0.95	0.14	-2.03	48,48,48,48	0
32	MG	0	8025	1/1	0.97	0.10	-2.12	37,37,37,37	0
32	MG	0	8010	1/1	0.98	0.11	-2.26	34,34,34,34	0
32	MG	Y	8086	1/1	0.97	0.10	-2.42	55,55,55,55	0
36	SR	0	8985	1/1	0.95	0.05	-2.44	148,148,148,148	0
38	CD	3	8704	1/1	0.99	0.06	-2.46	94,94,94,94	0
32	MG	0	8087	1/1	0.96	0.13	-2.59	36,36,36,36	0
36	SR	0	8984	1/1	0.75	0.07	-2.66	143,143,143,143	0
35	CL	B	8819	1/1	0.98	0.10	-2.78	57,57,57,57	0
32	MG	0	8052	1/1	0.84	0.06	-2.84	58,58,58,58	0
32	MG	T	8057	1/1	0.92	0.04	-2.92	72,72,72,72	0
36	SR	0	8970	1/1	0.93	0.06	-3.08	135,135,135,135	0
35	CL	3	8804	1/1	0.74	0.07	-3.26	76,76,76,76	0
36	SR	0	8936	1/1	0.98	0.07	-3.32	108,108,108,108	0
32	MG	0	8065	1/1	0.97	0.07	-3.78	41,41,41,41	0
38	CD	Z	8703	1/1	0.92	0.06	-3.80	172,172,172,172	0
35	CL	M	8818	1/1	0.98	0.04	-3.88	49,49,49,49	0
32	MG	0	8013	1/1	0.92	0.06	-4.27	30,30,30,30	0
34	NA	0	8557	1/1	0.80	0.04	-6.57	74,74,74,74	0
32	MG	0	8044	1/1	0.94	0.05	-6.61	55,55,55,55	0
34	NA	0	8517	1/1	0.97	0.10	-9.75	36,36,36,36	0
36	SR	9	8978	1/1	0.78	0.11	-	169,169,169,169	0
36	SR	0	9001	1/1	0.72	0.16	-	184,184,184,184	0
36	SR	0	8957	1/1	0.92	0.21	-	200,200,200,200	0
36	SR	0	8964	1/1	0.80	0.10	-	139,139,139,139	0
36	SR	0	8967	1/1	0.96	0.04	-	147,147,147,147	0
32	MG	0	8022	1/1	0.99	0.17	-	37,37,37,37	0
36	SR	0	8986	1/1	0.85	0.48	-	200,200,200,200	0
32	MG	0	8046	1/1	0.97	0.18	-	53,53,53,53	0
32	MG	0	8079	1/1	0.92	0.30	-	67,67,67,67	0
36	SR	R	8912	1/1	0.99	0.19	-	93,93,93,93	0
34	NA	0	8502	1/1	0.68	0.20	-	66,66,66,66	0
34	NA	0	8561	1/1	0.86	0.65	-	90,90,90,90	0
32	MG	0	8031	1/1	0.93	0.34	-	73,73,73,73	0
34	NA	0	8505	1/1	0.88	1.07	-	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	0	8032	1/1	0.95	0.06	-	42,42,42,42	0
32	MG	0	8007	1/1	0.97	0.19	-	40,40,40,40	0
34	NA	0	8548	1/1	0.76	0.29	-	67,67,67,67	0
34	NA	0	8546	1/1	0.94	0.73	-	85,85,85,85	0
36	SR	0	8909	1/1	0.87	0.17	-	99,99,99,99	0
32	MG	0	8038	1/1	0.77	0.09	-	70,70,70,70	0
36	SR	0	8995	1/1	0.78	0.14	-	142,142,142,142	0
36	SR	0	9008	1/1	0.75	0.24	-	111,111,111,111	0
32	MG	0	8071	1/1	0.93	0.12	-	71,71,71,71	0
32	MG	0	8016	1/1	0.96	0.16	-	30,30,30,30	0
36	SR	0	8911	1/1	0.99	0.08	-	95,95,95,95	0
32	MG	0	8026	1/1	0.99	0.12	-	55,55,55,55	0
35	CL	0	8817	1/1	0.98	0.05	-	68,68,68,68	0
32	MG	0	8063	1/1	0.87	0.22	-	80,80,80,80	0
32	MG	0	8020	1/1	0.91	0.16	-	57,57,57,57	0
36	SR	0	8906	1/1	0.99	0.23	-	67,67,67,67	0
35	CL	0	8813	1/1	0.98	0.02	-	54,54,54,54	0
32	MG	2	8060	1/1	0.92	0.10	-	65,65,65,65	0
32	MG	0	8082	1/1	0.90	0.30	-	81,81,81,81	0
