



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 12, 2024 – 05:07 PM EST

PDB ID : 3I55
Title : Co-crystal structure of Mycalamide A Bound to the Large Ribosomal Subunit
Authors : Gurel, G.; Blaha, G.; Steitz, T.A.; Moore, P.B.
Deposited on : 2009-07-03
Resolution : 3.11 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

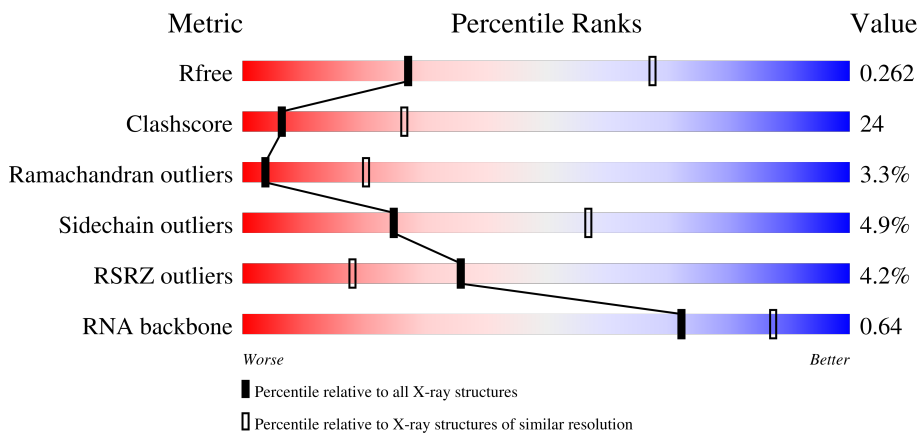
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.11 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.



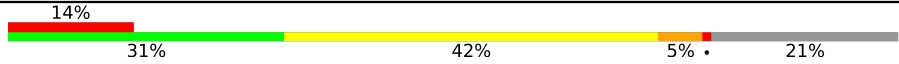



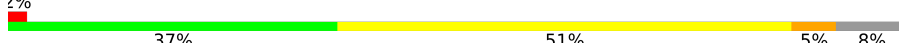


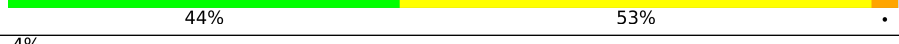
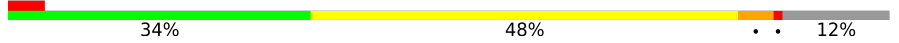
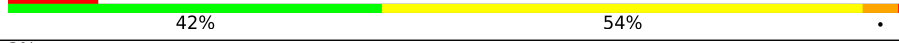


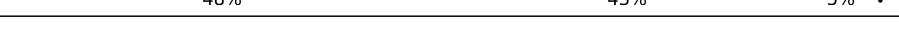


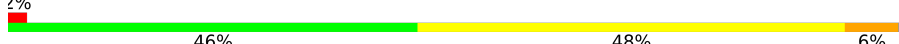
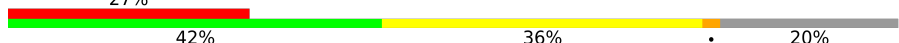


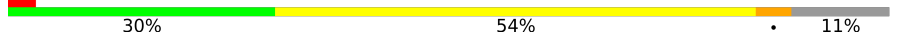
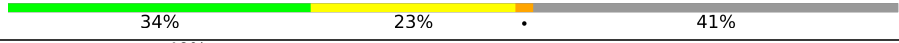




Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1292 (3.14-3.10)
Clashscore	141614	1389 (3.14-3.10)
Ramachandran outliers	138981	1337 (3.14-3.10)
Sidechain outliers	138945	1337 (3.14-3.10)
RSRZ outliers	127900	1260 (3.14-3.10)
RNA backbone	3102	1134 (3.44-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	
2	A	240	
3	B	338	
4	C	246	

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Mol	Chain	Length	Quality of chain
5	D	177	
6	E	178	
7	F	120	
8	G	348	
9	H	174	
10	I	162	
11	J	145	
12	K	132	
13	L	165	
14	M	194	
15	N	187	
16	O	116	
17	P	149	
18	Q	96	
19	R	155	
20	S	85	
21	T	120	
22	U	66	
23	V	71	
24	W	154	
25	X	92	
26	Y	241	
27	Z	116	
28	1	57	
29	2	50	

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Mol	Chain	Length	Quality of chain
30	3	92	
31	9	122	
32	4	8	

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	5AA	4	76	-	-	X	-
33	MG	0	8055	-	-	-	X
33	MG	0	8069	-	-	-	X
33	MG	0	8081	-	-	-	X
33	MG	0	8092	-	-	-	X
33	MG	3	8090	-	-	-	X
34	K	0	8402	-	-	-	X
35	NA	0	8506	-	-	-	X
35	NA	0	8508	-	-	-	X
35	NA	0	8509	-	-	-	X
35	NA	0	8513	-	-	-	X
35	NA	0	8521	-	-	-	X
35	NA	0	8528	-	-	-	X
35	NA	0	8530	-	-	-	X
35	NA	0	8544	-	-	-	X
35	NA	0	8551	-	-	-	X
35	NA	0	8554	-	-	-	X
35	NA	0	8556	-	-	-	X
35	NA	0	8558	-	-	-	X
35	NA	0	8560	-	-	-	X
35	NA	0	8563	-	-	-	X
35	NA	0	8567	-	-	-	X
35	NA	0	8568	-	-	-	X
35	NA	0	8574	-	-	-	X
35	NA	H	8518	-	-	-	X
36	CL	3	8804	-	-	-	X
37	SR	0	8922	-	-	-	X
37	SR	0	8949	-	-	-	X
37	SR	0	8953	-	-	-	X
37	SR	0	8962	-	-	-	X
37	SR	0	8986	-	-	-	X
37	SR	0	8997	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
37	SR	0	9000	-	-	-	X
37	SR	3	8999	-	-	-	X
37	SR	B	8987	-	-	-	X
37	SR	L	8969	-	-	-	X
38	MYL	0	2924	-	-	X	-
39	CD	3	8704	-	-	-	X

2 Entry composition [i](#)

There are 40 unique types of molecules in this entry. The entry contains 99287 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
9	H	160	1283	798	240	239	6	0	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	Z	73	Total	C	N	O	S	0	0	0
			573	343	113	112	5			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Z	1	MET	-	expression tag	UNP P60619
Z	2	SER	-	expression tag	UNP P60619
Z	3	PRO	-	expression tag	UNP P60619
Z	4	ARG	-	expression tag	UNP P60619
Z	5	ALA	-	expression tag	UNP P60619
Z	6	ARG	-	expression tag	UNP P60619
Z	7	ARG	-	expression tag	UNP P60619
Z	8	GLU	-	expression tag	UNP P60619
Z	9	PRO	-	expression tag	UNP P60619
Z	10	ASN	-	expression tag	UNP P60619
Z	11	LEU	-	expression tag	UNP P60619
Z	12	GLU	-	expression tag	UNP P60619
Z	13	GLY	-	expression tag	UNP P60619
Z	14	LEU	-	expression tag	UNP P60619
Z	15	MET	-	expression tag	UNP P60619
Z	16	TRP	-	expression tag	UNP P60619
Z	17	PRO	-	expression tag	UNP P60619
Z	18	LEU	-	expression tag	UNP P60619
Z	19	GLY	-	expression tag	UNP P60619
Z	20	GLY	-	expression tag	UNP P60619
Z	21	GLN	-	expression tag	UNP P60619
Z	22	GLN	-	expression tag	UNP P60619
Z	23	THR	-	expression tag	UNP P60619
Z	24	THR	-	expression tag	UNP P60619

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

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

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

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

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

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

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

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

- Molecule 32 is DNA/RNA hybrid called DNA/RNA (5'-R(*CP*CP*(5AA)P*(2OP)P*(PO2)P*AP*CP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
32	4	8	127	61	23	38	5	0	0	0

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	0	83	Total	Mg	0	0
			83	83		
33	A	2	Total	Mg	0	0
			2	2		
33	B	1	Total	Mg	0	0
			1	1		
33	K	1	Total	Mg	0	0
			1	1		
33	T	1	Total	Mg	0	0
			1	1		
33	Y	1	Total	Mg	0	0
			1	1		
33	2	1	Total	Mg	0	0
			1	1		
33	3	1	Total	Mg	0	0
			1	1		
33	9	2	Total	Mg	0	0
			2	2		

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

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

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	0	63	Total Na 63 63	0	0
35	B	1	Total Na 1 1	0	0
35	C	1	Total Na 1 1	0	0
35	H	1	Total Na 1 1	0	0
35	J	1	Total Na 1 1	0	0
35	M	1	Total Na 1 1	0	0
35	Q	1	Total Na 1 1	0	0
35	R	3	Total Na 3 3	0	0
35	S	1	Total Na 1 1	0	0
35	9	2	Total Na 2 2	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	0	10	Total Cl 10 10	0	0
36	A	1	Total Cl 1 1	0	0
36	B	1	Total Cl 1 1	0	0
36	J	3	Total Cl 3 3	0	0
36	L	1	Total Cl 1 1	0	0
36	M	1	Total Cl 1 1	0	0
36	N	1	Total Cl 1 1	0	0
36	O	1	Total Cl 1 1	0	0
36	R	1	Total Cl 1 1	0	0
36	Y	1	Total Cl 1 1	0	0

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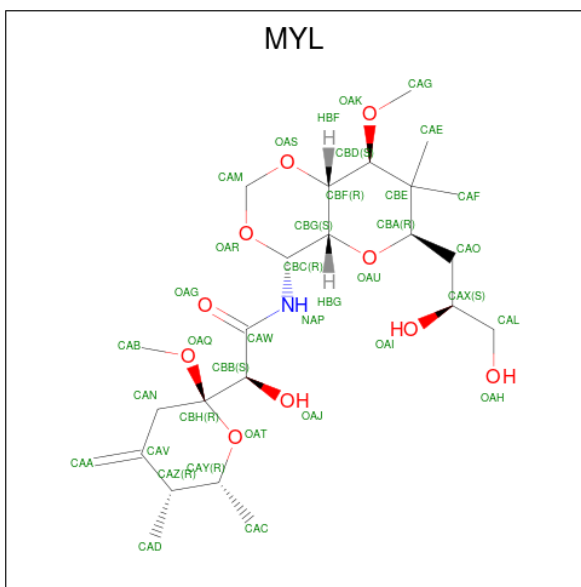
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	3	1	Total Cl 1 1	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	0	93	Total Sr 93 93	0	0
37	A	2	Total Sr 2 2	0	0
37	B	2	Total Sr 2 2	0	0
37	F	1	Total Sr 1 1	0	0
37	H	1	Total Sr 1 1	0	0
37	L	1	Total Sr 1 1	0	0
37	R	1	Total Sr 1 1	0	0
37	S	1	Total Sr 1 1	0	0
37	1	1	Total Sr 1 1	0	0
37	3	2	Total Sr 2 2	0	0
37	9	3	Total Sr 3 3	0	0

- Molecule 38 is Mycalamide A (three-letter code: MYL) (formula: C₂₄H₄₁NO₁₀).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
38	0	1	35	24	1	10	0	0

- Molecule 39 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
39	O	1	Total	Cd	0	0
			1	1		
39	U	1	Total	Cd	0	0
			1	1		
39	Z	1	Total	Cd	0	0
			1	1		
39	1	1	Total	Cd	0	0
			1	1		
39	3	1	Total	Cd	0	0
			1	1		

- Molecule 40 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
40	0	5841	Total	O	0	0
			5841	5841		
40	A	117	Total	O	0	0
			117	117		
40	B	151	Total	O	0	0
			151	151		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
40	C	175	Total 175	O 175	0	0
40	D	49	Total 49	O 49	0	0
40	E	40	Total 40	O 40	0	0
40	F	29	Total 29	O 29	0	0
40	G	18	Total 18	O 18	0	0
40	H	76	Total 76	O 76	0	0
40	I	10	Total 10	O 10	0	0
40	J	57	Total 57	O 57	0	0
40	K	62	Total 62	O 62	0	0
40	L	91	Total 91	O 91	0	0
40	M	148	Total 148	O 148	0	0
40	N	61	Total 61	O 61	0	0
40	O	41	Total 41	O 41	0	0
40	P	61	Total 61	O 61	0	0
40	Q	49	Total 49	O 49	0	0
40	R	83	Total 83	O 83	0	0
40	S	37	Total 37	O 37	0	0
40	T	36	Total 36	O 36	0	0
40	U	29	Total 29	O 29	0	0
40	V	13	Total 13	O 13	0	0
40	W	67	Total 67	O 67	0	0

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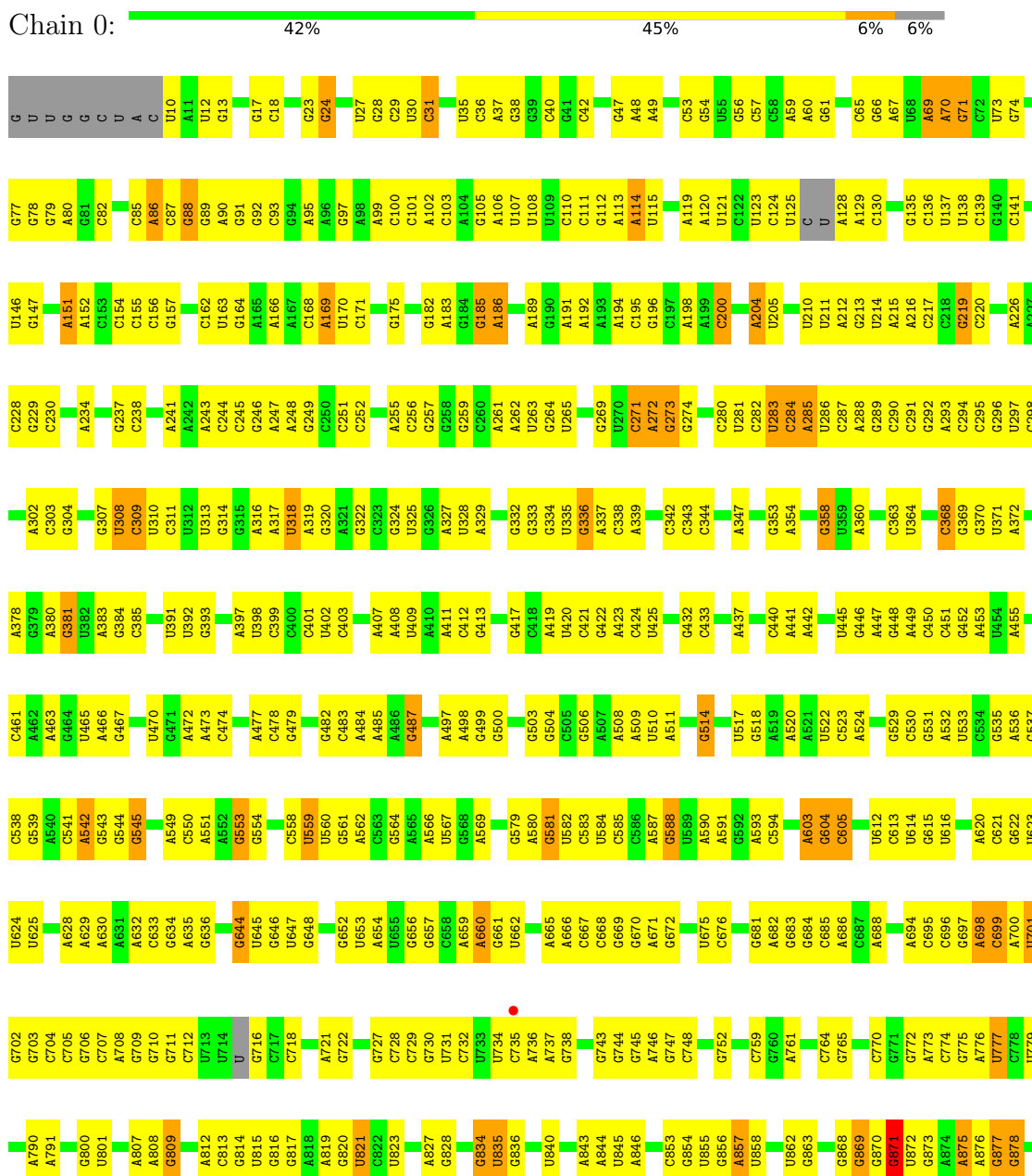
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
40	X	24	Total 24	O 24	0	0
40	Y	98	Total 98	O 98	0	0
40	Z	30	Total 30	O 30	0	0
40	1	58	Total 58	O 58	0	0
40	2	45	Total 45	O 45	0	0
40	3	70	Total 70	O 70	0	0
40	9	144	Total 144	O 144	0	0
40	4	13	Total 13	O 13	0	0

3 Residue-property plots

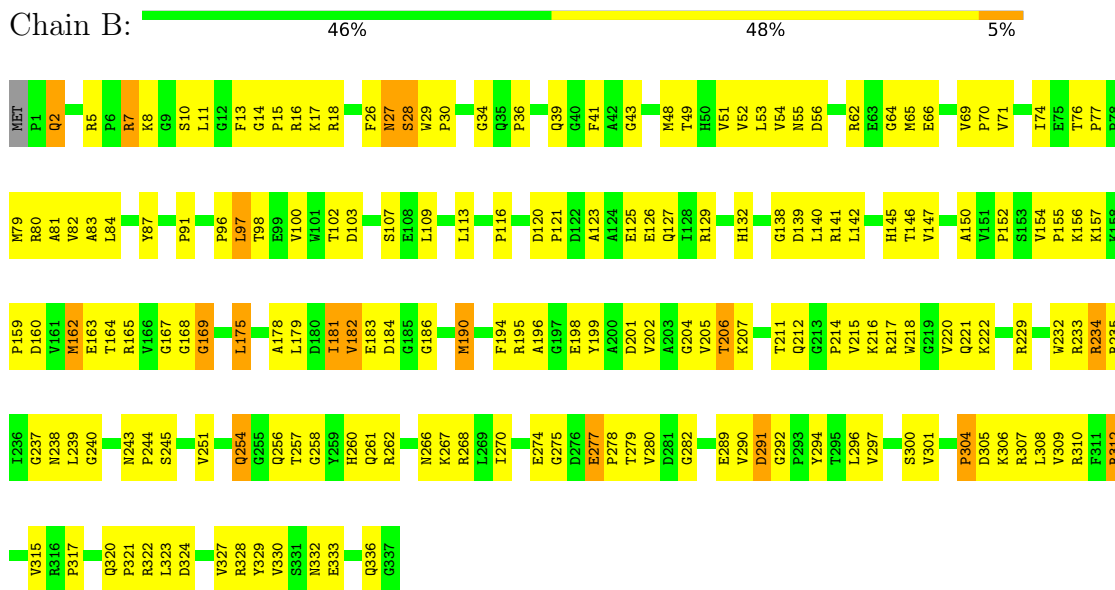
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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

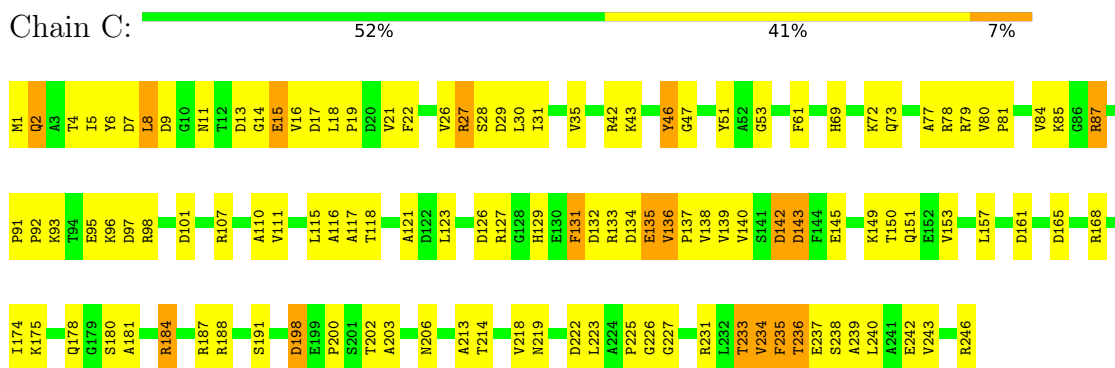


G2005	A1930	A1845	G1773	G1694	A1616	G1535	G1441	U1279	C1201	A1132	C1044	G969	A882
C2006	A1931	U1846	G1774	G1695	C1617	G1536	A1442	A1280	A1202	A1133	G1046	U970	G885
A2007	A1947	A1847	A1775	A1701	A1624	C1537	U1446	A1286	G1203	G1136	U1045	G	C890
G2009	C1936	U1850	A1776	U1702	U1625	G1541	U1447	U1287	C1204	U1135	G1046	U	G891
A2010	G1937	G1851	G1777	G1706	A1626	G1542	C1451	U1288	U1206	G1138	U1047	G	G892
A2011	G1938	A1852	A1778	G1706	G1627	G1543	C1451	C1289	A1207	U1139	G1048	C	C896
A2012	G1939	A1853	A1779	G1706	G1628	G1544	U1456	G1290	C1208	C1140	C1051	C	G897
G2013	A1940	C1854	A1780	A1710	G1629	G1545	U1457	A1291	C1209	U1149	G1052	G	G898
G2014	A1941	G1855	A1781	A1711	A1630	C1546	A1458	A1294	A1150	U1150	G1053	C	G899
U2016	A1942	C1856	G1785	A1712	A1631	G1546	A1458	A1294	C1211	A1151	G1054	C	G898
U2017	C1943	A1857	C1786	G1713	A1632	A1547	U1481	G1295	C1212	G1152	U1055	U	G901
G2026	G1948	A1858	C1787	C1714	C1633	C1548	C1482	U1297	C1213	C1153	A1057	C	G902
U2027	C1864	C1864	C1790	C1715	G1634	A1550	U1482	U1298	G1214	C1154	A1058	C	C905
U2028	A1865	G1635	U1791	U1722	G1636	A1551	U1473	G1299	G1215	A1154	G1059	A	G911
C2029	G1868	A1637	C1792	G1724	A1637	C1552	C1474	G1300	G1216	C1155	A1060	G	A912
G2033	U1871	C1640	G1793	U1724	C1640	C1553	C1474	U1300	U1219	C1156	C1061	G	G918
U2034	C1872	A1641	G1794	C1725	A1641	G1554	C1477	C1303	U1220	G1157	U1066	G	U919
C2035	G1873	A1642	A1796	G1726	A1642	G1555	U1478	C1304	G1221	U1158	A1067	A	C920
C2036	C1874	C1643	C1797	C1730	C1643	G1557	A1482	U1306	G1224	A1161	C1068	U	G921
G2037	G1875	C1644	C1798	G1731	C1644	C1558	C1483	A1307	C1225	G1162	C1069	U	A923
A2038	G1877	U1645	G1799	C1731	U1645	A1559	C1484	U1308	G1228	U1163	A1070	C	G924
A2039	G1878	U1645	G1799	C1731	U1645	A1559	C1484	U1308	G1229	U1164	G1071	G	A926
C2040	U1879	C1682	A1801	U1734	C1682	U1561	A1486	U1310	A1230	G1165	G1072	G	U932
G2041	C1882	A1653	G1802	G1736	A1653	C1564	A1492	G1312	U1234	A1166	A1081	A	C933
U2042	U1883	G1654	C1803	A1736	U1654	C1565	A1493	G1312	U1235	G1167	U1088	U	G938
U2043	G1884	G1655	A1804	A1737	G1655	C1566	A1494	U1307	C1236	U1168	A1090	U	G941
G2044	A1885	A1657	C1805	C1738	A1656	C1567	C1495	A1306	G1237	U1170	U1091	C	U942
G2045	U1886	A1657	G1806	G1739	A1657	G1567	C1495	U1309	U1237	A1171	U1095	U	A943
G2050	C1888	C1662	U1807	U1740	C1662	G1571	A1497	U1310	C1238	G1172	U1096	U	G944
G2051	U1889	A1663	C1808	U1741	A1663	A1572	G1498	U1311	C1239	A1173	A1097	U	U945
G2052	C1890	G1664	A1809	A1742	G1664	A1573	C1499	G1319	G1240	G1174	A1098	U	C946
G2053	G1891	G1665	C1810	G1743	G1665	C1574	U1500	G1325	G1241	G1175	U1099	U	U947
A2054	U1892	C1666	A1811	A1746	C1666	C1575	U1500	U1409	G1242	G1176	U1099	U	G948
A2055	C1893	A1667	G1812	U1747	A1667	G1586	A1504	A1328	A1242	U1178	U1095	U	A948
G2056	U1894	U1668	U1813	A1747	U1668	U1587	U1505	G1329	C1243	G1179	U1096	U	G944
G2057	A1895	G1669	G1814	U1748	G1669	U1588	U1506	A1330	C1244	U1180	A1097	U	U945
G2058	U1896	A1670	C1815	U1749	A1670	G1589	C1507	G1331	U1245	A1181	A1098	U	C946
G2059	G1897	C1671	A1816	C1750	A1670	G1589	C1507	C1332	A1246	C1182	U1099	U	U947
A2060	U1898	C1672	C1817	G1751	C1672	G1590	U1508	U1333	A1247	C1183	C1010	U	G948
U2063	C1899	C1673	G1818	G1752	C1673	G1591	U1508	C1334	U1248	C1184	C1102	U	A951
U2064	A1904	G1675	G1819	C1753	G1675	C1592	U1511	U1334	U1249	U1185	C1103	U	G952
C2065	U1905	G1676	C1820	C1753	G1676	C1593	G1512	G1339	C1250	C1186	A1013	U	G953
C2066	G1908	A1677	U1825	U1757	A1677	C1594	C1513	U1340	G1260	U1187	A1014	U	U954
G2070	U1909	C1678	C1826	U1758	C1678	C1595	A1514	G1340	A1261	U1188	C1015	U	G955
G2071	A1919	A1682	A1829	A1759	A1682	U1596	A1515	C1342	C1262	A1189	U1016	U	U956
G2072	C1920	G1683	C1830	C1762	G1683	A1597	U1516	C1343	C1263	U1190	A1020	U	G957
G2073	A1921	A1684	U1833	C1763	A1684	A1603	A1522	G1344	U1264	A1191	G1021	U	G958
A2074	U1922	G1685	C1834	C1764	A1685	G1604	A1522	A1341	C1268	A1192	C1025	U	C959
G2081	G1925	C1686	U1835	U1765	A1686	G1605	G1523	A1342	C1269	A1193	U1028	U	G960
C2087	G1926	G1687	U1836	C1766	A1687	A1606	U1524	C1342	C1269	A1194	U1029	U	A961
C2088	U1927	C1688	C1837	C1767	A1688	A1607	G1525	C1343	C1273	A1195	U1030	U	C962
A2089	C1928	G1688	U1838	U1769	G1688	A1607	A1526	G1344	U1264	A1196	G1031	U	C963
	U1840	C1692	U1839	U1770	G1688	C1613	A1527	U1428	U1276	U1197	U1114	U	G964
	U2004	A1693	U1840	C1772	A1693	A1614	A1528	U1429	C1277	U1198	U1115	U	A965
						A1615	G1529	U1440	A1278	A1200	U1130	U	G1039

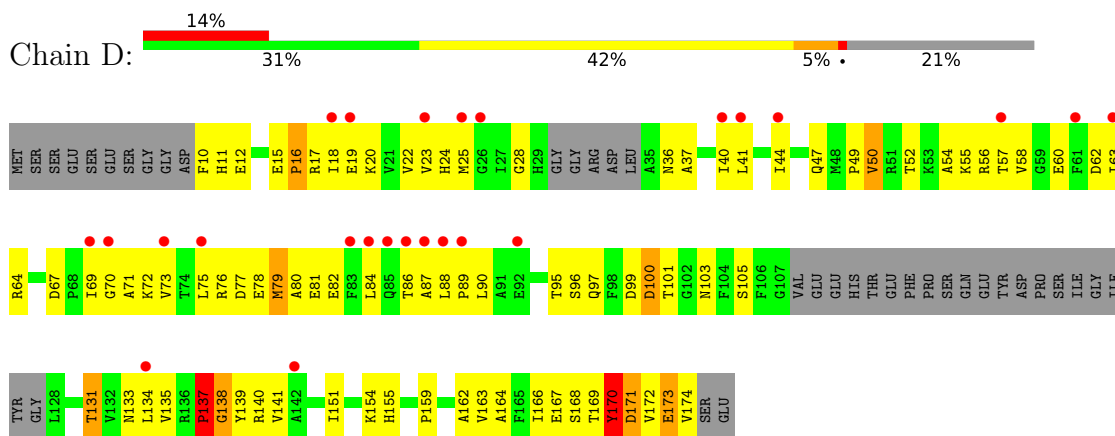
● Molecule 3: 50S ribosomal protein L3P



● Molecule 4: 50S ribosomal protein L4P

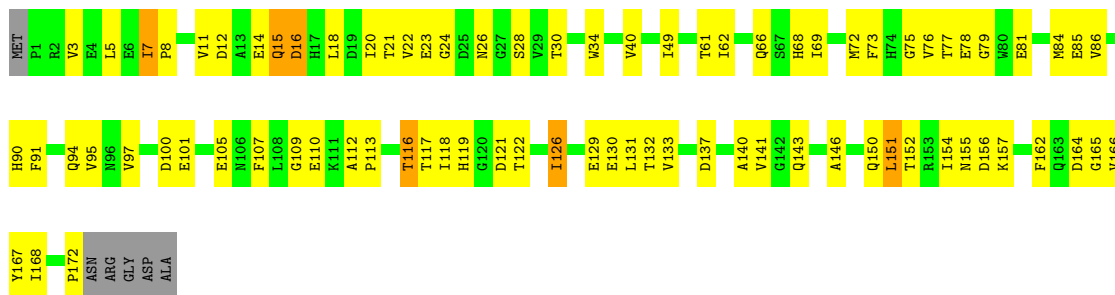


● Molecule 5: 50S ribosomal protein L5P

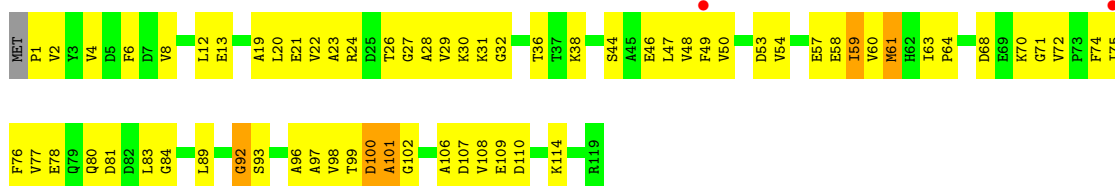


● Molecule 6: 50S ribosomal protein L6P

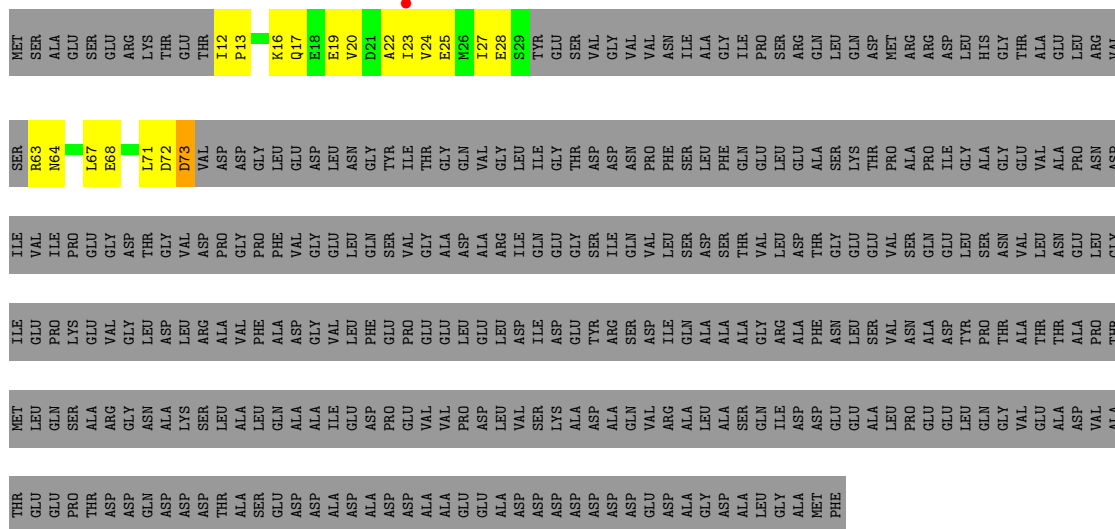




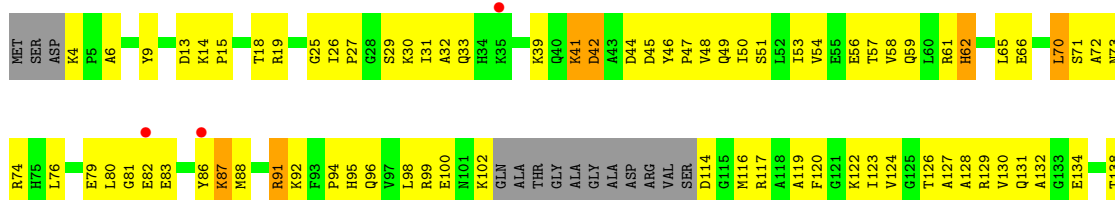
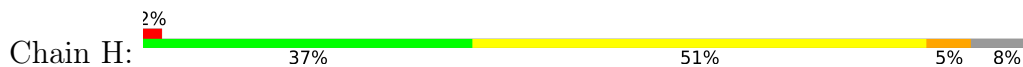
- Molecule 7: 50S ribosomal protein L7Ae

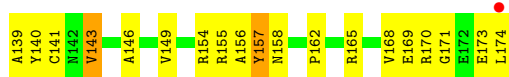


- Molecule 8: 50S ribosomal protein L10E

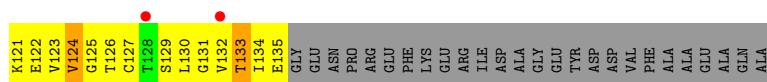
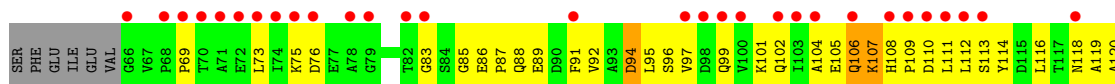
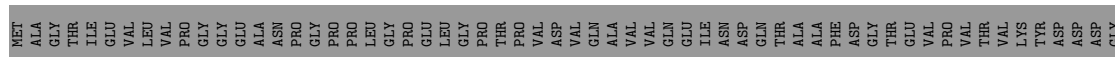


- Molecule 9: 50S ribosomal protein L10e





• Molecule 10: 50S ribosomal protein L11P



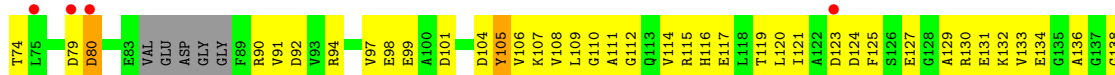
• Molecule 11: 50S ribosomal protein L13P



• Molecule 12: 50S ribosomal protein L14P



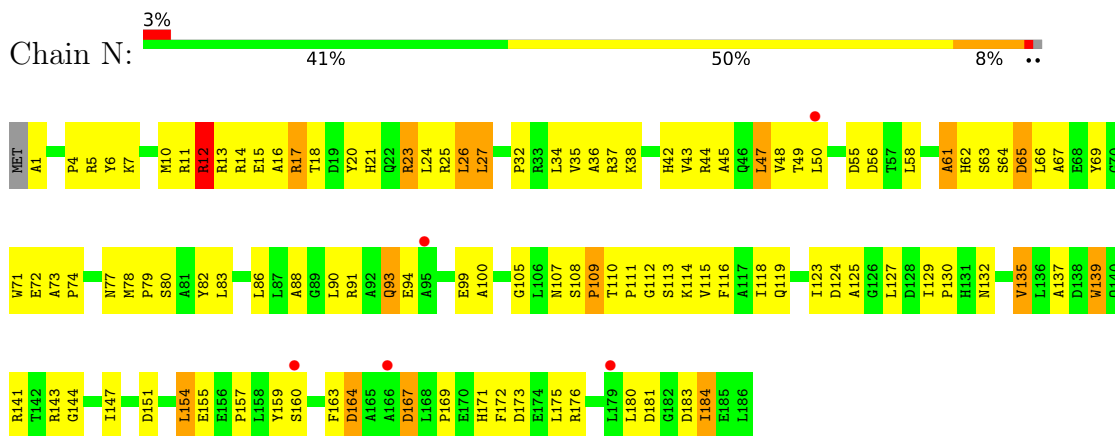
• Molecule 13: 50S ribosomal protein L15P



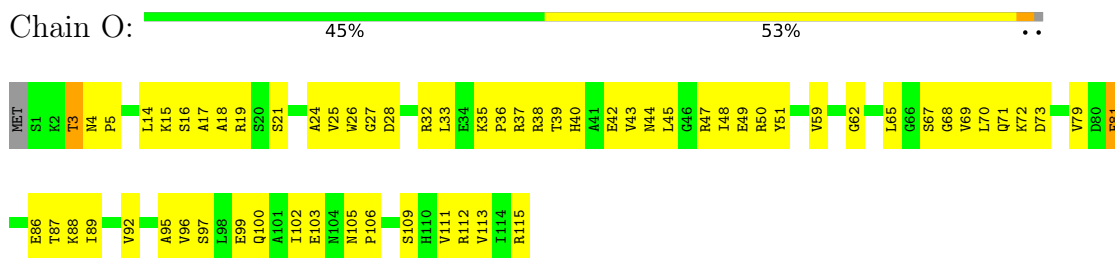
• Molecule 14: 50S ribosomal protein L15e



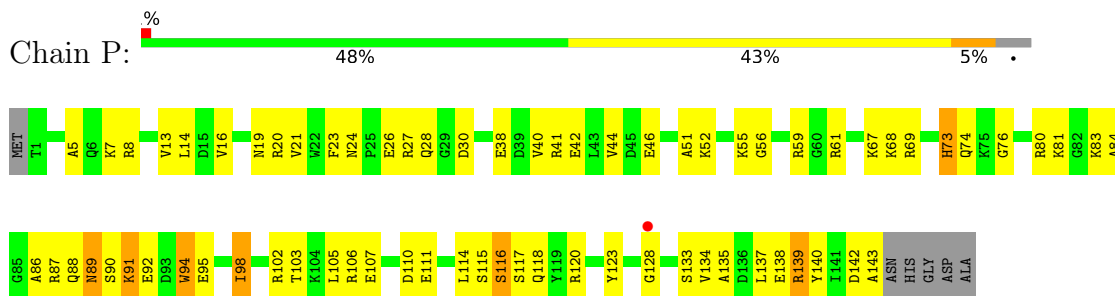
• Molecule 15: 50S ribosomal protein L18P



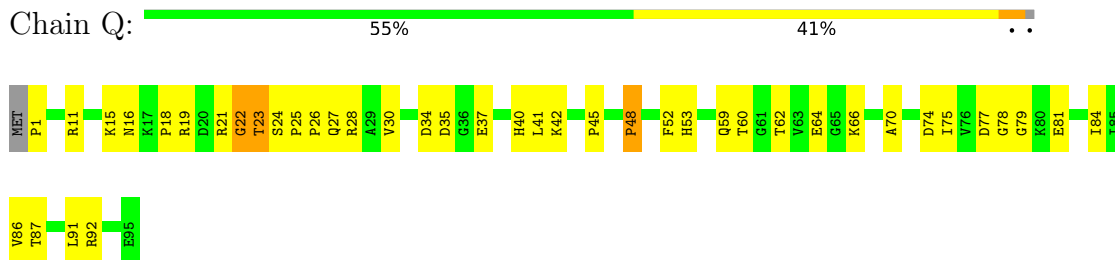
• Molecule 16: 50S ribosomal protein L18e



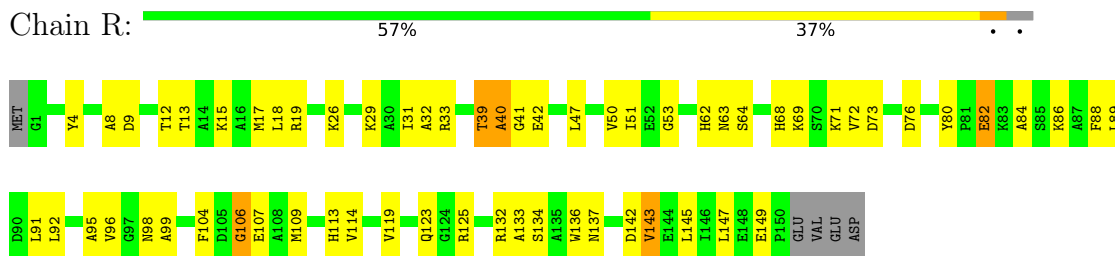
• Molecule 17: 50S ribosomal protein L19e



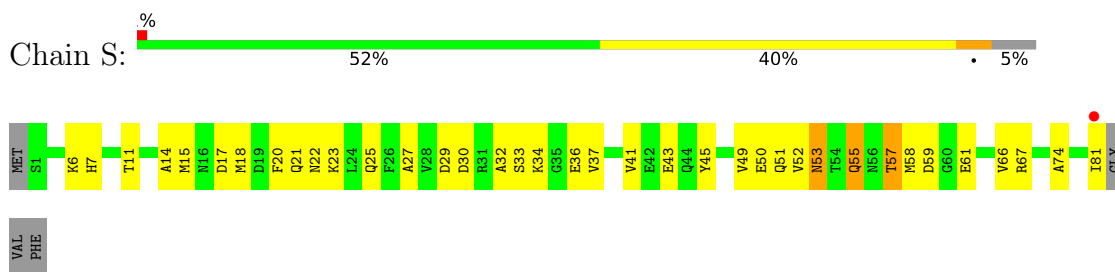
• Molecule 18: 50S ribosomal protein L21e



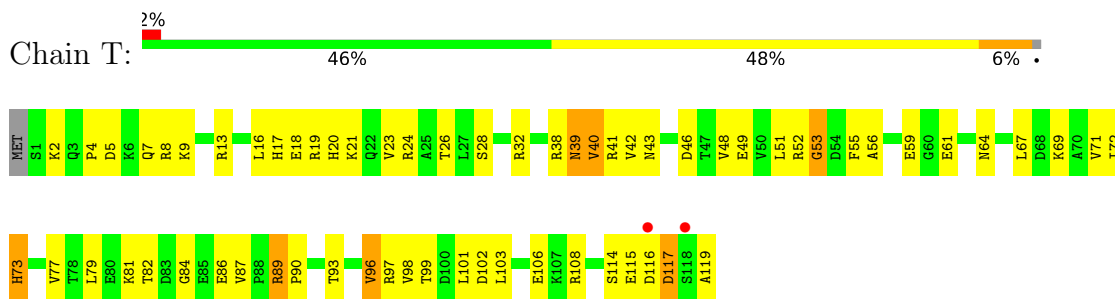
- Molecule 19: 50S ribosomal protein L22P



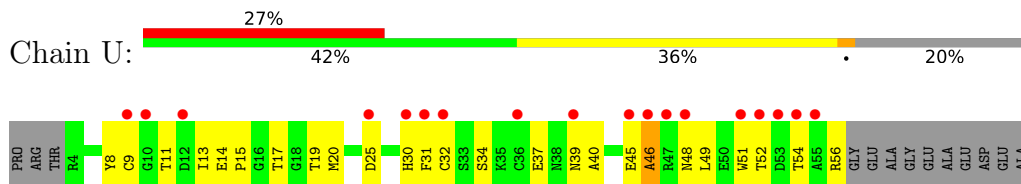
- Molecule 20: 50S ribosomal protein L23P



- Molecule 21: 50S ribosomal protein L24P



- Molecule 22: 50S ribosomal protein L24e

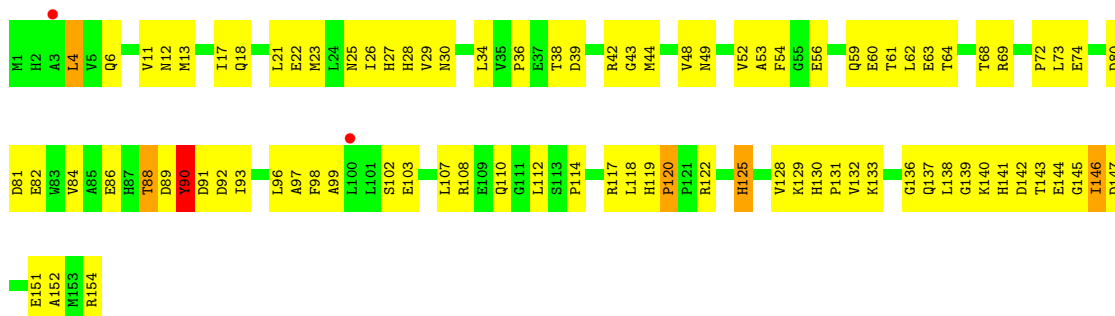


- Molecule 23: 50S ribosomal protein L29P

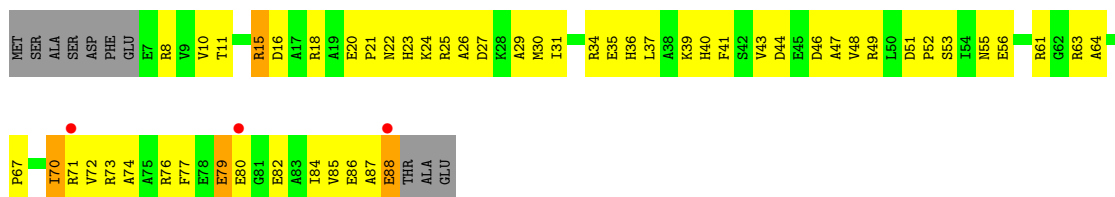




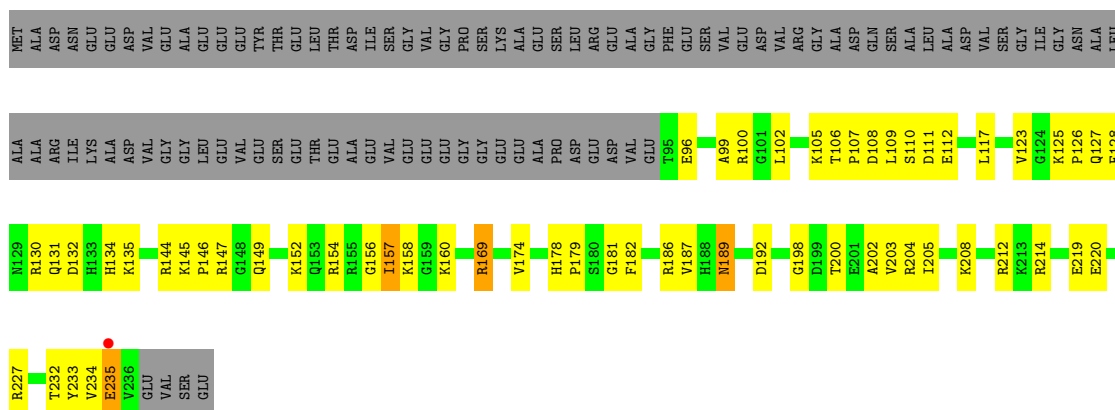
- Molecule 24: 50S ribosomal protein L30P



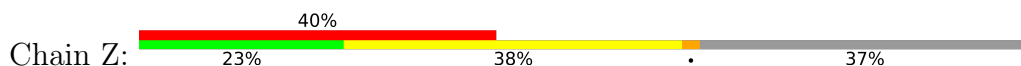
- Molecule 25: 50S ribosomal protein L31e

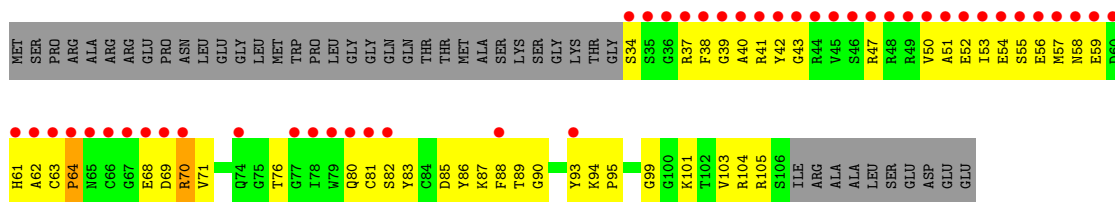


- Molecule 26: 50S ribosomal protein L32e

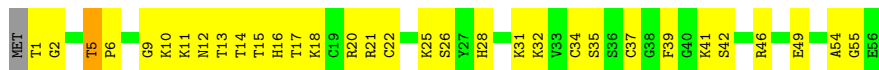


- Molecule 27: 50S ribosomal protein L37Ae





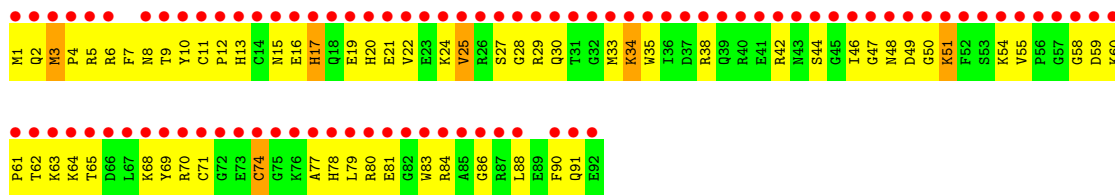
- Molecule 28: 50S ribosomal protein L37e



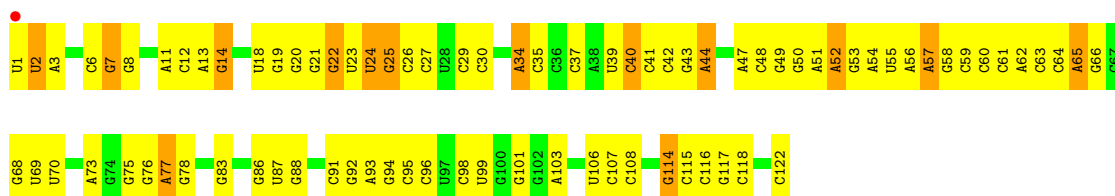
- Molecule 29: 50S ribosomal protein L39e



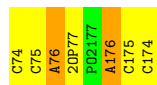
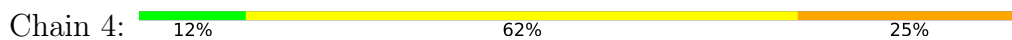
- Molecule 30: 50S ribosomal protein L44E



- Molecule 31: 5S ribosomal RNA



- Molecule 32: DNA/RNA (5'-R>(*CP*CP*(5AA)P*(2OP)P*(PO2)P*AP*CP*C)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	211.32Å 299.65Å 574.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.98 – 3.11 85.39 – 2.40	Depositor EDS
% Data completeness (in resolution range)	93.4 (49.98-3.11) 93.9 (85.39-2.40)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.00 (at 2.40Å)	Xtrriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.210 , 0.260 0.230 , 0.262	Depositor DCC
R_{free} test set	6547 reflections (0.98%)	wwPDB-VP
Wilson B-factor (Å ²)	62.5	Xtrriage
Anisotropy	0.119	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 92.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	99287	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.55% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: MYL, PSU, K, OMG, OMU, CD, PO2, UR3, 1MA, MG, CL, 2OP, NA, 5AA, SR

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	0	0.42	0/65958	0.68	6/102869 (0.0%)
2	A	0.33	0/1786	0.64	0/2408
3	B	0.36	0/2690	0.64	0/3652
4	C	0.38	0/1885	0.63	0/2552
5	D	0.31	0/1111	0.56	0/1498
6	E	0.35	0/1382	0.59	0/1880
7	F	0.32	0/901	0.59	0/1224
8	G	0.31	0/241	0.49	0/324
9	H	0.31	0/1303	0.63	0/1743
10	I	0.28	0/526	0.54	0/716
11	J	0.38	0/1136	0.62	0/1530
12	K	0.36	0/1004	0.65	0/1351
13	L	0.33	0/1130	0.62	0/1509
14	M	0.36	0/1583	0.59	0/2116
15	N	0.29	0/1474	0.62	0/1999
16	O	0.33	0/874	0.61	0/1181
17	P	0.36	0/1147	0.57	0/1528
18	Q	0.35	0/749	0.65	0/1005
19	R	0.40	0/1172	0.62	0/1578
20	S	0.35	0/648	0.58	0/875
21	T	0.33	0/958	0.63	0/1289
22	U	0.31	0/417	0.55	0/562
23	V	0.30	0/502	0.57	0/675
24	W	0.37	0/1219	0.66	0/1655
25	X	0.37	0/664	0.60	0/895
26	Y	0.38	0/1146	0.65	0/1536
27	Z	0.30	0/584	0.54	0/781
28	1	0.40	0/438	0.58	0/578
29	2	0.33	0/401	0.53	0/529
30	3	0.29	0/771	0.51	0/1024
31	9	0.35	0/2904	0.69	0/4526
32	4	0.46	0/102	0.73	0/149

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.39	0/98806	0.66	6/147737 (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	12
24	W	0	1
31	9	0	1
32	4	0	1
All	All	0	15

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	1504	A	N9-C1'-C2'	6.22	122.09	114.00
1	0	1819	G	C5'-C4'-C3'	5.93	125.50	116.00
1	0	2726	U	N1-C1'-C2'	5.42	121.04	114.00
1	0	871	G	C5'-C4'-O4'	-5.40	102.62	109.10
1	0	1942	A	C5'-C4'-C3'	5.19	124.30	116.00
1	0	2636	C	N1-C1'-C2'	-5.14	106.34	112.00

There are no chirality outliers.

All (15) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	1236	A	Sidechain
1	0	1430	G	Sidechain
1	0	1819	G	Sidechain
1	0	1829	A	Sidechain
1	0	1877	G	Sidechain
1	0	1878	G	Sidechain
1	0	24	G	Sidechain
1	0	2506	A	Sidechain
1	0	2526	C	Sidechain
1	0	2607	U	Sidechain
1	0	2636	C	Sidechain
1	0	2842	G	Sidechain

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Mol	Chain	Res	Type	Group
32	4	176	DA	Sidechain
31	9	94	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	1595	1
2	A	1753	0	1766	134	0
3	B	2625	0	2533	203	0
4	C	1860	0	1813	134	0
5	D	1094	0	1085	96	0
6	E	1357	0	1266	75	0
7	F	890	0	843	63	0
8	G	240	0	231	26	0
9	H	1283	0	1292	91	0
10	I	519	0	500	56	0
11	J	1120	0	1098	81	0
12	K	994	0	1027	84	0
13	L	1118	0	1076	94	0
14	M	1559	0	1573	155	0
15	N	1445	0	1401	122	0
16	O	865	0	873	59	0
17	P	1136	0	1123	84	0
18	Q	735	0	729	42	0
19	R	1149	0	1122	73	0
20	S	641	0	605	36	0
21	T	950	0	924	73	0
22	U	410	0	368	29	0
23	V	499	0	511	32	0
24	W	1196	0	1137	102	0
25	X	654	0	653	50	0
26	Y	1130	0	1133	62	0
27	Z	573	0	535	61	0
28	1	431	0	426	41	0
29	2	396	0	413	35	0
30	3	755	0	732	117	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	9	2599	0	1325	91	0
32	4	127	0	76	37	0
33	0	83	0	0	0	0
33	2	1	0	0	0	0
33	3	1	0	0	0	0
33	9	2	0	0	0	0
33	A	2	0	0	0	0
33	B	1	0	0	0	0
33	K	1	0	0	0	0
33	T	1	0	0	0	0
33	Y	1	0	0	0	0
34	0	2	0	0	0	0
35	0	63	0	0	0	0
35	9	2	0	0	0	0
35	B	1	0	0	0	0
35	C	1	0	0	0	0
35	H	1	0	0	0	0
35	J	1	0	0	0	0
35	M	1	0	0	0	0
35	Q	1	0	0	0	0
35	R	3	0	0	0	0
35	S	1	0	0	0	0
36	0	10	0	0	2	0
36	3	1	0	0	0	0
36	A	1	0	0	0	0
36	B	1	0	0	0	0
36	J	3	0	0	2	0
36	L	1	0	0	0	0
36	M	1	0	0	1	0
36	N	1	0	0	0	0
36	O	1	0	0	0	0
36	R	1	0	0	0	0
36	Y	1	0	0	0	0
37	0	93	0	0	0	0
37	1	1	0	0	0	0
37	3	2	0	0	0	0
37	9	3	0	0	0	0
37	A	2	0	0	0	0
37	B	2	0	0	0	0
37	F	1	0	0	0	0
37	H	1	0	0	0	0
37	L	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	R	1	0	0	0	0
37	S	1	0	0	0	0
38	0	35	0	41	22	0
39	1	1	0	0	0	0
39	3	1	0	0	0	0
39	O	1	0	0	0	0
39	U	1	0	0	0	0
39	Z	1	0	0	0	0
40	0	5841	0	0	203	0
40	1	58	0	0	4	0
40	2	45	0	0	2	0
40	3	70	0	0	6	0
40	4	13	0	0	7	0
40	9	144	0	0	7	0
40	A	117	0	0	8	0
40	B	151	0	0	16	0
40	C	175	0	0	21	0
40	D	49	0	0	6	0
40	E	40	0	0	7	0
40	F	29	0	0	5	0
40	G	18	0	0	1	0
40	H	76	0	0	11	0
40	I	10	0	0	3	0
40	J	57	0	0	2	0
40	K	62	0	0	7	0
40	L	91	0	0	12	0
40	M	148	0	0	13	0
40	N	61	0	0	8	0
40	O	41	0	0	2	0
40	P	61	0	0	3	0
40	Q	49	0	0	3	0
40	R	83	0	0	3	0
40	S	37	0	0	1	0
40	T	36	0	0	4	0
40	U	29	0	0	2	0
40	V	13	0	0	3	0
40	W	67	0	0	6	0
40	X	24	0	0	1	0
40	Y	98	0	0	5	0
40	Z	30	0	0	6	0
All	All	99287	0	60042	3609	1

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 24.