34	NA	0	8529	1/1	0.76	0.07	-	50,50,50,50	0
34	NA	0	8526	1/1	0.94	0.12	-	45,45,45,45	0
36	SR	9	9003	1/1	0.45	0.06	-	187,187,187,187	0
32	MG	0	8039	1/1	0.86	0.22	-	63,63,63,63	0
32	MG	0	8085	1/1	0.88	0.11	-	69,69,69,69	0
36	SR	0	8965	1/1	0.74	0.11	-	151,151,151,151	0
32	MG	0	8024	1/1	0.94	0.20	-	54,54,54,54	0
34	NA	0	8550	1/1	0.82	0.49	-	59,59,59,59	0
34	NA	0	8501	1/1	0.84	0.18	-	54,54,54,54	0
32	MG	0	8076	1/1	0.96	0.10	-	38,38,38,38	0
32	MG	0	8093	1/1	0.97	0.07	-	45,45,45,45	0
36	SR	3	8932	1/1	0.96	0.10	-	94,94,94,94	0
34	NA	0	8544	1/1	0.90	0.19	-	73,73,73,73	0
32	MG	0	8005	1/1	0.96	0.23	-	35,35,35,35	0
36	SR	0	8981	1/1	0.87	0.21	-	158,158,158,158	0
36	SR	S	8961	1/1	0.83	0.12	-	145,145,145,145	0
36	SR	0	8959	1/1	0.65	0.25	-	181,181,181,181	0
36	SR	0	8937	1/1	0.86	0.33	-	125,125,125,125	0
36	SR	0	8976	1/1	0.68	0.23	-	200,200,200,200	0
36	SR	0	8920	1/1	0.83	0.57	-	185,185,185,185	0
35	CL	0	8811	1/1	0.96	0.11	-	72,72,72,72	0
32	MG	0	8048	1/1	0.96	0.23	-	28,28,28,28	0
34	NA	0	8552	1/1	0.96	0.27	-	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
32	MG	0	8019	1/1	0.94	0.23	-	30,30,30,30	0
36	SR	0	8993	1/1	0.96	0.05	-	178,178,178,178	0
34	NA	0	8541	1/1	0.93	0.34	-	70,70,70,70	0
34	NA	0	8512	1/1	0.91	0.30	-	48,48,48,48	0
34	NA	0	8513	1/1	0.96	0.33	-	56,56,56,56	0
32	MG	0	8030	1/1	0.78	0.33	-	79,79,79,79	0
38	CD	O	8705	1/1	0.98	0.06	-	105,105,105,105	0
36	SR	0	8918	1/1	0.99	0.14	-	94,94,94,94	0
36	SR	1	8952	1/1	0.92	0.16	-	93,93,93,93	0
34	NA	R	8532	1/1	0.87	0.11	-	59,59,59,59	0
36	SR	0	8968	1/1	0.83	0.06	-	165,165,165,165	0
32	MG	0	8090	1/1	-0.01	0.56	-	121,121,121,121	0
32	MG	0	8018	1/1	0.88	0.28	-	54,54,54,54	0
36	SR	0	8953	1/1	0.99	0.19	-	164,164,164,164	0
36	SR	0	8917	1/1	0.56	0.22	-	151,151,151,151	0
36	SR	0	9007	1/1	0.96	0.69	-	199,199,199,199	0
36	SR	0	8947	1/1	0.96	0.25	-	200,200,200,200	0
36	SR	0	8933	1/1	0.63	0.09	-	143,143,143,143	0
36	SR	9	8980	1/1	0.78	0.05	-	175,175,175,175	0
36	SR	0	8974	1/1	0.95	0.22	-	179,179,179,179	0
32	MG	0	8089	1/1	0.65	0.16	-	64,64,64,64	0
36	SR	0	8928	1/1	0.70	0.09	-	151,151,151,151	0
36	SR	0	8991	1/1	0.71	0.26	-	195,195,195,195	0
36	SR	0	8983	1/1	0.62	0.12	-	199,199,199,199	0
35	CL	Y	8820	1/1	0.98	0.05	-	46,46,46,46	0
36	SR	0	8925	1/1	0.98	0.11	-	95,95,95,95	0
32	MG	0	8035	1/1	0.96	0.19	-	70,70,70,70	0
34	NA	0	8516	1/1	0.93	0.15	-	37,37,37,37	0
36	SR	0	8956	1/1	0.78	0.10	-	187,187,187,187	0
32	MG	0	8061	1/1	0.96	0.22	-	36,36,36,36	0
32	MG	0	8036	1/1	0.93	0.12	-	60,60,60,60	0