All (3609) 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)
40:0:4863:HOH:O	32:4:77:2OP:HB3	1.31	1.30
1:0:656:G:H5'	16:O:3:THR:HG22	1.20	1.15
1:0:871:G:C8	1:0:871:G:H5'	1.84	1.12
19:R:8:ALA:HB1	19:R:13:THR:HG21	1.28	1.11
1:0:1160:G:H5'	1:0:1161:A:H5'	1.28	1.10
14:M:71:SER:HB2	14:M:92:THR:HG22	1.31	1.10
1:0:2431:C:H42	38:0:2924:MYL:HAB	1.09	1.09
1:0:871:G:H5'	1:0:871:G:H8	0.98	1.08
1:0:1119:G:H2'	11:J:52:GLN:HE22	1.12	1.07
1:0:2717:C:H2'	1:0:2718:C:H5''	1.37	1.06
31:9:56:A:H2'	31:9:57:A:H5''	1.35	1.05
1:0:2637:A:N6	32:4:176:DA:H2'	1.70	1.05
30:3:38:ARG:HB3	30:3:42:ARG:HH12	1.19	1.05
27:Z:63:CYS:SG	27:Z:81:CYS:HB2	1.99	1.03
13:L:55:GLN:HA	13:L:58:GLN:HE21	1.25	1.01
14:M:99:ARG:HG2	14:M:99:ARG:HH11	1.25	1.01
11:J:19:MET:HE3	11:J:132:LEU:HD11	1.43	1.00
4:C:127:ARG:NH2	4:C:225:PRO:HG2	1.77	0.99
31:9:76:G:H3'	31:9:77:A:H5''	1.43	0.99
1:0:2717:C:C2'	1:0:2718:C:H5''	1.92	0.98
1:0:2890:A:C8	22:U:56:ARG:HD2	1.99	0.98
29:2:41:HIS:H	29:2:45:ASN:HD22	1.00	0.97
1:0:2637:A:H5''	32:4:175:C:OP2	1.65	0.97
14:M:70:GLY:HA3	14:M:73:ARG:NH2	1.79	0.96
1:0:1242:A:H5'	11:J:82:THR:HG23	1.45	0.95
30:3:21:GLU:HG2	30:3:22:VAL:H	1.30	0.95
12:K:10:GLN:HE21	12:K:10:GLN:H	1.12	0.95
1:0:656:G:H5'	16:O:3:THR:CG2	1.96	0.94
4:C:78:ARG:HH11	4:C:78:ARG:HG3	1.30	0.94
15:N:141:ARG:NH2	31:9:48:C:H4'	1.83	0.94
30:3:60:LYS:HG3	30:3:61:PRO:HD2	1.50	0.94
1:0:681:G:N3	1:0:681:G:H5'	1.82	0.93
17:P:135:ALA:HB1	17:P:139:ARG:HH12	1.33	0.93
1:0:1119:G:H2'	11:J:52:GLN:NE2	1.81	0.93
1:0:2502:C:H2'	1:0:2503:A:H5'	1.51	0.93
1:0:2503:A:H5''	9:H:155:ARG:HH12	1.29	0.93
5:D:28:GLY:HA2	5:D:69:ILE:HG23	1.50	0.93
5:D:17:ARG:HH12	5:D:137:PRO:HA	1.29	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:T:71:VAL:HG11	21:T:90:PRO:HB3	1.50	0.92
15:N:17:ARG:HB3	15:N:17:ARG:HH11	1.35	0.92
1:0:1684:A:H1'	29:2:43:ARG:HH22	1.34	0.92
9:H:72:ALA:HB2	9:H:156:ALA:HB2	1.51	0.91
1:0:823:U:H3'	40:0:3123:HOH:O	1.70	0.91
5:D:154:LYS:H	5:D:154:LYS:HD2	1.34	0.91
1:0:870:G:H2'	1:0:871:G:H5''	1.52	0.91
1:0:2506:A:HO2'	1:0:2507:G:H8	0.94	0.91
4:C:236:THR:HG22	4:C:239:ALA:H	1.36	0.90
1:0:1593:C:H5'	17:P:116:SER:O	1.71	0.90
2:A:153:ARG:HB2	2:A:153:ARG:HH11	1.33	0.90
11:J:131:THR:HB	11:J:134:GLU:HG3	1.53	0.89
24:W:137:GLN:HE21	24:W:141:HIS:HE1	1.17	0.89
12:K:10:GLN:H	12:K:10:GLN:NE2	1.71	0.89
1:0:2460:A:O4'	38:0:2924:MYL:HADB	1.72	0.89
30:3:3:MET:HG2	30:3:22:VAL:HG11	1.52	0.89
12:K:98:VAL:CG1	12:K:102:GLU:HA	2.03	0.89
1:0:2586:U:H3	1:0:2592:G:H22	1.16	0.89
15:N:141:ARG:HH21	31:9:48:C:H4'	1.38	0.89
23:V:12:THR:HG22	23:V:15:GLU:HG3	1.55	0.89
1:0:877:G:H5'	1:0:878:G:OP1	1.73	0.89
1:0:2468:A:H61	30:3:48:ASN:HD21	1.17	0.88
31:9:24:U:H3'	31:9:25:G:H5'	1.53	0.88
1:0:1205:U:H2'	1:0:1206:U:H5''	1.54	0.88
1:0:2618:G:O2'	32:4:76:5AA:H103	1.74	0.88
25:X:72:VAL:HG22	25:X:85:VAL:HG12	1.56	0.88
26:Y:187:VAL:HG23	26:Y:192:ASP:HB2	1.55	0.88
2:A:109:GLU:HG2	2:A:116:GLY:H	1.39	0.88
21:T:48:VAL:HG23	21:T:97:ARG:O	1.74	0.87
31:9:92:G:H2'	31:9:93:A:C8	2.10	0.87
1:0:381:G:H5''	40:M:2945:HOH:O	1.75	0.87
19:R:9:ASP:O	19:R:13:THR:HB	1.75	0.87
21:T:43:ASN:HD22	21:T:108:ARG:CZ	1.87	0.87
1:0:1328:A:OP1	26:Y:169:ARG:HD2	1.74	0.86
15:N:37:ARG:NH1	31:9:6:C:H5''	1.91	0.86
12:K:39:GLY:HA2	40:K:4183:HOH:O	1.72	0.86
23:V:1:THR:HG23	23:V:2:VAL:H	1.38	0.86
12:K:14:LYS:HB2	12:K:45:PRO:HG2	1.58	0.86
1:0:156:C:H5''	14:M:171:ARG:HD3	1.58	0.85
5:D:25:MET:HE3	5:D:37:ALA:HB1	1.57	0.85
1:0:2908:A:H2'	1:0:2909:G:O4'	1.77	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:F:2:VAL:HG22	7:F:57:GLU:OE1	1.73	0.85
17:P:115:SER:H	17:P:118:GLN:NE2	1.73	0.85
1:0:542:A:H5'	1:0:542:A:H8	1.40	0.85
1:0:2263:G:H4'	14:M:70:GLY:HA2	1.56	0.85
1:0:2533:C:H5'	1:0:2533:C:H6	1.38	0.85
1:0:2467:A:H1'	40:0:3036:HOH:O	1.76	0.85
1:0:2578:G:H5'	1:0:2578:G:H8	1.40	0.84
14:M:97:ILE:HD12	14:M:127:LYS:HD2	1.59	0.84
1:0:1701:A:H4'	1:0:1702:U:H5''	1.57	0.84
1:0:1116:U:O2'	1:0:1118:A:H2	1.57	0.84
3:B:320:GLN:HE21	3:B:321:PRO:HD2	1.42	0.84
1:0:2319:C:H3'	30:3:1:MET:N	1.92	0.84
1:0:735:C:H2'	1:0:736:A:O4'	1.78	0.84
31:9:14:G:H5'	31:9:14:G:H8	1.42	0.84
1:0:1160:G:C5'	1:0:1161:A:H5'	2.06	0.84
7:F:84:GLY:HA3	7:F:92:GLY:HA2	1.60	0.84
1:0:541:C:H2'	1:0:542:A:H5''	1.59	0.83
1:0:1835:U:H5	1:0:1840:A:N7	1.76	0.83
3:B:36:PRO:HA	3:B:168:GLY:HA3	1.58	0.83
19:R:96:VAL:HG13	19:R:106:GLY:HA3	1.60	0.83
31:9:56:A:C2'	31:9:57:A:H5''	2.07	0.83
1:0:506:G:H22	1:0:509:A:C5'	1.91	0.83
1:0:1701:A:H5'	40:0:5659:HOH:O	1.77	0.83
5:D:57:THR:HG23	5:D:63:ILE:HA	1.61	0.83
32:4:176:DA:OP1	40:4:334:HOH:O	1.94	0.83
1:0:819:A:H5'	27:Z:37:ARG:HD3	1.59	0.83
1:0:1667:A:H8	1:0:1667:A:H5'	1.43	0.83
3:B:62:ARG:HA	3:B:65:MET:HE2	1.58	0.83
6:E:116:THR:HG22	6:E:151:LEU:HD22	1.61	0.83
15:N:83:LEU:HD13	15:N:175:LEU:HD23	1.58	0.83
1:0:2503:A:H5''	9:H:155:ARG:NH1	1.94	0.82
11:J:39:VAL:HG22	11:J:106:GLY:O	1.79	0.82
22:U:46:ALA:HB1	22:U:52:THR:HG21	1.59	0.82
30:3:38:ARG:HB3	30:3:42:ARG:NH1	1.93	0.82
31:9:29:C:H2'	31:9:30:C:H5'	1.61	0.82
15:N:37:ARG:HH12	31:9:6:C:H5''	1.44	0.82
1:0:2502:C:C2'	1:0:2503:A:H5'	2.09	0.81
20:S:51:GLN:HE21	20:S:53:ASN:HD21	1.25	0.81
1:0:92:G:H4'	23:V:44:GLY:HA3	1.60	0.81
3:B:162:MET:CE	3:B:310:ARG:HD3	2.10	0.81
3:B:258:GLY:H	3:B:260:HIS:CE1	1.98	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:Y:235:GLU:CD	26:Y:235:GLU:H	1.83	0.81
1:O:200:C:H2'	40:O:7904:HOH:O	1.79	0.81
10:I:91:PHE:HD2	10:I:131:GLY:HA2	1.45	0.81
1:O:2419:U:H5''	1:O:2420:G:H5'	1.62	0.81
4:C:96:LYS:HB3	4:C:98:ARG:HH12	1.46	0.81
5:D:18:ILE:HG12	5:D:134:LEU:CD2	2.11	0.81
16:O:49:GLU:OE1	16:O:72:LYS:HG3	1.80	0.81
40:O:7291:HOH:O	3:B:211:THR:HG21	1.81	0.81
2:A:97:ALA:HA	2:A:131:HIS:NE2	1.95	0.81
20:S:11:THR:H	20:S:14:ALA:HB3	1.46	0.81
1:O:1160:G:H5'	1:O:1161:A:C5'	2.09	0.81
7:F:63:ILE:HB	7:F:64:PRO:HD3	1.62	0.80
19:R:99:ALA:HB1	19:R:109:MET:CE	2.11	0.80
21:T:9:LYS:HE3	21:T:13:ARG:NH1	1.96	0.80
1:O:506:G:H22	1:O:509:A:H5'	1.46	0.80
1:O:2846:C:H4'	3:B:156:LYS:HB3	1.63	0.80
14:M:83:SER:HB2	30:3:47:GLY:HA2	1.64	0.80
1:O:2431:C:N4	38:0:2924:MYL:HAB	1.93	0.80
1:O:2637:A:C5'	32:4:175:C:OP2	2.29	0.80
38:0:2924:MYL:HBG	38:0:2924:MYL:OAJ	1.82	0.80
11:J:74:ARG:HB3	11:J:74:ARG:HH11	1.47	0.80
1:O:1834:C:H2'	1:O:1840:A:N6	1.97	0.80
3:B:162:MET:HE2	3:B:310:ARG:HD3	1.62	0.80
14:M:69:LYS:HG2	14:M:70:GLY:H	1.47	0.79
32:4:75:C:C2'	40:4:6378:HOH:O	2.30	0.79
1:O:541:C:C2'	1:O:542:A:H5''	2.12	0.79
30:3:25:VAL:HG13	30:3:68:LYS:HE3	1.64	0.79
1:O:1446:U:H2'	20:S:55:GLN:NE2	1.97	0.79
1:O:870:G:C2'	1:O:871:G:H5''	2.12	0.79
1:O:1205:U:H2'	1:O:1206:U:C5'	2.12	0.79
7:F:29:VAL:HG12	7:F:98:VAL:HA	1.65	0.79
12:K:74:VAL:HG13	12:K:113:ILE:HG23	1.64	0.79
14:M:164:THR:HG22	14:M:166:ALA:N	1.97	0.79
1:O:710:G:OP1	16:O:24:ALA:HB3	1.83	0.79
17:P:103:THR:HA	17:P:106:ARG:NH1	1.98	0.79
1:O:871:G:H8	1:O:871:G:C5'	1.88	0.79
2:A:100:PRO:HG2	2:A:103:VAL:HG21	1.65	0.79
14:M:77:HIS:HE1	14:M:86:GLN:HE21	1.30	0.79
1:O:31:C:H4'	40:O:7242:HOH:O	1.82	0.78
1:O:380:A:OP2	14:M:9:ARG:HD2	1.83	0.78
1:O:2073:G:H5''	40:O:8371:HOH:O	1.83	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:275:GLY:O	3:B:291:ASP:HA	1.83	0.78
3:B:62:ARG:HA	3:B:65:MET:CE	2.14	0.78
1:0:420:U:H2'	1:0:421:C:H6	1.48	0.78
2:A:88:ILE:HD13	2:A:100:PRO:HD3	1.62	0.78
3:B:212:GLN:HB2	3:B:257:THR:HG21	1.64	0.78
14:M:164:THR:HG22	14:M:166:ALA:H	1.47	0.78
1:0:2541:U:H4'	1:0:2542:C:OP1	1.84	0.78
30:3:25:VAL:HG22	30:3:68:LYS:HG3	1.66	0.78
1:0:2263:G:H4'	14:M:70:GLY:CA	2.14	0.77
1:0:100:C:H5'	21:T:16:LEU:HD12	1.65	0.77
1:0:558:C:C2'	1:0:559:U:H5''	2.13	0.77
1:0:2431:C:H42	38:0:2924:MYL:CAB	1.93	0.77
16:O:47:ARG:HH11	16:O:47:ARG:HG3	1.48	0.77
17:P:135:ALA:HB1	17:P:139:ARG:NH1	2.00	0.77
5:D:58:VAL:HB	5:D:62:ASP:HB3	1.63	0.77
12:K:28:GLU:OE2	12:K:58:THR:HG21	1.85	0.77
15:N:86:LEU:O	15:N:90:LEU:HG	1.84	0.77
1:0:2364:A:H5''	18:Q:15:LYS:HD3	1.67	0.77
1:0:2382:A:H4'	30:3:12:PRO:HD3	1.66	0.77
12:K:81:ARG:HB2	12:K:87:ARG:HH11	1.50	0.77
25:X:76:ARG:HH11	25:X:76:ARG:HG3	1.49	0.77
1:0:1666:C:O2'	1:0:1667:A:H5''	1.84	0.77
1:0:1372:A:H3'	40:0:6923:HOH:O	1.85	0.77
16:O:32:ARG:O	16:O:32:ARG:HD3	1.83	0.77
17:P:55:LYS:HG2	17:P:56:GLY:N	2.00	0.76
19:R:39:THR:HB	19:R:42:GLU:HG3	1.66	0.76
7:F:27:GLY:HA3	7:F:101:ALA:O	1.85	0.76
24:W:108:ARG:HH21	24:W:114:PRO:HG2	1.50	0.76
1:0:1189:A:H3'	40:0:7609:HOH:O	1.85	0.76
15:N:110:THR:HB	15:N:113:SER:OG	1.86	0.76
21:T:9:LYS:HE3	21:T:13:ARG:CZ	2.15	0.76
5:D:103:ASN:ND2	5:D:133:ASN:HA	2.01	0.76
1:0:420:U:H2'	1:0:421:C:C6	2.20	0.76
1:0:1213:C:O2'	1:0:1214:G:H5'	1.86	0.76
9:H:62:HIS:HA	9:H:65:LEU:HD23	1.66	0.76
12:K:23:ASN:HD21	12:K:108:GLU:H	1.33	0.76
14:M:99:ARG:HH11	14:M:99:ARG:CG	1.98	0.76
2:A:217:ARG:HG2	2:A:229:ALA:HB2	1.66	0.76
3:B:162:MET:HE1	3:B:308:LEU:HD21	1.67	0.76
3:B:195:ARG:HG2	3:B:323:LEU:HD22	1.68	0.76
1:0:399:C:H5'	14:M:179:GLY:O	1.86	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:J:26:VAL:HG13	11:J:36:VAL:HG11	1.67	0.75
21:T:98:VAL:HG11	21:T:101:LEU:HD23	1.66	0.75
3:B:36:PRO:HG3	3:B:169:GLY:H	1.51	0.75
9:H:168:VAL:HG13	40:H:4963:HOH:O	1.86	0.75
24:W:21:LEU:HD21	24:W:48:VAL:HG11	1.67	0.75
19:R:99:ALA:HB1	19:R:109:MET:HE3	1.69	0.75
6:E:101:GLU:HB3	6:E:117:THR:HA	1.69	0.75
1:0:204:A:H2'	1:0:205:U:H5'	1.69	0.75
1:0:1759:A:N3	1:0:1818:C:H2'	2.01	0.75
1:0:2320:U:H5	30:3:1:MET:HE3	1.52	0.75
1:0:2420:G:O2'	1:0:2421:G:H5'	1.86	0.75
24:W:4:LEU:HD13	24:W:52:VAL:HG21	1.67	0.75
12:K:10:GLN:HE21	12:K:10:GLN:N	1.85	0.74
14:M:70:GLY:HA3	14:M:73:ARG:HH22	1.52	0.74
1:0:1166:A:H61	1:0:1180:U:H3	1.32	0.74
38:0:2924:MYL:HAZ	38:0:2924:MYL:HABB	1.68	0.74
15:N:169:PRO:O	15:N:172:PHE:HB3	1.88	0.74
1:0:1641:A:H2'	1:0:1642:A:H5'	1.68	0.74
15:N:38:LYS:HE2	15:N:107:ASN:ND2	2.02	0.74
13:L:90:ARG:HA	13:L:119:THR:HB	1.69	0.74
16:O:73:ASP:HA	16:O:92:VAL:O	1.87	0.74
7:F:58:GLU:CD	14:M:27:ARG:HH22	1.91	0.74
1:0:282:C:H1'	1:0:368:C:N4	2.03	0.74
1:0:545:G:H5'	1:0:545:G:H8	1.52	0.74
1:0:1528:A:H2'	1:0:1529:G:O4'	1.88	0.74
13:L:138:GLY:HA3	40:L:4360:HOH:O	1.87	0.74
3:B:18:ARG:HG3	3:B:256:GLN:HG3	1.68	0.74
14:M:68:ARG:NH2	14:M:73:ARG:HD3	2.03	0.74
7:F:61:MET:HB3	14:M:19:GLN:OE1	1.88	0.73
1:0:1300:G:H1'	40:0:3448:HOH:O	1.88	0.73
1:0:1679:C:H5'	40:0:3948:HOH:O	1.87	0.73
15:N:86:LEU:HD12	15:N:125:ALA:HB2	1.69	0.73
25:X:30:MET:HE1	25:X:55:ASN:HA	1.70	0.73
1:0:2055:A:H4'	19:R:132:ARG:NH2	2.02	0.73
1:0:2251:G:H2'	1:0:2252:A:C8	2.24	0.73
1:0:1116:U:H3	1:0:1246:A:H62	1.35	0.73
31:9:24:U:H3'	31:9:25:G:C5'	2.18	0.73
1:0:156:C:H5''	14:M:171:ARG:CD	2.18	0.73
1:0:2121:G:H21	14:M:86:GLN:HE22	1.35	0.73
1:0:1603:A:H5'	1:0:1605:G:O4'	1.89	0.72
1:0:2506:A:O2'	1:0:2507:G:H8	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:J:45:VAL:HG23	11:J:130:VAL:O	1.89	0.72
1:O:1183:C:N4	1:O:1184:C:H41	1.86	0.72
29:2:41:HIS:N	29:2:45:ASN:HD22	1.82	0.72
1:O:2588:OMG:O6	32:4:75:C:N4	2.15	0.72
6:E:84:MET:HG2	6:E:168:ILE:HA	1.69	0.72
8:G:16:LYS:O	8:G:20:VAL:HG23	1.89	0.72
9:H:61:ARG:HH11	9:H:61:ARG:HG3	1.54	0.72
12:K:74:VAL:HG11	12:K:113:ILE:HG12	1.71	0.72
2:A:192:VAL:HG11	2:A:208:HIS:N	2.05	0.72
5:D:105:SER:HB2	5:D:131:THR:HG23	1.72	0.72
32:4:175:C:OP1	40:4:334:HOH:O	2.07	0.72
1:O:2816:A:H5''	1:O:2817:G:H5'	1.69	0.72
5:D:41:LEU:HA	5:D:44:ILE:HG22	1.70	0.72
1:O:1130:U:H5'	40:0:7596:HOH:O	1.90	0.72
3:B:84:LEU:HD23	3:B:142:LEU:HD23	1.71	0.72
12:K:4:LEU:HD22	12:K:116:GLU:HB3	1.71	0.72
40:0:8828:HOH:O	2:A:200:PRO:HA	1.89	0.72
15:N:11:ARG:HD3	31:9:114:G:O6	1.88	0.72
1:O:447:A:OP1	21:T:2:LYS:HG2	1.90	0.72
6:E:7:ILE:HG13	6:E:11:VAL:HB	1.72	0.72
14:M:72:ALA:HB3	14:M:91:ILE:O	1.89	0.72
19:R:18:LEU:HG	19:R:91:LEU:HD13	1.70	0.72
1:O:2618:G:N3	32:4:76:5AA:C2	2.53	0.71
12:K:81:ARG:HB2	12:K:87:ARG:NH1	2.04	0.71
20:S:17:ASP:HB3	20:S:23:LYS:HB2	1.72	0.71
26:Y:219:GLU:HG3	26:Y:220:GLU:N	2.05	0.71
1:O:183:A:H1'	14:M:161:ARG:NH1	2.05	0.71
1:O:1771:U:H1'	27:Z:47:ARG:NH2	2.05	0.71
4:C:1:MET:HG2	4:C:2:GLN:H	1.55	0.71
27:Z:34:SER:HB2	40:Z:3188:HOH:O	1.90	0.71
24:W:63:GLU:HG2	24:W:93:ILE:HG22	1.73	0.71
1:O:558:C:H2'	1:O:559:U:H5''	1.72	0.71
1:O:926:A:H4'	13:L:39:GLU:HG2	1.71	0.71
22:U:34:SER:HA	22:U:37:GLU:HB2	1.72	0.71
32:4:75:C:H2'	40:4:6378:HOH:O	1.88	0.71
1:O:2533:C:H5'	1:O:2533:C:C6	2.24	0.71
4:C:236:THR:HA	40:C:6502:HOH:O	1.90	0.71
1:O:2618:G:N3	32:4:76:5AA:H2	2.06	0.71
4:C:129:HIS:CE1	4:C:231:ARG:HA	2.26	0.71
21:T:41:ARG:HG2	21:T:41:ARG:HH11	1.55	0.71
1:O:541:C:H2'	1:O:542:A:C5'	2.20	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2820:A:OP1	3:B:98:THR:HG22	1.91	0.71
3:B:27:ASN:HD22	3:B:27:ASN:H	1.39	0.71
4:C:236:THR:CG2	4:C:239:ALA:H	2.03	0.71
28:1:5:THR:N	28:1:6:PRO:HD2	2.05	0.71
1:0:450:C:OP1	4:C:184:ARG:NH2	2.23	0.71
38:0:2924:MYL:HBD	38:0:2924:MYL:OAR	1.89	0.71
21:T:48:VAL:HG21	21:T:96:VAL:HG13	1.72	0.71
1:0:853:C:H3'	40:0:3276:HOH:O	1.91	0.70
1:0:1973:A:H2'	1:0:1974:G:O4'	1.91	0.70
24:W:81:ASP:OD1	24:W:92:ASP:HB2	1.90	0.70
24:W:151:GLU:O	24:W:154:ARG:HG3	1.91	0.70
26:Y:187:VAL:HG23	26:Y:192:ASP:CB	2.21	0.70
1:0:2316:G:O2'	30:3:61:PRO:HG3	1.90	0.70
1:0:1118:A:C8	1:0:1118:A:H3'	2.25	0.70
1:0:2472:C:O2'	1:0:2634:G:H4'	1.91	0.70
11:J:107:ASN:ND2	11:J:109:TYR:H	1.89	0.70
19:R:18:LEU:HB2	19:R:143:VAL:HG13	1.74	0.70
21:T:16:LEU:HA	21:T:19:ARG:HG3	1.74	0.70
24:W:141:HIS:HB2	24:W:146:ILE:HG12	1.72	0.70
30:3:71:CYS:HB3	30:3:74:CYS:HB3	1.72	0.70
6:E:154:ILE:HD11	6:E:157:LYS:HB2	1.73	0.70
28:1:25:LYS:HD2	29:2:49:GLU:H	1.56	0.70
1:0:2320:U:H2'	30:3:2:GLN:HB2	1.74	0.70
4:C:115:LEU:HD21	4:C:243:VAL:HG22	1.72	0.70
14:M:72:ALA:HB2	14:M:92:THR:HA	1.72	0.70
31:9:13:A:O2'	31:9:14:G:H5''	1.91	0.70
1:0:1377:C:H5'	1:0:1377:C:H6	1.56	0.70
1:0:820:G:H3'	40:0:6474:HOH:O	1.92	0.70
1:0:1527:A:H1'	1:0:1528:A:C8	2.27	0.70
9:H:41:LYS:HE2	9:H:45:ASP:HB3	1.72	0.70
15:N:119:GLN:O	15:N:123:ILE:HG13	1.92	0.70
23:V:1:THR:HG23	23:V:2:VAL:N	2.07	0.70
1:0:2291:A:C8	1:0:2309:C:H5'	2.27	0.70
1:0:2542:C:H4'	32:4:75:C:O2'	1.92	0.70
40:0:4808:HOH:O	3:B:267:LYS:HD3	1.92	0.70
12:K:98:VAL:HG11	12:K:102:GLU:HA	1.72	0.70
25:X:79:GLU:CD	25:X:80:GLU:H	1.95	0.70
3:B:320:GLN:NE2	3:B:321:PRO:HD2	2.07	0.69
22:U:9:CYS:HA	22:U:52:THR:HG23	1.74	0.69
31:9:73:A:H61	31:9:108:C:H42	1.40	0.69
1:0:69:A:H5'	1:0:69:A:H8	1.56	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:N:61:ALA:CB	15:N:88:ALA:HB2	2.21	0.69
17:P:55:LYS:HG2	17:P:56:GLY:H	1.55	0.69
27:Z:51:ALA:HA	40:Z:3188:HOH:O	1.92	0.69
1:0:1474:C:H6	1:0:1474:C:H5'	1.58	0.69
1:0:1688:G:O2'	28:1:5:THR:HG23	1.92	0.69
3:B:312:ARG:HD3	3:B:315:VAL:HG13	1.72	0.69
12:K:82:ARG:NH2	12:K:115:ARG:HG2	2.08	0.69
31:9:3:A:N6	31:9:22:G:H1'	2.07	0.69
1:0:1224:G:H2'	1:0:1225:C:C6	2.27	0.69
15:N:48:VAL:CG1	15:N:55:ASP:HB3	2.22	0.69
30:3:24:LYS:HG3	30:3:90:PHE:CZ	2.28	0.69
31:9:54:A:O2'	31:9:55:U:H5'	1.93	0.69
18:Q:75:ILE:HG12	18:Q:84:ILE:HD12	1.74	0.69
19:R:12:THR:HG22	19:R:149:GLU:OE1	1.93	0.69
1:0:2353:A:H1'	18:Q:21:ARG:HH12	1.56	0.69
10:I:91:PHE:CD2	10:I:131:GLY:HA2	2.26	0.69
12:K:62:PRO:HG3	12:K:65:ARG:NH2	2.07	0.69
20:S:33:SER:O	20:S:37:VAL:HG23	1.93	0.69
27:Z:70:ARG:HH12	27:Z:82:SER:C	1.95	0.69
1:0:69:A:H5'	1:0:69:A:C8	2.28	0.69
1:0:447:A:O2'	1:0:448:G:H5'	1.92	0.69
1:0:902:G:N7	13:L:18:HIS:HD2	1.90	0.69
38:0:2924:MYL:OAJ	38:0:2924:MYL:CBC	2.40	0.69
3:B:162:MET:CE	3:B:308:LEU:HD21	2.21	0.69
4:C:139:VAL:HG13	40:C:6251:HOH:O	1.92	0.69
4:C:236:THR:HG22	4:C:239:ALA:N	2.07	0.69
10:I:95:LEU:HD23	10:I:99:GLN:OE1	1.93	0.69
11:J:19:MET:CE	11:J:132:LEU:HD11	2.21	0.69
1:0:1120:U:H5'	1:0:1121:G:OP2	1.92	0.69
1:0:1162:G:H1'	10:I:112:LEU:HD11	1.74	0.69
4:C:98:ARG:HG2	4:C:98:ARG:HH11	1.58	0.69
19:R:18:LEU:HB2	19:R:143:VAL:CG1	2.22	0.69
1:0:721:A:H4'	16:O:51:TYR:CD1	2.28	0.69
1:0:1132:A:N6	1:0:1229:C:H2'	2.07	0.69
1:0:533:U:H3'	40:0:8292:HOH:O	1.92	0.68
1:0:926:A:O2'	13:L:41:HIS:HD2	1.76	0.68
1:0:1762:C:H2'	1:0:1763:C:H6	1.57	0.68
18:Q:16:ASN:HD21	18:Q:45:PRO:HD2	1.59	0.68
1:0:1771:U:H1'	27:Z:47:ARG:HH21	1.58	0.68
1:0:1835:U:C5	1:0:1840:A:N7	2.60	0.68
1:0:1477:C:H5'	1:0:1868:G:H5'	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:78:ARG:HG3	4:C:78:ARG:NH1	2.02	0.68
11:J:95:ARG:O	11:J:99:GLU:HG3	1.93	0.68
13:L:145:LEU:O	13:L:148:GLU:HG3	1.92	0.68
38:0:2924:MYL:OAJ	38:0:2924:MYL:CBG	2.42	0.68
4:C:246:ARG:HB3	4:C:246:ARG:NH1	2.09	0.68
19:R:17:MET:HE1	19:R:19:ARG:NH2	2.09	0.68
1:0:1191:A:H2'	1:0:1193:A:H5'	1.76	0.68
1:0:280:C:H2'	1:0:281:U:O4'	1.94	0.68
1:0:2717:C:H2'	1:0:2718:C:C5'	2.20	0.68
4:C:246:ARG:HB3	4:C:246:ARG:HH11	1.58	0.68
11:J:107:ASN:C	11:J:107:ASN:HD22	1.96	0.68
22:U:52:THR:HG22	22:U:54:THR:H	1.59	0.68
25:X:25:ARG:HD3	25:X:64:ALA:O	1.93	0.68
30:3:78:HIS:O	30:3:79:LEU:HD23	1.94	0.68
1:0:56:G:H5''	23:V:50:ARG:HH12	1.58	0.68
1:0:2460:A:H5''	30:3:59:ASP:HA	1.75	0.68
1:0:2769:C:H2'	1:0:2770:G:O4'	1.93	0.68
27:Z:54:GLU:HG2	27:Z:57:MET:CE	2.23	0.68
29:2:41:HIS:H	29:2:45:ASN:ND2	1.84	0.68
1:0:42:C:H1'	40:0:3438:HOH:O	1.94	0.68
1:0:1166:A:H1'	1:0:1192:A:C2	2.29	0.68
24:W:52:VAL:HG22	24:W:53:ALA:N	2.09	0.67
24:W:110:GLN:HA	24:W:110:GLN:NE2	2.09	0.67
1:0:2005:G:H3'	1:0:2005:G:OP2	1.93	0.67
1:0:2904:U:H4'	25:X:8:ARG:NH1	2.08	0.67
2:A:30:ARG:HG2	2:A:31:LYS:N	2.09	0.67
29:2:35:ARG:HD3	29:2:37:HIS:NE2	2.08	0.67
1:0:877:G:H3'	40:0:6671:HOH:O	1.94	0.67
11:J:75:PRO:HG2	11:J:105:LEU:HD21	1.76	0.67
21:T:26:THR:HG23	21:T:97:ARG:HG3	1.75	0.67
2:A:51:ARG:NH2	2:A:53:ALA:HB3	2.08	0.67
9:H:59:GLN:HE21	9:H:129:ARG:HE	1.42	0.67
14:M:81:ARG:NH1	14:M:81:ARG:HB2	2.10	0.67
18:Q:21:ARG:HG2	18:Q:22:GLY:H	1.59	0.67
24:W:64:THR:O	24:W:68:THR:HG22	1.94	0.67
1:0:1206:U:H5'	1:0:1206:U:H6	1.60	0.67
12:K:29:LEU:HB3	12:K:55:VAL:HG11	1.75	0.67
14:M:91:ILE:HG21	40:M:533:HOH:O	1.95	0.67
1:0:656:G:C5'	16:O:3:THR:HG22	2.12	0.67
1:0:2081:A:H4'	11:J:69:TYR:CE1	2.29	0.67
3:B:30:PRO:HB2	3:B:39:GLN:NE2	2.08	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:9:12:C:H5'	31:9:70:U:O4'	1.94	0.67
1:0:1375:A:C2'	1:0:1376:G:H5'	2.24	0.67
1:0:1375:A:H2'	1:0:1376:G:H5'	1.77	0.67
1:0:2435:U:O2'	30:3:68:LYS:HE2	1.95	0.67
1:0:2491:G:H5'	40:0:4195:HOH:O	1.94	0.67
1:0:1119:G:H22	1:0:1246:A:H2	1.42	0.67
1:0:1500:U:P	17:P:41:ARG:HH22	2.18	0.67
2:A:192:VAL:HB	40:A:4780:HOH:O	1.94	0.67
9:H:102:LYS:HD3	9:H:122:LYS:HD3	1.77	0.67
10:I:91:PHE:HA	10:I:131:GLY:CA	2.25	0.67
13:L:30:ARG:HH11	13:L:30:ARG:HG3	1.60	0.67
21:T:98:VAL:HG11	21:T:101:LEU:CD2	2.25	0.67
1:0:559:U:H2'	1:0:560:U:O4'	1.94	0.66
1:0:1244:U:OP1	11:J:18:ILE:HD13	1.95	0.66
4:C:127:ARG:HH21	4:C:225:PRO:HG2	1.59	0.66
26:Y:189:ASN:C	26:Y:189:ASN:HD22	1.99	0.66
1:0:136:C:H2'	1:0:137:U:O4'	1.94	0.66
1:0:558:C:O2'	1:0:559:U:H5''	1.95	0.66
1:0:1118:A:H3'	1:0:1118:A:H8	1.60	0.66
11:J:107:ASN:HD21	11:J:109:TYR:HB2	1.61	0.66
15:N:62:HIS:HB3	15:N:65:ASP:OD1	1.95	0.66
17:P:105:LEU:HD21	17:P:137:LEU:HD21	1.77	0.66
25:X:21:PRO:HG2	25:X:24:LYS:HD3	1.77	0.66
30:3:11:CYS:HB2	30:3:20:HIS:NE2	2.10	0.66
1:0:559:U:H6	1:0:559:U:H5'	1.60	0.66
29:2:36:ASN:H	29:2:39:ARG:NH2	1.93	0.66
1:0:951:A:H5''	18:Q:42:LYS:HD3	1.75	0.66
1:0:2578:G:H5'	1:0:2578:G:C8	2.29	0.66
2:A:33:GLU:H	2:A:33:GLU:CD	1.99	0.66
4:C:26:VAL:HG22	4:C:117:ALA:HB2	1.77	0.66
6:E:20:ILE:HD11	6:E:40:VAL:HG11	1.77	0.66
1:0:297:U:H2'	1:0:298:C:C6	2.31	0.66
1:0:1939:U:H5''	2:A:237:GLY:O	1.94	0.66
1:0:2768:A:O2'	1:0:2769:C:H5'	1.95	0.66
10:I:120:ALA:O	10:I:124:VAL:HG23	1.95	0.66
14:M:77:HIS:CE1	14:M:86:GLN:HE21	2.13	0.66
14:M:84:LYS:HD3	40:M:674:HOH:O	1.96	0.66
1:0:1624:A:H4'	1:0:1626:A:H5''	1.77	0.66
1:0:2716:G:H5'	3:B:262:ARG:HG3	1.78	0.66
4:C:218:VAL:HG12	40:C:5065:HOH:O	1.95	0.66
1:0:1209:C:H2'	1:0:1210:G:H8	1.60	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1942:A:H2'	1:0:1943:C:H6	1.60	0.66
1:0:2460:A:H4'	30:3:58:GLY:O	1.96	0.66
1:0:2526:C:O2'	1:0:2527:U:H5'	1.96	0.66
1:0:2716:G:H5''	3:B:206:THR:HG21	1.76	0.66
3:B:5:ARG:HD2	3:B:8:LYS:HE2	1.78	0.66
1:0:10:U:H3'	1:0:10:U:H6	1.61	0.66
1:0:282:C:O2'	1:0:283:U:H5'	1.95	0.66
1:0:2253:G:H2'	1:0:2254:G:H8	1.61	0.66
13:L:79:ASP:HB3	40:L:4967:HOH:O	1.95	0.66
15:N:113:SER:HB2	40:N:6448:HOH:O	1.95	0.66
27:Z:101:LYS:HA	27:Z:104:ARG:NH1	2.10	0.66
1:0:281:U:H2'	1:0:282:C:O4'	1.96	0.66
1:0:2338:G:H1'	5:D:105:SER:OG	1.95	0.66
14:M:74:LYS:HD3	14:M:91:ILE:HD11	1.76	0.66
1:0:2694:A:H4'	6:E:91:PHE:HE1	1.60	0.65
11:J:39:VAL:CG2	11:J:107:ASN:HA	2.27	0.65
13:L:65:ASP:HA	13:L:109:LEU:O	1.96	0.65
14:M:74:LYS:HG3	40:M:3198:HOH:O	1.95	0.65
1:0:12:U:H2'	1:0:13:G:H5'	1.78	0.65
1:0:371:U:H2'	1:0:372:A:H8	1.61	0.65
1:0:1589:G:H22	1:0:1605:G:H1'	1.61	0.65
38:0:2924:MYL:HANA	38:0:2924:MYL:HACB	1.78	0.65
21:T:40:VAL:HG23	21:T:119:ALA:OXT	1.96	0.65
1:0:1118:A:H8	1:0:1119:G:H5''	1.61	0.65
1:0:2510:C:H42	1:0:2564:G:H22	1.44	0.65
2:A:153:ARG:HH11	2:A:153:ARG:CB	2.07	0.65
28:1:21:ARG:HD2	28:1:37:CYS:SG	2.37	0.65
1:0:10:U:O4	1:0:531:G:H2'	1.96	0.65
40:0:4078:HOH:O	28:1:1:THR:HA	1.96	0.65
3:B:41:PHE:CD1	3:B:79:MET:HE2	2.32	0.65
12:K:87:ARG:HB2	22:U:19:THR:HG23	1.78	0.65
20:S:33:SER:OG	20:S:36:GLU:HG3	1.96	0.65
1:0:558:C:H2'	1:0:559:U:C5'	2.26	0.65
13:L:80:ASP:HB2	13:L:90:ARG:O	1.97	0.65
1:0:657:G:OP1	4:C:27:ARG:NH2	2.28	0.65
1:0:1182:C:HO2'	1:0:1183:C:H5	1.44	0.65
1:0:1446:U:H2'	20:S:55:GLN:HE22	1.60	0.65
1:0:1654:U:H2'	2:A:47:HIS:HD2	1.60	0.65
4:C:77:ALA:O	4:C:78:ARG:HG3	1.97	0.65
15:N:49:THR:HG22	15:N:56:ASP:HB2	1.79	0.65
23:V:64:GLY:O	23:V:65:ASP:HB2	1.95	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1555:G:H4'	1:0:1630:A:H2	1.61	0.65
1:0:1838:U:H1'	1:0:2644:C:H5'	1.78	0.65
1:0:2114:C:O2'	1:0:2115:U:H5'	1.96	0.65
3:B:179:LEU:O	3:B:183:GLU:HG2	1.96	0.65
11:J:109:TYR:HE1	40:J:7556:HOH:O	1.80	0.65
15:N:27:LEU:HD21	15:N:50:LEU:HD13	1.77	0.65
30:3:21:GLU:HG2	30:3:22:VAL:N	2.08	0.65
1:0:523:C:H2'	1:0:524:A:C8	2.32	0.65
12:K:81:ARG:HD3	12:K:87:ARG:NH1	2.11	0.65
25:X:20:GLU:HG3	25:X:21:PRO:HD2	1.78	0.65
1:0:1477:C:H5'	1:0:1868:G:C5'	2.27	0.65
1:0:1589:G:N2	1:0:1605:G:H1'	2.12	0.65
1:0:2748:G:H5'	40:0:7410:HOH:O	1.97	0.65
2:A:76:VAL:HG23	27:Z:87:LYS:O	1.97	0.65
12:K:41:LYS:HE3	40:K:7871:HOH:O	1.97	0.65
23:V:39:ALA:N	23:V:40:PRO:HD2	2.12	0.65
1:0:706:G:HO2'	1:0:707:C:H6	1.42	0.64
1:0:2780:C:H1'	6:E:143:GLN:HE21	1.61	0.64
38:0:2924:MYL:HABB	38:0:2924:MYL:CAZ	2.25	0.64
40:0:5319:HOH:O	28:1:6:PRO:HB3	1.96	0.64
5:D:47:GLN:HE21	5:D:75:LEU:HD23	1.61	0.64
14:M:81:ARG:HG2	14:M:85:ARG:O	1.97	0.64
15:N:164:ASP:OD1	15:N:167:ASP:HA	1.96	0.64
1:0:182:G:H5'	40:0:4102:HOH:O	1.97	0.64
1:0:705:C:O2	1:0:705:C:H2'	1.97	0.64
1:0:1595:G:O2'	1:0:1596:U:H5'	1.97	0.64
6:E:7:ILE:HD11	6:E:11:VAL:O	1.96	0.64
7:F:21:GLU:O	7:F:24:ARG:HG3	1.97	0.64
13:L:12:THR:HG21	13:L:16:GLY:O	1.96	0.64
14:M:69:LYS:HB2	14:M:126:GLN:N	2.12	0.64
17:P:7:LYS:HD3	17:P:23:PHE:CE1	2.33	0.64
1:0:1441:G:H1'	40:0:7717:HOH:O	1.97	0.64
4:C:127:ARG:CZ	4:C:225:PRO:HG2	2.26	0.64
9:H:59:GLN:NE2	9:H:129:ARG:HE	1.95	0.64
24:W:132:VAL:HG21	24:W:140:LYS:O	1.97	0.64
1:0:1189:A:H1'	1:0:1209:C:O4'	1.97	0.64
3:B:205:VAL:HA	3:B:260:HIS:O	1.96	0.64
14:M:134:ILE:HG23	14:M:141:ILE:HD13	1.80	0.64
1:0:157:G:H4'	14:M:95:LYS:HE2	1.79	0.64
1:0:564:G:H1'	40:0:5694:HOH:O	1.95	0.64
2:A:167:LYS:HE2	27:Z:50:VAL:HG13	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:H:72:ALA:CB	9:H:156:ALA:HB2	2.27	0.64
1:0:871:G:C8	1:0:871:G:C5'	2.71	0.64
1:0:2469:A:H1'	40:0:7148:HOH:O	1.96	0.64
1:0:2613:G:O2'	1:0:2614:C:H5'	1.97	0.64
32:4:76:5AA:C4	40:4:6378:HOH:O	2.45	0.64
1:0:1741:U:H5'	1:0:1742:A:OP1	1.97	0.64
1:0:2382:A:O2'	30:3:12:PRO:HB3	1.98	0.64
9:H:146:ALA:O	9:H:149:VAL:HG12	1.97	0.64
26:Y:182:PHE:HD2	26:Y:200:THR:O	1.81	0.64
1:0:204:A:C2'	1:0:205:U:H5'	2.27	0.64
1:0:1201:C:H2'	1:0:1202:A:H5'	1.80	0.64
2:A:199:HIS:CD2	2:A:201:PHE:H	2.15	0.64
15:N:73:ALA:HB1	15:N:74:PRO:CD	2.28	0.64
1:0:262:A:C6	7:F:89:LEU:HD21	2.33	0.64
1:0:1015:C:H2'	1:0:1016:U:H6	1.61	0.64
3:B:56:ASP:HB2	3:B:322:ARG:HE	1.61	0.64
6:E:5:LEU:HD21	6:E:66:GLN:HG3	1.80	0.64
12:K:28:GLU:HG2	12:K:58:THR:HB	1.80	0.64
16:O:44:ASN:OD1	16:O:65:LEU:HB2	1.98	0.64
1:0:470:U:O2'	28:1:16:HIS:HD2	1.80	0.64
1:0:1295:G:H5''	13:L:14:GLY:O	1.98	0.64
2:A:48:ASP:HB3	40:A:5706:HOH:O	1.96	0.64
26:Y:234:VAL:HG12	26:Y:235:GLU:H	1.63	0.64
1:0:272:A:H5'	1:0:273:G:OP2	1.96	0.63
18:Q:66:LYS:HB2	18:Q:70:ALA:O	1.98	0.63
1:0:65:C:O2'	1:0:66:G:H5'	1.97	0.63
1:0:482:G:H4'	1:0:508:A:N1	2.13	0.63
3:B:201:ASP:HB2	3:B:312:ARG:HD2	1.80	0.63
9:H:42:ASP:HB2	9:H:45:ASP:OD1	1.98	0.63
11:J:131:THR:HB	11:J:134:GLU:CG	2.26	0.63
12:K:23:ASN:HD21	12:K:108:GLU:N	1.96	0.63
17:P:61:ARG:HH11	17:P:61:ARG:HB2	1.63	0.63
1:0:2618:G:O2'	32:4:76:5AA:C10	2.45	0.63
13:L:125:PHE:CZ	13:L:140:VAL:HG22	2.33	0.63
1:0:1596:U:H2'	1:0:1598:A:OP2	1.97	0.63
10:I:73:LEU:HD12	10:I:107:LYS:NZ	2.12	0.63
22:U:56:ARG:HH11	22:U:56:ARG:HG3	1.64	0.63
24:W:88:THR:C	24:W:90:TYR:H	2.00	0.63
1:0:2457:U:O3'	30:3:81:GLU:HA	1.98	0.63
2:A:42:VAL:HG21	2:A:74:VAL:CG1	2.29	0.63
17:P:38:GLU:HA	17:P:41:ARG:HH11	1.61	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:Z:64:PRO:HB2	27:Z:86:TYR:CE2	2.34	0.63
1:0:1118:A:H62	1:0:1244:U:H3	1.45	0.63
1:0:285:A:H2'	1:0:286:U:O4'	1.98	0.63
1:0:1015:C:H2'	1:0:1016:U:C6	2.33	0.63
1:0:1175:G:H1'	1:0:1193:A:H2'	1.80	0.63
1:0:1748:U:H4'	40:0:7383:HOH:O	1.99	0.63
2:A:190:ARG:NH2	2:A:207:GLN:OE1	2.32	0.63
4:C:165:ASP:OD2	4:C:191:SER:HB2	1.98	0.63
5:D:167:GLU:OE1	5:D:173:GLU:HB3	1.98	0.63
6:E:20:ILE:CD1	6:E:40:VAL:HG11	2.29	0.63
9:H:57:THR:HG23	9:H:131:GLN:HA	1.81	0.63
25:X:37:LEU:HD13	25:X:85:VAL:HG21	1.80	0.63
5:D:88:LEU:HB2	5:D:89:PRO:HD3	1.80	0.63
14:M:52:GLN:OE1	14:M:116:ASN:HB3	1.96	0.63
15:N:139:TRP:HA	15:N:139:TRP:CE3	2.34	0.63
1:0:1159:G:H21	1:0:1189:A:H8	1.45	0.63
1:0:1189:A:H1'	1:0:1209:C:C1'	2.28	0.63
1:0:1234:U:N3	3:B:244:PRO:HB3	2.13	0.63
1:0:1593:C:OP1	17:P:117:SER:HB3	1.99	0.63
1:0:1773:G:C8	27:Z:40:ALA:HA	2.32	0.63
1:0:2111:G:H1'	40:0:3046:HOH:O	1.97	0.63
1:0:2780:C:C1'	6:E:143:GLN:HE21	2.11	0.63
15:N:61:ALA:HB3	15:N:88:ALA:HB2	1.80	0.63
17:P:89:ASN:OD1	17:P:92:GLU:HG3	1.98	0.63
1:0:506:G:H22	1:0:509:A:H5''	1.63	0.62
1:0:821:U:H3'	40:0:8314:HOH:O	1.98	0.62
1:0:1632:A:H2'	1:0:1633:C:H5'	1.80	0.62
1:0:1778:A:H2'	1:0:1779:A:H5'	1.79	0.62
1:0:613:C:H2'	1:0:614:U:H6	1.64	0.62
6:E:95:VAL:O	6:E:126:ILE:HD12	1.99	0.62
15:N:48:VAL:HG11	15:N:55:ASP:HB3	1.79	0.62
27:Z:70:ARG:CB	27:Z:70:ARG:HH11	2.12	0.62
3:B:13:PHE:O	3:B:16:ARG:HD2	1.99	0.62
10:I:96:SER:OG	10:I:99:GLN:HG3	1.99	0.62
17:P:134:VAL:O	17:P:137:LEU:HB3	1.99	0.62
1:0:588:G:O6	24:W:154:ARG:NH1	2.32	0.62
1:0:1972:U:H2'	1:0:1973:A:C5'	2.30	0.62
38:0:2924:MYL:HBB	40:0:8226:HOH:O	1.97	0.62
3:B:305:ASP:O	3:B:306:LYS:HB2	1.99	0.62
20:S:53:ASN:HD22	20:S:53:ASN:N	1.97	0.62
30:3:4:PRO:HG2	30:3:7:PHE:HD2	1.65	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:3:44:SER:HA	30:3:49:ASP:OD1	1.98	0.62
1:0:10:U:O4	1:0:532:A:OP2	2.17	0.62
1:0:523:C:H2'	1:0:524:A:H8	1.64	0.62
1:0:1943:C:H4'	2:A:211:LYS:O	1.99	0.62
1:0:2426:G:H1'	40:0:5391:HOH:O	1.99	0.62
2:A:135:VAL:HG21	2:A:147:ARG:HB3	1.82	0.62
16:O:21:SER:OG	16:O:106:PRO:HB2	1.99	0.62
24:W:80:ASP:O	24:W:84:VAL:HG23	1.99	0.62
24:W:122:ARG:HG3	24:W:122:ARG:HH11	1.64	0.62
31:9:14:G:H5'	31:9:14:G:C8	2.30	0.62
1:0:1943:C:O4'	2:A:212:PRO:HA	2.00	0.62
1:0:2413:A:N7	15:N:109:PRO:HB3	2.15	0.62
40:0:4874:HOH:O	27:Z:41:ARG:HG2	1.99	0.62
3:B:80:ARG:HB2	3:B:145:HIS:CE1	2.34	0.62
4:C:79:ARG:O	4:C:87:ARG:HG2	1.99	0.62
1:0:1224:G:H2'	1:0:1225:C:H6	1.63	0.62
23:V:12:THR:HG22	23:V:15:GLU:CG	2.29	0.62
1:0:553:G:P	26:Y:204:ARG:HH22	2.21	0.62
1:0:1768:C:H2'	1:0:1769:C:O4'	2.00	0.62
1:0:2587:OMU:HM23	1:0:2589:U:C6	2.35	0.62
2:A:75:GLY:HA2	27:Z:88:PHE:HA	1.82	0.62
6:E:81:GLU:O	6:E:172:PRO:HD3	2.00	0.62
6:E:101:GLU:HB2	6:E:116:THR:O	1.99	0.62
15:N:55:ASP:OD2	31:9:7:G:H4'	2.00	0.62
1:0:2837:U:H2'	40:0:6433:HOH:O	1.99	0.62
7:F:50:VAL:HG13	7:F:60:VAL:HG11	1.81	0.62
27:Z:54:GLU:HB2	40:Z:3188:HOH:O	1.98	0.62
28:1:15:THR:HB	28:1:28:HIS:CD2	2.35	0.62
30:3:24:LYS:HG3	30:3:90:PHE:HZ	1.64	0.62
1:0:292:G:H2'	1:0:358:G:N2	2.15	0.62
1:0:960:G:H4'	40:0:7253:HOH:O	2.00	0.62
1:0:2521:A:OP2	9:H:6:ALA:HB3	2.00	0.62
4:C:1:MET:HG2	4:C:2:GLN:N	2.14	0.62
14:M:77:HIS:CE1	14:M:86:GLN:HG2	2.35	0.62
16:O:47:ARG:O	16:O:47:ARG:HG2	1.99	0.62
1:0:90:A:H2'	1:0:91:G:O4'	2.00	0.61
1:0:542:A:H5'	1:0:542:A:C8	2.29	0.61
1:0:1350:U:H4'	40:0:4055:HOH:O	2.00	0.61
10:I:126:THR:O	10:I:130:LEU:HG	2.00	0.61
21:T:48:VAL:HG23	21:T:97:ARG:C	2.19	0.61
1:0:450:C:H4'	4:C:46:TYR:CE1	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:819:A:C5'	27:Z:37:ARG:HD3	2.29	0.61
1:0:855:U:H3'	40:0:3915:HOH:O	2.00	0.61
1:0:1308:A:O4'	4:C:226:GLY:HA3	2.00	0.61
1:0:1819:G:H2'	1:0:1820:G:H4'	1.80	0.61
2:A:186:TRP:CG	2:A:187:PRO:HA	2.35	0.61
12:K:34:VAL:CG2	12:K:47:ALA:HB2	2.29	0.61
18:Q:62:THR:O	18:Q:64:GLU:HG2	1.99	0.61
1:0:1972:U:H2'	1:0:1973:A:H5'	1.82	0.61
1:0:2511:A:H2'	1:0:2512:U:O4'	2.00	0.61
1:0:2541:U:O2	32:4:77:2OP:HA	2.00	0.61
1:0:2795:C:O2'	1:0:2796:U:H5'	1.99	0.61
3:B:256:GLN:HG2	40:B:7358:HOH:O	1.99	0.61
14:M:77:HIS:HD2	14:M:81:ARG:H	1.46	0.61
15:N:17:ARG:HB3	15:N:17:ARG:NH1	2.12	0.61
17:P:7:LYS:HD2	17:P:21:VAL:CG2	2.30	0.61
1:0:500:G:H21	19:R:98:ASN:HD21	1.45	0.61
1:0:2321:A:H4'	1:0:2322:U:OP1	2.00	0.61
4:C:131:PHE:H	4:C:131:PHE:HD2	1.48	0.61
5:D:17:ARG:NH1	5:D:137:PRO:HA	2.07	0.61
19:R:4:TYR:CE2	19:R:15:LYS:HB3	2.34	0.61
1:0:100:C:H4'	21:T:16:LEU:HB2	1.82	0.61
15:N:79:PRO:HG3	15:N:143:ARG:O	2.00	0.61
15:N:154:LEU:HG	15:N:155:GLU:H	1.65	0.61
17:P:138:GLU:C	17:P:140:TYR:H	2.03	0.61
19:R:39:THR:HB	19:R:42:GLU:CG	2.29	0.61
20:S:37:VAL:O	20:S:41:VAL:HG23	2.01	0.61
1:0:603:A:H5''	1:0:604:G:OP1	2.00	0.61
1:0:1474:C:H5'	1:0:1474:C:C6	2.36	0.61
40:0:5298:HOH:O	3:B:254:GLN:HG3	1.99	0.61
3:B:258:GLY:H	3:B:260:HIS:HE1	1.45	0.61
4:C:27:ARG:NH2	16:O:4:ASN:ND2	2.48	0.61
5:D:76:ARG:NE	31:9:44:A:O4'	2.33	0.61
7:F:99:THR:HA	40:F:3461:HOH:O	1.99	0.61
11:J:107:ASN:HD22	11:J:109:TYR:H	1.45	0.61
14:M:68:ARG:O	14:M:68:ARG:HD3	2.01	0.61
18:Q:26:PRO:O	18:Q:30:VAL:HG22	2.01	0.61
29:2:25:VAL:O	29:2:29:THR:HG23	2.00	0.61
1:0:343:C:O2'	1:0:344:C:H5'	2.00	0.61
1:0:1205:U:C2'	1:0:1206:U:H5''	2.29	0.61
1:0:1447:U:H3'	1:0:1506:U:O2	1.99	0.61
2:A:95:PRO:HG2	2:A:98:GLU:HG2	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:84:LEU:HD23	3:B:142:LEU:CD2	2.30	0.61
13:L:121:ILE:HG12	13:L:141:GLU:HB2	1.82	0.61
17:P:80:ARG:HG2	17:P:87:ARG:CZ	2.30	0.61
31:9:39:U:H1'	31:9:44:A:H61	1.66	0.61
1:0:168:C:O5'	1:0:168:C:H6	1.84	0.61
1:0:271:C:H41	1:0:378:A:H2	1.49	0.61
1:0:946:C:H2'	1:0:947:U:C6	2.36	0.61
3:B:221:GLN:HE22	12:K:42:ASN:HD22	1.49	0.61
4:C:127:ARG:HD3	4:C:129:HIS:HE1	1.65	0.61
13:L:73:VAL:HG21	13:L:116:HIS:NE2	2.16	0.61
4:C:242:GLU:HB2	40:C:3133:HOH:O	2.00	0.61
7:F:53:ASP:OD1	7:F:80:GLN:HB2	2.00	0.61
13:L:66:VAL:HG22	13:L:111:ALA:H	1.65	0.61
23:V:49:LEU:O	23:V:53:ILE:HG13	2.01	0.61
27:Z:81:CYS:SG	27:Z:83:TYR:HB3	2.41	0.61
1:0:244:C:OP2	7:F:38:LYS:HE3	2.01	0.61
2:A:88:ILE:O	2:A:88:ILE:HG22	2.00	0.61
3:B:140:LEU:HA	40:B:3693:HOH:O	1.99	0.61
10:I:113:SER:HB2	10:I:118:ASN:HB2	1.83	0.61
11:J:6:PHE:HB3	11:J:109:TYR:OH	2.01	0.61
17:P:55:LYS:CG	17:P:56:GLY:H	2.14	0.61
19:R:47:LEU:HB2	19:R:89:LEU:HD21	1.82	0.61
1:0:157:G:H4'	14:M:95:LYS:CE	2.31	0.60
1:0:682:A:H2'	1:0:683:G:O4'	2.00	0.60
1:0:1615:A:H5'	40:0:8791:HOH:O	2.01	0.60
1:0:2717:C:OP1	3:B:207:LYS:HG3	2.00	0.60
1:0:2851:G:C2'	1:0:2852:A:H5'	2.31	0.60
3:B:41:PHE:CE1	3:B:79:MET:HG3	2.35	0.60
13:L:17:SER:C	13:L:19:LYS:H	2.05	0.60
17:P:59:ARG:HD3	40:P:5642:HOH:O	2.00	0.60
24:W:90:TYR:N	24:W:90:TYR:CD1	2.66	0.60
30:3:55:VAL:HG22	40:3:895:HOH:O	2.01	0.60
1:0:2564:G:OP2	1:0:2565:C:H5''	2.02	0.60
1:0:2851:G:O2'	1:0:2852:A:H5'	2.00	0.60
2:A:8:ARG:HG2	40:A:2279:HOH:O	2.01	0.60
5:D:135:VAL:HG21	5:D:139:TYR:CD1	2.36	0.60
6:E:14:GLU:HG2	6:E:15:GLN:N	2.15	0.60
31:9:2:U:OP2	31:9:3:A:H5'	2.01	0.60
1:0:259:G:H21	14:M:58:GLN:NE2	1.99	0.60
1:0:727:G:H3'	1:0:728:C:H6	1.66	0.60
1:0:947:U:H2'	1:0:948:G:C8	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1097:A:H5''	24:W:125:HIS:NE2	2.16	0.60
1:0:1641:A:H2'	1:0:1642:A:C5'	2.30	0.60
1:0:1682:A:O2'	1:0:1683:G:H5''	2.01	0.60
1:0:1981:A:H1'	1:0:1983:C:N4	2.16	0.60
1:0:2717:C:O2'	1:0:2718:C:H5''	2.00	0.60
2:A:192:VAL:HG11	2:A:208:HIS:H	1.65	0.60
9:H:57:THR:N	9:H:132:ALA:HB2	2.17	0.60
12:K:109:LEU:HD12	12:K:113:ILE:HD11	1.82	0.60
18:Q:64:GLU:HG3	18:Q:74:ASP:OD2	2.01	0.60
1:0:56:G:H5''	23:V:50:ARG:NH1	2.15	0.60
1:0:1120:U:H5''	1:0:1120:U:C6	2.36	0.60
1:0:2325:U:O2'	1:0:2411:C:H1'	2.00	0.60
1:0:2329:C:O2'	1:0:2330:U:H5'	2.01	0.60
2:A:36:ASP:O	2:A:38:ILE:N	2.33	0.60
2:A:51:ARG:HB2	40:A:5706:HOH:O	2.01	0.60
14:M:77:HIS:CD2	14:M:81:ARG:H	2.19	0.60
1:0:440:C:H2'	1:0:441:A:C8	2.37	0.60
1:0:1613:C:H2'	1:0:1614:G:O4'	2.00	0.60
5:D:58:VAL:CG1	5:D:60:GLU:HG2	2.31	0.60
15:N:27:LEU:HD22	15:N:50:LEU:HD22	1.84	0.60
25:X:22:ASN:HA	25:X:25:ARG:HG3	1.83	0.60
1:0:24:G:N2	1:0:518:G:H1'	2.15	0.60
1:0:291:C:H2'	1:0:292:G:O4'	2.02	0.60
1:0:2563:U:H2'	1:0:2565:C:O5'	2.01	0.60
1:0:2689:A:H2'	1:0:2690:U:H5'	1.83	0.60
3:B:7:ARG:HG2	3:B:7:ARG:HH11	1.65	0.60
4:C:188:ARG:HD3	40:C:2507:HOH:O	2.00	0.60
24:W:137:GLN:HE21	24:W:141:HIS:CE1	2.09	0.60
28:1:25:LYS:HD2	29:2:49:GLU:N	2.16	0.60
1:0:1733:A:H4'	3:B:212:GLN:HA	1.84	0.60
1:0:2542:C:H1'	40:4:6378:HOH:O	2.01	0.60
4:C:145:GLU:OE1	4:C:198:ASP:HB2	2.02	0.60
12:K:88:VAL:HG22	22:U:20:MET:HB3	1.82	0.60
19:R:72:VAL:HG12	19:R:73:ASP:N	2.16	0.60
24:W:59:GLN:HE22	24:W:98:PHE:N	1.98	0.60
26:Y:126:PRO:HG2	26:Y:128:PHE:CE1	2.37	0.60
31:9:76:G:C3'	31:9:77:A:H5''	2.24	0.60
1:0:1189:A:O2'	1:0:1208:C:H2'	2.02	0.60
1:0:1654:U:H2'	2:A:47:HIS:CD2	2.36	0.60
1:0:1687:C:O2	28:1:9:GLY:HA2	2.00	0.60
2:A:153:ARG:HB2	2:A:153:ARG:NH1	2.11	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:154:LYS:H	5:D:154:LYS:CD	2.10	0.60
6:E:24:GLY:HA3	6:E:76:VAL:HB	1.84	0.60
11:J:74:ARG:NH1	11:J:76:ASP:HB2	2.17	0.60
12:K:74:VAL:CG1	12:K:113:ILE:HG12	2.30	0.60
13:L:57:VAL:O	13:L:57:VAL:HG12	2.02	0.60
22:U:13:ILE:HG23	40:U:3194:HOH:O	2.00	0.60
24:W:119:HIS:HD2	24:W:120:PRO:O	1.83	0.60
1:0:1666:C:H2'	1:0:1667:A:H5'	1.84	0.60
1:0:2250:G:H2'	1:0:2251:G:O4'	2.02	0.60
1:0:2335:C:H2'	1:0:2336:G:C8	2.37	0.60
40:0:3857:HOH:O	14:M:125:ARG:HD2	2.01	0.60
12:K:13:GLU:O	12:K:16:SER:HB2	2.02	0.60
25:X:43:VAL:HG12	25:X:44:ASP:N	2.17	0.60
1:0:2055:A:H4'	19:R:132:ARG:HH21	1.67	0.60
1:0:2315:C:H5''	40:0:7987:HOH:O	2.02	0.60
3:B:274:GLU:HA	3:B:292:GLY:O	2.01	0.60
9:H:26:ILE:HA	9:H:123:ILE:HG21	1.84	0.60
13:L:17:SER:O	13:L:19:LYS:N	2.35	0.60
1:0:694:A:H2'	1:0:695:C:H5'	1.83	0.59
1:0:1308:A:C4'	4:C:226:GLY:HA3	2.32	0.59
1:0:1973:A:H5'	1:0:1973:A:H8	1.67	0.59
6:E:20:ILE:HD11	6:E:40:VAL:CG1	2.32	0.59
7:F:57:GLU:O	7:F:61:MET:HG3	2.02	0.59
10:I:85:GLY:O	10:I:86:GLU:HG3	2.02	0.59
10:I:88:GLN:HA	10:I:91:PHE:CE2	2.37	0.59
10:I:91:PHE:HA	10:I:131:GLY:HA3	1.83	0.59
17:P:115:SER:C	17:P:117:SER:H	2.05	0.59
21:T:43:ASN:ND2	21:T:108:ARG:CZ	2.61	0.59
1:0:333:G:O2'	1:0:334:G:H5'	2.02	0.59
8:G:64:ASN:HD22	8:G:64:ASN:N	2.00	0.59
1:0:308:U:H5'	1:0:309:C:OP1	2.02	0.59
1:0:1001:U:O2'	1:0:1002:G:H5'	2.02	0.59
1:0:2468:A:N6	30:3:50:GLY:HA2	2.17	0.59
1:0:2537:G:H5''	1:0:2538:A:H5''	1.84	0.59
1:0:2781:U:H2'	1:0:2782:G:H5'	1.84	0.59
5:D:84:LEU:HA	5:D:87:ALA:HB3	1.85	0.59
7:F:58:GLU:OE1	14:M:27:ARG:NH2	2.33	0.59
8:G:23:ILE:HD13	8:G:67:LEU:HD23	1.83	0.59
11:J:130:VAL:HG12	11:J:131:THR:N	2.16	0.59
31:9:107:C:H2'	31:9:108:C:C6	2.37	0.59
2:A:81:GLN:H	2:A:92:ASN:ND2	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:P:83:LYS:HG3	17:P:84:ALA:H	1.67	0.59
28:1:2:GLY:O	28:1:6:PRO:HG2	2.01	0.59
1:0:2735:U:H2'	1:0:2736:U:C6	2.37	0.59
5:D:50:VAL:O	5:D:71:ALA:HA	2.02	0.59
6:E:7:ILE:HD11	6:E:11:VAL:C	2.22	0.59
7:F:30:LYS:HB2	7:F:97:ALA:HB3	1.85	0.59
15:N:34:LEU:HD13	15:N:47:LEU:CD2	2.33	0.59
24:W:88:THR:HB	40:W:6679:HOH:O	2.03	0.59
1:0:316:A:N3	1:0:336:G:O2'	2.35	0.59
1:0:645:U:OP2	13:L:4:LYS:HE2	2.02	0.59
1:0:1940:C:H1'	40:0:4154:HOH:O	2.02	0.59
1:0:2301:A:H5''	1:0:2302:A:H5'	1.85	0.59
12:K:62:PRO:HG3	12:K:65:ARG:HH21	1.68	0.59
17:P:13:VAL:HG13	17:P:14:LEU:N	2.17	0.59
22:U:14:GLU:O	22:U:17:THR:HB	2.03	0.59
24:W:22:GLU:HG2	24:W:27:HIS:CD2	2.37	0.59
1:0:1681:G:H5''	1:0:1682:A:H5'	1.84	0.59
5:D:159:PRO:O	5:D:163:VAL:HG23	2.03	0.59
13:L:136:ALA:HB3	40:L:6166:HOH:O	2.02	0.59
15:N:154:LEU:O	15:N:155:GLU:HB3	2.03	0.59
1:0:2534:C:H1'	40:0:7954:HOH:O	2.02	0.59
5:D:138:GLY:HA2	31:9:29:C:O3'	2.03	0.59
1:0:1766:U:O2	1:0:1778:A:H5'	2.02	0.59
1:0:2880:A:H2'	1:0:2881:C:H5'	1.84	0.59
2:A:94:LEU:HD23	2:A:94:LEU:N	2.17	0.59
2:A:17:ARG:HD2	40:A:1373:HOH:O	2.02	0.59
3:B:97:LEU:O	3:B:98:THR:HG23	2.03	0.59
14:M:74:LYS:CD	14:M:91:ILE:HD11	2.33	0.59
15:N:73:ALA:HB1	15:N:74:PRO:HD2	1.85	0.59
15:N:77:ASN:OD1	15:N:79:PRO:HD2	2.02	0.59
1:0:1741:U:O2'	1:0:2723:G:H4'	2.03	0.58
40:0:4499:HOH:O	8:G:12:ILE:HG23	2.03	0.58
17:P:13:VAL:HG13	17:P:14:LEU:H	1.66	0.58
26:Y:117:LEU:HA	26:Y:174:VAL:HG11	1.85	0.58
30:3:34:LYS:HB2	30:3:34:LYS:NZ	2.18	0.58
1:0:195:C:H2'	1:0:196:G:H5'	1.85	0.58
2:A:167:LYS:HE3	27:Z:50:VAL:HA	1.85	0.58
4:C:27:ARG:NH1	4:C:30:LEU:HG	2.18	0.58
14:M:166:ALA:HB2	14:M:169:ARG:HH21	1.67	0.58
21:T:24:ARG:HH21	21:T:39:ASN:HD22	1.51	0.58
1:0:2437:A:H2'	1:0:2438:G:C8	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:125:ASN:HB3	2:A:158:VAL:HG12	1.84	0.58
2:A:167:LYS:CE	27:Z:50:VAL:HG13	2.34	0.58
5:D:58:VAL:HB	5:D:62:ASP:CB	2.33	0.58
5:D:134:LEU:HD11	5:D:166:ILE:HD11	1.83	0.58
10:I:107:LYS:HB3	10:I:110:ASP:HB2	1.84	0.58
14:M:47:ASP:CG	14:M:48:LYS:H	2.05	0.58
15:N:115:VAL:HG23	15:N:116:PHE:H	1.68	0.58
24:W:27:HIS:C	24:W:28:HIS:HD2	2.05	0.58
26:Y:106:THR:HG23	26:Y:107:PRO:HD2	1.84	0.58
26:Y:234:VAL:HG12	26:Y:235:GLU:N	2.19	0.58
1:O:290:C:O2'	1:O:291:C:H5'	2.02	0.58
1:O:2588:OMG:N1	32:4:75:C:N3	2.39	0.58
2:A:135:VAL:HG11	2:A:147:ARG:NH2	2.18	0.58
2:A:192:VAL:CG1	2:A:208:HIS:H	2.17	0.58
9:H:41:LYS:HD3	9:H:46:TYR:OH	2.03	0.58
1:O:1066:U:H2'	1:O:1067:A:C8	2.37	0.58
1:O:1119:G:H5'	11:J:52:GLN:HE21	1.68	0.58
1:O:2434:A:O2'	30:3:27:SER:HB3	2.04	0.58
1:O:2781:U:C2'	1:O:2782:G:H5'	2.33	0.58
7:F:13:GLU:OE2	7:F:78:GLU:HG2	2.02	0.58
26:Y:99:ALA:HB2	26:Y:233:TYR:CZ	2.38	0.58
30:3:70:ARG:HD3	30:3:77:ALA:HB2	1.84	0.58
31:9:91:C:H2'	31:9:92:G:O4'	2.03	0.58
1:O:308:U:H2'	21:T:52:ARG:NH2	2.18	0.58
1:O:933:C:H4'	1:O:1297:U:H4'	1.86	0.58
3:B:36:PRO:CG	3:B:169:GLY:H	2.16	0.58
13:L:55:GLN:HA	13:L:58:GLN:NE2	2.08	0.58
17:P:103:THR:O	17:P:107:GLU:HG3	2.04	0.58
14:M:133:LEU:O	14:M:134:ILE:HD13	2.04	0.58
15:N:61:ALA:HB2	15:N:88:ALA:HB2	1.86	0.58
18:Q:64:GLU:HG3	18:Q:74:ASP:CG	2.23	0.58
5:D:67:ASP:O	5:D:69:ILE:HG13	2.02	0.58
13:L:148:GLU:HA	40:L:6153:HOH:O	2.02	0.58
19:R:125:ARG:HG2	40:R:3539:HOH:O	2.04	0.58
23:V:11:MET:HB3	23:V:15:GLU:HB2	1.85	0.58
25:X:51:ASP:OD2	25:X:52:PRO:HD2	2.04	0.58
1:O:644:G:H5'	1:O:644:G:N3	2.19	0.58
1:O:926:A:C4'	13:L:39:GLU:HG2	2.33	0.58
1:O:1202:A:H2'	1:O:1203:G:O4'	2.03	0.58
4:C:14:GLY:O	4:C:15:GLU:HB3	2.04	0.58
4:C:136:VAL:HG22	4:C:137:PRO:HA	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:O:38:ARG:HD3	40:O:7674:HOH:O	2.03	0.58
21:T:48:VAL:HG21	21:T:96:VAL:CG1	2.33	0.58
1:O:247:A:H2'	40:O:8472:HOH:O	2.04	0.58
5:D:154:LYS:HD2	5:D:154:LYS:N	2.14	0.58
6:E:14:GLU:HG2	6:E:15:GLN:H	1.68	0.58
6:E:100:ASP:HB2	40:E:2789:HOH:O	2.04	0.58
9:H:41:LYS:HG2	9:H:42:ASP:H	1.69	0.58
10:I:94:ASP:OD1	10:I:133:THR:HB	2.04	0.58
20:S:6:LYS:NZ	20:S:61:GLU:HG2	2.19	0.58
1:O:420:U:H5'	1:O:1920:C:C2	2.39	0.57
3:B:147:VAL:O	3:B:147:VAL:HG12	2.04	0.57
5:D:86:THR:O	5:D:90:LEU:HG	2.04	0.57
9:H:76:LEU:HD21	9:H:149:VAL:HA	1.86	0.57
14:M:99:ARG:HG2	14:M:99:ARG:NH1	2.07	0.57
18:Q:27:GLN:HE21	31:9:8:G:H4'	1.69	0.57
27:Z:62:ALA:HA	27:Z:69:ASP:HA	1.84	0.57
1:O:2353:A:H4'	1:O:2354:A:O5'	2.04	0.57
1:O:2766:A:H5'	40:O:4808:HOH:O	2.03	0.57
24:W:84:VAL:HG12	40:W:6679:HOH:O	2.04	0.57
1:O:2321:A:H2	1:O:2378:U:H3	1.50	0.57
1:O:2345:A:H3'	1:O:2346:C:C6	2.38	0.57
1:O:2374:G:H2'	1:O:2375:A:C8	2.39	0.57
1:O:2533:C:H6	1:O:2533:C:C5'	2.14	0.57
1:O:2618:G:O2'	32:4:76:5AA:N1	2.33	0.57
17:P:105:LEU:CD2	17:P:137:LEU:HD21	2.33	0.57
1:O:1181:A:H2'	1:O:1182:C:H5'	1.87	0.57
1:O:2703:A:H2'	1:O:2704:C:H6	1.68	0.57
1:O:2769:C:O2'	1:O:2770:G:H5'	2.04	0.57
14:M:164:THR:CG2	14:M:165:GLY:N	2.66	0.57
17:P:103:THR:HA	17:P:106:ARG:HH12	1.69	0.57
26:Y:117:LEU:HD12	26:Y:174:VAL:HG13	1.87	0.57
1:O:297:U:H2'	1:O:298:C:H6	1.67	0.57
1:O:1183:C:H42	1:O:1184:C:H41	1.52	0.57
1:O:1451:C:H5'	1:O:1505:U:C5	2.38	0.57
1:O:1654:U:C2'	2:A:47:HIS:HD2	2.17	0.57
1:O:2676:C:H4'	11:J:70:PHE:CD1	2.40	0.57
3:B:56:ASP:CB	3:B:322:ARG:HE	2.17	0.57
3:B:238:ASN:HD22	3:B:240:GLY:H	1.52	0.57
5:D:49:PRO:HA	5:D:73:VAL:HG22	1.86	0.57
25:X:72:VAL:HG22	25:X:85:VAL:CG1	2.32	0.57
1:O:92:G:C4'	23:V:44:GLY:HA3	2.31	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:100:C:H2'	1:0:101:C:H6	1.68	0.57
40:0:6085:HOH:O	30:3:79:LEU:HB2	2.04	0.57
2:A:125:ASN:CB	2:A:158:VAL:HG12	2.35	0.57
5:D:10:PHE:CG	5:D:11:HIS:N	2.73	0.57
12:K:34:VAL:HG22	12:K:47:ALA:HB2	1.85	0.57
16:O:14:LEU:HD23	16:O:102:ILE:HD11	1.87	0.57
23:V:39:ALA:N	23:V:40:PRO:CD	2.68	0.57
23:V:44:GLY:O	23:V:48:GLU:HG2	2.05	0.57
24:W:34:LEU:HD12	24:W:107:LEU:HD11	1.86	0.57
1:0:228:C:H2'	1:0:229:G:H5'	1.85	0.57
1:0:1486:A:C5	29:2:2:LYS:HG3	2.39	0.57
1:0:1566:C:H2'	1:0:1567:G:H8	1.70	0.57
1:0:1829:A:H2'	1:0:1830:C:H5'	1.86	0.57
6:E:8:PRO:HB2	6:E:11:VAL:HG23	1.87	0.57
14:M:73:ARG:HD2	14:M:73:ARG:N	2.18	0.57
24:W:142:ASP:HB3	24:W:145:GLY:H	1.70	0.57
26:Y:235:GLU:CD	26:Y:235:GLU:N	2.54	0.57
31:9:116:C:O2'	31:9:117:G:H5'	2.05	0.57
1:0:1882:C:OP1	2:A:192:VAL:HG23	2.05	0.57
3:B:232:TRP:HD1	3:B:235:ARG:HD2	1.68	0.57
9:H:61:ARG:HG3	9:H:61:ARG:NH1	2.20	0.57
1:0:1829:A:N6	27:Z:42:TYR:HA	2.19	0.57
1:0:2737:C:OP2	17:P:61:ARG:NH2	2.37	0.57
3:B:199:TYR:HE2	3:B:268:ARG:HB2	1.70	0.57
15:N:114:LYS:O	15:N:118:ILE:HG13	2.05	0.57
1:0:57:C:H42	1:0:89:G:H1	1.53	0.57
1:0:1416:G:H2'	1:0:1417:G:H5'	1.86	0.57
1:0:1522:A:H1'	1:0:1665:G:N2	2.19	0.57
1:0:2457:U:H4'	30:3:80:ARG:O	2.04	0.57
3:B:215:VAL:HA	3:B:220:VAL:HG22	1.85	0.57
13:L:143:THR:HG22	13:L:144:ASP:N	2.19	0.57
17:P:55:LYS:CG	17:P:56:GLY:N	2.66	0.57
20:S:57:THR:HG22	20:S:58:MET:N	2.20	0.57
1:0:135:G:H5''	14:M:39:ARG:NH1	2.20	0.56
1:0:1183:C:H2'	40:0:5603:HOH:O	2.05	0.56
1:0:1441:G:O2'	1:0:1442:A:H5'	2.05	0.56
1:0:2507:G:H2'	1:0:2510:C:H42	1.69	0.56
38:0:2924:MYL:OAJ	38:0:2924:MYL:HBC	2.04	0.56
2:A:81:GLN:HB2	2:A:92:ASN:HD22	1.69	0.56
5:D:25:MET:HE3	5:D:37:ALA:CB	2.34	0.56
5:D:172:VAL:HG12	5:D:173:GLU:N	2.19	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:N:24:LEU:HD13	18:Q:26:PRO:HB3	1.86	0.56
15:N:181:ASP:O	15:N:184:ILE:HG22	2.04	0.56
1:0:581:G:O2'	1:0:582:U:H5'	2.04	0.56
1:0:952:G:OP1	18:Q:42:LYS:HE2	2.05	0.56
2:A:191:GLY:HA2	2:A:194:MET:HE3	1.87	0.56
3:B:195:ARG:N	3:B:198:GLU:OE1	2.36	0.56
8:G:71:LEU:O	8:G:73:ASP:N	2.38	0.56
12:K:64:MET:HA	12:K:67:GLN:HE21	1.69	0.56
1:0:164:G:H3'	40:0:8187:HOH:O	2.04	0.56
1:0:636:G:H1'	1:0:2058:G:C4	2.40	0.56
1:0:699:C:H5'	40:0:8623:HOH:O	2.05	0.56
1:0:779:U:H3'	40:0:4557:HOH:O	2.05	0.56
1:0:807:A:O2'	1:0:808:A:H5'	2.05	0.56
1:0:1625:U:H4'	40:0:3427:HOH:O	2.06	0.56
1:0:2488:A:H1'	40:0:3183:HOH:O	2.04	0.56
7:F:81:ASP:HA	7:F:92:GLY:HA3	1.87	0.56
14:M:111:ASN:HB2	40:M:1852:HOH:O	2.04	0.56
21:T:41:ARG:NH1	21:T:42:VAL:O	2.39	0.56
23:V:42:ASN:HB3	40:V:7247:HOH:O	2.04	0.56
26:Y:112:GLU:HA	26:Y:112:GLU:OE1	2.04	0.56
30:3:88:LEU:HD23	30:3:90:PHE:HE2	1.70	0.56
1:0:671:A:O2'	1:0:672:G:H2'	2.05	0.56
1:0:1268:C:O2'	1:0:1269:G:H5'	2.05	0.56
1:0:1387:G:H1'	17:P:28:GLN:HE22	1.68	0.56
1:0:2064:U:H5'	1:0:2652:U:H4'	1.87	0.56
1:0:2105:C:H4'	40:0:5147:HOH:O	2.05	0.56
40:0:5620:HOH:O	18:Q:11:ARG:HD3	2.04	0.56
2:A:30:ARG:HG2	2:A:31:LYS:H	1.70	0.56
3:B:56:ASP:HB2	3:B:322:ARG:HH21	1.70	0.56
4:C:35:VAL:HG21	4:C:227:GLY:HA2	1.88	0.56
13:L:104:ASP:O	13:L:105:TYR:HB3	2.04	0.56
25:X:72:VAL:CG2	25:X:85:VAL:HG12	2.32	0.56
1:0:210:U:O2'	1:0:211:U:H5'	2.05	0.56
1:0:1120:U:H5''	1:0:1120:U:H6	1.70	0.56
1:0:1667:A:H5'	1:0:1667:A:C8	2.32	0.56
1:0:2241:C:H2'	1:0:2242:U:C6	2.41	0.56
1:0:2460:A:H5''	30:3:59:ASP:OD1	2.06	0.56
1:0:2689:A:C2'	1:0:2690:U:H5'	2.35	0.56
7:F:46:GLU:OE1	7:F:100:ASP:HA	2.06	0.56
14:M:15:PRO:HA	14:M:20:LEU:HD23	1.86	0.56
15:N:67:ALA:HA	15:N:71:TRP:HB3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:W:99:ALA:HA	24:W:102:SER:OG	2.06	0.56
1:0:338:C:H4'	4:C:174:ILE:CD1	2.35	0.56
1:0:951:A:O2'	1:0:952:G:H5'	2.06	0.56
40:0:6374:HOH:O	28:1:46:ARG:HA	2.04	0.56
3:B:145:HIS:HD2	3:B:146:THR:O	1.88	0.56
8:G:68:GLU:HA	8:G:71:LEU:HD12	1.88	0.56
13:L:34:GLY:HA3	13:L:38:HIS:CE1	2.41	0.56
14:M:61:ILE:HD12	14:M:61:ILE:N	2.21	0.56
16:O:14:LEU:CD2	16:O:102:ILE:HD11	2.35	0.56
19:R:39:THR:O	19:R:42:GLU:N	2.38	0.56
28:1:26:SER:HB3	28:1:35:SER:OG	2.06	0.56
1:0:441:A:H1'	1:0:442:A:N7	2.21	0.56
1:0:745:G:O6	16:O:68:GLY:HA3	2.06	0.56
1:0:1714:C:O2'	1:0:1715:C:H5'	2.06	0.56
1:0:2252:A:C5	1:0:2253:G:H1'	2.41	0.56
14:M:84:LYS:HG2	30:3:46:ILE:O	2.05	0.56
15:N:147:ILE:HD12	40:9:4707:HOH:O	2.05	0.56
17:P:42:GLU:O	17:P:46:GLU:HG3	2.05	0.56
24:W:90:TYR:HE2	24:W:99:ALA:HB2	1.71	0.56
27:Z:54:GLU:HG2	27:Z:57:MET:HE2	1.88	0.56
30:3:25:VAL:HG22	30:3:68:LYS:HE3	1.87	0.56
1:0:736:A:H2'	1:0:737:A:O4'	2.05	0.56
1:0:1184:C:H1'	40:0:7308:HOH:O	2.04	0.56
1:0:2073:G:OP2	1:0:2490:A:H5'	2.05	0.56
1:0:2281:C:C2'	1:0:2282:U:H5'	2.34	0.56
40:0:4782:HOH:O	24:W:119:HIS:HE1	1.87	0.56
10:I:102:GLN:HA	10:I:105:GLU:OE2	2.06	0.56
14:M:138:HIS:ND1	14:M:139:PRO:HD2	2.20	0.56
15:N:132:ASN:O	15:N:135:VAL:HG12	2.06	0.56
15:N:143:ARG:HG2	15:N:172:PHE:CD2	2.41	0.56
17:P:14:LEU:HD13	17:P:51:ALA:HB2	1.87	0.56
20:S:14:ALA:HA	20:S:25:GLN:NE2	2.21	0.56
25:X:76:ARG:HG3	25:X:76:ARG:NH1	2.19	0.56
28:1:22:CYS:HA	40:1:2086:HOH:O	2.05	0.56
1:0:1038:G:O2'	1:0:1039:G:H5'	2.06	0.56
1:0:2006:C:H3'	1:0:2007:A:H2'	1.87	0.56
1:0:2438:G:H5'	40:0:5494:HOH:O	2.05	0.56
40:0:4808:HOH:O	3:B:267:LYS:HA	2.06	0.56
6:E:77:THR:OG1	6:E:78:GLU:N	2.34	0.56
11:J:25:GLN:HE22	11:J:116:LEU:HB3	1.69	0.56
17:P:138:GLU:O	17:P:140:TYR:N	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:T:115:GLU:HG3	21:T:116:ASP:N	2.21	0.56
1:0:1118:A:C8	1:0:1118:A:C3'	2.88	0.56
1:0:2565:C:H4'	40:0:3660:HOH:O	2.06	0.56
5:D:78:GLU:HB3	5:D:82:GLU:OE2	2.06	0.56
14:M:69:LYS:O	14:M:73:ARG:NH2	2.36	0.56
29:2:43:ARG:HG2	40:2:6577:HOH:O	2.06	0.56
1:0:1666:C:C2'	1:0:1667:A:H5''	2.36	0.55
1:0:2827:A:H2'	1:0:2828:G:O4'	2.05	0.55
3:B:14:GLY:HA2	3:B:15:PRO:C	2.26	0.55
5:D:23:VAL:HG23	5:D:23:VAL:O	2.06	0.55
9:H:174:LEU:HA	40:H:5702:HOH:O	2.06	0.55
10:I:124:VAL:O	10:I:124:VAL:HG12	2.06	0.55
14:M:31:TRP:HA	14:M:34:GLU:HG3	1.88	0.55
17:P:135:ALA:CB	17:P:139:ARG:HH12	2.12	0.55
21:T:28:SER:HA	21:T:97:ARG:HD3	1.88	0.55
26:Y:152:LYS:HB3	26:Y:160:LYS:HG3	1.88	0.55
1:0:1118:A:C8	1:0:1119:G:H5''	2.41	0.55
1:0:1701:A:H4'	1:0:1702:U:C5'	2.34	0.55
1:0:2345:A:H3'	1:0:2346:C:H6	1.72	0.55
1:0:2466:G:H2'	40:0:7450:HOH:O	2.06	0.55
1:0:2755:G:H1'	40:0:3447:HOH:O	2.06	0.55
12:K:24:THR:HG22	12:K:105:ARG:HG2	1.88	0.55
13:L:143:THR:HG22	13:L:145:LEU:H	1.71	0.55
14:M:183:THR:OG1	14:M:184:ARG:N	2.39	0.55
15:N:139:TRP:HA	15:N:139:TRP:HE3	1.70	0.55
30:3:25:VAL:HG12	30:3:27:SER:H	1.71	0.55
1:0:303:C:O2'	1:0:304:G:H5'	2.06	0.55
1:0:1586:G:O2'	1:0:1587:U:H5'	2.06	0.55
1:0:1940:C:H4'	40:0:7130:HOH:O	2.06	0.55
1:0:2044:G:OP1	25:X:23:HIS:HE1	1.89	0.55
1:0:2780:C:H2'	1:0:2781:U:H6	1.71	0.55
40:0:4939:HOH:O	14:M:68:ARG:HG3	2.06	0.55
4:C:127:ARG:HG2	4:C:127:ARG:HH11	1.71	0.55
4:C:153:VAL:O	4:C:157:LEU:HG	2.06	0.55
5:D:12:GLU:O	5:D:15:GLU:HG2	2.06	0.55
1:0:419:A:H1'	1:0:1921:A:C2	2.40	0.55
1:0:1014:A:H2'	1:0:1015:C:H5'	1.87	0.55
1:0:1477:C:O2'	1:0:1478:U:H5'	2.06	0.55
40:0:3422:HOH:O	30:3:50:GLY:HA3	2.06	0.55
40:0:7150:HOH:O	2:A:177:HIS:HE1	1.90	0.55
6:E:68:HIS:O	6:E:72:MET:HG3	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:J:22:VAL:O	11:J:26:VAL:HG23	2.06	0.55
13:L:73:VAL:HG23	13:L:74:THR:H	1.70	0.55
14:M:28:GLN:HA	14:M:31:TRP:HB2	1.89	0.55
31:9:61:C:H2'	31:9:62:A:H8	1.71	0.55
1:0:216:A:O2'	1:0:217:C:H5'	2.06	0.55
1:0:248:A:H5'	1:0:249:G:OP2	2.07	0.55
1:0:1162:G:H1'	10:I:112:LEU:CD1	2.35	0.55
1:0:1189:A:H1'	1:0:1209:C:H1'	1.87	0.55
1:0:1278:A:H4'	1:0:1279:U:C4	2.41	0.55
1:0:1398:G:H2'	1:0:1399:A:C8	2.41	0.55
1:0:1557:G:H2'	1:0:1558:C:H6	1.72	0.55
1:0:1616:A:H5''	1:0:1617:C:OP1	2.07	0.55
1:0:1921:A:O2'	1:0:1922:A:H5'	2.06	0.55
1:0:2240:U:O2'	1:0:2241:C:H5'	2.05	0.55
3:B:141:ARG:HD2	3:B:163:GLU:OE2	2.07	0.55
6:E:49:ILE:HD11	6:E:69:ILE:HD12	1.89	0.55
14:M:77:HIS:HB2	14:M:81:ARG:CZ	2.36	0.55
22:U:39:ASN:HD22	22:U:49:LEU:CD1	2.19	0.55
30:3:2:GLN:O	30:3:3:MET:HB2	2.06	0.55
31:9:35:C:H5''	40:9:4078:HOH:O	2.05	0.55
32:4:176:DA:O4'	32:4:175:C:H2'	2.06	0.55
1:0:1304:U:H2'	1:0:1305:C:C6	2.41	0.55
4:C:237:GLU:HB2	40:C:5218:HOH:O	2.07	0.55
11:J:43:ARG:HG2	40:J:5361:HOH:O	2.06	0.55
24:W:4:LEU:CD1	24:W:52:VAL:HG21	2.36	0.55
24:W:4:LEU:HD22	24:W:54:PHE:HB3	1.89	0.55
1:0:2090:G:H2'	1:0:2091:G:C8	2.42	0.55
1:0:2319:C:H3'	30:3:1:MET:H2	1.68	0.55
1:0:2409:C:H4'	30:3:17:HIS:CG	2.42	0.55
4:C:236:THR:HG22	4:C:239:ALA:CB	2.36	0.55
5:D:18:ILE:HG12	5:D:134:LEU:HD23	1.86	0.55
7:F:29:VAL:HA	7:F:99:THR:HG22	1.89	0.55
10:I:123:VAL:C	10:I:125:GLY:H	2.09	0.55
13:L:35:ARG:HB2	13:L:43:HIS:CD2	2.42	0.55
14:M:47:ASP:CG	14:M:48:LYS:N	2.60	0.55
16:O:15:LYS:O	16:O:16:SER:C	2.45	0.55
1:0:214:U:H5'	40:0:5454:HOH:O	2.06	0.55
5:D:19:GLU:HG3	40:D:6165:HOH:O	2.05	0.55
5:D:58:VAL:HG12	5:D:60:GLU:HG2	1.88	0.55
13:L:67:ARG:O	13:L:71:GLU:HG3	2.07	0.55
14:M:164:THR:HG22	14:M:165:GLY:N	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:241:A:C2	1:0:378:A:H4'	2.41	0.55
1:0:485:A:N3	1:0:487:G:H5''	2.22	0.55
1:0:952:G:N3	1:0:2302:A:H2'	2.21	0.55
1:0:1119:G:N2	1:0:1246:A:C2	2.65	0.55
1:0:2135:A:O2'	1:0:2136:G:H5'	2.06	0.55
1:0:2404:G:H5''	40:0:4170:HOH:O	2.06	0.55
1:0:2790:C:HO2'	1:0:2791:U:H6	1.55	0.55
1:0:2851:G:H2'	1:0:2902:A:H61	1.71	0.55
5:D:36:ASN:HA	40:D:7500:HOH:O	2.06	0.55
10:I:133:THR:HG22	10:I:134:ILE:H	1.72	0.55
12:K:58:THR:HG22	12:K:59:LYS:HG3	1.87	0.55
19:R:132:ARG:HG2	19:R:133:ALA:N	2.21	0.55
1:0:371:U:H2'	1:0:372:A:C8	2.41	0.55
1:0:1922:A:H2'	30:3:33:MET:HG2	1.89	0.55
1:0:2862:G:H4'	3:B:336:GLN:O	2.06	0.55
4:C:129:HIS:HA	4:C:165:ASP:OD1	2.07	0.55
18:Q:19:ARG:HH21	31:9:11:A:P	2.29	0.55
25:X:49:ARG:HD3	25:X:84:ILE:HG12	1.89	0.55
27:Z:62:ALA:HA	27:Z:68:GLU:O	2.07	0.55
29:2:36:ASN:HD22	29:2:39:ARG:HG2	1.71	0.55
1:0:834:G:H4'	1:0:835:U:OP2	2.06	0.54
1:0:1434:A:H2'	1:0:1436:C:C5	2.41	0.54
1:0:1825:U:O2'	1:0:1826:C:H5'	2.07	0.54
1:0:2363:G:H4'	18:Q:11:ARG:HE	1.71	0.54
2:A:191:GLY:HA2	2:A:194:MET:CE	2.38	0.54
5:D:95:THR:C	5:D:97:GLN:H	2.10	0.54
5:D:163:VAL:HA	40:D:6326:HOH:O	2.07	0.54
14:M:52:GLN:HE22	14:M:118:TYR:HB3	1.71	0.54
17:P:98:ILE:HD12	17:P:102:ARG:NE	2.21	0.54
1:0:113:A:H3'	1:0:114:A:H5''	1.88	0.54
1:0:383:A:H2'	1:0:384:G:O4'	2.07	0.54
1:0:1072:G:OP2	26:Y:154:ARG:NH2	2.40	0.54
1:0:1829:A:H61	27:Z:42:TYR:HA	1.71	0.54
1:0:2362:A:H2'	1:0:2363:G:C8	2.43	0.54
1:0:2442:G:H3'	40:0:6128:HOH:O	2.06	0.54
11:J:39:VAL:HG22	11:J:107:ASN:HA	1.88	0.54
15:N:78:MET:HB2	15:N:79:PRO:HD3	1.90	0.54
17:P:16:VAL:HG13	17:P:20:ARG:NH1	2.23	0.54
1:0:110:C:H2'	1:0:111:C:H6	1.72	0.54
1:0:1446:U:C2'	20:S:55:GLN:NE2	2.70	0.54
3:B:36:PRO:HA	3:B:167:GLY:O	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:I:96:SER:HB3	10:I:99:GLN:HE21	1.72	0.54
10:I:101:LYS:O	10:I:105:GLU:HG3	2.07	0.54
24:W:4:LEU:CD2	24:W:54:PHE:HB3	2.37	0.54
25:X:71:ARG:HD3	40:X:2171:HOH:O	2.08	0.54
29:2:22:PRO:HG2	29:2:25:VAL:HG23	1.89	0.54
30:3:62:THR:HG22	30:3:63:LYS:N	2.22	0.54
30:3:83:TRP:HA	40:3:4958:HOH:O	2.08	0.54
1:0:31:C:H2'	40:0:7619:HOH:O	2.06	0.54
1:0:1074:G:H4'	1:0:1260:G:C6	2.42	0.54
1:0:1187:U:O2'	1:0:1189:A:H2	1.89	0.54
1:0:1386:G:O2'	1:0:1387:G:H5'	2.07	0.54
1:0:1805:G:H2'	1:0:1806:G:H8	1.70	0.54
2:A:167:LYS:HD2	27:Z:53:ILE:HG21	1.90	0.54
3:B:199:TYR:CE2	3:B:268:ARG:HB2	2.42	0.54
14:M:122:GLN:OE1	14:M:127:LYS:HE2	2.07	0.54
19:R:50:VAL:O	19:R:53:GLY:N	2.40	0.54
22:U:13:ILE:HG12	22:U:32:CYS:HB3	1.90	0.54
1:0:613:C:H2'	1:0:614:U:C6	2.42	0.54
1:0:722:G:H22	1:0:938:G:P	2.30	0.54
40:0:3133:HOH:O	3:B:214:PRO:HD2	2.08	0.54
3:B:279:THR:HG22	3:B:280:VAL:N	2.23	0.54
5:D:163:VAL:O	5:D:167:GLU:HB2	2.08	0.54
14:M:134:ILE:CG2	14:M:141:ILE:HD13	2.36	0.54
15:N:100:ALA:O	15:N:129:ILE:HG23	2.06	0.54
21:T:48:VAL:HG22	21:T:49:GLU:N	2.23	0.54
24:W:29:VAL:O	24:W:30:ASN:HB2	2.07	0.54
31:9:57:A:H2'	31:9:58:G:H5'	1.89	0.54
1:0:2032:U:H2'	1:0:2033:G:C5'	2.38	0.54
1:0:2269:C:H2'	1:0:2270:G:O4'	2.08	0.54
1:0:2587:OMU:H2'	1:0:2589:U:H5''	1.89	0.54
1:0:2670:G:O2'	1:0:2671:U:H5'	2.07	0.54
2:A:70:ALA:HB1	27:Z:89:THR:HG21	1.89	0.54
4:C:19:PRO:HG2	4:C:22:PHE:CD1	2.43	0.54
8:G:20:VAL:O	8:G:24:VAL:HG23	2.07	0.54
27:Z:54:GLU:HG2	27:Z:57:MET:HE1	1.90	0.54
29:2:9:LYS:O	29:2:12:ALA:HB3	2.07	0.54
1:0:1181:A:C2'	1:0:1182:C:H5'	2.37	0.54
1:0:1419:U:H5'	1:0:1420:C:OP2	2.07	0.54
1:0:1666:C:H2'	1:0:1667:A:C5'	2.37	0.54
1:0:1942:A:H2'	1:0:1943:C:C6	2.42	0.54
1:0:2281:C:H2'	1:0:2282:U:H5'	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2505:G:O2'	1:0:2506:A:H5'	2.08	0.54
1:0:2588:OMG:C6	32:4:76:5AA:H102	2.43	0.54
4:C:26:VAL:HG21	4:C:123:LEU:HD11	1.88	0.54
6:E:3:VAL:HG22	6:E:49:ILE:HB	1.90	0.54
8:G:22:ALA:O	8:G:25:GLU:HB3	2.07	0.54
19:R:18:LEU:HD12	19:R:143:VAL:HG11	1.90	0.54
31:9:92:G:H2'	31:9:93:A:H8	1.64	0.54
1:0:820:G:O2'	1:0:856:G:H4'	2.07	0.54
1:0:1894:C:N4	1:0:1939:U:H2'	2.23	0.54
1:0:2459:G:OP1	30:3:64:LYS:HB2	2.08	0.54
1:0:2832:C:OP1	19:R:71:LYS:HE3	2.08	0.54
2:A:39:ALA:O	2:A:61:GLU:HG3	2.08	0.54
2:A:217:ARG:HH11	2:A:217:ARG:CG	2.20	0.54
12:K:118:ALA:HA	12:K:125:ALA:HB2	1.90	0.54
13:L:134:GLU:HG3	40:L:4812:HOH:O	2.07	0.54
19:R:123:GLN:HA	19:R:137:ASN:OD1	2.07	0.54
31:9:7:G:H5'	40:9:5071:HOH:O	2.06	0.54
1:0:138:U:OP2	1:0:139:C:H5	1.90	0.54
1:0:1213:C:C2'	1:0:1214:G:H5'	2.38	0.54
1:0:2812:A:H2	1:0:2814:A:H62	1.56	0.54
12:K:20:CYS:HB2	12:K:29:LEU:HG	1.90	0.54
12:K:45:PRO:HB2	40:K:7169:HOH:O	2.07	0.54
17:P:115:SER:O	17:P:117:SER:N	2.41	0.54
23:V:1:THR:CG2	23:V:2:VAL:H	2.17	0.54
24:W:131:PRO:O	24:W:136:GLY:N	2.41	0.54
1:0:105:G:O2'	1:0:106:A:H5'	2.07	0.54
1:0:1787:C:H4'	1:0:2883:A:O4'	2.08	0.54
1:0:2346:C:O2'	5:D:52:THR:HG21	2.06	0.54
1:0:2783:A:H3'	40:0:4201:HOH:O	2.08	0.54
2:A:171:LYS:HG2	2:A:174:ASN:ND2	2.23	0.54
3:B:36:PRO:HG3	3:B:169:GLY:N	2.20	0.54
3:B:41:PHE:HB3	3:B:190:MET:CE	2.38	0.54
21:T:23:VAL:HG23	21:T:41:ARG:HG3	1.90	0.54
25:X:20:GLU:CG	25:X:21:PRO:HD2	2.38	0.54
30:3:2:GLN:HG3	30:3:91:GLN:NE2	2.23	0.54
31:9:29:C:C2'	31:9:30:C:H5'	2.36	0.54
31:9:49:G:O2'	31:9:50:G:H5'	2.08	0.54
1:0:392:U:O2'	14:M:182:LYS:HE2	2.08	0.53
1:0:485:A:O2'	1:0:487:G:H5'	2.08	0.53
1:0:1244:U:H4'	1:0:1246:A:O4'	2.08	0.53
1:0:1641:A:C2'	1:0:1642:A:H5'	2.35	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1753:C:O2	3:B:229:ARG:NH2	2.39	0.53
1:0:2428:G:H5'	40:0:6155:HOH:O	2.07	0.53
3:B:162:MET:HE3	3:B:310:ARG:HD3	1.88	0.53
6:E:21:THR:HG23	6:E:30:THR:OG1	2.08	0.53
9:H:48:VAL:HA	9:H:170:ARG:O	2.07	0.53
12:K:23:ASN:ND2	12:K:108:GLU:H	2.01	0.53
17:P:7:LYS:HD3	17:P:23:PHE:CZ	2.43	0.53
21:T:51:LEU:O	21:T:52:ARG:HD3	2.08	0.53
27:Z:101:LYS:HG2	27:Z:104:ARG:HH12	1.72	0.53
1:0:1377:C:H5'	1:0:1377:C:C6	2.40	0.53
1:0:1603:A:H5''	1:0:1605:G:H5'	1.90	0.53
1:0:1794:G:P	17:P:133:SER:HB2	2.47	0.53
1:0:1856:C:H5'	1:0:1858:A:O4'	2.08	0.53
3:B:51:VAL:HG23	3:B:330:VAL:HG22	1.91	0.53
12:K:98:VAL:HG13	12:K:102:GLU:HA	1.85	0.53
15:N:38:LYS:HE2	15:N:107:ASN:HD22	1.70	0.53
22:U:14:GLU:OE1	22:U:15:PRO:HD2	2.08	0.53
1:0:170:U:H5'	30:3:48:ASN:HB3	1.91	0.53
1:0:1555:G:H4'	1:0:1630:A:C2	2.43	0.53
1:0:2320:U:C2'	30:3:2:GLN:HB2	2.38	0.53
1:0:2825:C:H4'	1:0:2826:G:O5'	2.09	0.53
3:B:162:MET:HG3	3:B:310:ARG:NH1	2.23	0.53
5:D:63:ILE:HG13	5:D:64:ARG:N	2.23	0.53
18:Q:59:GLN:OE1	18:Q:75:ILE:HB	2.08	0.53
24:W:13:MET:HE3	24:W:17:ILE:HG22	1.90	0.53
31:9:95:C:O2'	31:9:96:C:H5'	2.09	0.53
1:0:420:U:H5'	1:0:1920:C:O2	2.09	0.53
1:0:1664:A:H8	1:0:1664:A:OP1	1.91	0.53
1:0:2893:C:O2'	1:0:2894:C:H5'	2.08	0.53
2:A:9:ARG:HG2	2:A:16:PHE:CD2	2.43	0.53
7:F:26:THR:HG21	7:F:102:GLY:C	2.28	0.53
8:G:67:LEU:O	8:G:71:LEU:HG	2.08	0.53
15:N:4:PRO:HG3	31:9:69:U:OP1	2.08	0.53
19:R:47:LEU:O	19:R:51:ILE:HG13	2.09	0.53
21:T:49:GLU:HB3	21:T:59:GLU:HG2	1.90	0.53
23:V:39:ALA:C	23:V:41:GLU:H	2.11	0.53
26:Y:107:PRO:HB3	26:Y:182:PHE:CD2	2.44	0.53
1:0:1008:C:H5''	9:H:19:ARG:HH12	1.73	0.53
1:0:1735:C:OP2	3:B:234:ARG:HG3	2.08	0.53
1:0:2768:A:H2'	1:0:2769:C:O4'	2.07	0.53
6:E:172:PRO:HB3	40:E:6931:HOH:O	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:H:128:ALA:HA	40:H:175:HOH:O	2.09	0.53
11:J:64:GLY:HA3	36:J:8821:CL:CL	2.45	0.53
11:J:74:ARG:O	11:J:78:ILE:HG12	2.08	0.53
12:K:105:ARG:HD2	40:K:3385:HOH:O	2.08	0.53
17:P:40:VAL:O	17:P:44:VAL:HG23	2.08	0.53
28:1:18:LYS:HA	28:1:25:LYS:HA	1.90	0.53
28:1:25:LYS:O	28:1:25:LYS:HG2	2.09	0.53
30:3:2:GLN:HB3	30:3:91:GLN:HG3	1.90	0.53
30:3:11:CYS:HA	40:3:3538:HOH:O	2.07	0.53
1:0:338:C:H4'	4:C:174:ILE:HD11	1.90	0.53
1:0:703:G:O2'	1:0:704:C:H5'	2.09	0.53
1:0:2780:C:H2'	1:0:2781:U:C6	2.43	0.53
3:B:215:VAL:HB	40:B:5430:HOH:O	2.09	0.53
5:D:47:GLN:NE2	5:D:75:LEU:HD23	2.23	0.53
5:D:60:GLU:HG3	5:D:60:GLU:O	2.08	0.53
9:H:50:ILE:HG12	9:H:168:VAL:HG22	1.90	0.53
20:S:18:MET:HG3	20:S:74:ALA:HB1	1.90	0.53
20:S:49:VAL:HG13	20:S:66:VAL:HG13	1.91	0.53
1:0:1839:A:H5'	1:0:2643:G:H4'	1.90	0.53
1:0:2421:G:H1'	40:0:8242:HOH:O	2.07	0.53
1:0:2842:G:H2'	1:0:2843:A:H5'	1.91	0.53
2:A:192:VAL:O	2:A:192:VAL:HG12	2.09	0.53
7:F:46:GLU:HG3	40:F:3461:HOH:O	2.08	0.53
30:3:64:LYS:HE2	30:3:84:ARG:NH1	2.24	0.53
31:9:1:U:H4'	31:9:3:A:OP1	2.08	0.53
1:0:196:G:H2'	40:L:6170:HOH:O	2.08	0.53
1:0:363:C:H2'	1:0:364:U:H6	1.72	0.53
1:0:1521:C:H2'	1:0:1522:A:O4'	2.09	0.53
1:0:1544:U:O4	1:0:1640:C:H2'	2.09	0.53
1:0:2819:C:O4'	3:B:96:PRO:HB2	2.09	0.53
1:0:2860:G:H1'	40:0:6383:HOH:O	2.09	0.53
2:A:88:ILE:HD13	2:A:100:PRO:CD	2.35	0.53
3:B:30:PRO:HB2	3:B:39:GLN:HE21	1.72	0.53
5:D:141:VAL:HG21	31:9:57:A:C8	2.44	0.53
7:F:53:ASP:OD1	7:F:80:GLN:N	2.42	0.53
13:L:108:VAL:HB	13:L:125:PHE:HD2	1.74	0.53
21:T:55:PHE:CD2	21:T:77:VAL:HG13	2.44	0.53
26:Y:117:LEU:N	26:Y:174:VAL:HG21	2.23	0.53
1:0:421:C:H4'	1:0:1919:A:C6	2.44	0.53
1:0:424:C:H2'	1:0:425:U:H6	1.72	0.53
1:0:449:A:N7	4:C:43:LYS:HG2	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:708:A:H2'	1:0:709:G:O4'	2.09	0.53
1:0:1166:A:OP1	1:0:1174:A:H4'	2.09	0.53
1:0:1508:C:H5'	20:S:21:GLN:NE2	2.24	0.53
1:0:1803:C:H2'	1:0:1804:A:C8	2.44	0.53
1:0:1857:A:N6	1:0:2247:C:H1'	2.24	0.53
1:0:2372:A:H2'	1:0:2373:U:C6	2.44	0.53
1:0:2507:G:H2'	1:0:2510:C:N4	2.24	0.53
1:0:2614:C:O2'	1:0:2615:U:H5'	2.09	0.53
1:0:2659:U:H5''	40:0:8735:HOH:O	2.09	0.53
1:0:2824:C:H5''	1:0:2825:C:H5'	1.91	0.53
4:C:236:THR:HG22	4:C:239:ALA:HB2	1.91	0.53
8:G:24:VAL:O	8:G:28:GLU:HG3	2.09	0.53
11:J:69:TYR:CD2	11:J:69:TYR:O	2.62	0.53
14:M:166:ALA:HB2	14:M:169:ARG:NH2	2.23	0.53
20:S:20:PHE:N	20:S:20:PHE:CD2	2.72	0.53
24:W:52:VAL:HG22	24:W:53:ALA:H	1.73	0.53
1:0:932:U:O2'	1:0:1296:A:H1'	2.08	0.53
1:0:2415:A:N3	15:N:26:LEU:HD13	2.24	0.53
10:I:108:HIS:H	10:I:109:PRO:HD2	1.74	0.53
14:M:102:GLU:OE1	14:M:164:THR:HG21	2.09	0.53
15:N:34:LEU:HD13	15:N:47:LEU:HD21	1.90	0.53
28:1:42:SER:HB2	40:1:354:HOH:O	2.09	0.53
30:3:69:TYR:HB2	30:3:78:HIS:CE1	2.44	0.53
31:9:115:C:H2'	31:9:116:C:H6	1.74	0.53
1:0:424:C:H2'	1:0:425:U:C6	2.43	0.52
1:0:834:G:H3'	1:0:835:U:H4'	1.91	0.52
1:0:1262:C:O2'	24:W:120:PRO:HD3	2.08	0.52
1:0:1496:A:H2'	1:0:1497:G:O4'	2.09	0.52
1:0:1566:C:H2'	1:0:1567:G:C8	2.44	0.52
1:0:2325:U:H2'	1:0:2326:C:C6	2.44	0.52
1:0:2612:A:H4'	40:0:8224:HOH:O	2.09	0.52
1:0:2714:U:H4'	3:B:10:SER:HB2	1.90	0.52
1:0:2830:U:O2'	1:0:2831:C:H5'	2.09	0.52
2:A:217:ARG:HH11	2:A:217:ARG:HG3	1.75	0.52
8:G:63:ARG:N	40:G:2569:HOH:O	2.41	0.52
14:M:159:VAL:HG12	36:M:8818:CL:CL	2.47	0.52
15:N:37:ARG:NH1	31:9:6:C:OP1	2.42	0.52
16:O:62:GLY:O	16:O:79:VAL:HG23	2.09	0.52
22:U:20:MET:HG3	22:U:30:HIS:CE1	2.44	0.52
26:Y:145:LYS:O	26:Y:147:ARG:HG2	2.08	0.52
30:3:10:TYR:HB2	30:3:17:HIS:HE1	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1008:C:O2'	1:0:1009:U:H5'	2.09	0.52
1:0:1815:A:H2'	1:0:1816:C:O4'	2.10	0.52
1:0:2055:A:H5'	19:R:134:SER:HB2	1.91	0.52
1:0:2740:G:H2'	1:0:2741:A:O4'	2.08	0.52
10:I:95:LEU:HD22	10:I:99:GLN:HB3	1.89	0.52
10:I:133:THR:HG22	10:I:134:ILE:N	2.23	0.52
21:T:41:ARG:HG2	21:T:41:ARG:NH1	2.23	0.52
1:0:93:C:H5''	23:V:1:THR:HB	1.90	0.52
1:0:621:C:H2'	1:0:622:G:C8	2.45	0.52
1:0:857:A:H4'	2:A:176:HIS:CD2	2.45	0.52
1:0:1114:A:O2'	1:0:1115:U:H5'	2.09	0.52
1:0:1416:G:C2'	1:0:1417:G:H5'	2.39	0.52
1:0:2371:G:H5'	40:0:3898:HOH:O	2.08	0.52
1:0:2609:G:N2	3:B:238:ASN:HD21	2.07	0.52
3:B:51:VAL:HG23	3:B:329:TYR:O	2.08	0.52
6:E:69:ILE:HA	6:E:72:MET:HE2	1.90	0.52
9:H:73:ASN:HB2	9:H:88:MET:CE	2.39	0.52
21:T:71:VAL:CG1	21:T:90:PRO:HB3	2.30	0.52
25:X:34:ARG:NH1	25:X:48:VAL:O	2.42	0.52
1:0:635:A:H2'	1:0:636:G:H5''	1.90	0.52
1:0:911:G:H5'	1:0:932:U:OP1	2.09	0.52
1:0:1170:U:H2'	1:0:1172:G:OP2	2.10	0.52
1:0:1294:A:H2'	1:0:1295:G:O4'	2.10	0.52
1:0:1925:G:OP1	30:3:29:ARG:CZ	2.58	0.52
5:D:18:ILE:HG12	5:D:134:LEU:HD21	1.91	0.52
6:E:101:GLU:CB	6:E:117:THR:HA	2.39	0.52
11:J:17:CYS:HA	11:J:119:THR:O	2.10	0.52
11:J:19:MET:HE2	11:J:79:PHE:HA	1.92	0.52
1:0:1594:C:OP2	17:P:120:ARG:HD2	2.09	0.52
1:0:1762:C:O2'	1:0:1763:C:H5'	2.10	0.52
1:0:2909:G:H2'	1:0:2910:A:H8	1.75	0.52
4:C:131:PHE:CD2	4:C:131:PHE:N	2.77	0.52
13:L:112:GLY:H	13:L:132:LYS:NZ	2.07	0.52
24:W:48:VAL:O	24:W:48:VAL:HG12	2.09	0.52
27:Z:61:HIS:HB2	27:Z:71:VAL:HB	1.91	0.52
31:9:73:A:N6	31:9:108:C:H42	2.05	0.52
1:0:70:A:H4'	1:0:71:G:O5'	2.10	0.52
1:0:154:C:H2'	1:0:155:C:C6	2.45	0.52
1:0:1185:U:OP1	10:I:121:LYS:HD3	2.10	0.52
1:0:2016:U:H2'	1:0:2017:U:O4'	2.09	0.52
1:0:2320:U:O5'	30:3:1:MET:HA	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2766:A:O2'	1:0:2767:C:H5'	2.09	0.52
40:0:3741:HOH:O	30:3:25:VAL:HG11	2.09	0.52
40:0:7968:HOH:O	4:C:80:VAL:HA	2.09	0.52
4:C:135:GLU:O	4:C:136:VAL:HB	2.10	0.52
5:D:140:ARG:HH11	5:D:140:ARG:HG3	1.74	0.52
6:E:15:GLN:HG2	6:E:16:ASP:N	2.25	0.52
9:H:4:LYS:HE3	9:H:100:GLU:OE2	2.10	0.52
12:K:21:ALA:O	12:K:22:ASP:HB3	2.10	0.52
13:L:17:SER:C	13:L:19:LYS:N	2.60	0.52
13:L:73:VAL:HG23	13:L:74:THR:N	2.24	0.52
14:M:34:GLU:HB3	14:M:38:GLU:HG3	1.92	0.52
14:M:83:SER:CB	30:3:47:GLY:HA2	2.37	0.52
17:P:7:LYS:HD2	17:P:21:VAL:HG21	1.92	0.52
21:T:102:ASP:O	21:T:103:LEU:HD23	2.10	0.52
22:U:45:GLU:HB2	22:U:48:ASN:ND2	2.24	0.52
1:0:157:G:H3'	40:0:8533:HOH:O	2.09	0.52
1:0:463:A:H5'	1:0:465:U:O4'	2.10	0.52
1:0:524:A:C5'	19:R:29:LYS:HE2	2.40	0.52
1:0:918:G:H5''	40:0:3194:HOH:O	2.10	0.52
1:0:1052:G:H2'	1:0:1052:G:N3	2.24	0.52
1:0:1279:U:O2	1:0:1279:U:H2'	2.09	0.52
1:0:1315:G:C4	26:Y:212:ARG:HB2	2.45	0.52
36:0:8812:CL:CL	12:K:14:LYS:NZ	2.78	0.52
2:A:36:ASP:CB	2:A:85:SER:HB2	2.39	0.52
5:D:103:ASN:HD22	5:D:133:ASN:HA	1.75	0.52
10:I:127:CYS:HB3	10:I:132:VAL:HB	1.92	0.52
15:N:49:THR:CG2	15:N:56:ASP:HB2	2.39	0.52
31:9:3:A:H2	31:9:21:G:N3	2.08	0.52
1:0:2278:U:H5'	40:0:4522:HOH:O	2.09	0.52
1:0:2311:A:H5'	9:H:120:PHE:CD1	2.45	0.52
40:0:4499:HOH:O	8:G:12:ILE:HA	2.10	0.52
11:J:80:LYS:HE2	11:J:98:PHE:CZ	2.45	0.52
13:L:144:ASP:HA	13:L:147:GLU:OE1	2.10	0.52
18:Q:41:LEU:HB3	18:Q:52:PHE:CZ	2.44	0.52
27:Z:53:ILE:HG23	27:Z:93:TYR:HB3	1.91	0.52
1:0:1069:C:H2'	1:0:1070:A:O4'	2.10	0.52
1:0:2050:G:H5''	19:R:80:TYR:O	2.10	0.52
12:K:114:ALA:HB3	12:K:117:VAL:HG23	1.91	0.52
27:Z:38:PHE:HB3	27:Z:42:TYR:CD1	2.45	0.52
1:0:451:C:O2'	1:0:452:G:H5'	2.09	0.52
1:0:561:G:H2'	1:0:562:A:H8	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:704:C:H2'	1:0:705:C:H6	1.75	0.52
1:0:1020:A:H2'	1:0:1021:G:C8	2.45	0.52
1:0:1948:G:H1	1:0:1964:U:H3	1.57	0.52
1:0:2394:A:H5'	40:0:6767:HOH:O	2.10	0.52
1:0:2401:A:H2'	1:0:2402:A:C8	2.45	0.52
2:A:72:GLU:HG3	27:Z:90:GLY:HA2	1.92	0.52
40:K:7438:HOH:O	22:U:20:MET:HE2	2.09	0.52
16:O:47:ARG:HG3	16:O:47:ARG:NH1	2.20	0.52
1:0:363:C:H2'	1:0:364:U:C6	2.45	0.51
1:0:517:U:H2'	1:0:518:G:H5'	1.91	0.51
1:0:727:G:H3'	1:0:728:C:C6	2.45	0.51
1:0:1168:C:H5'	10:I:83:GLY:HA3	1.92	0.51
1:0:1246:A:O2'	1:0:1247:A:H3'	2.10	0.51
1:0:2344:G:H2'	1:0:2344:G:N3	2.25	0.51
1:0:2375:A:H2'	1:0:2376:C:C6	2.45	0.51
1:0:2433:A:O4'	38:0:2924:MYL:HBF	2.10	0.51
1:0:2498:C:O2'	1:0:2499:U:H5'	2.10	0.51
1:0:2721:U:H4'	12:K:87:ARG:HG3	1.91	0.51
38:0:2924:MYL:HAGA	38:0:2924:MYL:OAS	2.11	0.51
3:B:157:LYS:O	3:B:159:PRO:HD3	2.09	0.51
14:M:184:ARG:HG3	14:M:185:PRO:HA	1.91	0.51
19:R:39:THR:CB	19:R:42:GLU:HG3	2.39	0.51
1:0:453:A:H4'	1:0:455:A:N7	2.25	0.51
1:0:1167:G:H2'	1:0:1168:C:C6	2.45	0.51
1:0:2414:A:H2'	1:0:2415:A:C8	2.45	0.51
4:C:16:VAL:HG12	4:C:17:ASP:H	1.76	0.51
11:J:45:VAL:HG22	11:J:46:ILE:N	2.24	0.51
21:T:43:ASN:HB2	21:T:108:ARG:NH1	2.25	0.51
26:Y:149:GLN:HB3	40:Y:6589:HOH:O	2.09	0.51
26:Y:187:VAL:CG2	26:Y:192:ASP:HB2	2.35	0.51
31:9:75:G:H1	31:9:106:U:H3	1.56	0.51
1:0:259:G:H21	14:M:58:GLN:HE22	1.58	0.51
1:0:746:A:C6	16:O:65:LEU:HD13	2.46	0.51
1:0:1020:A:H2'	1:0:1021:G:H8	1.76	0.51
1:0:2319:C:H3'	30:3:1:MET:H1	1.72	0.51
1:0:2541:U:H5'	40:0:4280:HOH:O	2.09	0.51
3:B:102:THR:HG23	3:B:182:VAL:HG12	1.91	0.51
4:C:140:VAL:HB	40:C:6502:HOH:O	2.08	0.51
6:E:69:ILE:HA	6:E:72:MET:CE	2.40	0.51
6:E:126:ILE:HA	6:E:131:LEU:HD23	1.93	0.51
11:J:52:GLN:HG3	11:J:53:ILE:N	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:L:107:LYS:HA	13:L:124:ASP:O	2.11	0.51
31:9:39:U:H3	31:9:42:C:H5''	1.76	0.51
1:0:2316:G:H4'	40:0:5391:HOH:O	2.10	0.51
1:0:2416:G:H2'	1:0:2417:C:C6	2.44	0.51
1:0:2436:U:H5''	30:3:70:ARG:HH22	1.75	0.51
4:C:31:ILE:HA	4:C:110:ALA:HB1	1.93	0.51
7:F:1:PRO:H3	7:F:4:VAL:HG23	1.75	0.51
9:H:157:TYR:CD1	9:H:157:TYR:C	2.84	0.51
13:L:92:ASP:HA	13:L:121:ILE:HB	1.92	0.51
19:R:132:ARG:HD3	40:R:248:HOH:O	2.10	0.51
24:W:82:GLU:HB2	40:W:2749:HOH:O	2.11	0.51
25:X:61:ARG:HH12	25:X:67:PRO:HD3	1.76	0.51
25:X:70:ILE:HG23	25:X:70:ILE:O	2.11	0.51
1:0:95:A:H5''	1:0:97:G:O4'	2.09	0.51
1:0:119:A:H2'	1:0:120:A:H5''	1.92	0.51
1:0:470:U:O2'	28:1:16:HIS:CD2	2.62	0.51
1:0:775:G:OP1	28:1:16:HIS:HE1	1.93	0.51
1:0:2594:C:O2'	1:0:2595:U:H5'	2.10	0.51
3:B:233:ARG:HG2	3:B:233:ARG:HH11	1.75	0.51
10:I:87:PRO:HB3	40:I:6825:HOH:O	2.10	0.51
17:P:115:SER:H	17:P:118:GLN:HE21	1.55	0.51
21:T:81:LYS:HD2	21:T:87:VAL:HG11	1.92	0.51
24:W:13:MET:HE1	24:W:18:GLN:HA	1.91	0.51
30:3:6:ARG:HG2	30:3:6:ARG:HH11	1.75	0.51
30:3:25:VAL:HG22	30:3:68:LYS:CG	2.38	0.51
1:0:154:C:H2'	1:0:155:C:H6	1.75	0.51
1:0:545:G:H5'	1:0:545:G:C8	2.39	0.51
1:0:553:G:H2'	1:0:554:G:H5'	1.93	0.51
1:0:790:A:H1'	1:0:1710:A:H2'	1.92	0.51
1:0:2276:U:H2'	1:0:2277:U:C6	2.45	0.51
3:B:51:VAL:CG2	3:B:327:VAL:HG13	2.40	0.51
4:C:8:LEU:HD11	4:C:143:ASP:O	2.10	0.51
8:G:71:LEU:C	8:G:73:ASP:N	2.62	0.51
13:L:134:GLU:HA	13:L:138:GLY:O	2.09	0.51
14:M:84:LYS:HA	30:3:46:ILE:O	2.10	0.51
14:M:157:ASP:HB3	14:M:160:PHE:HD1	1.76	0.51
18:Q:25:PRO:HB2	40:9:4350:HOH:O	2.09	0.51
21:T:64:ASN:HB3	21:T:73:HIS:HB2	1.92	0.51
30:3:65:THR:HG21	30:3:88:LEU:HD22	1.93	0.51
1:0:155:C:OP1	14:M:189:SER:HB3	2.11	0.51
1:0:853:C:H2'	1:0:854:G:O4'	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:963:C:H2'	1:0:964:G:C8	2.45	0.51
1:0:1299:G:O6	13:L:6:ARG:HD3	2.11	0.51
1:0:1437:A:O2'	1:0:1438:G:H5'	2.10	0.51
1:0:1592:G:H2'	1:0:1593:C:H6	1.75	0.51
1:0:1855:G:H4'	1:0:1856:C:O5'	2.10	0.51
1:0:1996:U:H6	1:0:2586:U:O2	1.94	0.51
1:0:2089:A:O2'	1:0:2090:G:H5'	2.11	0.51
1:0:2119:C:O2'	1:0:2120:U:H5'	2.11	0.51
1:0:2515:C:H2'	1:0:2516:G:O4'	2.10	0.51
1:0:2676:C:H4'	11:J:70:PHE:CE1	2.45	0.51
3:B:150:ALA:O	3:B:152:PRO:HD3	2.11	0.51
16:O:25:VAL:O	16:O:28:ASP:N	2.44	0.51
18:Q:27:GLN:HE21	31:9:8:G:C5'	2.24	0.51
21:T:106:GLU:HG3	40:T:4913:HOH:O	2.11	0.51
22:U:13:ILE:HG12	22:U:32:CYS:CB	2.41	0.51
1:0:10:U:H3'	1:0:10:U:C6	2.44	0.51
1:0:269:G:O3'	1:0:274:G:H4'	2.11	0.51
1:0:308:U:C4	1:0:342:C:H1'	2.46	0.51
1:0:412:C:O2'	1:0:413:G:H5'	2.10	0.51
1:0:629:A:H2'	1:0:630:A:O4'	2.11	0.51
1:0:1333:U:H2'	1:0:1334:C:H6	1.75	0.51
1:0:1514:C:H2'	1:0:1515:A:C8	2.45	0.51
1:0:2134:G:N2	1:0:2242:U:C2	2.78	0.51
1:0:2319:C:H3'	30:3:1:MET:CA	2.40	0.51
40:0:7242:HOH:O	21:T:9:LYS:HD2	2.10	0.51
3:B:217:ARG:HG3	3:B:257:THR:HG22	1.91	0.51
4:C:123:LEU:O	4:C:126:ASP:HB2	2.11	0.51
4:C:165:ASP:O	4:C:168:ARG:HB3	2.10	0.51
5:D:81:GLU:O	5:D:84:LEU:N	2.44	0.51
9:H:49:GLN:O	9:H:169:GLU:HB2	2.11	0.51
12:K:113:ILE:HD12	12:K:128:ALA:HB2	1.91	0.51
18:Q:91:LEU:O	18:Q:92:ARG:HD2	2.09	0.51
26:Y:126:PRO:HG2	26:Y:128:PHE:CZ	2.45	0.51
1:0:329:A:OP2	4:C:206:ASN:HB2	2.09	0.51
1:0:1180:U:H4'	10:I:86:GLU:HG2	1.92	0.51
1:0:1634:G:H2'	1:0:1635:U:C6	2.45	0.51
1:0:1792:C:H2'	1:0:1793:C:H6	1.75	0.51
1:0:2363:G:O2'	18:Q:11:ARG:HG3	2.10	0.51
1:0:2508:C:H2'	40:0:6319:HOH:O	2.10	0.51
4:C:18:LEU:HD12	4:C:19:PRO:HD2	1.93	0.51
1:0:423:A:H2'	1:0:424:C:H6	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1636:G:O2'	1:0:1637:A:H5'	2.11	0.51
1:0:1666:C:C2'	1:0:1667:A:C5'	2.89	0.51
1:0:2782:G:O6	1:0:2790:C:H5''	2.11	0.51
1:0:2796:U:H1'	6:E:143:GLN:OE1	2.10	0.51
1:0:2821:C:H4'	3:B:116:PRO:HB3	1.93	0.51
1:0:2840:A:OP1	3:B:211:THR:HG23	2.11	0.51
40:0:5660:HOH:O	26:Y:158:LYS:HD3	2.11	0.51
4:C:123:LEU:O	4:C:126:ASP:N	2.43	0.51
9:H:81:GLY:C	9:H:83:GLU:H	2.15	0.51
9:H:117:ARG:HB3	40:H:7374:HOH:O	2.10	0.51
12:K:109:LEU:CD1	12:K:113:ILE:HD11	2.40	0.51
22:U:39:ASN:HD22	22:U:49:LEU:HD11	1.75	0.51
27:Z:64:PRO:HB2	27:Z:86:TYR:HE2	1.73	0.51
30:3:60:LYS:CG	30:3:61:PRO:HD2	2.32	0.51
1:0:284:C:H4'	1:0:285:A:H8	1.74	0.50
1:0:1178:G:H2'	1:0:1179:C:C6	2.45	0.50
1:0:1504:A:H4'	1:0:1506:U:C5	2.46	0.50
1:0:1552:G:H2'	1:0:1553:C:C6	2.46	0.50
1:0:1829:A:C2'	1:0:1830:C:H5'	2.41	0.50
1:0:1966:U:H2'	1:0:1967:U:C6	2.46	0.50
1:0:1980:U:O2'	1:0:1981:A:H5'	2.10	0.50
1:0:2510:C:H42	1:0:2564:G:N2	2.09	0.50
3:B:55:ASN:HB3	3:B:64:GLY:H	1.75	0.50
7:F:19:ALA:O	7:F:22:VAL:HG22	2.11	0.50
8:G:23:ILE:HG22	8:G:27:ILE:HD11	1.93	0.50
11:J:131:THR:HG22	11:J:133:GLY:N	2.25	0.50
13:L:94:ARG:NH1	13:L:143:THR:HG21	2.26	0.50
15:N:80:SER:HB2	40:N:4257:HOH:O	2.11	0.50
16:O:21:SER:HB2	16:O:106:PRO:O	2.10	0.50
19:R:33:ARG:NH1	19:R:33:ARG:HB2	2.26	0.50
1:0:162:C:H2'	1:0:163:U:H5'	1.94	0.50
1:0:334:G:H2'	1:0:335:U:O4'	2.11	0.50
1:0:1183:C:N3	1:0:1184:C:C5	2.79	0.50
1:0:1206:U:H2'	1:0:1207:A:O4'	2.11	0.50
1:0:1289:C:O2'	1:0:1290:G:H5'	2.12	0.50
1:0:2057:U:O5'	1:0:2057:U:H6	1.93	0.50
1:0:2584:G:H4'	40:0:6824:HOH:O	2.10	0.50
2:A:109:GLU:HG2	2:A:116:GLY:N	2.20	0.50
2:A:164:ARG:HA	27:Z:93:TYR:CE1	2.45	0.50
12:K:32:ILE:HD11	12:K:56:SER:HB3	1.94	0.50
13:L:129:ALA:O	13:L:133:VAL:HG23	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:R:95:ALA:HB1	19:R:147:LEU:HD11	1.92	0.50
24:W:80:ASP:C	24:W:84:VAL:HG23	2.31	0.50
1:0:398:U:H2'	1:0:399:C:C6	2.45	0.50
1:0:1342:C:C2'	1:0:1343:C:H5'	2.42	0.50
1:0:1594:C:C5	17:P:120:ARG:NH1	2.79	0.50
1:0:1735:C:O2'	1:0:1736:A:H5'	2.10	0.50
1:0:2590:U:O2	32:4:74:C:H1'	2.12	0.50
1:0:2712:G:OP1	12:K:43:ARG:NH1	2.44	0.50
4:C:21:VAL:HG13	40:C:3779:HOH:O	2.12	0.50
25:X:22:ASN:OD1	25:X:25:ARG:HD2	2.11	0.50
1:0:445:U:H2'	1:0:446:G:H8	1.75	0.50
1:0:711:G:C2	1:0:718:C:C2	2.99	0.50
1:0:877:G:C5'	1:0:878:G:OP1	2.55	0.50
1:0:1057:A:H1'	1:0:2492:U:O2'	2.12	0.50
1:0:2320:U:P	30:3:2:GLN:HG2	2.52	0.50
1:0:2694:A:H5''	6:E:90:HIS:CE1	2.47	0.50
1:0:2869:G:H5'	40:0:4548:HOH:O	2.11	0.50
4:C:4:THR:HA	4:C:15:GLU:HB3	1.93	0.50
4:C:111:VAL:HB	40:C:721:HOH:O	2.10	0.50
9:H:79:GLU:O	9:H:80:LEU:HD23	2.11	0.50
14:M:69:LYS:CG	14:M:70:GLY:H	2.18	0.50
21:T:19:ARG:HD3	21:T:67:LEU:O	2.11	0.50
23:V:7:GLU:O	23:V:11:MET:HG3	2.11	0.50
24:W:88:THR:HG21	24:W:96:LEU:HD13	1.93	0.50
1:0:219:G:O2'	30:3:51:LYS:HB3	2.11	0.50
1:0:310:U:H2'	1:0:311:C:C6	2.46	0.50
1:0:836:G:H1'	40:0:7509:HOH:O	2.10	0.50
1:0:1201:C:H5''	40:0:5584:HOH:O	2.10	0.50
1:0:1314:U:H5''	1:0:1316:G:O4'	2.11	0.50
1:0:1774:G:O2'	1:0:1775:A:H5'	2.12	0.50
1:0:1783:A:O2'	1:0:1784:U:H5'	2.11	0.50
1:0:2510:C:N4	1:0:2564:G:H22	2.07	0.50
3:B:53:LEU:HD21	3:B:270:ILE:HD12	1.93	0.50
4:C:5:ILE:HG22	4:C:6:TYR:N	2.27	0.50
5:D:99:ASP:HB3	5:D:103:ASN:H	1.77	0.50
12:K:30:LYS:O	12:K:55:VAL:HG13	2.11	0.50
23:V:4:HIS:HB3	40:V:6622:HOH:O	2.12	0.50
30:3:64:LYS:HA	30:3:83:TRP:O	2.10	0.50
1:0:80:A:H3'	21:T:43:ASN:OD1	2.12	0.50
1:0:612:U:H2'	1:0:613:C:C6	2.47	0.50
1:0:1003:U:H4'	9:H:91:ARG:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2028:U:H2'	1:0:2029:C:H6	1.76	0.50
1:0:2769:C:C2'	1:0:2770:G:H5'	2.42	0.50
3:B:238:ASN:ND2	3:B:240:GLY:H	2.09	0.50
5:D:75:LEU:HB3	5:D:80:ALA:HA	1.93	0.50
7:F:100:ASP:O	7:F:101:ALA:O	2.30	0.50
10:I:111:LEU:HD22	10:I:122:GLU:OE1	2.11	0.50
10:I:119:ALA:O	10:I:123:VAL:HG23	2.12	0.50
12:K:55:VAL:HG12	12:K:56:SER:N	2.27	0.50
12:K:66:ARG:HG2	12:K:66:ARG:HH11	1.77	0.50
26:Y:182:PHE:CG	26:Y:202:ALA:HB2	2.47	0.50
29:2:40:ARG:HA	29:2:45:ASN:ND2	2.27	0.50
1:0:583:C:H2'	1:0:584:U:H6	1.76	0.50
1:0:685:C:O2	1:0:748:C:H4'	2.12	0.50
1:0:945:U:O2'	24:W:43:GLY:HA3	2.11	0.50
1:0:1119:G:OP2	11:J:49:ARG:HD3	2.12	0.50
1:0:1351:G:H1'	40:0:3441:HOH:O	2.10	0.50
1:0:1593:C:H5''	17:P:120:ARG:HG2	1.92	0.50
1:0:2904:U:H4'	25:X:8:ARG:HH12	1.77	0.50
3:B:305:ASP:O	3:B:306:LYS:CB	2.59	0.50
3:B:332:ASN:HB3	40:B:2649:HOH:O	2.12	0.50
4:C:133:ARG:HG2	4:C:134:ASP:N	2.27	0.50
8:G:64:ASN:N	8:G:64:ASN:ND2	2.59	0.50
20:S:57:THR:CG2	20:S:58:MET:N	2.75	0.50
23:V:27:LEU:HA	23:V:49:LEU:HD13	1.93	0.50
24:W:60:GLU:O	24:W:63:GLU:HB2	2.11	0.50
1:0:292:G:H1'	1:0:360:A:N6	2.27	0.50
1:0:1157:C:H2'	1:0:1158:G:H8	1.75	0.50
1:0:1674:C:P	20:S:34:LYS:HG3	2.52	0.50
1:0:2335:C:H2'	1:0:2336:G:H8	1.75	0.50
1:0:2439:C:H5'	40:0:4534:HOH:O	2.12	0.50
40:0:6935:HOH:O	28:1:41:LYS:HD3	2.11	0.50
2:A:217:ARG:HG2	2:A:229:ALA:CB	2.37	0.50
3:B:212:GLN:HB2	3:B:257:THR:CG2	2.38	0.50
9:H:32:ALA:C	9:H:33:GLN:HG3	2.31	0.50
9:H:49:GLN:HG3	9:H:140:TYR:CE2	2.47	0.50
11:J:25:GLN:NE2	11:J:116:LEU:HB3	2.27	0.50
15:N:160:SER:HB2	31:9:51:A:H5'	1.94	0.50
18:Q:27:GLN:HB3	40:9:4350:HOH:O	2.12	0.50
21:T:69:LYS:O	21:T:71:VAL:HG23	2.12	0.50
26:Y:189:ASN:HB2	40:Y:651:HOH:O	2.11	0.50
32:4:74:C:H2'	32:4:75:C:H5'	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:79:G:N2	1:0:97:G:H1'	2.27	0.50
1:0:536:A:H3'	40:0:3958:HOH:O	2.12	0.50
1:0:614:U:H2'	1:0:615:G:H8	1.77	0.50
1:0:656:G:OP2	16:O:37:ARG:HD2	2.12	0.50
1:0:1797:A:H4'	1:0:1798:C:C5	2.47	0.50
1:0:2070:G:H4'	40:0:2976:HOH:O	2.12	0.50
1:0:2407:G:O2'	1:0:2408:A:H5'	2.12	0.50
1:0:2898:G:H1'	3:B:282:GLY:O	2.12	0.50
3:B:5:ARG:HD2	3:B:8:LYS:CE	2.41	0.50
5:D:78:GLU:O	5:D:80:ALA:N	2.44	0.50
14:M:82:ARG:O	14:M:86:GLN:HG3	2.12	0.50
15:N:35:VAL:HG13	40:N:3863:HOH:O	2.12	0.50
15:N:115:VAL:HG23	15:N:116:PHE:N	2.27	0.50
16:O:25:VAL:HG23	16:O:26:TRP:H	1.77	0.50
17:P:91:LYS:O	17:P:95:GLU:HG3	2.12	0.50
17:P:138:GLU:C	17:P:140:TYR:N	2.65	0.50
28:1:37:CYS:SG	28:1:39:PHE:HB2	2.52	0.50
1:0:1091:U:H4'	26:Y:123:VAL:HG13	1.94	0.49
1:0:1163:G:H2'	1:0:1164:U:C5	2.47	0.49
1:0:1185:U:H2'	1:0:1186:C:C6	2.47	0.49
1:0:1928:C:H2'	1:0:1929:G:O4'	2.12	0.49
1:0:2703:A:H2'	1:0:2704:C:C6	2.47	0.49
3:B:279:THR:OG1	3:B:290:VAL:HB	2.12	0.49
4:C:47:GLY:HA2	4:C:92:PRO:HB2	1.92	0.49
5:D:41:LEU:HA	5:D:44:ILE:CG2	2.40	0.49
8:G:64:ASN:O	8:G:68:GLU:HG3	2.12	0.49
9:H:25:GLY:O	9:H:27:PRO:HD3	2.12	0.49
12:K:76:GLN:HA	12:K:93:ASN:HA	1.94	0.49
14:M:57:LYS:HZ3	14:M:144:ASP:HB2	1.77	0.49
14:M:71:SER:HB2	14:M:92:THR:CG2	2.22	0.49
14:M:186:SER:HB3	14:M:189:SER:HB3	1.94	0.49
16:O:81:PHE:HB2	16:O:86:GLU:HB2	1.93	0.49
17:P:98:ILE:O	17:P:98:ILE:HD13	2.12	0.49
21:T:38:ARG:HG3	21:T:38:ARG:HH11	1.76	0.49
26:Y:96:GLU:O	26:Y:235:GLU:HA	2.12	0.49
1:0:151:A:H2'	1:0:152:A:O4'	2.13	0.49
1:0:264:G:H1'	1:0:265:U:H5	1.76	0.49
1:0:484:A:N1	1:0:506:G:H4'	2.28	0.49
1:0:920:C:H4'	1:0:921:G:C2	2.47	0.49
1:0:2635:A:O2'	1:0:2636:C:H5'	2.12	0.49
2:A:36:ASP:HB2	2:A:85:SER:H	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:139:ASP:HB2	3:B:165:ARG:HE	1.78	0.49
4:C:233:THR:HG22	4:C:234:VAL:H	1.77	0.49
13:L:40:PHE:CD1	13:L:40:PHE:C	2.84	0.49
16:O:49:GLU:OE2	16:O:71:GLN:HB2	2.12	0.49
17:P:24:ASN:OD1	17:P:26:GLU:N	2.43	0.49
18:Q:28:ARG:HG2	40:9:4350:HOH:O	2.11	0.49
24:W:52:VAL:CG2	24:W:53:ALA:N	2.75	0.49
29:2:41:HIS:HD2	29:2:44:ARG:H	1.60	0.49
1:0:229:G:O2'	1:0:230:C:H5'	2.12	0.49
1:0:1553:C:H2'	1:0:1554:C:H6	1.77	0.49
1:0:2323:G:H5'	40:0:6692:HOH:O	2.12	0.49
1:0:2597:U:H2'	1:0:2598:U:H5'	1.93	0.49
1:0:2748:G:H2'	40:0:7410:HOH:O	2.10	0.49
3:B:297:VAL:HB	40:B:4810:HOH:O	2.12	0.49
4:C:96:LYS:HB3	4:C:98:ARG:NH1	2.22	0.49
5:D:25:MET:SD	5:D:40:ILE:HD11	2.52	0.49
9:H:54:VAL:HG13	9:H:162:PRO:HG3	1.94	0.49
16:O:89:ILE:HG21	16:O:95:ALA:HB2	1.94	0.49
19:R:18:LEU:HD12	19:R:143:VAL:CG1	2.43	0.49
24:W:146:ILE:HG22	24:W:147:ASP:N	2.26	0.49
26:Y:205:ILE:HD12	26:Y:214:ARG:NH1	2.27	0.49
31:9:37:C:O2	31:9:47:A:H1'	2.13	0.49
1:0:79:G:H22	1:0:97:G:H1'	1.78	0.49
1:0:398:U:O3'	14:M:179:GLY:HA3	2.12	0.49
1:0:423:A:H2'	1:0:424:C:C6	2.47	0.49
1:0:1180:U:H2'	1:0:1181:A:O4'	2.13	0.49
1:0:1211:G:O2'	1:0:1212:C:H5'	2.12	0.49
1:0:1494:A:H1'	1:0:1495:C:C6	2.47	0.49
1:0:2576:A:H4'	1:0:2799:A:C2	2.47	0.49
1:0:2642:G:H2'	1:0:2643:G:O4'	2.12	0.49
1:0:2694:A:H4'	6:E:91:PHE:CE1	2.43	0.49
1:0:2854:A:H2'	1:0:2855:G:H8	1.77	0.49
3:B:205:VAL:HB	3:B:307:ARG:HD3	1.95	0.49
3:B:304:PRO:HD2	3:B:307:ARG:NE	2.27	0.49
7:F:36:THR:HG23	7:F:97:ALA:HB2	1.95	0.49
8:G:12:ILE:N	8:G:13:PRO:HD3	2.28	0.49
14:M:122:GLN:HG3	14:M:122:GLN:O	2.12	0.49
24:W:122:ARG:HG3	24:W:122:ARG:NH1	2.27	0.49
1:0:566:A:H2'	1:0:567:U:O4'	2.12	0.49
1:0:951:A:C2'	1:0:952:G:H5'	2.42	0.49
1:0:1235:G:C1'	11:J:63:ILE:HG23	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2783:A:H2'	1:0:2784:A:C8	2.48	0.49
3:B:41:PHE:HA	3:B:79:MET:CE	2.42	0.49
3:B:43:GLY:O	3:B:308:LEU:HD12	2.12	0.49
3:B:294:TYR:HE2	40:B:7123:HOH:O	1.95	0.49
10:I:106:GLN:O	10:I:108:HIS:N	2.46	0.49
10:I:118:ASN:HA	10:I:121:LYS:HD2	1.94	0.49
11:J:54:VAL:HG11	11:J:138:THR:HG21	1.93	0.49
15:N:15:GLU:OE1	15:N:17:ARG:HD2	2.13	0.49
18:Q:21:ARG:HG2	18:Q:22:GLY:N	2.26	0.49
30:3:7:PHE:HE1	30:3:9:THR:HG21	1.77	0.49
31:9:26:C:H2'	31:9:27:C:C6	2.48	0.49
1:0:1119:G:H5'	11:J:52:GLN:NE2	2.27	0.49
1:0:1787:C:OP1	17:P:68:LYS:HE2	2.12	0.49
1:0:2473:U:O3'	1:0:2474:A:H3'	2.13	0.49
38:0:2924:MYL:HACB	38:0:2924:MYL:CAN	2.42	0.49
2:A:54:PRO:HG2	2:A:160:ALA:HB3	1.94	0.49
3:B:54:VAL:HB	40:B:5136:HOH:O	2.12	0.49
3:B:140:LEU:HD13	3:B:175:LEU:HA	1.95	0.49
4:C:127:ARG:HG2	4:C:127:ARG:NH1	2.27	0.49
5:D:170:TYR:O	5:D:171:ASP:HB3	2.12	0.49
12:K:97:ILE:HG22	12:K:98:VAL:N	2.27	0.49
14:M:48:LYS:HE3	14:M:52:GLN:HE21	1.76	0.49
15:N:143:ARG:HG2	15:N:172:PHE:CE2	2.48	0.49
31:9:59:C:O5'	31:9:59:C:H6	1.95	0.49
1:0:654:A:OP2	16:O:38:ARG:HD2	2.13	0.49
1:0:926:A:H1'	13:L:38:HIS:O	2.13	0.49
1:0:2906:A:H5'	1:0:2907:C:O4'	2.13	0.49
2:A:21:HIS:CE1	2:A:22:ARG:HG3	2.48	0.49
3:B:84:LEU:HD23	3:B:178:ALA:HB1	1.94	0.49
7:F:20:LEU:O	7:F:23:ALA:HB3	2.12	0.49
8:G:12:ILE:HG22	8:G:17:GLN:NE2	2.28	0.49
14:M:74:LYS:HG2	14:M:87:GLY:O	2.13	0.49
14:M:181:GLU:OE1	14:M:181:GLU:N	2.39	0.49
15:N:90:LEU:O	15:N:93:GLN:HB2	2.12	0.49
17:P:137:LEU:O	17:P:140:TYR:HB3	2.13	0.49
31:9:73:A:H61	31:9:108:C:N4	2.07	0.49
1:0:1573:A:H2'	1:0:1574:C:O4'	2.13	0.49
2:A:33:GLU:O	2:A:34:ASP:HB2	2.12	0.49
9:H:54:VAL:HG13	9:H:162:PRO:CG	2.42	0.49
12:K:64:MET:HA	12:K:67:GLN:NE2	2.28	0.49
13:L:120:LEU:HB2	13:L:140:VAL:HG23	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:M:77:HIS:CG	14:M:81:ARG:HB3	2.48	0.49
17:P:27:ARG:O	17:P:28:GLN:C	2.50	0.49
17:P:83:LYS:O	17:P:86:ALA:HB3	2.12	0.49
31:9:115:C:H2'	31:9:116:C:C6	2.48	0.49
1:0:30:U:OP2	4:C:181:ALA:HB2	2.11	0.49
1:0:263:U:C2	7:F:59:ILE:CD1	2.96	0.49
1:0:295:C:H2'	1:0:296:G:O4'	2.12	0.49
1:0:363:C:O2'	1:0:364:U:H5'	2.13	0.49
1:0:892:G:H5''	28:1:54:ALA:HB2	1.93	0.49
1:0:1634:G:H2'	1:0:1635:U:H6	1.78	0.49
1:0:2807:U:P	3:B:27:ASN:HD21	2.36	0.49
3:B:87:TYR:O	3:B:138:GLY:N	2.43	0.49
5:D:37:ALA:O	5:D:40:ILE:HG12	2.12	0.49
7:F:1:PRO:H3	7:F:4:VAL:CG2	2.25	0.49
9:H:88:MET:HA	9:H:139:ALA:HA	1.95	0.49
11:J:39:VAL:HG13	11:J:40:ASN:ND2	2.28	0.49
15:N:69:TYR:CD2	15:N:184:ILE:HD11	2.48	0.49
21:T:61:GLU:HG3	40:T:3851:HOH:O	2.11	0.49
25:X:43:VAL:CG1	25:X:47:ALA:HB3	2.43	0.49
1:0:699:C:H6	1:0:744:G:O4'	1.96	0.49
1:0:946:C:H2'	1:0:947:U:H6	1.76	0.49
1:0:969:G:H1	1:0:999:C:N4	2.11	0.49
1:0:1187:U:H2'	40:0:6517:HOH:O	2.13	0.49
1:0:1310:U:OP2	4:C:168:ARG:NH1	2.46	0.49
1:0:2894:C:O2'	1:0:2895:C:H5'	2.12	0.49
4:C:28:SER:HB2	40:C:7195:HOH:O	2.13	0.49
6:E:11:VAL:HG12	6:E:12:ASP:N	2.28	0.49
12:K:125:ALA:C	12:K:127:ALA:H	2.16	0.49
13:L:10:SER:O	13:L:11:ARG:HB3	2.12	0.49
20:S:43:GLU:HB3	40:S:7106:HOH:O	2.13	0.49
24:W:110:GLN:HA	24:W:110:GLN:HE21	1.76	0.49
26:Y:156:GLY:O	26:Y:157:ILE:C	2.52	0.49
30:3:4:PRO:HG2	30:3:7:PHE:CD2	2.48	0.49
30:3:54:LYS:HE2	40:3:4294:HOH:O	2.12	0.49
1:0:503:G:H2'	1:0:504:G:H8	1.77	0.48
1:0:777:U:O2'	28:1:11:LYS:HG2	2.13	0.48
1:0:1010:C:H4'	15:N:4:PRO:HB2	1.95	0.48
1:0:1299:G:N7	13:L:6:ARG:NH1	2.61	0.48
1:0:1363:G:H2'	1:0:1364:G:C8	2.48	0.48
1:0:1500:U:OP2	17:P:41:ARG:NH2	2.46	0.48
1:0:1829:A:C8	1:0:1885:A:C8	3.01	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2038:A:H5''	3:B:222:LYS:HG3	1.95	0.48
1:0:2241:C:O2'	1:0:2242:U:H5'	2.13	0.48
1:0:2909:G:H2'	1:0:2910:A:C8	2.47	0.48
40:0:7267:HOH:O	2:A:211:LYS:HE3	2.13	0.48
11:J:48:GLY:HA3	11:J:53:ILE:HD11	1.94	0.48
17:P:94:TRP:CZ2	17:P:98:ILE:HG13	2.47	0.48
24:W:11:VAL:O	24:W:12:ASN:HB2	2.13	0.48
24:W:27:HIS:C	24:W:28:HIS:CD2	2.86	0.48
28:1:13:THR:HG22	28:1:14:THR:N	2.28	0.48
1:0:694:A:C2'	1:0:695:C:H5'	2.42	0.48
1:0:947:U:H2'	1:0:948:G:H8	1.77	0.48
1:0:1166:A:P	1:0:1174:A:H4'	2.52	0.48
1:0:1426:C:H2'	40:0:4918:HOH:O	2.13	0.48
1:0:2028:U:H2'	1:0:2029:C:C6	2.48	0.48
1:0:2899:A:H4'	3:B:289:GLU:OE1	2.14	0.48
4:C:96:LYS:CB	4:C:98:ARG:HH12	2.22	0.48
9:H:39:LYS:HD3	40:H:6292:HOH:O	2.12	0.48
21:T:24:ARG:NH2	21:T:39:ASN:HD22	2.11	0.48
30:3:24:LYS:HE2	30:3:65:THR:HG23	1.95	0.48
31:9:39:U:H3'	31:9:40:C:H5''	1.95	0.48
1:0:243:A:H61	1:0:269:G:H1'	1.78	0.48
1:0:499:G:O2'	1:0:500:G:H5'	2.13	0.48
1:0:2032:U:H2'	1:0:2033:G:H5''	1.94	0.48
1:0:2478:U:O2'	1:0:2479:A:H5'	2.12	0.48
1:0:2636:C:H4'	32:4:174:C:H4'	1.95	0.48
1:0:2897:C:H2'	1:0:2898:G:H8	1.77	0.48
3:B:310:ARG:HD2	40:B:4128:HOH:O	2.13	0.48
6:E:101:GLU:HA	6:E:118:ILE:HG13	1.95	0.48
9:H:27:PRO:HD3	9:H:123:ILE:HG22	1.95	0.48
14:M:57:LYS:NZ	14:M:144:ASP:HB2	2.28	0.48
15:N:160:SER:CB	31:9:51:A:H5'	2.42	0.48
15:N:184:ILE:HG23	15:N:184:ILE:O	2.13	0.48
24:W:13:MET:CE	24:W:17:ILE:HG22	2.43	0.48
25:X:43:VAL:CG1	25:X:44:ASP:N	2.75	0.48
26:Y:131:GLN:O	26:Y:132:ASP:HB2	2.13	0.48
26:Y:189:ASN:ND2	26:Y:192:ASP:H	2.12	0.48
1:0:77:G:O2'	1:0:78:G:H5'	2.13	0.48
1:0:107:U:H2'	1:0:108:U:H5'	1.95	0.48
1:0:535:G:C5	1:0:2063:U:C4	3.01	0.48
1:0:553:G:O4'	1:0:1325:G:H5'	2.12	0.48
1:0:812:A:H2'	1:0:813:C:O4'	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1029:U:O2'	1:0:1273:C:OP1	2.27	0.48
1:0:1303:C:O2	1:0:1353:C:H1'	2.13	0.48
1:0:1353:C:H4'	40:0:5388:HOH:O	2.13	0.48
1:0:1513:C:O2'	1:0:1514:C:H5'	2.12	0.48
1:0:1514:C:H2'	1:0:1515:A:H8	1.77	0.48
1:0:1904:A:H2'	1:0:1905:U:O4'	2.12	0.48
1:0:2112:A:H2'	1:0:2113:G:C8	2.48	0.48
1:0:2614:C:H5''	3:B:232:TRP:CZ3	2.49	0.48
1:0:2637:A:O5'	32:4:175:C:OP2	2.30	0.48
3:B:232:TRP:CD1	3:B:235:ARG:HD2	2.47	0.48
7:F:13:GLU:OE1	7:F:77:VAL:HG13	2.13	0.48
14:M:24:GLN:HE22	14:M:27:ARG:HH11	1.59	0.48
25:X:20:GLU:HG3	25:X:21:PRO:CD	2.42	0.48
30:3:65:THR:HG21	30:3:88:LEU:CD2	2.44	0.48
1:0:790:A:H2'	1:0:791:A:O4'	2.14	0.48
1:0:2321:A:H8	1:0:2322:U:O2'	1.96	0.48
1:0:2626:C:H2'	1:0:2627:G:C8	2.48	0.48
2:A:81:GLN:HB2	2:A:92:ASN:ND2	2.28	0.48
3:B:307:ARG:HH11	3:B:307:ARG:HG3	1.78	0.48
13:L:108:VAL:HB	13:L:125:PHE:CD2	2.49	0.48
14:M:91:ILE:HB	40:M:7419:HOH:O	2.13	0.48
19:R:72:VAL:CG1	19:R:73:ASP:N	2.76	0.48
23:V:23:LEU:HD22	23:V:49:LEU:HD23	1.95	0.48
27:Z:101:LYS:HA	27:Z:104:ARG:HH11	1.78	0.48
29:2:35:ARG:HB3	40:2:2691:HOH:O	2.12	0.48
1:0:314:G:N2	1:0:317:A:C8	2.82	0.48
1:0:1016:U:H1'	40:0:8202:HOH:O	2.12	0.48
1:0:1180:U:O2'	10:I:87:PRO:HD2	2.14	0.48
2:A:123:GLY:HA2	2:A:159:VAL:O	2.14	0.48
3:B:36:PRO:CA	3:B:168:GLY:HA3	2.35	0.48
5:D:173:GLU:O	5:D:174:VAL:O	2.32	0.48
6:E:137:ASP:O	6:E:141:VAL:HG23	2.13	0.48
13:L:115:ARG:O	13:L:116:HIS:CG	2.67	0.48
17:P:27:ARG:HH21	17:P:30:ASP:CG	2.17	0.48
30:3:3:MET:CG	30:3:22:VAL:HG11	2.35	0.48
30:3:5:ARG:HG3	30:3:6:ARG:HG3	1.95	0.48
1:0:401:C:O2'	14:M:92:THR:HB	2.13	0.48
1:0:590:A:H2'	1:0:591:A:O4'	2.13	0.48
1:0:1060:C:H6	1:0:1060:C:H5'	1.78	0.48
1:0:1938:G:O2'	1:0:1939:U:H5'	2.13	0.48
1:0:2549:C:H1'	40:B:342:HOH:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2725:G:N1	1:0:2756:U:OP2	2.37	0.48
9:H:143:VAL:HG11	9:H:173:GLU:HG2	1.95	0.48
12:K:23:ASN:ND2	12:K:108:GLU:HB2	2.28	0.48
15:N:6:TYR:HB3	31:9:11:A:N6	2.28	0.48
19:R:99:ALA:CB	19:R:109:MET:HE3	2.41	0.48
26:Y:106:THR:CG2	26:Y:107:PRO:HD2	2.44	0.48
1:0:120:A:C6	28:1:17:THR:HG21	2.48	0.48
1:0:228:C:C2'	1:0:229:G:H5'	2.43	0.48
1:0:622:G:O2'	1:0:623:U:H5'	2.14	0.48
1:0:646:G:H5''	4:C:96:LYS:HD2	1.96	0.48
1:0:962:C:H2'	1:0:963:C:H5'	1.95	0.48
1:0:1548:U:O2'	1:0:1549:C:H5'	2.14	0.48
1:0:1774:G:H2'	1:0:1775:A:O4'	2.13	0.48
1:0:2590:U:H1'	32:4:74:C:C2	2.49	0.48
1:0:2634:G:OP2	2:A:204:GLY:N	2.47	0.48
3:B:160:ASP:CB	3:B:308:LEU:HD22	2.44	0.48
6:E:34:TRP:HB3	40:E:1053:HOH:O	2.13	0.48
9:H:29:SER:HA	9:H:62:HIS:HD2	1.78	0.48
13:L:34:GLY:C	13:L:36:ASP:H	2.16	0.48
26:Y:152:LYS:CB	26:Y:160:LYS:HG3	2.43	0.48
28:1:12:ASN:OD1	28:1:12:ASN:C	2.52	0.48
1:0:123:U:O2'	1:0:124:C:H5'	2.14	0.48
1:0:661:G:C5	1:0:686:A:C2	3.02	0.48
1:0:800:G:H4'	40:0:6743:HOH:O	2.14	0.48
1:0:843:A:C2	1:0:846:A:C8	3.01	0.48
1:0:1801:A:H3'	40:0:7513:HOH:O	2.14	0.48
3:B:147:VAL:HG12	3:B:150:ALA:H	1.79	0.48
3:B:268:ARG:HH21	3:B:322:ARG:HB2	1.78	0.48
6:E:26:ASN:HB3	6:E:76:VAL:O	2.13	0.48
11:J:26:VAL:HG13	11:J:36:VAL:CG1	2.41	0.48
13:L:143:THR:O	13:L:147:GLU:HG3	2.13	0.48
15:N:36:ALA:N	40:N:3863:HOH:O	2.47	0.48
15:N:72:GLU:O	15:N:72:GLU:HG2	2.13	0.48
19:R:39:THR:HB	19:R:42:GLU:CD	2.35	0.48
19:R:39:THR:HG22	19:R:42:GLU:H	1.79	0.48
24:W:133:LYS:HG3	40:W:5904:HOH:O	2.13	0.48
1:0:53:C:H2'	1:0:54:G:O4'	2.14	0.48
1:0:113:A:H3'	1:0:114:A:C5'	2.43	0.48
1:0:449:A:C8	4:C:43:LYS:HG2	2.48	0.48
1:0:1617:C:C4	1:0:1643:C:H4'	2.49	0.48
1:0:1617:C:C5	1:0:1643:C:H4'	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1625:U:H3'	1:0:1625:U:C6	2.48	0.48
1:0:2002:C:H2'	1:0:2003:U:H5'	1.95	0.48
1:0:2114:C:OP1	2:A:1:GLY:HA2	2.13	0.48
1:0:2483:A:H4'	1:0:2484:U:OP2	2.12	0.48
1:0:2588:OMG:N2	32:4:76:5AA:C2	2.77	0.48
2:A:35:GLY:O	2:A:36:ASP:HB2	2.14	0.48
2:A:121:ALA:O	2:A:124:VAL:HG22	2.14	0.48
3:B:15:PRO:HG2	3:B:17:LYS:HG2	1.96	0.48
6:E:75:GLY:O	6:E:79:GLY:HA2	2.14	0.48
6:E:81:GLU:HG3	6:E:133:VAL:O	2.14	0.48
7:F:50:VAL:CG2	7:F:63:ILE:HG21	2.44	0.48
9:H:91:ARG:NH1	9:H:138:THR:OG1	2.47	0.48
12:K:113:ILE:HG22	12:K:114:ALA:N	2.28	0.48
14:M:66:SER:HB2	14:M:128:TRP:CD1	2.49	0.48
15:N:171:HIS:CE1	40:N:6988:HOH:O	2.67	0.48
19:R:31:ILE:O	19:R:32:ALA:C	2.52	0.48
21:T:38:ARG:HG3	21:T:38:ARG:NH1	2.28	0.48
1:0:35:U:H5'	4:C:47:GLY:O	2.14	0.47
1:0:517:U:C2'	1:0:518:G:H5'	2.44	0.47
1:0:862:U:H2'	1:0:863:G:H8	1.79	0.47
1:0:926:A:O2'	13:L:41:HIS:CD2	2.62	0.47
1:0:958:G:O2'	1:0:959:C:H5'	2.14	0.47
1:0:1366:C:H1'	40:0:3715:HOH:O	2.14	0.47
1:0:1684:A:O2'	1:0:1685:A:H5''	2.14	0.47
1:0:1739:G:O2'	1:0:1740:U:H5'	2.13	0.47
1:0:2088:C:H1'	1:0:2841:A:C2	2.49	0.47
1:0:2271:G:P	2:A:223:ARG:HH12	2.37	0.47
1:0:2499:U:H2'	1:0:2500:C:H6	1.79	0.47
1:0:2590:U:O2	32:4:74:C:C1'	2.61	0.47
1:0:2840:A:H3'	40:0:7562:HOH:O	2.13	0.47
2:A:207:GLN:O	2:A:208:HIS:HB3	2.14	0.47
2:A:231:LYS:O	2:A:232:ARG:HB3	2.14	0.47
4:C:219:ASN:O	4:C:222:ASP:HB2	2.14	0.47
4:C:236:THR:H	4:C:239:ALA:HB3	1.78	0.47
11:J:107:ASN:ND2	11:J:107:ASN:C	2.64	0.47
17:P:69:ARG:HA	17:P:73:HIS:O	2.13	0.47
21:T:38:ARG:NH1	40:T:6217:HOH:O	2.45	0.47
21:T:48:VAL:HG22	21:T:96:VAL:HG22	1.96	0.47
21:T:49:GLU:OE2	21:T:97:ARG:NH1	2.46	0.47
30:3:10:TYR:CG	30:3:11:CYS:N	2.81	0.47
1:0:17:G:H2'	1:0:18:C:C6	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:88:G:C8	29:2:28:LYS:HB2	2.49	0.47
1:0:1149:U:C5	1:0:1215:A:C5	3.02	0.47
1:0:1205:U:H2'	1:0:1206:U:H5'	1.96	0.47
1:0:2704:C:H1'	6:E:110:GLU:OE1	2.14	0.47
4:C:73:GLN:HE21	4:C:73:GLN:HA	1.79	0.47
7:F:50:VAL:HG21	7:F:63:ILE:HG21	1.95	0.47
9:H:41:LYS:HD3	9:H:46:TYR:CZ	2.48	0.47
13:L:90:ARG:CA	13:L:119:THR:HB	2.42	0.47
20:S:20:PHE:N	20:S:20:PHE:HD2	2.11	0.47
24:W:39:ASP:OD1	24:W:42:ARG:NH1	2.46	0.47
25:X:52:PRO:O	25:X:55:ASN:N	2.48	0.47
27:Z:70:ARG:HH11	27:Z:70:ARG:HB3	1.77	0.47
1:0:319:A:H2'	1:0:320:G:C8	2.49	0.47
1:0:1116:U:HO2'	1:0:1118:A:H2	0.74	0.47
1:0:1358:A:N7	1:0:1360:C:C2	2.82	0.47
1:0:1497:G:H2'	1:0:1498:G:H8	1.78	0.47
1:0:1701:A:H5''	1:0:1702:U:H3'	1.95	0.47
2:A:199:HIS:CD2	2:A:201:PHE:HB2	2.49	0.47
5:D:55:LYS:O	5:D:56:ARG:HB2	2.14	0.47
7:F:101:ALA:HA	40:F:5413:HOH:O	2.14	0.47
10:I:108:HIS:N	10:I:109:PRO:HD2	2.29	0.47
40:M:674:HOH:O	30:3:46:ILE:HB	2.14	0.47
19:R:33:ARG:CB	19:R:33:ARG:HH11	2.27	0.47
22:U:8:TYR:CE1	22:U:40:ALA:HB2	2.48	0.47
22:U:39:ASN:ND2	22:U:49:LEU:CD1	2.77	0.47
24:W:147:ASP:O	24:W:151:GLU:HB2	2.15	0.47
31:9:75:G:H2'	31:9:76:G:O4'	2.14	0.47
1:0:228:C:H2'	1:0:229:G:C5'	2.44	0.47
1:0:579:G:H2'	1:0:580:A:C8	2.49	0.47
1:0:702:G:O2'	1:0:703:G:H5'	2.15	0.47
1:0:709:G:O3'	16:O:25:VAL:HG13	2.15	0.47
1:0:820:G:C6	2:A:171:LYS:HB2	2.48	0.47
1:0:2604:A:H5'	40:0:4959:HOH:O	2.13	0.47
1:0:2637:A:O5'	32:4:175:C:P	2.72	0.47
1:0:2887:G:H2'	1:0:2888:U:C6	2.49	0.47
2:A:100:PRO:O	2:A:103:VAL:HG23	2.14	0.47
3:B:162:MET:HG3	3:B:310:ARG:HH11	1.79	0.47
3:B:202:VAL:HG11	3:B:301:VAL:HG13	1.96	0.47
4:C:214:THR:HG23	40:C:5535:HOH:O	2.15	0.47
5:D:170:TYR:CD1	5:D:170:TYR:N	2.83	0.47
9:H:87:LYS:HG2	9:H:140:TYR:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:R:26:LYS:HD3	19:R:62:HIS:CG	2.49	0.47
24:W:117:ARG:HB3	24:W:117:ARG:HH11	1.79	0.47
25:X:76:ARG:O	25:X:77:PHE:HB3	2.14	0.47
29:2:16:ASN:C	29:2:18:ASN:N	2.67	0.47
29:2:16:ASN:C	29:2:18:ASN:H	2.18	0.47
31:9:20:G:O2'	31:9:21:G:H5'	2.14	0.47
31:9:107:C:H2'	31:9:108:C:H6	1.79	0.47
1:0:23:G:H1'	1:0:520:A:N6	2.30	0.47
1:0:29:C:H5'	1:0:1342:C:OP1	2.13	0.47
1:0:111:C:O2'	28:1:20:ARG:HG2	2.14	0.47
1:0:194:A:H2'	1:0:195:C:O4'	2.15	0.47
1:0:660:A:H4'	1:0:661:G:O5'	2.14	0.47
1:0:944:G:H21	24:W:44:MET:CE	2.27	0.47
1:0:1149:U:H5''	1:0:1151:G:O4'	2.14	0.47
1:0:1219:U:H2'	1:0:1220:U:C6	2.50	0.47
1:0:1333:U:H2'	1:0:1334:C:C6	2.48	0.47
1:0:1632:A:C2'	1:0:1633:C:H5'	2.43	0.47
1:0:2831:C:H2'	1:0:2832:C:H5'	1.97	0.47
40:0:3944:HOH:O	27:Z:40:ALA:HB3	2.14	0.47
2:A:164:ARG:HB2	40:Z:292:HOH:O	2.13	0.47
3:B:217:ARG:HG3	3:B:257:THR:CG2	2.44	0.47
7:F:4:VAL:HA	7:F:76:PHE:CZ	2.49	0.47
9:H:123:ILE:HD12	9:H:123:ILE:N	2.30	0.47
10:I:116:LEU:O	10:I:119:ALA:HB3	2.13	0.47
11:J:77:GLY:O	11:J:78:ILE:C	2.53	0.47
21:T:32:ARG:NH1	21:T:38:ARG:HH12	2.12	0.47
23:V:12:THR:CG2	23:V:15:GLU:HG3	2.36	0.47
30:3:25:VAL:HG13	30:3:68:LYS:CE	2.41	0.47
1:0:100:C:C4'	21:T:16:LEU:HB2	2.44	0.47
1:0:721:A:H5''	16:O:51:TYR:CE1	2.50	0.47
1:0:1163:G:H2'	1:0:1164:U:H5	1.79	0.47
1:0:1174:A:C6	1:0:1201:C:H4'	2.50	0.47
1:0:1574:C:H2'	1:0:1575:C:H6	1.78	0.47
40:0:8330:HOH:O	14:M:189:SER:HB2	2.13	0.47
2:A:33:GLU:OE1	2:A:33:GLU:N	2.42	0.47
5:D:15:GLU:HA	5:D:16:PRO:HD3	1.75	0.47
7:F:8:VAL:HG13	7:F:12:LEU:HD13	1.96	0.47
8:G:71:LEU:C	8:G:73:ASP:H	2.18	0.47
14:M:74:LYS:HE2	40:M:444:HOH:O	2.14	0.47
28:1:28:HIS:ND1	28:1:31:LYS:HG3	2.30	0.47
1:0:17:G:H2'	1:0:18:C:H6	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:110:C:H2'	1:0:111:C:C6	2.48	0.47
1:0:422:G:O2'	1:0:423:A:H5'	2.15	0.47
1:0:477:A:C6	1:0:478:C:C4	3.02	0.47
1:0:561:G:O2'	1:0:562:A:H5'	2.15	0.47
1:0:734:U:O2'	1:0:736:A:N7	2.40	0.47
1:0:1634:G:H3'	40:0:8442:HOH:O	2.15	0.47
1:0:1800:G:H1'	17:P:88:GLN:NE2	2.30	0.47
1:0:2065:C:O2'	1:0:2066:C:H5'	2.15	0.47
1:0:2321:A:C2	1:0:2378:U:N3	2.76	0.47
1:0:2639:G:O2'	1:0:2640:U:H5'	2.14	0.47
40:0:4371:HOH:O	17:P:117:SER:HB2	2.13	0.47
2:A:69:LEU:HD23	2:A:107:ASN:HB2	1.96	0.47
2:A:134:ASN:O	2:A:150:PRO:CD	2.63	0.47
3:B:29:TRP:CH2	3:B:164:THR:HA	2.50	0.47
3:B:80:ARG:HA	3:B:186:GLY:O	2.15	0.47
3:B:91:PRO:HA	11:J:144:THR:OG1	2.14	0.47
3:B:275:GLY:C	3:B:291:ASP:HA	2.35	0.47
5:D:151:ILE:CG2	5:D:155:HIS:HB3	2.45	0.47
10:I:96:SER:O	10:I:99:GLN:HB2	2.15	0.47
14:M:52:GLN:NE2	14:M:118:TYR:HB3	2.30	0.47
15:N:11:ARG:O	15:N:13:ARG:N	2.47	0.47
16:O:69:VAL:HG12	16:O:70:LEU:N	2.29	0.47
18:Q:34:ASP:O	18:Q:37:GLU:HG3	2.15	0.47
19:R:8:ALA:CB	19:R:13:THR:HG21	2.21	0.47
19:R:13:THR:HA	19:R:147:LEU:O	2.15	0.47
19:R:33:ARG:HB2	19:R:33:ARG:HH11	1.80	0.47
24:W:88:THR:C	24:W:90:TYR:N	2.66	0.47
30:3:70:ARG:HA	30:3:77:ALA:HB2	1.97	0.47
1:0:10:U:C6	1:0:10:U:C3'	2.97	0.47
1:0:125:U:H2'	40:0:8310:HOH:O	2.15	0.47
1:0:812:A:H1'	40:0:8538:HOH:O	2.14	0.47
1:0:1296:A:O2'	1:0:1297:U:H5'	2.15	0.47
1:0:1850:U:O4'	1:0:1941:A:C2	2.68	0.47
1:0:2256:G:O2'	1:0:2257:G:H5'	2.14	0.47
1:0:2504:A:H4'	9:H:74:ARG:HH11	1.80	0.47
1:0:2590:U:C2	32:4:74:C:N1	2.83	0.47
3:B:26:PHE:HD2	3:B:312:ARG:HH21	1.63	0.47
3:B:125:GLU:O	3:B:129:ARG:HG3	2.14	0.47
9:H:30:LYS:H	9:H:62:HIS:CD2	2.33	0.47
9:H:73:ASN:HB2	9:H:88:MET:HE1	1.95	0.47
10:I:118:ASN:HA	10:I:121:LYS:CD	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:K:115:ARG:HG3	12:K:116:GLU:N	2.29	0.47
14:M:75:ARG:NH2	14:M:78:LYS:NZ	2.62	0.47
20:S:6:LYS:HE3	20:S:29:ASP:HA	1.97	0.47
24:W:107:LEU:O	24:W:112:LEU:HB2	2.15	0.47
27:Z:81:CYS:O	27:Z:85:ASP:HA	2.14	0.47
29:2:20:ARG:HG3	29:2:20:ARG:HH11	1.79	0.47
1:0:307:G:H3'	1:0:342:C:OP2	2.14	0.47
1:0:697:G:H4'	1:0:730:G:O3'	2.15	0.47
1:0:1603:A:C5'	1:0:1605:G:H5'	2.45	0.47
1:0:1972:U:C2'	1:0:1973:A:H5''	2.45	0.47
1:0:2735:U:H2'	1:0:2736:U:H6	1.79	0.47
1:0:2831:C:C2'	1:0:2832:C:H5'	2.45	0.47
3:B:27:ASN:HD22	3:B:27:ASN:N	2.06	0.47
3:B:109:LEU:HD11	3:B:113:LEU:HD12	1.97	0.47
3:B:195:ARG:O	3:B:196:ALA:C	2.52	0.47
3:B:198:GLU:HA	40:B:7384:HOH:O	2.13	0.47
7:F:32:GLY:N	40:F:3111:HOH:O	2.47	0.47
11:J:77:GLY:O	11:J:80:LYS:N	2.48	0.47
24:W:27:HIS:O	24:W:28:HIS:HD2	1.98	0.47
24:W:90:TYR:CE2	24:W:99:ALA:HB2	2.50	0.47
26:Y:144:ARG:CZ	40:Y:7277:HOH:O	2.62	0.47
1:0:256:C:H2'	1:0:257:G:O4'	2.14	0.47
1:0:500:G:H21	19:R:98:ASN:ND2	2.12	0.47
1:0:522:U:O2'	1:0:1366:C:H5'	2.15	0.47
1:0:716:G:H1'	40:0:4890:HOH:O	2.15	0.47
1:0:1006:A:N1	1:0:2311:A:H1'	2.30	0.47
1:0:1115:U:O2'	1:0:1116:U:H5'	2.15	0.47
1:0:1603:A:H5''	1:0:1604:G:H3'	1.97	0.47
1:0:1706:G:H1'	1:0:1712:A:H61	1.80	0.47
1:0:1878:G:O2'	1:0:1879:U:OP2	2.33	0.47
1:0:1972:U:H2'	1:0:1973:A:H5''	1.97	0.47
1:0:2289:G:O2'	1:0:2290:U:H5'	2.15	0.47
5:D:76:ARG:O	5:D:77:ASP:HB2	2.15	0.47
10:I:73:LEU:HD12	10:I:107:LYS:HZ1	1.78	0.47
12:K:14:LYS:HG3	12:K:32:ILE:O	2.14	0.47
13:L:143:THR:CG2	13:L:144:ASP:N	2.77	0.47
15:N:23:ARG:NH2	15:N:55:ASP:OD2	2.48	0.47
16:O:43:VAL:HG11	16:O:115:ARG:HA	1.97	0.47
17:P:115:SER:N	17:P:118:GLN:NE2	2.53	0.47
21:T:18:GLU:O	21:T:21:LYS:HG2	2.15	0.47
21:T:40:VAL:HG23	21:T:119:ALA:C	2.35	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:V:33:VAL:O	23:V:33:VAL:HG12	2.15	0.47
1:0:86:A:C2	29:2:25:VAL:HG13	2.50	0.46
1:0:453:A:H3'	40:0:4941:HOH:O	2.14	0.46
1:0:1564:C:H1'	1:0:2738:G:C2	2.51	0.46
1:0:1972:U:C2'	1:0:1973:A:C5'	2.93	0.46
1:0:2542:C:C1'	40:4:6378:HOH:O	2.62	0.46
40:0:6342:HOH:O	15:N:4:PRO:HD2	2.15	0.46
2:A:32:VAL:HG22	2:A:38:ILE:HG13	1.97	0.46
2:A:186:TRP:CD1	2:A:187:PRO:HA	2.50	0.46
3:B:195:ARG:O	3:B:198:GLU:HG3	2.14	0.46
7:F:29:VAL:CA	7:F:99:THR:HG22	2.45	0.46
17:P:16:VAL:HG13	17:P:20:ARG:CZ	2.45	0.46
25:X:72:VAL:HG23	25:X:86:GLU:O	2.15	0.46
30:3:10:TYR:HB2	30:3:17:HIS:CE1	2.50	0.46
31:9:117:G:H2'	31:9:118:C:C6	2.49	0.46
1:0:185:G:O3'	1:0:186:A:H4'	2.15	0.46
1:0:195:C:H5''	40:M:4431:HOH:O	2.13	0.46
1:0:709:G:O2'	16:O:25:VAL:CG1	2.63	0.46
1:0:770:C:OP1	14:M:79:ALA:HB1	2.14	0.46
1:0:1525:G:H5'	1:0:1526:A:OP2	2.15	0.46
1:0:1883:U:H5''	1:0:2013:G:OP2	2.15	0.46
1:0:2346:C:H5'	5:D:54:ALA:HB2	1.96	0.46
1:0:2421:G:H3'	1:0:2422:U:C5'	2.45	0.46
3:B:84:LEU:CD2	3:B:178:ALA:HB1	2.45	0.46
3:B:204:GLY:O	3:B:261:GLN:HA	2.15	0.46
4:C:72:LYS:HG2	4:C:77:ALA:HA	1.97	0.46
9:H:44:ASP:HA	9:H:170:ARG:HH12	1.79	0.46
11:J:36:VAL:HG12	11:J:37:ALA:N	2.29	0.46
14:M:60:VAL:C	14:M:61:ILE:HD12	2.36	0.46
14:M:83:SER:C	14:M:85:ARG:H	2.17	0.46
23:V:12:THR:HG23	23:V:14:ALA:H	1.80	0.46
30:3:34:LYS:HB2	30:3:34:LYS:HZ3	1.78	0.46
31:9:52:A:H2'	31:9:53:G:O4'	2.15	0.46
1:0:220:C:H2'	13:L:48:LYS:HE3	1.97	0.46
1:0:558:C:C2'	1:0:559:U:C5'	2.87	0.46
1:0:816:G:C6	1:0:817:G:N1	2.83	0.46
1:0:901:G:OP2	13:L:18:HIS:HE1	1.98	0.46
1:0:2244:A:H1'	40:M:2788:HOH:O	2.14	0.46
1:0:2389:U:H4'	18:Q:53:HIS:CD2	2.50	0.46
1:0:2694:A:C6	1:0:2702:A:C8	3.04	0.46
3:B:16:ARG:NH2	40:B:2268:HOH:O	2.43	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:41:PHE:HB3	3:B:190:MET:HE3	1.97	0.46
3:B:71:VAL:HG11	3:B:296:LEU:HB3	1.97	0.46
3:B:194:PHE:HA	3:B:198:GLU:OE1	2.15	0.46
5:D:105:SER:CB	5:D:131:THR:HG23	2.45	0.46
7:F:110:ASP:O	7:F:114:LYS:N	2.35	0.46
8:G:23:ILE:HG22	8:G:27:ILE:CD1	2.46	0.46
15:N:63:SER:O	15:N:66:LEU:HB3	2.15	0.46
21:T:24:ARG:HH21	21:T:39:ASN:ND2	2.13	0.46
29:2:22:PRO:HG2	29:2:25:VAL:CG2	2.45	0.46
1:0:1365:C:H4'	40:0:3354:HOH:O	2.16	0.46
1:0:1473:U:C1'	28:1:42:SER:HB3	2.46	0.46
1:0:1626:A:H2'	1:0:1627:G:C5'	2.45	0.46
1:0:2438:G:H2'	1:0:2439:C:C6	2.51	0.46
1:0:2910:A:H5''	40:0:8739:HOH:O	2.15	0.46
4:C:142:ASP:OD1	4:C:237:GLU:HB3	2.15	0.46
6:E:18:LEU:HD13	6:E:34:TRP:CG	2.50	0.46
6:E:132:THR:HB	40:E:2227:HOH:O	2.15	0.46
12:K:41:LYS:O	12:K:42:ASN:HB2	2.16	0.46
14:M:89:THR:O	14:M:89:THR:HG22	2.15	0.46
17:P:83:LYS:HG3	17:P:84:ALA:N	2.31	0.46
19:R:113:HIS:O	19:R:145:LEU:HA	2.16	0.46
22:U:31:PHE:CD2	22:U:37:GLU:HA	2.49	0.46
24:W:130:HIS:NE2	31:9:88:G:OP1	2.46	0.46
30:3:25:VAL:CG2	30:3:68:LYS:HG3	2.43	0.46
30:3:83:TRP:HZ2	30:3:88:LEU:HD21	1.81	0.46
1:0:79:G:H4'	21:T:20:HIS:CE1	2.50	0.46
1:0:604:G:H4'	1:0:605:C:O5'	2.15	0.46
1:0:647:U:H2'	1:0:648:G:C8	2.50	0.46
1:0:960:G:H3'	1:0:960:G:N3	2.31	0.46
1:0:1427:A:H61	1:0:1440:U:H1'	1.79	0.46
1:0:1574:C:O5'	1:0:1574:C:H6	1.98	0.46
1:0:2045:G:H5''	40:0:6966:HOH:O	2.15	0.46
1:0:2087:C:O2'	1:0:2088:C:H5'	2.15	0.46
3:B:36:PRO:CD	3:B:169:GLY:H	2.29	0.46
4:C:16:VAL:HG12	4:C:17:ASP:N	2.31	0.46
4:C:73:GLN:HA	4:C:73:GLN:NE2	2.31	0.46
11:J:84:ARG:HB2	11:J:98:PHE:CE1	2.51	0.46
14:M:172:GLY:HA2	40:M:199:HOH:O	2.15	0.46
15:N:144:GLY:O	15:N:147:ILE:CG2	2.63	0.46
1:0:86:A:H3'	1:0:86:A:OP2	2.16	0.46
1:0:453:A:H4'	1:0:455:A:C8	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:941:G:C5	1:0:942:U:C4	3.03	0.46
1:0:1131:G:C6	1:0:1230:A:C4	3.04	0.46
1:0:1163:G:H5'	10:I:110:ASP:O	2.15	0.46
1:0:1377:C:O2'	1:0:1378:G:H5''	2.16	0.46
1:0:1702:U:H5'	40:0:7857:HOH:O	2.16	0.46
1:0:1762:C:H2'	1:0:1763:C:C6	2.44	0.46
1:0:2135:A:O4'	1:0:2243:C:N4	2.49	0.46
1:0:2300:A:H4'	1:0:2301:A:O5'	2.16	0.46
40:0:3360:HOH:O	16:O:39:THR:HB	2.15	0.46
2:A:14:SER:O	2:A:15:THR:C	2.54	0.46
2:A:179:MET:HG2	2:A:186:TRP:HB2	1.98	0.46
3:B:56:ASP:HB2	3:B:322:ARG:NE	2.30	0.46
14:M:167:GLY:O	14:M:171:ARG:HG3	2.16	0.46
21:T:48:VAL:CG2	21:T:49:GLU:N	2.79	0.46
1:0:86:A:O4'	29:2:29:THR:HG22	2.16	0.46
1:0:212:A:O4'	1:0:214:U:C6	2.69	0.46
1:0:402:U:H2'	1:0:403:C:C6	2.51	0.46
1:0:553:G:H5'	40:0:7958:HOH:O	2.15	0.46
1:0:711:G:O2'	1:0:712:C:H5'	2.16	0.46
1:0:772:G:H2'	1:0:773:A:O4'	2.16	0.46
1:0:1167:G:H2'	1:0:1168:C:O4'	2.16	0.46
1:0:1181:A:H2'	1:0:1182:C:C5'	2.45	0.46
1:0:1393:A:C2	1:0:1726:G:H4'	2.51	0.46
1:0:1496:A:H5'	1:0:1572:A:H1'	1.97	0.46
1:0:2011:A:H5'	1:0:2013:G:H1'	1.97	0.46
1:0:2438:G:H2'	1:0:2439:C:H6	1.81	0.46
1:0:2590:U:C2	32:4:74:C:C6	3.03	0.46
1:0:2720:C:O2	12:K:87:ARG:NH2	2.48	0.46
3:B:268:ARG:NH2	3:B:322:ARG:HB2	2.31	0.46
4:C:107:ARG:O	4:C:111:VAL:HG23	2.16	0.46
4:C:235:PHE:CD1	4:C:235:PHE:N	2.84	0.46
9:H:18:THR:HG22	9:H:95:HIS:O	2.15	0.46
9:H:31:ILE:HG23	40:H:6314:HOH:O	2.15	0.46
9:H:53:ILE:HG23	9:H:134:GLU:O	2.16	0.46
14:M:28:GLN:O	14:M:32:ARG:HG3	2.15	0.46
19:R:39:THR:O	19:R:40:ALA:C	2.53	0.46
22:U:56:ARG:HG3	22:U:56:ARG:NH1	2.29	0.46
23:V:25:THR:CG2	23:V:29:ASN:ND2	2.79	0.46
1:0:401:C:H2'	1:0:402:U:O4'	2.16	0.46
1:0:669:G:O2'	1:0:670:G:H5'	2.15	0.46
1:0:698:A:C5'	13:L:110:GLY:O	2.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1098:A:H2'	1:0:1099:G:O4'	2.16	0.46
1:0:1154:A:H2'	1:0:1155:G:C8	2.50	0.46
1:0:1495:C:H1'	1:0:1573:A:H1'	1.97	0.46
1:0:1850:U:H2'	1:0:1851:G:H8	1.80	0.46
1:0:1925:G:O2'	1:0:1926:G:H5'	2.15	0.46
40:0:3432:HOH:O	3:B:300:SER:HB3	2.15	0.46
3:B:233:ARG:HG2	3:B:233:ARG:NH1	2.31	0.46
4:C:27:ARG:NH1	4:C:29:ASP:OD1	2.47	0.46
4:C:84:VAL:HG12	4:C:85:LYS:HG2	1.97	0.46
5:D:159:PRO:O	5:D:162:ALA:HB3	2.15	0.46
9:H:154:ARG:HA	9:H:157:TYR:CE2	2.51	0.46
11:J:29:GLN:O	11:J:32:ASP:N	2.49	0.46
12:K:125:ALA:O	12:K:127:ALA:N	2.40	0.46
13:L:73:VAL:HG21	13:L:116:HIS:CD2	2.50	0.46
14:M:5:TYR:O	14:M:7:TYR:N	2.49	0.46
15:N:64:SER:C	15:N:66:LEU:H	2.19	0.46
20:S:32:ALA:HA	20:S:36:GLU:OE1	2.16	0.46
1:0:137:U:OP1	1:0:259:G:O2'	2.34	0.46
1:0:272:A:N1	1:0:369:G:H5''	2.31	0.46
1:0:542:A:H2'	1:0:543:G:O4'	2.16	0.46
1:0:700:A:H5''	1:0:701:U:O5'	2.16	0.46
1:0:705:C:O2	1:0:705:C:C2'	2.64	0.46
1:0:710:G:O2'	1:0:711:G:H5'	2.16	0.46
1:0:1209:C:H2'	1:0:1210:G:C8	2.47	0.46
1:0:1330:A:H5''	1:0:1331:G:OP2	2.16	0.46
1:0:1332:C:O2'	1:0:1333:U:H5'	2.16	0.46
1:0:1545:C:H2'	1:0:1546:G:O4'	2.16	0.46
1:0:1550:A:H2'	1:0:1551:C:O4'	2.15	0.46
1:0:1652:C:H4'	27:Z:76:THR:HG21	1.98	0.46
1:0:1909:A:H1'	1:0:2267:G:H5'	1.97	0.46
1:0:2416:G:O2'	15:N:25:ARG:HG2	2.15	0.46
1:0:2551:C:O2'	1:0:2552:C:H5'	2.16	0.46
1:0:2624:A:H1'	40:0:5545:HOH:O	2.15	0.46
7:F:83:LEU:HD11	7:F:96:ALA:HB3	1.96	0.46
9:H:98:LEU:HD11	9:H:127:ALA:HB2	1.96	0.46
10:I:102:GLN:C	10:I:104:ALA:H	2.19	0.46
14:M:97:ILE:CD1	14:M:127:LYS:HD2	2.40	0.46
14:M:102:GLU:OE2	14:M:164:THR:HG21	2.16	0.46
14:M:139:PRO:HA	14:M:142:GLN:HB2	1.98	0.46
14:M:180:SER:N	14:M:181:GLU:OE1	2.49	0.46
15:N:157:PRO:HA	40:N:2957:HOH:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:O:18:ALA:HB2	16:O:27:GLY:N	2.31	0.46
20:S:50:GLU:HB3	20:S:67:ARG:HH21	1.81	0.46
28:1:34:CYS:HB3	28:1:39:PHE:H	1.81	0.46
31:9:29:C:H2'	31:9:30:C:C5'	2.41	0.46
1:0:136:C:H4'	14:M:138:HIS:CD2	2.51	0.46
1:0:675:U:H2'	1:0:676:C:H5'	1.98	0.46
1:0:923:A:H2'	40:0:4815:HOH:O	2.16	0.46
1:0:955:A:H2'	1:0:956:G:O4'	2.15	0.46
1:0:1296:A:H3'	40:0:6001:HOH:O	2.16	0.46
1:0:1351:G:H3'	40:0:4676:HOH:O	2.16	0.46
1:0:1497:G:H2'	1:0:1498:G:C8	2.51	0.46
1:0:1987:C:O2'	1:0:1988:C:H5'	2.16	0.46
1:0:1992:U:H2'	1:0:1994:A:OP2	2.16	0.46
1:0:2072:G:C6	1:0:2533:C:H1'	2.50	0.46
1:0:2461:U:O2	1:0:2466:G:H1'	2.16	0.46
1:0:2749:U:H5'	40:0:7896:HOH:O	2.15	0.46
40:0:6414:HOH:O	4:C:175:LYS:HE3	2.16	0.46
3:B:13:PHE:CD1	3:B:13:PHE:N	2.83	0.46
9:H:56:GLU:C	9:H:132:ALA:HB2	2.37	0.46
11:J:75:PRO:HG2	11:J:105:LEU:CD2	2.46	0.46
12:K:63:GLU:HB2	40:K:6344:HOH:O	2.16	0.46
13:L:66:VAL:HG13	13:L:110:GLY:HA2	1.98	0.46