36	SR	0	8926	1/1	0.97	0.12	-	142,142,142,142	0
32	MG	0	8027	1/1	0.85	0.17	-	47,47,47,47	0
34	NA	0	8551	1/1	0.96	0.20	-	60,60,60,60	0
34	NA	0	8536	1/1	0.82	0.06	-	65,65,65,65	0
36	SR	0	8988	1/1	0.89	0.12	-	158,158,158,158	0
36	SR	0	8989	1/1	0.87	0.17	-	185,185,185,185	0
36	SR	0	8998	1/1	0.54	0.24	-	175,175,175,175	0
36	SR	0	8982	1/1	0.62	0.96	-	200,200,200,200	0
32	MG	0	8069	1/1	0.82	0.19	-	49,49,49,49	0
32	MG	0	8033	1/1	0.95	0.20	-	63,63,63,63	0
36	SR	0	8955	1/1	0.72	0.10	-	198,198,198,198	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
36	SR	0	8940	1/1	0.96	0.10	-	94,94,94,94	0
32	MG	0	8078	1/1	0.93	0.29	-	54,54,54,54	0
36	SR	0	8915	1/1	0.67	0.10	-	136,136,136,136	0
34	NA	0	8571	1/1	0.86	0.30	-	98,98,98,98	0
32	MG	0	8080	1/1	0.88	0.30	-	87,87,87,87	0
34	NA	0	8509	1/1	0.90	0.27	-	77,77,77,77	0
32	MG	0	8073	1/1	0.95	0.08	-	80,80,80,80	0
32	MG	0	8083	1/1	0.99	0.27	-	74,74,74,74	0
33	K	0	8401	1/1	0.78	0.89	-	123,123,123,123	0
36	SR	0	8922	1/1	0.81	0.28	-	156,156,156,156	0
36	SR	0	8960	1/1	0.94	0.10	-	151,151,151,151	0
34	NA	0	8567	1/1	0.88	0.51	-	87,87,87,87	0
36	SR	0	8905	1/1	0.99	0.26	-	73,73,73,73	0
36	SR	F	9005	1/1	0.93	0.04	-	149,149,149,149	0
36	SR	0	8979	1/1	0.93	0.10	-	195,195,195,195	0
36	SR	0	8938	1/1	0.62	0.06	-	191,191,191,191	0
36	SR	0	8946	1/1	0.96	0.17	-	129,129,129,129	0
36	SR	0	8971	1/1	0.89	0.06	-	185,185,185,185	0
36	SR	0	8944	1/1	0.34	0.16	-	178,178,178,178	0
32	MG	0	8092	1/1	0.82	0.10	-	80,80,80,80	0
36	SR	0	8919	1/1	0.93	0.08	-	179,179,179,179	0
34	NA	0	8554	1/1	0.43	0.43	-	70,70,70,70	0
36	SR	0	8924	1/1	0.77	0.21	-	149,149,149,149	0
36	SR	0	8934	1/1	0.85	0.32	-	166,166,166,166	0
32	MG	0	8066	1/1	0.87	0.34	-	88,88,88,88	0
34	NA	0	8525	1/1	0.36	0.27	-	93,93,93,93	0
36	SR	0	8966	1/1	0.49	0.14	-	120,120,120,120	0
34	NA	0	8573	1/1	0.89	0.13	-	87,87,87,87	0
34	NA	0	8507	1/1	0.90	0.17	-	46,46,46,46	0
36	SR	0	8916	1/1	0.88	0.10	-	129,129,129,129	0
32	MG	0	8068	1/1	0.92	0.09	-	67,67,67,67	0
35	CL	A	8809	1/1	0.94	0.31	-	96,96,96,96	0
36	SR	3	8999	1/1	0.98	0.10	-	140,140,140,140	0
32	MG	0	8015	1/1	0.98	0.14	-	33,33,33,33	0
35	CL	R	8806	1/1	1.00	0.11	-	55,55,55,55	0
34	NA	0	8508	1/1	0.91	0.20	-	63,63,63,63	0
36	SR	0	9006	1/1	0.56	0.57	-	200,200,200,200	0
35	CL	J	8802	1/1	0.98	0.08	-	79,79,79,79	0
36	SR	0	8914	1/1	0.91	0.30	-	127,127,127,127	0
34	NA	0	8531	1/1	0.75	0.23	-	50,50,50,50	0
32	MG	0	8023	1/1	0.96	0.20	-	30,30,30,30	0
32	MG	0	8017	1/1	0.98	0.08	-	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	0	8056	1/1	0.95	0.15	-	62,62,62,62	0