15:N:34:LEU:HD13	15:N:47:LEU:HD22	1.98	0.46
15:N:86:LEU:HD12	15:N:125:ALA:CB	2.45	0.46
24:W:125:HIS:HE1	40:W:3071:HOH:O	1.99	0.46
27:Z:52:GLU:O	27:Z:55:SER:HB3	2.16	0.46
28:1:28:HIS:O	28:1:32:LYS:N	2.47	0.46
31:9:63:C:O2'	31:9:64:C:H5'	2.16	0.46
1:0:263:U:C4	7:F:54:VAL:HG13	2.50	0.45
1:0:407:A:H2'	1:0:408:A:C8	2.50	0.45
1:0:875:A:C2	2:A:194:MET:SD	3.10	0.45
1:0:2002:C:H2'	1:0:2003:U:C5'	2.46	0.45
1:0:2089:A:C2'	1:0:2090:G:H5'	2.46	0.45
1:0:2421:G:H3'	1:0:2422:U:H5''	1.97	0.45
1:0:2514:U:OP1	1:0:2572:G:H1'	2.16	0.45
1:0:2793:A:H2'	1:0:2794:G:H5'	1.97	0.45
3:B:217:ARG:HD3	3:B:218:TRP:NE1	2.31	0.45
6:E:14:GLU:CG	6:E:15:GLN:H	2.29	0.45
7:F:48:VAL:CG2	7:F:74:PHE:HB3	2.45	0.45
13:L:91:VAL:CG1	13:L:120:LEU:HD23	2.46	0.45
15:N:144:GLY:O	15:N:147:ILE:HG22	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:R:114:VAL:HG13	19:R:114:VAL:O	2.15	0.45
20:S:6:LYS:HZ3	20:S:61:GLU:HG2	1.80	0.45
1:0:273:G:H2'	1:0:274:G:C8	2.51	0.45
1:0:319:A:H4'	1:0:338:C:C5	2.51	0.45
1:0:944:G:H21	24:W:44:MET:HE2	1.82	0.45
1:0:1181:A:N1	1:0:1192:A:O2'	2.48	0.45
1:0:1891:G:H1'	1:0:1972:U:C2	2.52	0.45
1:0:2382:A:H1'	30:3:10:TYR:CE2	2.51	0.45
1:0:2878:U:H2'	1:0:2879:A:O4'	2.16	0.45
4:C:161:ASP:HA	40:C:2972:HOH:O	2.16	0.45
4:C:246:ARG:NE	40:C:5065:HOH:O	2.50	0.45
14:M:152:ALA:O	14:M:155:GLN:N	2.46	0.45
15:N:48:VAL:HG13	15:N:56:ASP:O	2.16	0.45
15:N:143:ARG:HE	15:N:143:ARG:HB3	1.49	0.45
18:Q:86:VAL:HG13	18:Q:91:LEU:HD11	1.98	0.45
21:T:79:LEU:HG	21:T:89:ARG:HB2	1.98	0.45
29:2:40:ARG:HG3	29:2:45:ASN:CB	2.45	0.45
30:3:60:LYS:C	30:3:62:THR:H	2.19	0.45
1:0:432:G:O2'	1:0:433:C:H5'	2.16	0.45
1:0:653:U:H3	1:0:752:G:H1	1.64	0.45
1:0:729:C:C2	1:0:743:G:C2	3.04	0.45
1:0:1182:C:H1'	1:0:1192:A:H8	1.81	0.45
1:0:1306:U:OP1	4:C:184:ARG:NH1	2.48	0.45
1:0:1805:G:H2'	1:0:1806:G:C8	2.50	0.45
1:0:2133:U:H4'	1:0:2134:G:H5'	1.97	0.45
1:0:2408:A:HO2'	30:3:10:TYR:HD1	1.59	0.45
1:0:2779:G:N7	1:0:2790:C:C2	2.84	0.45
2:A:26:ASP:O	2:A:28:GLU:HG3	2.15	0.45
2:A:135:VAL:CG2	2:A:147:ARG:HB3	2.45	0.45
2:A:199:HIS:HD2	2:A:201:PHE:HB2	1.80	0.45
3:B:87:TYR:HD1	40:B:3693:HOH:O	1.99	0.45
3:B:175:LEU:O	3:B:175:LEU:HD23	2.17	0.45
12:K:12:LEU:HB2	12:K:47:ALA:O	2.16	0.45
15:N:183:ASP:O	15:N:184:ILE:C	2.54	0.45
17:P:111:GLU:O	17:P:111:GLU:HG2	2.15	0.45
1:0:368:C:H2'	1:0:369:G:H5'	1.99	0.45
1:0:524:A:H5''	19:R:29:LYS:HE2	1.97	0.45
1:0:1163:G:H1	1:0:1184:C:N4	2.14	0.45
1:0:1535:G:H2'	1:0:1536:C:C6	2.52	0.45
1:0:1813:U:O2'	17:P:81:LYS:HE3	2.16	0.45
1:0:2807:U:OP2	3:B:28:SER:HB2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:2842:G:H5'	19:R:68:HIS:O	2.16	0.45
2:A:76:VAL:CG2	27:Z:87:LYS:HB3	2.46	0.45
4:C:7:ASP:C	4:C:9:ASP:H	2.20	0.45
5:D:23:VAL:HG22	5:D:73:VAL:HB	1.98	0.45
6:E:94:GLN:HG3	40:E:4917:HOH:O	2.17	0.45
15:N:49:THR:HG22	15:N:56:ASP:CB	2.46	0.45
24:W:142:ASP:O	24:W:143:THR:C	2.54	0.45
26:Y:108:ASP:OD1	26:Y:108:ASP:N	2.47	0.45
27:Z:43:GLY:O	27:Z:47:ARG:NE	2.49	0.45
31:9:55:U:H4'	31:9:56:A:C8	2.52	0.45
31:9:98:C:H2'	31:9:99:U:H6	1.81	0.45
1:O:219:G:O5'	1:O:220:C:H5''	2.16	0.45
1:O:317:A:OP1	21:T:52:ARG:O	2.34	0.45
1:O:558:C:HO2'	1:O:559:U:H5''	1.80	0.45
1:O:614:U:H2'	1:O:615:G:C8	2.51	0.45
1:O:633:C:O2'	1:O:634:G:H5'	2.15	0.45
1:O:764:C:H2'	1:O:765:G:O4'	2.17	0.45
1:O:1477:C:H4'	1:O:1868:G:OP1	2.16	0.45
1:O:2248:C:H2'	1:O:2249:G:H8	1.82	0.45
1:O:2379:G:N3	1:O:2418:G:H2'	2.31	0.45
1:O:2502:C:H4'	9:H:158:ASN:ND2	2.31	0.45
1:O:2503:A:C5'	9:H:155:ARG:HH12	2.13	0.45
1:O:2637:A:C6	32:4:176:DA:H2'	2.48	0.45
1:O:2706:A:H2'	1:O:2707:C:O4'	2.17	0.45
2:A:45:ILE:HD12	27:Z:89:THR:CG2	2.46	0.45
2:A:173:GLY:O	2:A:176:HIS:HB3	2.15	0.45
4:C:138:VAL:O	4:C:234:VAL:HA	2.16	0.45
5:D:23:VAL:O	5:D:72:LYS:HA	2.16	0.45
9:H:49:GLN:NE2	9:H:170:ARG:HE	2.15	0.45
9:H:91:ARG:H	9:H:91:ARG:HG2	1.44	0.45
12:K:34:VAL:O	12:K:35:HIS:C	2.55	0.45
14:M:120:VAL:HG11	14:M:130:GLU:HG3	1.98	0.45
15:N:43:VAL:HG13	15:N:118:ILE:HD11	1.97	0.45
20:S:15:MET:O	20:S:18:MET:HB3	2.16	0.45
26:Y:178:HIS:CG	26:Y:179:PRO:HD2	2.52	0.45
31:9:56:A:C3'	31:9:57:A:H5''	2.46	0.45
1:O:380:A:H2'	40:O:6974:HOH:O	2.15	0.45
1:O:473:A:O2'	1:O:474:C:H5'	2.17	0.45
1:O:1928:C:C2'	1:O:1929:G:H5'	2.47	0.45
1:O:2506:A:O2'	1:O:2507:G:O5'	2.35	0.45
1:O:2507:G:H22	1:O:2512:U:H5''	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2602:G:H2'	1:0:2603:G:C8	2.52	0.45
1:0:2828:G:O5'	1:0:2828:G:H8	2.00	0.45
2:A:1:GLY:HA2	2:A:197:VAL:HG23	1.98	0.45
4:C:7:ASP:O	4:C:9:ASP:N	2.49	0.45
9:H:48:VAL:HB	9:H:141:CYS:O	2.16	0.45
14:M:74:LYS:O	14:M:88:VAL:HG12	2.16	0.45
14:M:186:SER:HB3	14:M:189:SER:CB	2.47	0.45
40:M:533:HOH:O	30:3:46:ILE:HD12	2.17	0.45
15:N:154:LEU:O	15:N:155:GLU:CB	2.65	0.45
16:O:33:LEU:HA	16:O:40:HIS:NE2	2.32	0.45
16:O:45:LEU:HD11	16:O:88:LYS:HB2	1.99	0.45
16:O:112:ARG:HG3	16:O:113:VAL:N	2.32	0.45
24:W:73:LEU:O	24:W:74:GLU:HG2	2.17	0.45
24:W:117:ARG:HH11	24:W:117:ARG:CB	2.29	0.45
24:W:139:GLY:O	24:W:141:HIS:HD2	1.99	0.45
1:0:292:G:H1'	1:0:360:A:H61	1.82	0.45
1:0:293:A:O2'	1:0:294:C:H5'	2.16	0.45
1:0:353:G:H2'	1:0:354:A:C8	2.51	0.45
1:0:466:A:H2'	1:0:467:G:O4'	2.17	0.45
1:0:747:G:H3'	40:0:4594:HOH:O	2.15	0.45
1:0:1088:A:C6	1:0:1291:A:H1'	2.51	0.45
1:0:1412:U:O4	1:0:1681:G:H2'	2.16	0.45
1:0:1839:A:H3'	40:0:5104:HOH:O	2.17	0.45
1:0:1890:U:H4'	1:0:2010:A:C6	2.52	0.45
1:0:2781:U:H2'	1:0:2782:G:C5'	2.45	0.45
38:0:2924:MYL:HBG	40:0:5669:HOH:O	2.17	0.45
4:C:142:ASP:OD2	4:C:238:SER:OG	2.35	0.45
13:L:97:VAL:HG12	13:L:98:GLU:O	2.16	0.45
13:L:133:VAL:HG13	40:L:4360:HOH:O	2.16	0.45
14:M:118:TYR:CZ	14:M:130:GLU:HB2	2.52	0.45
15:N:11:ARG:HA	15:N:14:ARG:NE	2.32	0.45
15:N:42:HIS:CG	15:N:62:HIS:HE1	2.34	0.45
25:X:41:PHE:CZ	25:X:74:ALA:HB3	2.51	0.45
26:Y:117:LEU:CD1	26:Y:181:GLY:HA2	2.46	0.45
27:Z:53:ILE:HG12	40:Z:5979:HOH:O	2.15	0.45
31:9:14:G:N2	31:9:68:G:H1'	2.32	0.45
1:0:12:U:C2'	1:0:13:G:H5'	2.46	0.45
1:0:59:A:H5'	40:0:2959:HOH:O	2.16	0.45
1:0:1069:C:H4'	1:0:1081:A:O2'	2.17	0.45
1:0:1456:C:H2'	1:0:1457:U:C6	2.51	0.45
1:0:2283:G:C5	9:H:116:MET:HB3	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2330:U:H4'	1:0:2331:C:OP1	2.17	0.45
1:0:2443:C:H3'	40:0:7933:HOH:O	2.17	0.45
1:0:2524:G:H21	1:0:2526:C:N4	2.15	0.45
1:0:2804:C:H2'	1:0:2805:A:O4'	2.17	0.45
40:0:8798:HOH:O	26:Y:186:ARG:HD2	2.15	0.45
2:A:217:ARG:CG	2:A:217:ARG:NH1	2.79	0.45
3:B:98:THR:HG21	3:B:127:GLN:OE1	2.16	0.45
4:C:78:ARG:NH1	4:C:78:ARG:CG	2.73	0.45
5:D:63:ILE:HG13	5:D:64:ARG:H	1.81	0.45
5:D:169:THR:C	5:D:170:TYR:HD1	2.20	0.45
6:E:162:PHE:N	6:E:162:PHE:CD1	2.84	0.45
19:R:92:LEU:HD23	19:R:145:LEU:HD21	1.99	0.45
1:0:244:C:H6	1:0:244:C:O5'	1.99	0.45
1:0:624:U:H3'	40:0:8802:HOH:O	2.16	0.45
1:0:1183:C:C2	1:0:1184:C:C5	3.05	0.45
1:0:1287:A:C5	1:0:1288:U:C5	3.05	0.45
1:0:1378:G:C6	1:0:2747:C:H2'	2.52	0.45
1:0:1387:G:C1'	17:P:28:GLN:HE22	2.30	0.45
1:0:1516:U:H2'	1:0:1517:C:C6	2.52	0.45
1:0:1785:G:OP1	17:P:76:GLY:HA3	2.16	0.45
1:0:1968:A:H2'	1:0:1969:A:C8	2.51	0.45
1:0:2100:A:H5'	40:C:7192:HOH:O	2.16	0.45
1:0:2134:G:C6	1:0:2258:A:C8	3.04	0.45
4:C:61:PHE:HB3	40:C:6056:HOH:O	2.15	0.45
12:K:82:ARG:O	12:K:85:GLY:N	2.43	0.45
13:L:43:HIS:O	13:L:44:GLU:C	2.55	0.45
13:L:90:ARG:NH2	13:L:121:ILE:HD11	2.32	0.45
13:L:148:GLU:OE1	13:L:148:GLU:C	2.55	0.45
14:M:50:ARG:N	14:M:54:TYR:HB3	2.31	0.45
15:N:37:ARG:CZ	40:N:3863:HOH:O	2.65	0.45
18:Q:48:PRO:HD2	40:Q:5227:HOH:O	2.16	0.45
21:T:71:VAL:HG11	21:T:90:PRO:CB	2.34	0.45
24:W:142:ASP:O	24:W:145:GLY:N	2.50	0.45
27:Z:57:MET:HE3	40:Z:5656:HOH:O	2.17	0.45
1:0:820:G:C5	2:A:171:LYS:HB2	2.51	0.45
1:0:944:G:O2'	1:0:945:U:H5'	2.17	0.45
1:0:1010:C:OP1	15:N:5:ARG:NH1	2.49	0.45
1:0:1025:C:H5'	24:W:23:MET:O	2.17	0.45
1:0:1055:G:N2	1:0:1057:A:H3'	2.32	0.45
1:0:1200:A:H3'	40:0:4912:HOH:O	2.17	0.45
1:0:1523:G:H2'	1:0:1524:U:O4'	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1743:G:H1'	40:0:3739:HOH:O	2.17	0.45
1:0:1815:A:H4'	1:0:2751:C:O4'	2.16	0.45
1:0:2361:A:H2'	1:0:2362:A:C8	2.51	0.45
1:0:2908:A:O5'	1:0:2908:A:H8	2.00	0.45
40:0:4366:HOH:O	2:A:215:ILE:HD12	2.16	0.45
4:C:7:ASP:OD1	4:C:11:ASN:N	2.49	0.45
6:E:22:VAL:O	6:E:28:SER:HA	2.17	0.45
6:E:146:ALA:O	6:E:150:GLN:HG2	2.17	0.45
7:F:28:ALA:CB	7:F:99:THR:HG23	2.47	0.45
7:F:58:GLU:OE2	14:M:27:ARG:NH2	2.49	0.45
9:H:70:LEU:O	9:H:72:ALA:N	2.50	0.45
11:J:71:TYR:CD1	11:J:72:PRO:HD2	2.52	0.45
12:K:130:MET:SD	22:U:25:ASP:O	2.75	0.45
26:Y:117:LEU:HD11	26:Y:181:GLY:HA2	1.98	0.45
26:Y:219:GLU:CG	26:Y:220:GLU:N	2.77	0.45
1:0:220:C:H5'	40:L:166:HOH:O	2.17	0.44
1:0:309:C:H42	1:0:322:G:H1	1.65	0.44
1:0:1766:U:H2'	1:0:1776:A:N6	2.31	0.44
1:0:1771:U:O2	27:Z:43:GLY:HA2	2.17	0.44
1:0:2435:U:OP1	30:3:28:GLY:HA3	2.17	0.44
1:0:2645:U:OP2	1:0:2645:U:H6	2.00	0.44
2:A:65:ARG:O	2:A:66:ARG:HG3	2.17	0.44
3:B:279:THR:CG2	3:B:280:VAL:N	2.79	0.44
7:F:28:ALA:C	7:F:99:THR:HG23	2.37	0.44
9:H:6:ALA:HA	9:H:61:ARG:NH1	2.32	0.44
12:K:74:VAL:HG21	12:K:96:VAL:HG23	2.00	0.44
14:M:176:LYS:HE2	14:M:176:LYS:HB3	1.85	0.44
24:W:117:ARG:CB	24:W:117:ARG:NH1	2.80	0.44
1:0:245:C:H2'	1:0:246:G:H5'	1.99	0.44
1:0:316:A:H1'	1:0:336:G:N3	2.32	0.44
1:0:862:U:H2'	1:0:863:G:C8	2.52	0.44
1:0:1164:U:OP1	10:I:69:PRO:HA	2.18	0.44
1:0:1278:A:O2'	1:0:1279:U:H3'	2.17	0.44
1:0:1523:G:C5	1:0:1524:U:C4	3.05	0.44
1:0:1557:G:H2'	1:0:1558:C:C6	2.51	0.44
1:0:1747:A:H5''	1:0:2585:G:OP1	2.17	0.44
1:0:1864:C:H2'	1:0:1865:A:O4'	2.17	0.44
1:0:2004:U:H2'	40:0:6540:HOH:O	2.16	0.44
1:0:2103:A:O2'	1:0:2104:C:OP1	2.32	0.44
1:0:2432:C:H2'	40:0:5669:HOH:O	2.16	0.44
1:0:2719:A:C2	3:B:70:PRO:HG3	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:111:C:H2'	1:0:112:G:O4'	2.17	0.44
1:0:1053:G:OP1	9:H:15:PRO:HG3	2.16	0.44
1:0:1190:G:H4'	1:0:1207:A:N1	2.33	0.44
1:0:1350:U:H1'	40:0:5164:HOH:O	2.16	0.44
1:0:2471:G:H4'	40:0:7361:HOH:O	2.16	0.44
1:0:2576:A:H4'	1:0:2799:A:N1	2.33	0.44
1:0:2765:C:H2'	1:0:2766:A:H8	1.82	0.44
1:0:2887:G:H2'	1:0:2888:U:O4'	2.16	0.44
2:A:132:ASP:OD2	2:A:133:ARG:N	2.45	0.44
5:D:172:VAL:HG12	5:D:173:GLU:H	1.82	0.44
7:F:60:VAL:O	7:F:61:MET:C	2.56	0.44
12:K:34:VAL:HB	40:K:7169:HOH:O	2.17	0.44
24:W:99:ALA:HA	24:W:102:SER:HG	1.81	0.44
30:3:2:GLN:HG3	30:3:91:GLN:CD	2.38	0.44
1:0:113:A:OP2	1:0:114:A:H2'	2.17	0.44
1:0:684:G:H2'	1:0:685:C:C6	2.52	0.44
1:0:776:A:H1'	1:0:779:U:O4	2.18	0.44
1:0:816:G:H5'	1:0:1598:A:H4'	1.98	0.44
1:0:933:C:H5''	40:0:7590:HOH:O	2.17	0.44
1:0:1014:A:H5''	31:9:101:G:O2'	2.18	0.44
1:0:1587:U:H2'	1:0:1588:G:O4'	2.18	0.44
1:0:1675:C:H5''	29:2:5:LYS:HD2	1.99	0.44
1:0:1845:A:OP2	2:A:190:ARG:NH1	2.50	0.44
1:0:2509:A:H2'	1:0:2510:C:O4'	2.18	0.44
9:H:30:LYS:H	9:H:62:HIS:HD2	1.66	0.44
9:H:61:ARG:HG3	40:H:3845:HOH:O	2.17	0.44
10:I:102:GLN:C	10:I:104:ALA:N	2.71	0.44
12:K:34:VAL:HG21	12:K:46:LYS:O	2.18	0.44
16:O:25:VAL:HG23	16:O:26:TRP:N	2.32	0.44
17:P:115:SER:C	17:P:117:SER:N	2.69	0.44
20:S:22:ASN:OD1	20:S:74:ALA:N	2.43	0.44
28:1:5:THR:N	28:1:6:PRO:CD	2.79	0.44
30:3:11:CYS:SG	30:3:12:PRO:HD2	2.58	0.44
31:9:3:A:OP2	31:9:25:G:N2	2.50	0.44
31:9:39:U:C2'	31:9:40:C:OP1	2.66	0.44
1:0:102:A:H2'	1:0:103:C:O4'	2.17	0.44
1:0:146:U:O2'	1:0:147:G:H5'	2.17	0.44
1:0:262:A:O2'	7:F:93:SER:HB2	2.16	0.44
1:0:869:G:H1'	40:0:7376:HOH:O	2.17	0.44
1:0:2133:U:H4'	1:0:2134:G:C5'	2.48	0.44
1:0:2672:C:O2'	1:0:2673:U:H5'	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:150:THR:HA	4:C:203:ALA:O	2.18	0.44
5:D:20:LYS:HG2	5:D:133:ASN:HB3	2.00	0.44
5:D:167:GLU:C	5:D:169:THR:H	2.20	0.44
6:E:152:THR:HG21	6:E:165:GLY:HA2	1.98	0.44
7:F:47:LEU:O	7:F:98:VAL:HG23	2.18	0.44
10:I:129:SER:O	10:I:130:LEU:HD23	2.18	0.44
17:P:5:ALA:O	17:P:8:ARG:HB3	2.18	0.44
20:S:15:MET:O	20:S:18:MET:N	2.50	0.44
24:W:88:THR:HG22	24:W:90:TYR:CD1	2.52	0.44
24:W:99:ALA:O	24:W:103:GLU:N	2.50	0.44
26:Y:189:ASN:C	26:Y:189:ASN:ND2	2.70	0.44
1:O:327:A:OP1	4:C:149:LYS:NZ	2.41	0.44
1:O:1683:G:C2	1:O:1693:A:O4'	2.71	0.44
1:O:1935:C:H2'	1:O:1936:C:C6	2.53	0.44
1:O:2299:G:O6	18:Q:1:PRO:HA	2.16	0.44
2:A:192:VAL:O	2:A:207:GLN:HG2	2.18	0.44
2:A:215:ILE:HG13	2:A:216:SER:N	2.33	0.44
3:B:175:LEU:C	3:B:175:LEU:CD2	2.86	0.44
3:B:279:THR:OG1	3:B:290:VAL:O	2.34	0.44
3:B:329:TYR:CE2	22:U:15:PRO:HG2	2.52	0.44
11:J:59:LYS:O	11:J:63:ILE:HG13	2.17	0.44
14:M:83:SER:C	14:M:85:ARG:N	2.71	0.44
20:S:18:MET:HA	20:S:23:LYS:O	2.17	0.44
28:1:15:THR:HB	28:1:28:HIS:NE2	2.33	0.44
29:2:36:ASN:O	29:2:39:ARG:HG3	2.17	0.44
1:O:506:G:N2	1:O:509:A:H5'	2.25	0.44
1:O:1187:U:C2	1:O:1189:A:OP2	2.70	0.44
1:O:1205:U:C2'	1:O:1206:U:C5'	2.89	0.44
1:O:2765:C:H2'	1:O:2766:A:C8	2.53	0.44
2:A:55:VAL:O	2:A:55:VAL:HG13	2.18	0.44
4:C:5:ILE:CG2	4:C:6:TYR:N	2.81	0.44
4:C:121:ALA:HA	4:C:136:VAL:HG11	2.00	0.44
7:F:96:ALA:HA	40:F:3111:HOH:O	2.18	0.44
21:T:82:THR:C	21:T:84:GLY:H	2.20	0.44
24:W:59:GLN:NE2	24:W:97:ALA:HB3	2.33	0.44
1:O:313:U:H2'	1:O:314:G:O4'	2.17	0.44
1:O:328:U:O4'	4:C:202:THR:HG22	2.17	0.44
1:O:645:U:O2	1:O:761:A:H2	2.01	0.44
1:O:1180:U:H1'	40:I:1549:HOH:O	2.17	0.44
1:O:1249:U:H2'	1:O:1250:C:C6	2.52	0.44
1:O:1593:C:H1'	40:O:5409:HOH:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:0:2924:MYL:OAR	38:0:2924:MYL:CBD	2.55	0.44
2:A:93:THR:HG23	2:A:154:ALA:O	2.18	0.44
3:B:62:ARG:HA	3:B:65:MET:HE3	1.96	0.44
6:E:94:GLN:HB2	6:E:105:GLU:HB2	1.99	0.44
10:I:87:PRO:C	10:I:89:GLU:H	2.21	0.44
12:K:34:VAL:HG21	12:K:47:ALA:HB2	1.98	0.44
13:L:17:SER:H	13:L:20:ASN:ND2	2.15	0.44
14:M:66:SER:HB2	14:M:128:TRP:NE1	2.32	0.44
17:P:89:ASN:ND2	17:P:89:ASN:C	2.70	0.44
18:Q:40:HIS:HD2	18:Q:60:THR:HG23	1.82	0.44
20:S:59:ASP:C	20:S:61:GLU:H	2.21	0.44
24:W:6:GLN:CB	24:W:26:ILE:HD11	2.48	0.44
1:0:289:G:O2'	1:0:290:C:H5'	2.17	0.44
1:0:302:A:O2'	1:0:303:C:H5'	2.18	0.44
1:0:514:G:OP1	1:0:514:G:H2'	2.17	0.44
1:0:659:A:H5''	40:O:6799:HOH:O	2.17	0.44
1:0:1174:A:C5	1:0:1201:C:H4'	2.53	0.44
1:0:1279:U:H5''	1:0:1280:A:OP2	2.18	0.44
1:0:1541:G:O2'	1:0:1542:G:H5'	2.18	0.44
1:0:1551:C:H2'	1:0:1552:G:H8	1.83	0.44
1:0:1574:C:H2'	1:0:1575:C:C6	2.52	0.44
1:0:1625:U:C6	1:0:1625:U:C3'	3.00	0.44
1:0:1746:A:H5''	40:O:5395:HOH:O	2.17	0.44
1:0:1994:A:P	12:K:66:ARG:HH22	2.40	0.44
1:0:2717:C:C2'	1:0:2718:C:C5'	2.82	0.44
1:0:2734:G:O2'	1:0:2735:U:H5'	2.18	0.44
3:B:48:MET:N	40:B:2534:HOH:O	2.50	0.44
3:B:74:ILE:HG13	40:B:4810:HOH:O	2.18	0.44
3:B:102:THR:CG2	3:B:182:VAL:HG12	2.48	0.44
3:B:141:ARG:HG2	3:B:165:ARG:HA	1.98	0.44
4:C:96:LYS:HD3	4:C:98:ARG:NH1	2.33	0.44
6:E:21:THR:HA	6:E:30:THR:HA	2.00	0.44
11:J:40:ASN:N	11:J:106:GLY:O	2.50	0.44
14:M:71:SER:OG	14:M:72:ALA:N	2.50	0.44
16:O:48:ILE:C	16:O:50:ARG:N	2.72	0.44
19:R:96:VAL:HA	19:R:99:ALA:HB3	2.00	0.44
19:R:99:ALA:O	19:R:104:PHE:HB2	2.18	0.44
24:W:13:MET:HE3	24:W:17:ILE:CG2	2.47	0.44
31:9:18:U:H2'	31:9:19:G:H8	1.81	0.44
31:9:114:G:H2'	31:9:115:C:C6	2.53	0.44
1:0:1305:C:O2'	1:0:1306:U:H5'	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1594:C:H5	17:P:120:ARG:NH1	2.15	0.43
1:0:2006:C:H2'	1:0:2007:A:C8	2.53	0.43
1:0:2103:A:HO2'	1:0:2104:C:P	2.40	0.43
1:0:2324:G:N2	1:0:2377:U:H1'	2.33	0.43
3:B:123:ALA:O	3:B:126:GLU:HB3	2.17	0.43
4:C:2:GLN:HB3	40:C:3249:HOH:O	2.18	0.43
4:C:35:VAL:HG11	4:C:227:GLY:N	2.33	0.43
6:E:23:GLU:HG2	6:E:28:SER:HB3	2.00	0.43
6:E:116:THR:CG2	6:E:151:LEU:HD22	2.39	0.43
7:F:20:LEU:HD13	7:F:49:PHE:CZ	2.53	0.43
13:L:66:VAL:HG23	13:L:67:ARG:N	2.33	0.43
14:M:146:ASP:O	14:M:147:LEU:HD23	2.18	0.43
14:M:159:VAL:HG13	14:M:160:PHE:N	2.33	0.43
15:N:44:ARG:HG3	15:N:45:ALA:N	2.32	0.43
17:P:114:LEU:HA	17:P:118:GLN:NE2	2.33	0.43
18:Q:25:PRO:HA	18:Q:26:PRO:HD3	1.83	0.43
19:R:84:ALA:O	19:R:88:PHE:HD1	2.01	0.43
23:V:12:THR:HG22	23:V:15:GLU:OE2	2.18	0.43
1:0:35:U:O2'	1:0:36:C:H5'	2.18	0.43
1:0:57:C:N4	1:0:89:G:H1	2.15	0.43
1:0:524:A:H5'	19:R:29:LYS:HE2	2.00	0.43
1:0:808:A:C5	1:0:809:G:H1'	2.54	0.43
1:0:1264:U:P	24:W:117:ARG:HH22	2.40	0.43
1:0:1626:A:H2'	1:0:1627:G:H5'	1.99	0.43
1:0:1819:G:H2'	1:0:1820:G:C4'	2.47	0.43
1:0:2504:A:H4'	9:H:74:ARG:NH1	2.34	0.43
1:0:2596:A:H3'	40:0:8372:HOH:O	2.18	0.43
40:0:3998:HOH:O	3:B:216:LYS:HA	2.18	0.43
4:C:46:TYR:H	4:C:98:ARG:HH21	1.65	0.43
10:I:134:ILE:HG22	10:I:135:GLU:N	2.33	0.43
13:L:114:VAL:HG21	13:L:132:LYS:HB3	2.00	0.43
16:O:97:SER:C	16:O:99:GLU:H	2.21	0.43
17:P:89:ASN:HD22	17:P:90:SER:N	2.16	0.43
20:S:6:LYS:O	20:S:7:HIS:HB3	2.18	0.43
21:T:17:HIS:O	21:T:20:HIS:HD2	2.00	0.43
21:T:82:THR:C	21:T:84:GLY:N	2.72	0.43
1:0:37:A:C2	1:0:446:G:C2	3.07	0.43
1:0:65:C:H2'	1:0:66:G:C8	2.53	0.43
1:0:686:A:O2'	1:0:747:G:H4'	2.18	0.43
1:0:1319:G:H1'	40:0:3460:HOH:O	2.17	0.43
1:0:1375:A:O2'	1:0:1376:G:H5'	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1677:U:OP2	29:2:8:LYS:NZ	2.43	0.43
1:0:1750:C:H5''	40:0:8211:HOH:O	2.17	0.43
1:0:2026:C:H2'	1:0:2027:U:H6	1.81	0.43
1:0:2053:G:H4'	19:R:136:TRP:CE2	2.53	0.43
4:C:95:GLU:HG3	40:C:7650:HOH:O	2.18	0.43
4:C:246:ARG:HH11	4:C:246:ARG:CB	2.27	0.43
5:D:169:THR:O	5:D:170:TYR:HB2	2.18	0.43
6:E:166:VAL:HB	40:E:6341:HOH:O	2.17	0.43
16:O:96:VAL:HG12	16:O:97:SER:N	2.33	0.43
28:1:10:LYS:HG3	40:1:2979:HOH:O	2.18	0.43
1:0:170:U:H2'	1:0:171:C:H5'	1.99	0.43
1:0:912:A:C4	1:0:1294:A:C2	3.05	0.43
1:0:1028:U:H5'	1:0:1031:G:O4'	2.18	0.43
1:0:1311:G:C2	1:0:1312:G:C8	3.06	0.43
1:0:1629:G:N2	1:0:1632:A:OP2	2.52	0.43
1:0:1899:C:H5''	2:A:216:SER:N	2.33	0.43
1:0:2615:U:C5	1:0:2616:G:C6	3.07	0.43
1:0:2779:G:H21	6:E:143:GLN:NE2	2.16	0.43
4:C:72:LYS:HD2	40:C:5079:HOH:O	2.18	0.43
4:C:98:ARG:HG2	4:C:98:ARG:NH1	2.31	0.43
4:C:132:ASP:HB3	40:C:2669:HOH:O	2.18	0.43
9:H:92:LYS:HG3	9:H:130:VAL:HG22	2.00	0.43
11:J:130:VAL:CG1	11:J:131:THR:N	2.81	0.43
13:L:41:HIS:O	13:L:42:ASN:HB2	2.17	0.43
14:M:4:ALA:O	14:M:7:TYR:HB2	2.18	0.43
14:M:120:VAL:CG1	14:M:130:GLU:HG3	2.48	0.43
15:N:27:LEU:CD2	15:N:50:LEU:HD22	2.47	0.43
20:S:52:VAL:HG22	20:S:66:VAL:HG22	2.01	0.43
24:W:88:THR:O	24:W:90:TYR:N	2.52	0.43
27:Z:70:ARG:NH1	27:Z:82:SER:C	2.68	0.43
27:Z:90:GLY:HA3	27:Z:95:PRO:O	2.18	0.43
1:0:553:G:C2'	1:0:554:G:H5'	2.49	0.43
1:0:827:A:H2'	1:0:828:G:O4'	2.18	0.43
1:0:1738:C:O2'	1:0:1739:G:H5'	2.18	0.43
1:0:1786:C:OP1	17:P:74:GLN:HG2	2.18	0.43
40:0:7516:HOH:O	2:A:21:HIS:HB2	2.19	0.43
2:A:170:VAL:HG21	27:Z:50:VAL:HG21	2.00	0.43
3:B:266:ASN:OD1	3:B:317:PRO:HA	2.19	0.43
9:H:122:LYS:O	9:H:124:VAL:HG13	2.18	0.43
12:K:27:ARG:HD2	12:K:60:GLY:HA2	2.01	0.43
15:N:15:GLU:HB3	15:N:17:ARG:HG3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:324:G:O2'	1:0:325:U:H5'	2.19	0.43
1:0:391:U:H5''	40:0:5416:HOH:O	2.18	0.43
1:0:550:C:H2'	1:0:551:A:O4'	2.18	0.43
1:0:1051:C:H2'	1:0:1052:G:O4'	2.18	0.43
1:0:1171:A:H2'	1:0:1172:G:H5'	2.00	0.43
1:0:1286:A:H5''	40:0:7804:HOH:O	2.18	0.43
1:0:1537:C:H1'	40:0:6076:HOH:O	2.18	0.43
1:0:1695:G:N3	28:1:9:GLY:HA3	2.33	0.43
1:0:1808:C:O2'	1:0:1809:G:H5'	2.19	0.43
1:0:2433:A:H8	1:0:2433:A:O5'	2.01	0.43
1:0:2529:G:H3'	40:0:6917:HOH:O	2.19	0.43
1:0:2541:U:O2'	32:4:76:5AA:H4'	2.18	0.43
2:A:140:LEU:HB3	2:A:141:PRO:HD2	2.00	0.43
2:A:213:LYS:HB2	40:A:242:HOH:O	2.18	0.43
3:B:26:PHE:HE1	3:B:310:ARG:HB3	1.82	0.43
3:B:71:VAL:HG11	3:B:296:LEU:HD22	2.01	0.43
11:J:19:MET:HE3	11:J:132:LEU:CD1	2.30	0.43
13:L:30:ARG:HG3	13:L:30:ARG:NH1	2.30	0.43
14:M:81:ARG:HB2	14:M:81:ARG:HH11	1.80	0.43
15:N:159:TYR:HE1	31:9:50:G:H5''	1.84	0.43
21:T:114:SER:OG	21:T:117:ASP:HB2	2.19	0.43
22:U:9:CYS:HA	22:U:52:THR:CG2	2.47	0.43
24:W:122:ARG:NH1	24:W:152:ALA:O	2.49	0.43
24:W:128:VAL:HG12	24:W:138:LEU:HD21	2.01	0.43
30:3:62:THR:CG2	30:3:63:LYS:N	2.81	0.43
1:0:74:G:H5'	23:V:9:ARG:HH22	1.83	0.43
1:0:251:C:H2'	1:0:252:C:H6	1.83	0.43
1:0:1186:C:H42	1:0:1190:G:H22	1.66	0.43
1:0:1342:C:O2'	1:0:1343:C:H5'	2.19	0.43
1:0:1441:G:H2'	1:0:1442:A:H8	1.83	0.43
1:0:1553:C:O5'	1:0:1553:C:H6	2.02	0.43
1:0:1730:G:H4'	1:0:1731:C:H6	1.82	0.43
1:0:2415:A:H2'	1:0:2416:G:H5'	1.99	0.43
3:B:139:ASP:CB	3:B:165:ARG:HE	2.31	0.43
5:D:52:THR:N	5:D:70:GLY:O	2.52	0.43
5:D:75:LEU:HB3	5:D:80:ALA:CA	2.49	0.43
6:E:14:GLU:CG	6:E:15:GLN:N	2.80	0.43
6:E:26:ASN:CB	6:E:76:VAL:O	2.67	0.43
7:F:28:ALA:HB3	7:F:99:THR:HG23	2.00	0.43
9:H:49:GLN:O	9:H:49:GLN:HG2	2.18	0.43
9:H:53:ILE:HA	9:H:134:GLU:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:H:96:GLN:NE2	9:H:129:ARG:NH2	2.66	0.43
11:J:131:THR:HG22	11:J:134:GLU:H	1.84	0.43
20:S:6:LYS:HB2	20:S:27:ALA:O	2.19	0.43
1:0:82:C:H4'	1:0:99:A:O2'	2.19	0.43
1:0:125:U:C2	1:0:128:A:C2	3.07	0.43
1:0:255:A:H2'	1:0:256:C:C6	2.54	0.43
1:0:281:U:O2'	1:0:282:C:H5'	2.19	0.43
1:0:304:G:H1'	1:0:347:A:N6	2.33	0.43
1:0:593:A:H2'	1:0:594:C:H5'	2.01	0.43
1:0:945:U:H2'	1:0:946:C:C6	2.54	0.43
1:0:1166:A:H2'	1:0:1166:A:N3	2.33	0.43
1:0:1220:U:O2'	1:0:1221:G:H5'	2.18	0.43
1:0:1262:C:O2	24:W:120:PRO:HG2	2.19	0.43
1:0:1515:A:H2'	1:0:1516:U:C6	2.53	0.43
1:0:1594:C:O2'	1:0:1607:A:H4'	2.18	0.43
1:0:2237:G:H1'	1:0:2238:A:C8	2.54	0.43
1:0:2647:C:H1'	40:0:5844:HOH:O	2.18	0.43
1:0:2834:G:OP1	25:X:39:LYS:HE2	2.18	0.43
2:A:135:VAL:HG22	2:A:136:ALA:N	2.33	0.43
5:D:23:VAL:O	5:D:23:VAL:CG2	2.66	0.43
5:D:25:MET:HE2	5:D:41:LEU:HD11	2.01	0.43
5:D:137:PRO:O	5:D:139:TYR:N	2.52	0.43
8:G:64:ASN:ND2	8:G:64:ASN:H	2.16	0.43
11:J:75:PRO:HB3	11:J:132:LEU:HB3	2.01	0.43
15:N:7:LYS:HB2	40:Q:5853:HOH:O	2.19	0.43
15:N:164:ASP:CG	15:N:167:ASP:HA	2.39	0.43
17:P:80:ARG:HG2	17:P:87:ARG:NH2	2.33	0.43
26:Y:109:LEU:HA	40:Y:4541:HOH:O	2.18	0.43
30:3:11:CYS:SG	30:3:13:HIS:CD2	3.11	0.43
31:9:52:A:O2'	31:9:53:G:H5'	2.19	0.43
1:0:17:G:O2'	1:0:18:C:H5'	2.18	0.43
1:0:85:C:H3'	1:0:86:A:H2'	2.00	0.43
1:0:696:C:H2'	1:0:697:G:O4'	2.18	0.43
1:0:699:C:C2	1:0:743:G:N2	2.86	0.43
1:0:1095:U:O2	24:W:120:PRO:HG2	2.18	0.43
1:0:1409:G:C2	1:0:1410:G:C8	3.07	0.43
1:0:1430:G:H5''	40:0:3794:HOH:O	2.18	0.43
1:0:1741:U:C4	1:0:2033:G:C8	3.07	0.43
1:0:1800:G:H2'	1:0:1801:A:H8	1.83	0.43
1:0:1804:A:H2'	1:0:1805:G:C8	2.53	0.43
1:0:1850:U:H2'	1:0:1851:G:C8	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1935:C:H2'	1:0:1936:C:H6	1.84	0.43
1:0:2387:U:H2'	1:0:2388:C:C6	2.53	0.43
1:0:2502:C:H2'	1:0:2503:A:C5'	2.35	0.43
1:0:2631:U:H5''	40:0:5654:HOH:O	2.19	0.43
3:B:278:PRO:HD3	3:B:294:TYR:CZ	2.53	0.43
4:C:22:PHE:HA	4:C:116:ALA:HA	2.01	0.43
4:C:79:ARG:O	4:C:87:ARG:N	2.51	0.43
11:J:42:GLU:O	11:J:131:THR:HG23	2.19	0.43
13:L:32:ASP:O	13:L:35:ARG:HB3	2.19	0.43
14:M:74:LYS:O	14:M:88:VAL:HA	2.18	0.43
14:M:101:ALA:O	14:M:102:GLU:C	2.56	0.43
15:N:180:LEU:HD12	15:N:180:LEU:N	2.34	0.43
21:T:53:GLY:HA3	40:T:6384:HOH:O	2.18	0.43
24:W:142:ASP:C	24:W:144:GLU:N	2.71	0.43
26:Y:160:LYS:HD3	26:Y:160:LYS:HA	1.79	0.43
27:Z:81:CYS:HB3	27:Z:86:TYR:H	1.83	0.43
28:1:20:ARG:N	40:1:513:HOH:O	2.52	0.43
28:1:25:LYS:HD2	29:2:48:ASP:HA	2.01	0.43
31:9:34:A:H2'	31:9:35:C:O4'	2.19	0.43
1:0:195:C:C2'	1:0:196:G:H5'	2.46	0.43
1:0:220:C:H2'	40:L:166:HOH:O	2.18	0.43
1:0:226:A:H1'	1:0:393:G:C5	2.54	0.43
1:0:603:A:H1'	1:0:605:C:C2	2.53	0.43
1:0:667:C:H2'	1:0:668:C:H6	1.84	0.43
1:0:675:U:O2'	4:C:42:ARG:NH1	2.52	0.43
1:0:844:A:C6	1:0:882:A:C6	3.06	0.43
1:0:920:C:OP1	13:L:37:LYS:NZ	2.52	0.43
1:0:1055:G:OP2	9:H:99:ARG:NH1	2.52	0.43
1:0:1102:C:H1'	1:0:1109:U:C4	2.54	0.43
1:0:2271:G:N3	1:0:2271:G:H2'	2.34	0.43
1:0:2758:G:H2'	1:0:2759:C:C6	2.54	0.43
1:0:2911:C:H2'	1:0:2912:C:C6	2.54	0.43
40:0:8286:HOH:O	16:O:42:GLU:HB2	2.18	0.43
11:J:74:ARG:HH11	11:J:74:ARG:CB	2.25	0.43
11:J:131:THR:HG22	11:J:133:GLY:H	1.83	0.43
13:L:130:ARG:O	13:L:131:GLU:C	2.57	0.43
14:M:24:GLN:NE2	14:M:27:ARG:NH1	2.67	0.43
17:P:67:LYS:O	17:P:68:LYS:C	2.57	0.43
18:Q:16:ASN:ND2	18:Q:45:PRO:HD2	2.29	0.43
19:R:4:TYR:CZ	19:R:15:LYS:HB3	2.54	0.43
23:V:5:VAL:HG23	40:V:2271:HOH:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:Y:146:PRO:O	26:Y:154:ARG:HG3	2.19	0.43
27:Z:99:GLY:O	27:Z:103:VAL:HG23	2.19	0.43
1:0:107:U:C2'	1:0:108:U:H5'	2.49	0.42
1:0:121:U:OP2	29:2:10:ARG:NH2	2.47	0.42
1:0:1116:U:O2'	1:0:1118:A:C2	2.47	0.42
1:0:1388:U:H2'	1:0:1389:G:O4'	2.19	0.42
1:0:1477:C:C5'	1:0:1868:G:C5'	2.97	0.42
1:0:1838:U:O2'	1:0:2644:C:H5'	2.19	0.42
1:0:1908:G:N1	1:0:1930:A:OP2	2.51	0.42
1:0:2103:A:O2'	1:0:2104:C:P	2.77	0.42
1:0:2493:C:O2	1:0:2493:C:H2'	2.19	0.42
1:0:2505:G:C2'	1:0:2506:A:H5'	2.49	0.42
1:0:2526:C:C6	1:0:2526:C:H5'	2.54	0.42
3:B:181:ILE:HG22	3:B:186:GLY:HA2	2.01	0.42
4:C:80:VAL:HA	4:C:81:PRO:HD3	1.88	0.42
4:C:149:LYS:O	4:C:150:THR:C	2.57	0.42
40:C:2822:HOH:O	21:T:2:LYS:HE2	2.18	0.42
7:F:107:ASP:O	7:F:108:VAL:C	2.57	0.42
10:I:97:VAL:HG12	10:I:101:LYS:HE3	2.00	0.42
14:M:23:LEU:HD13	14:M:27:ARG:NH2	2.34	0.42
18:Q:23:THR:HG22	18:Q:24:SER:N	2.34	0.42
19:R:39:THR:HB	19:R:42:GLU:OE1	2.19	0.42
21:T:49:GLU:HG2	21:T:99:THR:CG2	2.49	0.42
24:W:131:PRO:O	24:W:136:GLY:CA	2.67	0.42
30:3:34:LYS:HG3	30:3:35:TRP:H	1.84	0.42
1:0:48:A:H2'	1:0:49:A:C8	2.53	0.42
1:0:699:C:C2'	1:0:744:G:N3	2.82	0.42
1:0:2317:C:P	30:3:61:PRO:HG2	2.58	0.42
1:0:2332:A:H3'	1:0:2333:G:H8	1.84	0.42
1:0:2474:A:N7	1:0:2621:PSU:H4'	2.34	0.42
1:0:2545:U:OP2	3:B:2:GLN:NE2	2.46	0.42
1:0:2617:G:H4'	40:0:3214:HOH:O	2.18	0.42
3:B:52:VAL:N	3:B:329:TYR:O	2.43	0.42
3:B:160:ASP:HB3	3:B:308:LEU:HD22	2.01	0.42
6:E:18:LEU:HD13	6:E:34:TRP:CD1	2.53	0.42
7:F:48:VAL:HG23	7:F:74:PHE:CB	2.49	0.42
13:L:110:GLY:HA3	13:L:129:ALA:HA	2.01	0.42
16:O:71:GLN:HA	16:O:92:VAL:HG11	2.01	0.42
18:Q:77:ASP:O	18:Q:79:GLY:N	2.51	0.42
19:R:68:HIS:CG	19:R:76:ASP:HB2	2.54	0.42
24:W:23:MET:C	24:W:25:ASN:H	2.23	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:W:56:GLU:O	24:W:143:THR:HG23	2.19	0.42
24:W:80:ASP:O	24:W:81:ASP:C	2.57	0.42
25:X:52:PRO:O	25:X:53:SER:C	2.58	0.42
28:1:49:GLU:HA	28:1:49:GLU:OE2	2.19	0.42
31:9:54:A:C2'	31:9:55:U:H5'	2.48	0.42
1:0:212:A:O3'	1:0:213:G:H4'	2.19	0.42
1:0:215:A:OP1	13:L:52:LYS:NZ	2.45	0.42
1:0:1185:U:H5'	40:0:7308:HOH:O	2.17	0.42
1:0:1397:C:H1'	17:P:28:GLN:OE1	2.19	0.42
1:0:2070:G:H2'	1:0:2072:G:OP1	2.19	0.42
1:0:2546:U:O2'	3:B:237:GLY:N	2.52	0.42
1:0:2637:A:N6	32:4:176:DA:C2'	2.62	0.42
40:0:6068:HOH:O	31:9:83:G:H4'	2.18	0.42
40:0:8389:HOH:O	9:H:14:LYS:HD3	2.19	0.42
3:B:147:VAL:CG1	3:B:150:ALA:HB2	2.49	0.42
3:B:258:GLY:N	3:B:260:HIS:CE1	2.78	0.42
4:C:131:PHE:HD2	4:C:131:PHE:N	2.09	0.42
5:D:10:PHE:N	40:D:7345:HOH:O	2.53	0.42
8:G:73:ASP:N	8:G:73:ASP:OD1	2.52	0.42
14:M:98:GLN:NE2	14:M:117:SER:OG	2.49	0.42
15:N:20:TYR:HA	15:N:23:ARG:HB3	2.01	0.42
17:P:68:LYS:O	17:P:73:HIS:HB2	2.20	0.42
19:R:39:THR:O	19:R:41:GLY:N	2.52	0.42
23:V:25:THR:HG23	23:V:29:ASN:ND2	2.34	0.42
26:Y:125:LYS:HB2	26:Y:126:PRO:HD2	2.01	0.42
26:Y:132:ASP:OD1	26:Y:135:LYS:HD2	2.18	0.42
30:3:6:ARG:HG2	30:3:6:ARG:NH1	2.34	0.42
1:0:272:A:C2	1:0:369:G:H5'	2.55	0.42
1:0:472:A:O4'	1:0:774:C:H4'	2.18	0.42
1:0:665:A:H2'	1:0:666:A:C8	2.54	0.42
1:0:1135:G:C6	1:0:1136:U:C4	3.07	0.42
1:0:1184:C:O2'	1:0:1185:U:OP2	2.27	0.42
1:0:1427:A:O2'	1:0:1428:C:H5'	2.19	0.42
1:0:2036:C:H1'	12:K:44:HIS:CD2	2.54	0.42
2:A:134:ASN:O	2:A:150:PRO:HD3	2.20	0.42
2:A:181:ALA:O	2:A:182:ARG:HG2	2.19	0.42
5:D:166:ILE:HB	40:D:6326:HOH:O	2.20	0.42
13:L:61:ALA:HB2	13:L:105:TYR:CZ	2.54	0.42
14:M:76:ARG:NH1	14:M:77:HIS:CE1	2.88	0.42
14:M:164:THR:HG22	14:M:167:GLY:H	1.85	0.42
17:P:55:LYS:HA	40:P:4732:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:Q:81:GLU:HG3	40:Q:3458:HOH:O	2.20	0.42
24:W:68:THR:HG23	24:W:69:ARG:HG2	2.01	0.42
30:3:59:ASP:CG	30:3:63:LYS:HZ1	2.22	0.42
31:9:61:C:H2'	31:9:62:A:C8	2.53	0.42
31:9:78:G:H22	31:9:103:A:P	2.42	0.42
1:0:163:U:O3'	1:0:896:C:H4'	2.20	0.42
1:0:213:G:HO2'	1:0:214:U:P	2.42	0.42
1:0:710:G:P	16:O:24:ALA:HB3	2.59	0.42
1:0:737:A:H2'	1:0:738:G:C8	2.54	0.42
1:0:1167:G:H4'	10:I:130:LEU:HD22	2.00	0.42
1:0:2382:A:H1'	30:3:10:TYR:HE2	1.84	0.42
1:0:2533:C:O2'	1:0:2534:C:H5'	2.20	0.42
1:0:2663:U:C4	1:0:2664:A:C6	3.08	0.42
1:0:2748:G:H1'	40:0:7865:HOH:O	2.18	0.42
1:0:2811:A:C4'	1:0:2812:A:H5''	2.49	0.42
1:0:2838:A:H2'	1:0:2839:C:O4'	2.20	0.42
1:0:2896:A:OP1	25:X:15:ARG:NH1	2.52	0.42
1:0:2898:G:O2'	1:0:2899:A:H5'	2.19	0.42
40:0:5147:HOH:O	32:4:176:DA:H2	2.02	0.42
4:C:200:PRO:HA	40:C:3887:HOH:O	2.19	0.42
4:C:236:THR:O	4:C:239:ALA:HB3	2.18	0.42
6:E:126:ILE:HB	6:E:131:LEU:CD2	2.49	0.42
7:F:1:PRO:N	7:F:4:VAL:HG23	2.33	0.42
10:I:95:LEU:CD2	10:I:99:GLN:HB3	2.49	0.42
13:L:21:ARG:HA	13:L:26:HIS:HD2	1.85	0.42
13:L:73:VAL:HG21	13:L:116:HIS:CE1	2.54	0.42
14:M:94:ARG:HG2	14:M:94:ARG:HH11	1.84	0.42
14:M:112:LEU:HB3	14:M:133:LEU:HB3	2.02	0.42
15:N:151:ASP:O	15:N:154:LEU:HB2	2.19	0.42
21:T:23:VAL:C	21:T:93:THR:HG21	2.40	0.42
22:U:14:GLU:HA	22:U:15:PRO:HD2	1.91	0.42
24:W:82:GLU:O	24:W:86:GLU:HG3	2.20	0.42
26:Y:107:PRO:HB3	26:Y:182:PHE:CE2	2.53	0.42
32:4:74:C:C2'	32:4:75:C:H5'	2.49	0.42
1:0:37:A:H2'	1:0:38:G:C8	2.55	0.42
1:0:483:C:C4	1:0:484:A:C6	3.08	0.42
1:0:541:C:O2'	1:0:542:A:H5''	2.19	0.42
1:0:549:A:O2'	1:0:550:C:H5'	2.20	0.42
1:0:652:G:H5''	40:0:6351:HOH:O	2.18	0.42
1:0:706:G:N2	1:0:707:C:N4	2.66	0.42
1:0:921:G:H4'	1:0:924:G:N1	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1380:U:O4	1:0:2043:U:H4'	2.19	0.42
1:0:1898:G:H2'	1:0:1899:C:C6	2.55	0.42
40:0:8598:HOH:O	21:T:82:THR:HA	2.20	0.42
3:B:270:ILE:HD13	3:B:270:ILE:HA	1.87	0.42
4:C:97:ASP:OD2	4:C:97:ASP:C	2.58	0.42
7:F:6:PHE:O	7:F:6:PHE:CD1	2.72	0.42
9:H:46:TYR:HA	9:H:47:PRO:HD3	1.86	0.42
9:H:94:PRO:HB2	9:H:126:THR:HB	2.00	0.42
10:I:114:TYR:CD1	10:I:114:TYR:N	2.87	0.42
13:L:142:LEU:HD21	13:L:146:GLY:O	2.19	0.42
14:M:14:ASN:C	14:M:16:GLY:H	2.22	0.42
14:M:99:ARG:CG	14:M:99:ARG:NH1	2.67	0.42
15:N:26:LEU:HD12	15:N:26:LEU:HA	1.82	0.42
16:O:35:LYS:HB3	16:O:36:PRO:HD2	2.00	0.42
16:O:59:VAL:HG23	16:O:111:VAL:HG21	2.01	0.42
16:O:100:GLN:O	16:O:103:GLU:N	2.52	0.42
19:R:95:ALA:HB1	19:R:147:LEU:CD1	2.50	0.42
24:W:108:ARG:NH2	24:W:114:PRO:HG2	2.27	0.42
24:W:129:LYS:HD3	31:9:87:U:H2'	2.00	0.42
26:Y:187:VAL:CG1	26:Y:205:ILE:HA	2.49	0.42
1:0:183:A:H1'	14:M:161:ARG:HH11	1.82	0.42
1:0:1589:G:H4'	40:0:6458:HOH:O	2.19	0.42
1:0:1878:G:O2'	1:0:1879:U:P	2.78	0.42
1:0:1965:C:O5'	1:0:1965:C:H6	2.01	0.42
4:C:53:GLY:O	4:C:79:ARG:HA	2.20	0.42
9:H:51:SER:HA	9:H:138:THR:HA	2.01	0.42
11:J:39:VAL:HG13	11:J:40:ASN:HD22	1.84	0.42
11:J:39:VAL:O	11:J:40:ASN:HB2	2.19	0.42
13:L:144:ASP:HA	13:L:147:GLU:CD	2.40	0.42
21:T:4:PRO:O	21:T:8:ARG:HG3	2.20	0.42
22:U:39:ASN:ND2	22:U:51:TRP:HZ2	2.18	0.42
24:W:90:TYR:N	24:W:90:TYR:HD1	2.17	0.42
30:3:3:MET:HE3	30:3:4:PRO:HD2	2.02	0.42
1:0:164:G:H4'	13:L:30:ARG:HD2	2.01	0.42
1:0:585:C:H5''	40:0:3708:HOH:O	2.20	0.42
1:0:661:G:C6	1:0:686:A:C2	3.07	0.42
1:0:1067:A:O2'	24:W:12:ASN:HA	2.20	0.42
1:0:1441:G:H2'	1:0:1442:A:C8	2.54	0.42
1:0:1855:G:N7	2:A:142:SER:OG	2.43	0.42
1:0:1882:C:H2'	1:0:1883:U:C6	2.54	0.42
1:0:1941:A:H5''	40:0:7014:HOH:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2548:C:OP2	3:B:5:ARG:NH2	2.52	0.42
1:0:2607:U:OP2	3:B:243:ASN:HB2	2.19	0.42
1:0:2757:A:C4	1:0:2896:A:C2	3.08	0.42
38:0:2924:MYL:HABB	38:0:2924:MYL:CAV	2.50	0.42
2:A:109:GLU:HG2	2:A:114:ASP:OD1	2.19	0.42
3:B:320:GLN:NE2	3:B:321:PRO:CD	2.80	0.42
7:F:70:LYS:O	7:F:72:VAL:N	2.44	0.42
8:G:19:GLU:O	8:G:23:ILE:HG13	2.20	0.42
8:G:23:ILE:C	8:G:25:GLU:N	2.72	0.42
9:H:9:TYR:O	9:H:59:GLN:HB2	2.20	0.42
9:H:165:ARG:NH1	40:H:6571:HOH:O	2.53	0.42
12:K:18:ILE:HG22	12:K:93:ASN:HB2	2.00	0.42
15:N:1:ALA:HB2	31:9:14:G:O2'	2.20	0.42
15:N:58:LEU:N	15:N:58:LEU:HD12	2.35	0.42
15:N:108:SER:C	15:N:110:THR:H	2.23	0.42
31:9:60:C:O2'	31:9:61:C:H5'	2.19	0.42
1:0:88:G:N7	29:2:28:LYS:HD2	2.35	0.42
1:0:453:A:C4	1:0:479:G:C8	3.08	0.42
1:0:544:G:H2'	1:0:545:G:H5'	2.01	0.42
1:0:1047:U:H2'	1:0:1048:G:C8	2.54	0.42
1:0:1158:G:O2'	1:0:1159:G:H5'	2.20	0.42
1:0:1311:G:C5	1:0:1344:G:C6	3.08	0.42
1:0:1486:A:C4	29:2:2:LYS:HG3	2.55	0.42
1:0:1942:A:O2'	1:0:1943:C:H5'	2.20	0.42
1:0:2319:C:H3'	30:3:1:MET:HA	2.02	0.42
1:0:2324:G:H4'	1:0:2418:G:O2'	2.19	0.42
1:0:2349:G:H5'	5:D:133:ASN:HD22	1.85	0.42
1:0:2378:U:OP1	30:3:8:ASN:HB3	2.20	0.42
1:0:2820:A:H2'	1:0:2821:C:C6	2.55	0.42
3:B:120:ASP:CG	3:B:123:ALA:HB2	2.40	0.42
3:B:154:VAL:HA	3:B:155:PRO:HD3	1.87	0.42
3:B:280:VAL:HG13	3:B:333:GLU:O	2.20	0.42
4:C:178:GLN:C	4:C:180:SER:N	2.69	0.42
8:G:24:VAL:HA	8:G:27:ILE:HD12	2.02	0.42
13:L:117:GLU:O	13:L:117:GLU:CG	2.68	0.42
17:P:87:ARG:HG2	17:P:87:ARG:HH11	1.85	0.42
19:R:63:ASN:OD1	19:R:63:ASN:N	2.53	0.42
25:X:16:ASP:C	25:X:18:ARG:H	2.23	0.42
25:X:21:PRO:CG	25:X:24:LYS:HD3	2.49	0.42
25:X:41:PHE:O	25:X:43:VAL:HG23	2.20	0.42
30:3:3:MET:CE	30:3:4:PRO:HD2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:3:8:ASN:ND2	30:3:17:HIS:HD2	2.18	0.42
1:0:65:C:H2'	1:0:66:G:H8	1.85	0.42
1:0:261:A:OP1	14:M:42:ARG:NH2	2.53	0.42
1:0:332:G:H4'	21:T:2:LYS:O	2.20	0.42
1:0:645:U:O2	4:C:93:LYS:NZ	2.52	0.42
1:0:1013:A:H5''	1:0:2302:A:N6	2.35	0.42
1:0:1150:A:C2	8:G:20:VAL:HG21	2.54	0.42
1:0:1384:C:H5'	25:X:30:MET:HG2	2.02	0.42
1:0:1457:U:O2'	1:0:1458:A:H5'	2.20	0.42
1:0:1552:G:C6	1:0:1634:G:C6	3.08	0.42
1:0:1630:A:H2'	1:0:1631:A:O4'	2.20	0.42
1:0:1790:C:H2'	1:0:1791:U:C6	2.55	0.42
1:0:2001:G:O2'	1:0:2002:C:H5'	2.20	0.42
1:0:2248:C:H3'	40:0:4476:HOH:O	2.20	0.42
1:0:2542:C:O2'	32:4:75:C:H1'	2.19	0.42
1:0:2815:G:H4'	1:0:2816:A:OP2	2.20	0.42
40:0:3586:HOH:O	2:A:11:ARG:HD3	2.19	0.42
2:A:95:PRO:HG2	2:A:98:GLU:CG	2.50	0.42
2:A:188:ASN:HA	40:A:3459:HOH:O	2.19	0.42
4:C:243:VAL:HG22	4:C:243:VAL:O	2.20	0.42
5:D:22:VAL:HA	5:D:73:VAL:O	2.20	0.42
5:D:169:THR:O	5:D:169:THR:HG22	2.20	0.42
7:F:12:LEU:HD22	7:F:75:ILE:HD11	2.02	0.42
9:H:14:LYS:HG2	40:H:714:HOH:O	2.19	0.42
11:J:54:VAL:O	11:J:58:GLU:HB2	2.19	0.42
11:J:107:ASN:HD22	11:J:108:PRO:N	2.16	0.42
12:K:8:VAL:HG12	12:K:9:THR:N	2.35	0.42
15:N:69:TYR:CE2	15:N:184:ILE:HD11	2.55	0.42
24:W:52:VAL:CG2	24:W:53:ALA:H	2.32	0.42
26:Y:110:SER:O	26:Y:111:ASP:C	2.58	0.42
30:3:30:GLN:HB3	40:3:5866:HOH:O	2.19	0.42
31:9:55:U:H4'	31:9:56:A:H8	1.84	0.42
1:0:408:A:O2'	1:0:409:U:H5'	2.19	0.41
1:0:473:A:O2'	1:0:890:C:H5'	2.19	0.41
1:0:560:U:H2'	1:0:561:G:H8	1.84	0.41
1:0:873:G:H2'	1:0:875:A:N7	2.35	0.41
1:0:958:G:H2'	1:0:959:C:C6	2.54	0.41
1:0:1260:G:H3'	1:0:1261:A:C8	2.56	0.41
1:0:1329:G:N2	40:0:3448:HOH:O	2.50	0.41
1:0:1564:C:H1'	1:0:2738:G:N2	2.34	0.41
1:0:2499:U:H2'	1:0:2500:C:C6	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2756:U:N3	1:0:2896:A:C2	2.87	0.41
2:A:18:ALA:O	2:A:20:SER:N	2.46	0.41
2:A:192:VAL:HG12	2:A:207:GLN:HG2	2.03	0.41
3:B:5:ARG:HD2	3:B:8:LYS:NZ	2.35	0.41
4:C:213:ALA:CB	4:C:218:VAL:HG23	2.50	0.41
13:L:34:GLY:C	13:L:36:ASP:N	2.73	0.41
13:L:34:GLY:HA2	40:L:4728:HOH:O	2.20	0.41
15:N:37:ARG:NE	40:N:3863:HOH:O	2.53	0.41
16:O:73:ASP:O	16:O:73:ASP:CG	2.58	0.41
25:X:76:ARG:NH1	25:X:76:ARG:CG	2.83	0.41
30:3:11:CYS:SG	30:3:13:HIS:HD2	2.42	0.41
1:0:40:C:H4'	40:0:6666:HOH:O	2.19	0.41
1:0:411:A:H4'	1:0:412:C:OP2	2.20	0.41
1:0:653:U:H2'	1:0:654:A:C8	2.55	0.41
1:0:1090:A:C6	1:0:1091:U:C4	3.08	0.41
1:0:1553:C:O2'	1:0:1554:C:H5'	2.19	0.41
1:0:1571:G:C2'	1:0:1626:A:H61	2.33	0.41
1:0:1654:U:H5''	40:0:7237:HOH:O	2.19	0.41
1:0:1656:A:H2'	1:0:1657:A:O4'	2.20	0.41
1:0:2346:C:O3'	5:D:52:THR:CG2	2.69	0.41
1:0:2900:G:H2'	1:0:2901:C:O4'	2.20	0.41
40:0:7242:HOH:O	21:T:9:LYS:HB2	2.20	0.41
2:A:62:ASP:OD1	2:A:62:ASP:N	2.52	0.41
2:A:207:GLN:HA	40:A:2643:HOH:O	2.20	0.41
3:B:215:VAL:CA	3:B:220:VAL:HG22	2.48	0.41
5:D:100:ASP:OD1	5:D:100:ASP:N	2.53	0.41
6:E:154:ILE:HG13	6:E:156:ASP:OD1	2.20	0.41
11:J:47:THR:HA	11:J:129:PHE:HA	2.01	0.41
14:M:5:TYR:C	14:M:7:TYR:H	2.23	0.41
18:Q:41:LEU:HD12	18:Q:41:LEU:N	2.34	0.41
19:R:82:GLU:O	19:R:86:LYS:HG3	2.20	0.41
23:V:64:GLY:O	23:V:65:ASP:CB	2.64	0.41
25:X:26:ALA:HB3	25:X:63:ARG:HG3	2.02	0.41
27:Z:59:GLU:HB2	27:Z:61:HIS:CE1	2.55	0.41
1:0:287:C:H2'	1:0:288:A:H8	1.84	0.41
1:0:308:U:C2'	21:T:52:ARG:NH2	2.83	0.41
1:0:876:A:N3	1:0:876:A:H2'	2.35	0.41
1:0:1339:G:C6	1:0:1340:G:N1	2.89	0.41
1:0:1343:C:C2'	26:Y:208:LYS:HZ1	2.33	0.41
1:0:1351:G:OP1	4:C:96:LYS:NZ	2.40	0.41
1:0:1355:A:H2'	1:0:1355:A:N3	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1405:U:H2'	40:0:6435:HOH:O	2.20	0.41
1:0:1688:G:C6	1:0:1692:C:C6	3.09	0.41
1:0:1765:G:O2'	1:0:1766:U:H5'	2.20	0.41
1:0:1784:U:O2'	1:0:1812:G:H2'	2.20	0.41
1:0:1994:A:OP1	12:K:66:ARG:NH2	2.54	0.41
1:0:2112:A:H2'	1:0:2113:G:H8	1.85	0.41
1:0:2676:C:H4'	11:J:70:PHE:HD1	1.85	0.41
2:A:135:VAL:HG11	2:A:147:ARG:HH21	1.86	0.41
3:B:66:GLU:OE1	3:B:328:ARG:HD2	2.20	0.41
3:B:215:VAL:N	3:B:220:VAL:HG22	2.35	0.41
6:E:107:PHE:C	6:E:109:GLY:N	2.74	0.41
7:F:70:LYS:C	7:F:72:VAL:H	2.22	0.41
9:H:30:LYS:N	9:H:62:HIS:HD2	2.18	0.41
13:L:65:ASP:O	13:L:66:VAL:C	2.59	0.41
14:M:43:PRO:HG3	14:M:62:VAL:HG21	2.02	0.41
14:M:81:ARG:HB2	14:M:81:ARG:CZ	2.50	0.41
15:N:108:SER:HA	15:N:109:PRO:HD3	1.75	0.41
16:O:14:LEU:HG	16:O:102:ILE:HD11	2.02	0.41
19:R:18:LEU:HB2	19:R:143:VAL:HG12	1.99	0.41
19:R:92:LEU:HD23	19:R:145:LEU:CD2	2.51	0.41
25:X:43:VAL:HG12	25:X:47:ALA:HB3	2.01	0.41
25:X:47:ALA:HB1	25:X:82:GLU:HB3	2.02	0.41
1:0:407:A:C2	1:0:408:A:C4	3.08	0.41
1:0:1060:C:H2'	1:0:1061:C:H6	1.86	0.41
1:0:1544:U:H1'	1:0:1642:A:C2	2.55	0.41
1:0:1669:G:H2'	1:0:1670:A:C8	2.56	0.41
1:0:1833:U:O2'	1:0:1834:C:H5'	2.20	0.41
1:0:1930:A:H2'	1:0:1931:A:C8	2.56	0.41
1:0:2362:A:O5'	1:0:2362:A:H8	2.02	0.41
1:0:2715:G:O2'	3:B:262:ARG:HD2	2.20	0.41
1:0:2796:U:H2'	1:0:2797:C:O5'	2.21	0.41
1:0:2818:A:O2'	3:B:96:PRO:HD2	2.20	0.41
2:A:76:VAL:HG23	27:Z:87:LYS:HB3	2.01	0.41
2:A:88:ILE:CD1	2:A:100:PRO:HD3	2.43	0.41
2:A:114:ASP:OD1	2:A:115:GLY:N	2.53	0.41
2:A:165:THR:O	2:A:165:THR:HG22	2.19	0.41
3:B:16:ARG:NH1	40:B:5367:HOH:O	2.52	0.41
3:B:62:ARG:HG2	3:B:62:ARG:HH11	1.85	0.41
3:B:277:GLU:N	3:B:278:PRO:HD2	2.35	0.41
9:H:114:ASP:HA	40:H:3102:HOH:O	2.19	0.41
11:J:69:TYR:O	11:J:70:PHE:C	2.58	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:K:121:PHE:CD1	12:K:121:PHE:N	2.88	0.41
13:L:3:LYS:O	13:L:4:LYS:C	2.59	0.41
14:M:55:LYS:HZ2	14:M:146:ASP:HB2	1.84	0.41
15:N:32:PRO:HD2	15:N:99:GLU:O	2.21	0.41
15:N:110:THR:HA	15:N:111:PRO:HD3	1.87	0.41
25:X:73:ARG:NH1	25:X:88:GLU:HB2	2.35	0.41
26:Y:132:ASP:C	26:Y:134:HIS:N	2.72	0.41
1:0:40:C:H6	1:0:40:C:O5'	2.04	0.41
1:0:154:C:C2	1:0:155:C:C5	3.08	0.41
1:0:243:A:H61	1:0:269:G:C1'	2.33	0.41
1:0:661:G:C6	1:0:662:U:C4	3.08	0.41
1:0:1461:U:H2'	1:0:1462:C:C6	2.56	0.41
1:0:1588:G:C6	1:0:1589:G:N1	2.88	0.41
1:0:2092:G:O3'	3:B:239:LEU:HD12	2.20	0.41
1:0:2372:A:H2'	1:0:2373:U:H6	1.84	0.41
1:0:2379:G:H4'	1:0:2380:A:C5'	2.50	0.41
1:0:2383:G:C6	1:0:2384:U:C4	3.08	0.41
5:D:78:GLU:O	5:D:79:MET:C	2.59	0.41
6:E:112:ALA:HA	6:E:113:PRO:HD3	1.88	0.41
6:E:121:ASP:O	6:E:122:THR:C	2.59	0.41
9:H:157:TYR:C	9:H:157:TYR:HD1	2.23	0.41
12:K:74:VAL:HG12	12:K:75:ARG:HG3	2.02	0.41
13:L:22:ARG:HG3	40:L:2203:HOH:O	2.20	0.41
15:N:91:ARG:O	15:N:94:GLU:HB2	2.20	0.41
20:S:45:TYR:HE2	20:S:81:ILE:HG12	1.84	0.41
21:T:89:ARG:O	21:T:89:ARG:HG3	2.20	0.41
27:Z:54:GLU:HB3	27:Z:58:ASN:ND2	2.36	0.41
1:0:314:G:N2	1:0:316:A:H3'	2.36	0.41
1:0:613:C:C2	1:0:614:U:C5	3.09	0.41
1:0:696:C:O2'	1:0:697:G:H5'	2.20	0.41
1:0:814:G:C2	1:0:815:U:C2	3.08	0.41
1:0:905:C:H3'	40:0:4139:HOH:O	2.19	0.41
1:0:960:G:N3	1:0:960:G:C2'	2.82	0.41
1:0:1175:G:H1'	1:0:1193:A:C2'	2.47	0.41
1:0:1186:C:H42	1:0:1190:G:N2	2.19	0.41
1:0:1747:A:O3'	1:0:2584:G:H5'	2.21	0.41
1:0:1757:U:H6	1:0:1757:U:O5'	2.03	0.41
1:0:2042:U:H2'	1:0:2043:U:C6	2.56	0.41
1:0:2312:G:H2'	1:0:2313:C:H5'	2.02	0.41
1:0:2514:U:H5''	1:0:2572:G:O4'	2.21	0.41
3:B:76:THR:N	3:B:77:PRO:HD3	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:277:GLU:N	3:B:278:PRO:CD	2.83	0.41
6:E:86:VAL:O	6:E:86:VAL:HG13	2.21	0.41
9:H:66:GLU:O	9:H:70:LEU:HB2	2.21	0.41
11:J:116:LEU:HB2	11:J:119:THR:HG21	2.03	0.41
13:L:91:VAL:HG12	13:L:120:LEU:HD23	2.02	0.41
17:P:8:ARG:HG3	40:P:5725:HOH:O	2.21	0.41
17:P:89:ASN:C	17:P:89:ASN:HD22	2.23	0.41
24:W:91:ASP:HB2	40:W:5425:HOH:O	2.21	0.41
1:0:437:A:H3'	40:0:4828:HOH:O	2.20	0.41
1:0:569:A:H5''	1:0:587:A:N1	2.35	0.41
1:0:706:G:N2	1:0:707:C:H41	2.18	0.41
1:0:941:G:O2'	1:0:942:U:H5'	2.20	0.41
1:0:1170:U:H1'	1:0:1172:G:N7	2.35	0.41
1:0:1363:G:H1'	40:0:4299:HOH:O	2.20	0.41
1:0:1551:C:H2'	1:0:1552:G:C8	2.56	0.41
1:0:1662:C:H2'	1:0:1663:G:O4'	2.20	0.41
1:0:1871:U:O4'	1:0:1873:G:C8	2.74	0.41
1:0:1883:U:O2'	1:0:1884:G:H5'	2.20	0.41
1:0:2064:U:H4'	1:0:2652:U:O3'	2.21	0.41
1:0:2240:U:H2'	1:0:2241:C:O4'	2.21	0.41
1:0:2468:A:H62	30:3:50:GLY:HA2	1.86	0.41
1:0:2588:OMG:O6	32:4:76:5AA:H102	2.21	0.41
1:0:2653:A:H2'	1:0:2654:C:C6	2.56	0.41
3:B:294:TYR:CD1	3:B:294:TYR:C	2.93	0.41
5:D:95:THR:C	5:D:97:GLN:N	2.74	0.41
6:E:85:GLU:HG2	6:E:130:GLU:HG2	2.02	0.41
7:F:106:ALA:O	7:F:109:GLU:HB3	2.21	0.41
11:J:127:ILE:HG22	36:J:8801:CL:CL	2.57	0.41
11:J:130:VAL:HG12	11:J:131:THR:H	1.86	0.41
12:K:2:GLU:O	12:K:3:ALA:C	2.59	0.41
12:K:99:ASP:OD1	12:K:99:ASP:C	2.59	0.41
13:L:56:LYS:NZ	40:L:6170:HOH:O	2.53	0.41
14:M:27:ARG:O	14:M:30:GLU:N	2.54	0.41
15:N:67:ALA:HA	15:N:71:TRP:H	1.85	0.41
15:N:112:GLY:HA2	15:N:137:ALA:HB2	2.02	0.41
16:O:97:SER:C	16:O:99:GLU:N	2.73	0.41
17:P:142:ASP:O	17:P:143:ALA:HB3	2.21	0.41
19:R:15:LYS:HE3	40:R:6682:HOH:O	2.21	0.41
20:S:53:ASN:N	20:S:53:ASN:ND2	2.68	0.41
24:W:4:LEU:HD22	24:W:4:LEU:HA	1.88	0.41
25:X:10:VAL:HG12	25:X:11:THR:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:X:26:ALA:O	25:X:29:ALA:HB3	2.20	0.41
26:Y:102:LEU:O	26:Y:227:ARG:HG3	2.20	0.41
29:2:9:LYS:HE2	29:2:9:LYS:HB3	1.86	0.41
29:2:35:ARG:HA	29:2:39:ARG:HH22	1.84	0.41
31:9:107:C:O2'	31:9:108:C:H5'	2.21	0.41
1:0:27:U:H2'	1:0:28:G:C8	2.56	0.41
1:0:314:G:C2	1:0:317:A:C8	3.08	0.41
1:0:332:G:O2'	21:T:7:GLN:HG3	2.21	0.41
1:0:445:U:H2'	1:0:446:G:C8	2.55	0.41
1:0:593:A:C2'	1:0:594:C:H5'	2.49	0.41
1:0:621:C:H2'	1:0:622:G:H8	1.84	0.41
1:0:765:G:H4'	4:C:69:HIS:HB2	2.03	0.41
1:0:800:G:H2'	1:0:801:U:C6	2.56	0.41
1:0:1370:G:O5'	19:R:62:HIS:HB3	2.20	0.41
1:0:2032:U:C2'	1:0:2033:G:H5''	2.51	0.41
1:0:2238:A:O2'	1:0:2239:C:H5'	2.21	0.41
1:0:2265:U:H2'	1:0:2266:A:C8	2.56	0.41
1:0:2421:G:H2'	40:0:8689:HOH:O	2.19	0.41
1:0:2681:A:H4'	1:0:2682:C:OP1	2.20	0.41
3:B:51:VAL:CG2	3:B:330:VAL:HG22	2.50	0.41
3:B:80:ARG:O	3:B:82:VAL:N	2.53	0.41
9:H:119:ALA:O	9:H:120:PHE:C	2.57	0.41
12:K:97:ILE:HG22	12:K:98:VAL:H	1.86	0.41
14:M:5:TYR:C	14:M:7:TYR:N	2.74	0.41
14:M:61:ILE:N	14:M:61:ILE:CD1	2.84	0.41
26:Y:105:LYS:HE2	26:Y:198:GLY:O	2.20	0.41
27:Z:70:ARG:NH1	27:Z:83:TYR:N	2.68	0.41
27:Z:80:GLN:HG2	27:Z:81:CYS:N	2.35	0.41
1:0:73:U:H2'	1:0:74:G:C8	2.55	0.41
1:0:175:G:O6	14:M:94:ARG:NH2	2.52	0.41
1:0:369:G:O2'	1:0:370:G:H5'	2.21	0.41
1:0:385:C:O5'	1:0:385:C:H6	2.03	0.41
1:0:524:A:OP1	19:R:29:LYS:NZ	2.52	0.41
1:0:660:A:N6	1:0:746:A:O4'	2.54	0.41
1:0:1103:C:O2	11:J:86:MET:HG2	2.20	0.41
1:0:1119:G:C5	1:0:1243:C:C4	3.08	0.41
1:0:1153:C:N3	1:0:2786:G:O6	2.53	0.41
1:0:1195:G:N2	1:0:1205:U:C2	2.89	0.41
1:0:1308:A:H4'	4:C:226:GLY:HA3	2.02	0.41
1:0:1342:C:C4	1:0:1343:C:C5	3.09	0.41
1:0:1497:G:H4'	1:0:1627:G:O2'	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1592:G:O2'	1:0:1593:C:O5'	2.39	0.41
1:0:1790:C:H2'	1:0:1791:U:H6	1.85	0.41
1:0:1809:G:H2'	1:0:1811:A:OP2	2.21	0.41
1:0:1853:C:O2'	2:A:217:ARG:NH2	2.54	0.41
1:0:1896:G:C6	1:0:1897:U:C4	3.09	0.41
1:0:2043:U:O2'	1:0:2044:G:H5'	2.21	0.41
1:0:2245:C:H6	1:0:2245:C:O5'	2.03	0.41
1:0:2252:A:H2'	1:0:2253:G:H5'	2.02	0.41
1:0:2377:U:O2'	1:0:2378:U:H5'	2.20	0.41
1:0:2645:U:OP2	1:0:2645:U:C6	2.74	0.41
1:0:2781:U:O2'	1:0:2782:G:H5'	2.20	0.41
1:0:2842:G:H2'	1:0:2843:A:C5'	2.51	0.41
1:0:2883:A:H2'	1:0:2884:G:O4'	2.21	0.41
3:B:120:ASP:OD2	3:B:123:ALA:HB2	2.21	0.41
4:C:51:TYR:HE1	28:1:55:GLY:O	2.04	0.41
5:D:101:THR:O	5:D:101:THR:HG22	2.20	0.41
5:D:140:ARG:HG3	5:D:140:ARG:NH1	2.36	0.41
5:D:170:TYR:O	5:D:171:ASP:CB	2.68	0.41
5:D:173:GLU:HG3	5:D:174:VAL:HG23	2.02	0.41
6:E:24:GLY:CA	6:E:76:VAL:HB	2.49	0.41
6:E:73:PHE:O	6:E:76:VAL:HG22	2.21	0.41
6:E:166:VAL:HG12	6:E:167:TYR:N	2.36	0.41
7:F:63:ILE:HB	7:F:64:PRO:CD	2.43	0.41
9:H:141:CYS:HB2	40:H:2934:HOH:O	2.21	0.41
10:I:85:GLY:C	10:I:86:GLU:HG3	2.41	0.41
10:I:123:VAL:C	10:I:125:GLY:N	2.74	0.41
11:J:80:LYS:HE3	11:J:101:VAL:O	2.21	0.41
13:L:144:ASP:O	13:L:147:GLU:HB2	2.21	0.41
14:M:164:THR:CG2	14:M:166:ALA:H	2.27	0.41
15:N:10:MET:O	15:N:11:ARG:C	2.59	0.41
15:N:37:ARG:HH21	15:N:105:GLY:CA	2.33	0.41
15:N:154:LEU:HG	15:N:155:GLU:N	2.32	0.41
16:O:4:ASN:HA	16:O:5:PRO:HD3	1.95	0.41
16:O:49:GLU:O	16:O:49:GLU:HG3	2.20	0.41
16:O:87:THR:C	16:O:89:ILE:H	2.25	0.41
18:Q:86:VAL:HG22	18:Q:87:THR:N	2.35	0.41
19:R:39:THR:HG23	19:R:107:GLU:O	2.21	0.41
21:T:55:PHE:O	21:T:56:ALA:C	2.58	0.41
24:W:117:ARG:NH1	24:W:117:ARG:HB2	2.35	0.41
25:X:31:ILE:O	25:X:35:GLU:HG3	2.21	0.41
26:Y:100:ARG:HD2	26:Y:232:THR:HB	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:2:29:THR:O	29:2:30:ASP:C	2.59	0.41
30:3:6:ARG:HB3	30:3:19:GLU:CD	2.41	0.41
31:9:64:C:H2'	31:9:65:A:H5'	2.03	0.41
1:0:168:C:O2'	1:0:169:A:H5'	2.21	0.41
1:0:210:U:H2'	1:0:211:U:O4'	2.20	0.41
1:0:581:G:H5'	40:0:7612:HOH:O	2.21	0.41
1:0:625:U:H5''	1:0:1044:C:N4	2.36	0.41
1:0:711:G:H1'	40:0:6793:HOH:O	2.19	0.41
1:0:941:G:C6	1:0:942:U:C4	3.09	0.41
1:0:1316:G:H1'	1:0:1340:G:N2	2.36	0.41
1:0:1511:U:O2'	1:0:1512:G:H5'	2.20	0.41
1:0:1795:G:H2'	1:0:1796:A:O4'	2.21	0.41
1:0:1804:A:H2'	1:0:1805:G:H8	1.85	0.41
1:0:2092:G:H5''	1:0:2613:G:OP1	2.21	0.41
1:0:2474:A:H4'	1:0:2475:C:O5'	2.21	0.41
1:0:2720:C:H3'	40:0:5838:HOH:O	2.21	0.41
3:B:69:VAL:HA	3:B:70:PRO:HD3	1.75	0.41
9:H:80:LEU:HD12	9:H:86:TYR:CD2	2.56	0.41
11:J:62:ASP:O	11:J:63:ILE:C	2.59	0.41
14:M:48:LYS:HG3	14:M:52:GLN:HE21	1.86	0.41
15:N:129:ILE:HA	15:N:130:PRO:HD3	1.98	0.41
15:N:176:ARG:HG3	15:N:176:ARG:HH11	1.86	0.41
16:O:105:ASN:HD21	16:O:109:SER:N	2.19	0.41
18:Q:75:ILE:HG12	18:Q:84:ILE:CD1	2.49	0.41
22:U:30:HIS:HB3	40:U:6215:HOH:O	2.20	0.41
24:W:13:MET:HE2	24:W:18:GLN:N	2.36	0.41
24:W:27:HIS:O	24:W:28:HIS:CD2	2.74	0.41
26:Y:127:GLN:O	26:Y:128:PHE:HB2	2.20	0.41
30:3:25:VAL:HG22	30:3:68:LYS:CE	2.50	0.41
30:3:69:TYR:N	30:3:69:TYR:CD1	2.89	0.41
1:0:615:G:H2'	1:0:616:U:C6	2.57	0.40
1:0:845:U:OP1	28:1:5:THR:OG1	2.37	0.40
1:0:1263:C:H5'	24:W:118:LEU:O	2.21	0.40
1:0:1342:C:H2'	1:0:1343:C:H5'	2.02	0.40
1:0:2088:C:H1'	1:0:2841:A:N1	2.36	0.40
1:0:2263:G:H4'	14:M:70:GLY:HA3	2.00	0.40
1:0:2320:U:H4'	1:0:2321:A:O4'	2.21	0.40
1:0:2718:C:H6	1:0:2718:C:H5'	1.87	0.40
1:0:2839:C:H2'	1:0:2840:A:H5''	2.02	0.40
1:0:2896:A:H5''	40:0:5399:HOH:O	2.21	0.40
40:0:3518:HOH:O	15:N:21:HIS:HD2	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:0:3623:HOH:O	7:F:31:LYS:HD2	2.20	0.40
40:0:4400:HOH:O	27:Z:37:ARG:HD2	2.21	0.40
2:A:75:GLY:HA3	27:Z:86:TYR:CZ	2.56	0.40
3:B:202:VAL:HA	3:B:310:ARG:O	2.22	0.40
6:E:97:VAL:HG12	40:E:4191:HOH:O	2.21	0.40
12:K:53:ILE:HG13	12:K:55:VAL:HG23	2.02	0.40
15:N:82:TYR:CD2	15:N:82:TYR:C	2.94	0.40
17:P:120:ARG:NH2	17:P:123:TYR:CD2	2.89	0.40
19:R:63:ASN:O	19:R:64:SER:C	2.59	0.40
19:R:69:LYS:HB2	19:R:72:VAL:HG23	2.04	0.40
22:U:9:CYS:CA	22:U:52:THR:HG23	2.46	0.40
25:X:36:HIS:CE1	25:X:40:HIS:CD2	3.09	0.40
25:X:73:ARG:HH12	25:X:88:GLU:HB2	1.86	0.40
27:Z:56:GLU:CD	27:Z:94:LYS:HZ2	2.25	0.40
30:3:86:GLY:HA2	40:3:3274:HOH:O	2.21	0.40
1:0:29:C:O2'	1:0:30:U:H5'	2.21	0.40
1:0:170:U:H4'	30:3:48:ASN:O	2.22	0.40
1:0:401:C:H1'	14:M:92:THR:OG1	2.21	0.40
1:0:731:U:O2'	1:0:732:C:H5'	2.21	0.40
1:0:1139:U:H2'	1:0:1140:C:H6	1.86	0.40
1:0:1508:C:H5'	20:S:21:GLN:HE22	1.85	0.40
1:0:1598:A:N6	36:0:8815:CL:CL	2.91	0.40
1:0:1644:C:H2'	1:0:1645:U:H6	1.86	0.40
1:0:2039:A:H2'	1:0:2040:C:C6	2.56	0.40
1:0:2291:A:N9	1:0:2309:C:H5'	2.35	0.40
1:0:2408:A:H4'	30:3:15:ASN:C	2.42	0.40
1:0:2608:C:H2'	40:0:8118:HOH:O	2.21	0.40
1:0:2636:C:H1'	40:0:3790:HOH:O	2.20	0.40
1:0:2761:A:C4	1:0:2763:G:C8	3.09	0.40
40:0:6597:HOH:O	18:Q:16:ASN:HB2	2.21	0.40
40:0:7968:HOH:O	4:C:81:PRO:HD3	2.20	0.40
2:A:172:ALA:O	2:A:173:GLY:C	2.58	0.40
10:I:127:CYS:N	40:I:5371:HOH:O	2.53	0.40
11:J:92:GLN:O	11:J:93:ARG:C	2.59	0.40
11:J:115:VAL:O	11:J:115:VAL:HG12	2.21	0.40
13:L:106:VAL:O	13:L:123:ASP:HB2	2.21	0.40
13:L:110:GLY:N	13:L:129:ALA:HB2	2.36	0.40
15:N:72:GLU:HG2	15:N:163:PHE:HD1	1.87	0.40
16:O:26:TRP:HA	16:O:26:TRP:CE3	2.56	0.40
19:R:39:THR:CG2	19:R:42:GLU:HG3	2.51	0.40
24:W:61:THR:O	24:W:62:LEU:C	2.59	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:1:28:HIS:ND1	28:1:31:LYS:HE2	2.36	0.40
31:9:86:G:C2	31:9:88:G:C8	3.10	0.40
1:0:154:C:O2'	1:0:155:C:H5'	2.21	0.40
1:0:189:A:OP1	14:M:171:ARG:NH2	2.54	0.40
1:0:965:A:C2	1:0:1004:C:C2	3.09	0.40
1:0:1398:G:H2'	1:0:1399:A:H8	1.83	0.40
1:0:1711:A:H3'	40:0:5721:HOH:O	2.21	0.40
1:0:1758:U:H2'	1:0:1759:A:O4'	2.21	0.40
1:0:1847:A:OP1	2:A:175:LYS:HG3	2.21	0.40
1:0:1888:C:H2'	1:0:1889:C:O4'	2.20	0.40
1:0:2050:G:H4'	19:R:82:GLU:HG2	2.03	0.40
1:0:2059:U:H2'	1:0:2060:A:C8	2.56	0.40
1:0:2103:A:O2'	1:0:2104:C:H5'	2.21	0.40
1:0:2353:A:O2'	15:N:7:LYS:HB3	2.21	0.40
1:0:2459:G:H2'	38:0:2924:MYL:HAA	2.04	0.40
1:0:2504:A:H2'	1:0:2505:G:O4'	2.21	0.40
1:0:2512:U:H4'	1:0:2514:U:O4	2.21	0.40
38:0:2924:MYL:CAL	30:3:51:LYS:O	2.70	0.40
38:0:2924:MYL:HAC	38:0:2924:MYL:HADA	1.86	0.40
3:B:254:GLN:NE2	40:B:4243:HOH:O	2.54	0.40
3:B:309:VAL:O	3:B:310:ARG:HG2	2.20	0.40
5:D:56:ARG:N	40:D:6752:HOH:O	2.54	0.40
5:D:173:GLU:CG	5:D:174:VAL:H	2.29	0.40
7:F:38:LYS:NZ	14:M:3:SER:HA	2.36	0.40
7:F:50:VAL:CG1	7:F:60:VAL:HG11	2.50	0.40
12:K:82:ARG:HH21	12:K:115:ARG:HG2	1.84	0.40
15:N:15:GLU:O	15:N:16:ALA:HB3	2.22	0.40
15:N:18:THR:HG21	40:9:5071:HOH:O	2.21	0.40
18:Q:75:ILE:HD12	18:Q:75:ILE:C	2.42	0.40
25:X:26:ALA:HB2	25:X:63:ARG:HA	2.02	0.40
26:Y:130:ARG:HD2	40:Y:3314:HOH:O	2.21	0.40
26:Y:132:ASP:C	26:Y:134:HIS:H	2.24	0.40
1:0:47:G:N3	1:0:114:A:C2	2.90	0.40
1:0:234:A:H4'	1:0:437:A:O4'	2.21	0.40
1:0:238:C:H4'	1:0:287:C:OP1	2.21	0.40
1:0:319:A:H2'	1:0:320:G:H8	1.86	0.40
1:0:421:C:H4'	1:0:1919:A:N6	2.36	0.40
1:0:529:G:C5	1:0:530:C:C5	3.09	0.40
1:0:801:U:O4'	17:P:128:GLY:HA3	2.22	0.40
1:0:812:A:H2'	1:0:813:C:C6	2.56	0.40
1:0:1103:C:C2	1:0:1241:G:N2	2.90	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1187:U:HO2'	1:0:1189:A:H2	1.70	0.40
1:0:1276:U:H3'	16:O:19:ARG:NH1	2.36	0.40
1:0:1314:U:H2'	40:0:5081:HOH:O	2.21	0.40
1:0:1482:A:O2'	1:0:1483:C:H5'	2.21	0.40
1:0:1805:G:O2'	1:0:1806:G:H5'	2.21	0.40
1:0:2408:A:O3'	30:3:16:GLU:HA	2.21	0.40
1:0:2582:G:O3'	12:K:41:LYS:HA	2.21	0.40
1:0:2618:G:O6	1:0:2619:UR3:H3U2	2.22	0.40
1:0:2754:G:H2'	1:0:2755:G:O4'	2.22	0.40
1:0:2829:G:O2'	1:0:2830:U:H5'	2.22	0.40
3:B:8:LYS:HG3	3:B:220:VAL:HG12	2.03	0.40
3:B:83:ALA:HA	3:B:100:VAL:O	2.21	0.40
6:E:61:THR:O	6:E:62:ILE:C	2.59	0.40
6:E:86:VAL:CG1	6:E:129:GLU:HA	2.51	0.40
6:E:119:HIS:O	6:E:140:ALA:HB1	2.20	0.40
10:I:127:CYS:C	10:I:129:SER:N	2.74	0.40
14:M:125:ARG:O	14:M:126:GLN:HB3	2.22	0.40
15:N:12:ARG:NH2	31:9:6:C:C5	2.90	0.40
15:N:159:TYR:CE1	31:9:50:G:H5''	2.56	0.40
25:X:84:ILE:C	25:X:85:VAL:CG2	2.89	0.40
26:Y:117:LEU:HD12	26:Y:174:VAL:CG1	2.50	0.40
31:9:57:A:H2'	31:9:58:G:C5'	2.52	0.40
1:0:60:A:C2	1:0:61:G:C8	3.09	0.40
1:0:100:C:H2'	1:0:101:C:C6	2.52	0.40
1:0:318:U:H5'	1:0:339:A:C2	2.57	0.40
1:0:497:A:H5''	40:0:8141:HOH:O	2.21	0.40
1:0:1121:G:H21	1:0:1248:A:C4'	2.35	0.40
1:0:1196:C:H2'	1:0:1197:G:H5'	2.03	0.40
1:0:1228:C:H2'	1:0:1229:C:O4'	2.22	0.40
1:0:1483:C:O2'	1:0:1484:G:H5'	2.21	0.40
1:0:1523:G:C6	1:0:1524:U:C4	3.09	0.40
1:0:1544:U:H1'	1:0:1642:A:N1	2.37	0.40
1:0:1926:G:C2	1:0:1927:A:C4	3.10	0.40
1:0:2102:G:N2	1:0:2104:C:C2	2.90	0.40
1:0:2408:A:H1'	30:3:10:TYR:CD1	2.57	0.40
1:0:2478:U:H2'	1:0:2479:A:C8	2.56	0.40
1:0:2750:G:H2'	1:0:2751:C:C6	2.56	0.40
3:B:26:PHE:HD2	3:B:312:ARG:NH2	2.19	0.40
4:C:116:ALA:C	4:C:118:THR:N	2.75	0.40
5:D:99:ASP:N	5:D:103:ASN:O	2.49	0.40
10:I:92:VAL:N	10:I:131:GLY:O	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:M:1445:HOH:O	30:3:46:ILE:HG12	2.21	0.40
16:O:81:PHE:CD1	16:O:81:PHE:N	2.90	0.40
21:T:71:VAL:HG12	21:T:72:ILE:N	2.37	0.40
23:V:1:THR:CG2	23:V:2:VAL:N	2.77	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1171:A:N3	1:0:1964:U:O5'[3_655]	1.73	0.47