34	NA	9	8543	1/1	0.96	0.17	-	57,57,57,57	0
32	MG	0	8077	1/1	0.98	0.06	-	43,43,43,43	0
34	NA	0	8514	1/1	0.89	0.71	-	54,54,54,54	0
34	NA	0	8566	1/1	0.75	0.59	-	59,59,59,59	0
32	MG	0	8037	1/1	0.84	0.16	-	80,80,80,80	0
32	MG	0	8029	1/1	0.96	0.17	-	69,69,69,69	0
32	MG	0	8091	1/1	0.60	0.13	-	89,89,89,89	0
36	SR	0	8990	1/1	0.90	0.11	-	116,116,116,116	0
36	SR	0	9000	1/1	0.76	0.20	-	200,200,200,200	0
32	MG	9	8074	1/1	0.95	0.14	-	101,101,101,101	0
36	SR	0	8994	1/1	0.80	0.40	-	199,199,199,199	0
36	SR	0	8901	1/1	0.85	0.14	-	96,96,96,96	0
35	CL	0	8822	1/1	0.97	0.35	-	86,86,86,86	0
35	CL	N	8807	1/1	0.97	0.17	-	72,72,72,72	0
36	SR	0	8997	1/1	0.80	1.16	-	200,200,200,200	0
36	SR	0	8941	1/1	0.59	0.23	-	131,131,131,131	0
36	SR	B	8950	1/1	0.75	0.12	-	119,119,119,119	0
32	MG	0	8064	1/1	0.93	0.18	-	51,51,51,51	0
36	SR	0	8996	1/1	0.63	0.47	-	200,200,200,200	0
34	NA	S	8510	1/1	0.97	0.15	-	50,50,50,50	0
35	CL	J	8801	1/1	0.93	0.09	-	82,82,82,82	0
34	NA	H	8518	1/1	0.76	0.50	-	95,95,95,95	0
36	SR	0	8927	1/1	0.97	0.11	-	167,167,167,167	0
35	CL	0	8814	1/1	0.97	0.09	-	66,66,66,66	0
36	SR	0	8923	1/1	0.91	0.15	-	112,112,112,112	0
36	SR	0	8954	1/1	0.87	0.11	-	109,109,109,109	0
36	SR	0	8977	1/1	0.11	0.06	-	197,197,197,197	0
36	SR	0	8939	1/1	0.93	0.06	-	145,145,145,145	0
36	SR	0	9004	1/1	0.95	0.47	-	200,200,200,200	0
36	SR	0	8931	1/1	0.92	0.09	-	136,136,136,136	0
36	SR	0	9002	1/1	0.84	0.15	-	183,183,183,183	0
36	SR	0	8973	1/1	0.97	0.11	-	141,141,141,141	0
34	NA	0	8506	1/1	0.52	0.22	-	76,76,76,76	0
35	CL	0	8803	1/1	0.95	0.07	-	62,62,62,62	0
36	SR	0	8921	1/1	0.94	0.11	-	99,99,99,99	0
36	SR	0	8913	1/1	0.54	0.82	-	200,200,200,200	0
36	SR	0	8945	1/1	0.95	0.07	-	131,131,131,131	0
36	SR	0	8907	1/1	1.00	0.14	-	62,62,62,62	0
32	MG	0	8059	1/1	0.91	0.12	-	52,52,52,52	0
32	MG	0	8049	1/1	0.93	0.53	-	116,116,116,116	0
36	SR	0	8948	1/1	0.93	0.16	-	122,122,122,122	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
34	NA	0	8549	1/1	0.76	0.91	-	60,60,60,60	0
34	NA	0	8574	1/1	0.93	0.40	-	69,69,69,69	0
32	MG	K	8054	1/1	0.82	0.21	-	47,47,47,47	0
34	NA	0	8570	1/1	0.96	0.08	-	59,59,59,59	0
34	NA	0	8524	1/1	0.55	0.62	-	73,73,73,73	0
36	SR	0	8958	1/1	0.76	0.12	-	121,121,121,121	0
36	SR	0	8963	1/1	0.96	0.08	-	133,133,133,133	0
36	SR	0	8942	1/1	0.75	0.18	-	144,144,144,144	0
36	SR	0	8951	1/1	0.77	0.05	-	149,149,149,149	0
32	MG	0	8053	1/1	0.88	0.06	-	69,69,69,69	0
32	MG	0	8081	1/1	0.94	0.17	-	81,81,81,81	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.