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	A	235/240 (98%)	193 (82%)	32 (14%)	10 (4%)	2	15
3	B	335/338 (99%)	285 (85%)	38 (11%)	12 (4%)	3	19
4	C	244/246 (99%)	204 (84%)	35 (14%)	5 (2%)	7	30
5	D	134/177 (76%)	91 (68%)	33 (25%)	10 (8%)	1	5
6	E	170/178 (96%)	149 (88%)	20 (12%)	1 (1%)	25	59
7	F	117/120 (98%)	95 (81%)	15 (13%)	7 (6%)	1	9
8	G	25/348 (7%)	18 (72%)	6 (24%)	1 (4%)	3	16
9	H	156/174 (90%)	134 (86%)	15 (10%)	7 (4%)	2	14
10	I	68/162 (42%)	43 (63%)	20 (29%)	5 (7%)	1	6
11	J	140/145 (97%)	120 (86%)	15 (11%)	5 (4%)	3	19
12	K	130/132 (98%)	113 (87%)	15 (12%)	2 (2%)	10	38
13	L	141/165 (86%)	105 (74%)	31 (22%)	5 (4%)	3	19
14	M	192/194 (99%)	153 (80%)	29 (15%)	10 (5%)	2	12

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	N	184/187 (98%)	147 (80%)	27 (15%)	10 (5%)	2	11
16	O	113/116 (97%)	89 (79%)	23 (20%)	1 (1%)	17	51
17	P	141/149 (95%)	118 (84%)	20 (14%)	3 (2%)	7	29
18	Q	93/96 (97%)	78 (84%)	10 (11%)	5 (5%)	2	11
19	R	148/155 (96%)	130 (88%)	16 (11%)	2 (1%)	11	39
20	S	79/85 (93%)	66 (84%)	12 (15%)	1 (1%)	12	41
21	T	117/120 (98%)	99 (85%)	15 (13%)	3 (3%)	5	25
22	U	51/66 (77%)	43 (84%)	6 (12%)	2 (4%)	3	17
23	V	63/71 (89%)	52 (82%)	11 (18%)	0	100	100
24	W	152/154 (99%)	121 (80%)	27 (18%)	4 (3%)	5	25
25	X	80/92 (87%)	65 (81%)	13 (16%)	2 (2%)	5	26
26	Y	140/241 (58%)	126 (90%)	13 (9%)	1 (1%)	22	56
27	Z	71/116 (61%)	58 (82%)	10 (14%)	3 (4%)	3	15
28	1	54/57 (95%)	46 (85%)	8 (15%)	0	100	100
29	2	42/50 (84%)	34 (81%)	7 (17%)	1 (2%)	6	26
30	3	90/92 (98%)	64 (71%)	23 (26%)	3 (3%)	4	20
All	All	3705/4466 (83%)	3039 (82%)	545 (15%)	121 (3%)	4	20

All (121) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	36	ASP
2	A	37	VAL
3	B	184	ASP
3	B	206	THR
4	C	8	LEU
5	D	16	PRO
5	D	137	PRO
7	F	101	ALA
9	H	70	LEU
10	I	107	LYS
14	M	82	ARG
15	N	154	LEU
15	N	184	ILE
17	P	116	SER
24	W	36	PRO

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Mol	Chain	Res	Type
27	Z	105	ARG
30	3	74	CYS
2	A	74	VAL
3	B	169	GLY
4	C	15	GLU
5	D	79	MET
6	E	151	LEU
7	F	59	ILE
7	F	92	GLY
8	G	72	ASP
9	H	41	LYS
13	L	21	ARG
14	M	35	GLY
14	M	79	ALA
17	P	139	ARG
18	Q	48	PRO
18	Q	78	GLY
20	S	57	THR
21	T	46	ASP
21	T	53	GLY
22	U	11	THR
24	W	49	ASN
25	X	70	ILE
25	X	87	ALA
26	Y	157	ILE
27	Z	64	PRO
30	3	25	VAL
2	A	15	THR
2	A	34	ASP
3	B	107	SER
4	C	142	ASP
5	D	96	SER
5	D	138	GLY
5	D	171	ASP
7	F	61	MET
7	F	100	ASP
9	H	71	SER
10	I	75	LYS
10	I	106	GLN
11	J	7	ASP
11	J	78	ILE
12	K	127	ALA

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Mol	Chain	Res	Type
13	L	18	HIS
13	L	35	ARG
13	L	105	TYR
14	M	6	SER
14	M	76	ARG
15	N	12	ARG
15	N	27	LEU
15	N	61	ALA
15	N	164	ASP
19	R	40	ALA
24	W	72	PRO
24	W	89	ASP
29	2	37	HIS
2	A	119	ALA
3	B	245	SER
5	D	164	ALA
5	D	173	GLU
9	H	143	VAL
12	K	126	SER
13	L	101	ASP
14	M	88	VAL
15	N	139	TRP
15	N	167	ASP
22	U	46	ALA
2	A	14	SER
2	A	208	HIS
3	B	2	GLN
3	B	34	GLY
3	B	81	ALA
3	B	121	PRO
5	D	168	SER
5	D	170	TYR
7	F	44	SER
7	F	71	GLY
9	H	82	GLU
11	J	18	ILE
11	J	76	ASP
11	J	89	HIS
14	M	15	PRO
14	M	49	ALA
14	M	110	PRO
15	N	65	ASP

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Mol	Chain	Res	Type
16	O	17	ALA
18	Q	23	THR
2	A	232	ARG
3	B	182	VAL
3	B	291	ASP
4	C	13	ASP
10	I	124	VAL
10	I	133	THR
14	M	78	LYS
17	P	19	ASN
30	3	3	MET
3	B	181	ILE
4	C	136	VAL
15	N	109	PRO
19	R	106	GLY
2	A	150	PRO
9	H	58	VAL
9	H	171	GLY
18	Q	18	PRO
21	T	40	VAL
18	Q	22	GLY
27	Z	39	GLY

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	A	179/182 (98%)	170 (95%)	9 (5%)	24 56
3	B	282/283 (100%)	264 (94%)	18 (6%)	17 47
4	C	193/193 (100%)	174 (90%)	19 (10%)	8 29
5	D	117/148 (79%)	111 (95%)	6 (5%)	24 55
6	E	152/156 (97%)	145 (95%)	7 (5%)	27 59
7	F	93/94 (99%)	92 (99%)	1 (1%)	73 88
8	G	27/282 (10%)	26 (96%)	1 (4%)	34 66

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	H	134/143 (94%)	128 (96%)	6 (4%)	27	59
10	I	58/130 (45%)	56 (97%)	2 (3%)	37	68
11	J	118/121 (98%)	114 (97%)	4 (3%)	37	68
12	K	106/106 (100%)	101 (95%)	5 (5%)	26	58
13	L	113/127 (89%)	103 (91%)	10 (9%)	10	35
14	M	158/158 (100%)	153 (97%)	5 (3%)	39	69
15	N	149/150 (99%)	139 (93%)	10 (7%)	16	45
16	O	93/94 (99%)	90 (97%)	3 (3%)	39	69
17	P	113/117 (97%)	106 (94%)	7 (6%)	18	48
18	Q	79/80 (99%)	78 (99%)	1 (1%)	69	86
19	R	117/122 (96%)	112 (96%)	5 (4%)	29	61
20	S	71/74 (96%)	68 (96%)	3 (4%)	30	62
21	T	105/106 (99%)	98 (93%)	7 (7%)	16	45
22	U	44/52 (85%)	44 (100%)	0	100	100
23	V	51/57 (90%)	51 (100%)	0	100	100
24	W	130/130 (100%)	123 (95%)	7 (5%)	22	53
25	X	66/74 (89%)	60 (91%)	6 (9%)	9	33
26	Y	120/196 (61%)	116 (97%)	4 (3%)	38	68
27	Z	60/94 (64%)	59 (98%)	1 (2%)	60	83
28	1	46/47 (98%)	45 (98%)	1 (2%)	52	77
29	2	42/46 (91%)	40 (95%)	2 (5%)	25	57
30	3	79/79 (100%)	76 (96%)	3 (4%)	33	65
All	All	3095/3641 (85%)	2942 (95%)	153 (5%)	25	57

All (153) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	3	ARG
2	A	33	GLU
2	A	62	ASP
2	A	78	ASP
2	A	94	LEU
2	A	131	HIS
2	A	153	ARG

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Mol	Chain	Res	Type
2	A	179	MET
2	A	217	ARG
3	B	7	ARG
3	B	11	LEU
3	B	27	ASN
3	B	28	SER
3	B	49	THR
3	B	97	LEU
3	B	103	ASP
3	B	132	HIS
3	B	162	MET
3	B	175	LEU
3	B	190	MET
3	B	234	ARG
3	B	251	VAL
3	B	254	GLN
3	B	277	GLU
3	B	304	PRO
3	B	312	ARG
3	B	324	ASP
4	C	2	GLN
4	C	27	ARG
4	C	46	TYR
4	C	87	ARG
4	C	91	PRO
4	C	101	ASP
4	C	131	PHE
4	C	135	GLU
4	C	143	ASP
4	C	151	GLN
4	C	184	ARG
4	C	187	ARG
4	C	198	ASP
4	C	223	LEU
4	C	233	THR
4	C	234	VAL
4	C	235	PHE
4	C	236	THR
4	C	240	LEU
5	D	24	HIS
5	D	50	VAL
5	D	100	ASP

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Mol	Chain	Res	Type
5	D	131	THR
5	D	137	PRO
5	D	170	TYR
6	E	7	ILE
6	E	15	GLN
6	E	16	ASP
6	E	116	THR
6	E	126	ILE
6	E	155	ASN
6	E	164	ASP
7	F	68	ASP
8	G	73	ASP
9	H	13	ASP
9	H	42	ASP
9	H	62	HIS
9	H	87	LYS
9	H	91	ARG
9	H	157	TYR
10	I	76	ASP
10	I	94	ASP
11	J	39	VAL
11	J	52	GLN
11	J	74	ARG
11	J	107	ASN
12	K	4	LEU
12	K	7	ASP
12	K	10	GLN
12	K	16	SER
12	K	83	PRO
13	L	18	HIS
13	L	26	HIS
13	L	35	ARG
13	L	40	PHE
13	L	70	ASP
13	L	80	ASP
13	L	99	GLU
13	L	127	GLU
13	L	140	VAL
13	L	148	GLU
14	M	46	LEU
14	M	68	ARG
14	M	88	VAL

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Mol	Chain	Res	Type
14	M	99	ARG
14	M	120	VAL
15	N	12	ARG
15	N	17	ARG
15	N	23	ARG
15	N	26	LEU
15	N	47	LEU
15	N	93	GLN
15	N	124	ASP
15	N	127	LEU
15	N	135	VAL
15	N	173	ASP
16	O	3	THR
16	O	67	SER
16	O	81	PHE
17	P	52	LYS
17	P	73	HIS
17	P	89	ASN
17	P	91	LYS
17	P	94	TRP
17	P	98	ILE
17	P	110	ASP
18	Q	35	ASP
19	R	39	THR
19	R	82	GLU
19	R	119	VAL
19	R	142	ASP
19	R	143	VAL
20	S	30	ASP
20	S	53	ASN
20	S	55	GLN
21	T	5	ASP
21	T	39	ASN
21	T	73	HIS
21	T	86	GLU
21	T	89	ARG
21	T	96	VAL
21	T	117	ASP
24	W	4	LEU
24	W	38	THR
24	W	88	THR
24	W	90	TYR

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Mol	Chain	Res	Type
24	W	120	PRO
24	W	125	HIS
24	W	146	ILE
25	X	15	ARG
25	X	27	ASP
25	X	46	ASP
25	X	56	GLU
25	X	79	GLU
25	X	88	GLU
26	Y	169	ARG
26	Y	189	ASN
26	Y	203	VAL
26	Y	235	GLU
27	Z	70	ARG
28	1	5	THR
29	2	16	ASN
29	2	18	ASN
30	3	17	HIS
30	3	34	LYS
30	3	51	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (107) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	29	HIS
2	A	47	HIS
2	A	92	ASN
2	A	176	HIS
2	A	199	HIS
3	B	27	ASN
3	B	39	GLN
3	B	106	HIS
3	B	145	HIS
3	B	221	GLN
3	B	238	ASN
3	B	260	HIS
3	B	320	GLN
4	C	2	GLN
4	C	11	ASN
4	C	73	GLN
4	C	129	HIS
4	C	151	GLN

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Mol	Chain	Res	Type
5	D	29	HIS
5	D	47	GLN
5	D	133	ASN
6	E	55	ASN
6	E	74	HIS
6	E	90	HIS
6	E	106	ASN
6	E	143	GLN
7	F	80	GLN
8	G	17	GLN
8	G	64	ASN
9	H	34	HIS
9	H	49	GLN
9	H	59	GLN
9	H	62	HIS
10	I	88	GLN
10	I	106	GLN
11	J	25	GLN
11	J	40	ASN
11	J	52	GLN
11	J	107	ASN
11	J	126	ASN
12	K	10	GLN
12	K	44	HIS
12	K	67	GLN
13	L	18	HIS
13	L	20	ASN
13	L	41	HIS
13	L	42	ASN
13	L	43	HIS
13	L	58	GLN
14	M	24	GLN
14	M	52	GLN
14	M	58	GLN
14	M	77	HIS
14	M	86	GLN
14	M	98	GLN
14	M	170	ASN
15	N	93	GLN
15	N	107	ASN
16	O	91	GLN
17	P	28	GLN

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Mol	Chain	Res	Type
17	P	50	GLN
17	P	66	GLN
17	P	88	GLN
17	P	89	ASN
17	P	118	GLN
18	Q	16	ASN
18	Q	27	GLN
18	Q	40	HIS
19	R	94	ASN
19	R	98	ASN
19	R	123	GLN
20	S	25	GLN
20	S	44	GLN
20	S	53	ASN
20	S	55	GLN
21	T	39	ASN
21	T	43	ASN
22	U	39	ASN
22	U	48	ASN
23	V	4	HIS
23	V	29	ASN
23	V	34	GLN
23	V	60	GLN
24	W	27	HIS
24	W	28	HIS
24	W	59	GLN
24	W	110	GLN
24	W	119	HIS
24	W	141	HIS
25	X	23	HIS
26	Y	149	GLN
26	Y	189	ASN
27	Z	61	HIS
28	1	8	GLN
28	1	16	HIS
29	2	16	ASN
29	2	18	ASN
29	2	36	ASN
29	2	41	HIS
29	2	45	ASN
30	3	2	GLN
30	3	8	ASN

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Mol	Chain	Res	Type
30	3	13	HIS
30	3	15	ASN
30	3	30	GLN
30	3	43	ASN
30	3	48	ASN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2745/2923 (93%)	248 (9%)	18 (0%)
31	9	121/122 (99%)	18 (14%)	1 (0%)
32	4	1/8 (12%)	0	0
All	All	2867/3053 (93%)	266 (9%)	19 (0%)

All (266) 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	130	C
1	0	141	C
1	0	151	A
1	0	166	A
1	0	169	A
1	0	185	G
1	0	186	A
1	0	191	A
1	0	192	A
1	0	198	A
1	0	200	C
1	0	204	A
1	0	219	G
1	0	237	G

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Mol	Chain	Res	Type
1	0	271	C
1	0	272	A
1	0	273	G
1	0	283	U
1	0	284	C
1	0	285	A
1	0	308	U
1	0	309	C
1	0	318	U
1	0	336	G
1	0	337	A
1	0	358	G
1	0	368	C
1	0	381	G
1	0	397	A
1	0	417	G
1	0	461	C
1	0	487	G
1	0	498	A
1	0	510	U
1	0	511	A
1	0	514	G
1	0	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	605	C
1	0	620	A
1	0	632	A
1	0	644	G
1	0	660	A
1	0	688	A
1	0	698	A
1	0	701	U
1	0	759	C
1	0	777	U

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Mol	Chain	Res	Type
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	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	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
1	0	1165	G
1	0	1166	A
1	0	1174	A

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Mol	Chain	Res	Type
1	0	1175	G
1	0	1185	U
1	0	1192	A
1	0	1193	A
1	0	1205	U
1	0	1206	U
1	0	1208	C
1	0	1216	G
1	0	1238	C
1	0	1239	G
1	0	1242	A
1	0	1279	U
1	0	1289	C
1	0	1331	G
1	0	1342	C
1	0	1353	C
1	0	1360	C
1	0	1377	C
1	0	1378	G
1	0	1407	A
1	0	1474	C
1	0	1492	A
1	0	1505	U
1	0	1506	U
1	0	1524	U
1	0	1525	G
1	0	1526	A
1	0	1559	A
1	0	1592	G
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
1	0	1701	A
1	0	1722	U
1	0	1723	G
1	0	1725	C

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Mol	Chain	Res	Type
1	0	1730	G
1	0	1731	C
1	0	1752	G
1	0	1778	A
1	0	1779	A
1	0	1798	C
1	0	1820	G
1	0	1829	A
1	0	1856	C
1	0	1873	G
1	0	1879	U
1	0	1919	A
1	0	1942	A
1	0	1968	A
1	0	1971	G
1	0	1973	A
1	0	1978	A
1	0	1979	G
1	0	1996	U
1	0	2004	U
1	0	2006	C
1	0	2008	U
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	2103	A
1	0	2104	C
1	0	2110	G
1	0	2238	A
1	0	2243	C
1	0	2258	A
1	0	2271	G
1	0	2272	G
1	0	2291	A

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Mol	Chain	Res	Type
1	0	2317	C
1	0	2321	A
1	0	2322	U
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	2465	A
1	0	2467	A
1	0	2476	C
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	2542	C
1	0	2553	A
1	0	2564	G
1	0	2570	G
1	0	2589	U
1	0	2601	A
1	0	2602	G
1	0	2607	U
1	0	2608	C
1	0	2609	G
1	0	2613	G
1	0	2637	A
1	0	2638	G
1	0	2644	C
1	0	2649	A
1	0	2664	A
1	0	2681	A
1	0	2682	C
1	0	2726	U
1	0	2747	C
1	0	2748	G
1	0	2749	U
1	0	2750	G

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Mol	Chain	Res	Type
1	0	2762	C
1	0	2768	A
1	0	2792	A
1	0	2800	A
1	0	2811	A
1	0	2812	A
1	0	2825	C
1	0	2852	A
1	0	2876	G
1	0	2890	A
1	0	2896	A
1	0	2903	C
1	0	2912	C
1	0	2914	A
31	9	2	U
31	9	7	G
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 (19) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	69	A
1	0	129	A
1	0	603	A
1	0	604	G
1	0	644	G
1	0	699	C

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Mol	Chain	Res	Type
1	0	834	G
1	0	857	A
1	0	871	G
1	0	1352	A
1	0	2011	A
1	0	2103	A
1	0	2526	C
1	0	2536	C
1	0	2541	U
1	0	2718	C
1	0	2726	U
1	0	2791	U
31	9	65	A

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

6 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	OMG	0	2588	32,1	18,26,27	1.06	3 (16%)	19,38,41	0.76	1 (5%)
1	1MA	0	628	1	16,25,26	1.40	3 (18%)	18,37,40	1.23	3 (16%)
1	UR3	0	2619	1	19,22,23	0.41	0	26,32,35	0.64	1 (3%)
1	OMU	0	2587	1,35	19,22,23	0.25	0	26,31,34	0.38	0
1	PSU	0	2621	1	18,21,22	1.60	2 (11%)	22,30,33	1.32	3 (13%)
32	5AA	4	76	32,1	18,26,27	0.76	0	15,38,41	0.80	1 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMG	0	2588	32,1	-	0/5/27/28	0/3/3/3
1	1MA	0	628	1	-	0/3/25/26	0/3/3/3
1	UR3	0	2619	1	-	0/7/25/26	0/2/2/2
1	OMU	0	2587	1,35	-	0/9/27/28	0/2/2/2
1	PSU	0	2621	1	-	0/7/25/26	0/2/2/2
32	5AA	4	76	32,1	-	0/7/29/30	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	0	2621	PSU	C2-N1	5.30	1.43	1.36
1	0	628	1MA	C2-N3	3.78	1.33	1.29
1	0	2621	PSU	C6-C5	3.11	1.38	1.35
1	0	2588	OMG	C5-C6	-2.85	1.41	1.47
1	0	628	1MA	C6-N6	2.67	1.34	1.27
1	0	2588	OMG	C8-N7	-2.35	1.31	1.35
1	0	2588	OMG	C5-C4	-2.11	1.37	1.43
1	0	628	1MA	C8-N7	-2.09	1.31	1.35

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	2621	PSU	C6-C5-C4	3.55	120.68	118.20
1	0	628	1MA	N1-C2-N3	2.89	129.39	126.02
1	0	2621	PSU	C6-N1-C2	-2.83	119.79	122.68
1	0	2621	PSU	O2-C2-N1	2.68	125.74	122.79
1	0	628	1MA	C5-C6-N1	2.44	117.53	113.90
1	0	628	1MA	CM1-N1-C6	2.40	123.90	120.27
1	0	2619	UR3	C4-N3-C2	2.35	126.78	124.56
1	0	2588	OMG	O6-C6-C5	2.23	128.73	124.37
32	4	76	5AA	C9-N6-C6	2.21	126.20	119.51

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	0	2588	OMG	5	0
1	0	2619	UR3	1	0
1	0	2587	OMU	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	0	2621	PSU	1	0
32	4	76	5AA	10	0

5.5 Carbohydrates [i](#)

There are no monosaccharides 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
38	MYL	0	2924	-	34,37,37	1.19	4 (11%)	38,56,56	1.64	10 (26%)

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
38	MYL	0	2924	-	-	7/23/77/77	1/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	0	2924	MYL	CBC-NAP	4.80	1.49	1.43
38	0	2924	MYL	CAA-CAV	2.97	1.39	1.32
38	0	2924	MYL	OAR-CAM	2.14	1.44	1.41
38	0	2924	MYL	OAS-CAM	2.14	1.44	1.41

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	0	2924	MYL	OAT-CAY-CAC	4.10	110.94	105.85
38	0	2924	MYL	CAN-CAV-CAZ	3.78	116.96	112.10
38	0	2924	MYL	CBC-NAP-CAW	3.04	126.58	122.69
38	0	2924	MYL	OAR-CBC-NAP	2.71	110.89	107.15
38	0	2924	MYL	OAR-CBC-CBG	-2.68	104.64	109.35
38	0	2924	MYL	CAB-OAQ-CBH	-2.41	110.45	116.33
38	0	2924	MYL	OAS-CBF-CBG	-2.36	106.40	110.68
38	0	2924	MYL	CAG-OAK-CBD	-2.14	110.75	114.44
38	0	2924	MYL	CAF-CBE-CAE	2.09	110.69	107.72
38	0	2924	MYL	CAM-OAR-CBC	-2.01	108.21	111.62

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
38	0	2924	MYL	OAG-CAW-NAP-CBC
38	0	2924	MYL	CBB-CAW-NAP-CBC
38	0	2924	MYL	OAR-CBC-NAP-CAW
38	0	2924	MYL	CBG-CBC-NAP-CAW
38	0	2924	MYL	CAN-CBH-OAQ-CAB
38	0	2924	MYL	OAT-CBH-OAQ-CAB
38	0	2924	MYL	CBB-CBH-OAQ-CAB

All (1) ring outliers are listed below:

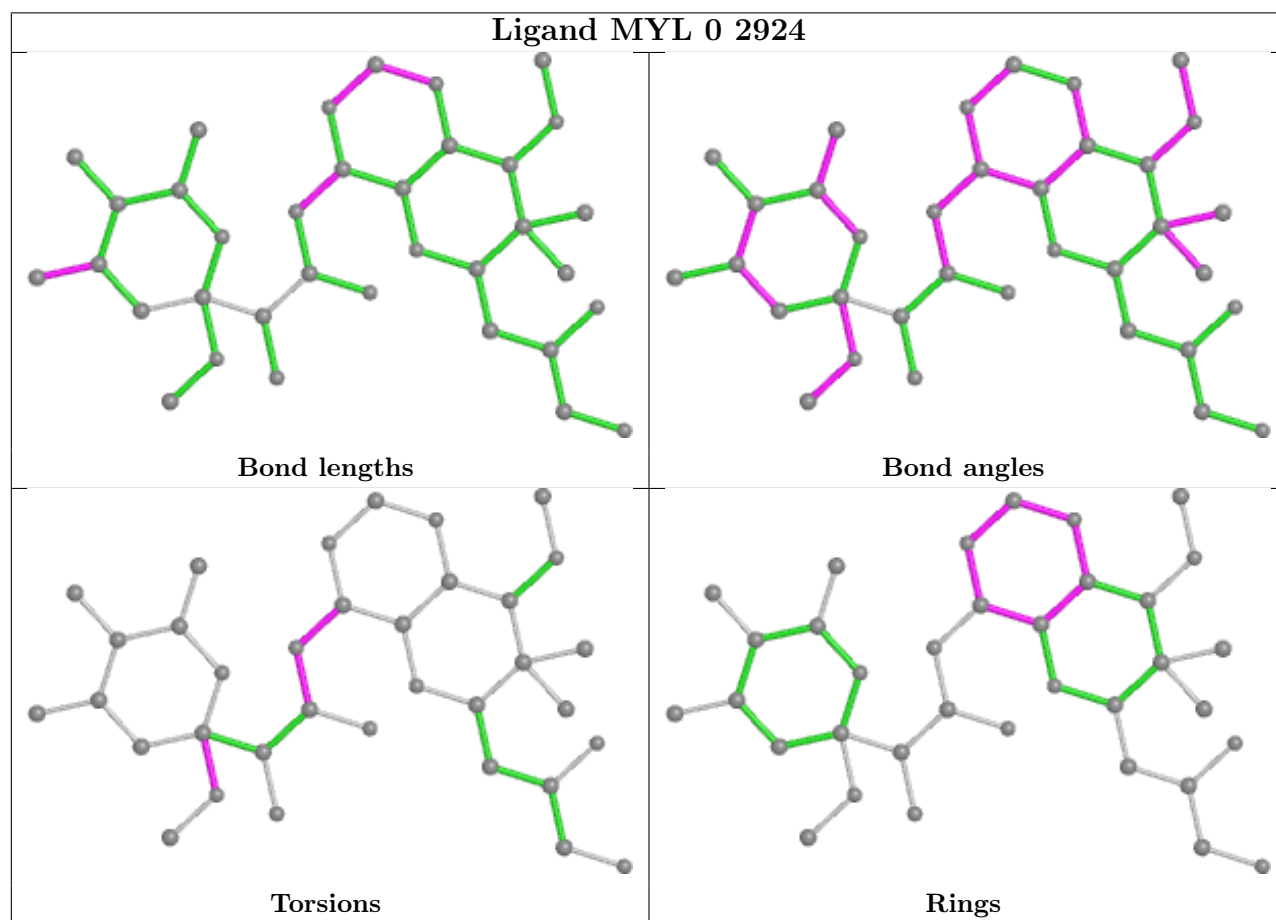
Mol	Chain	Res	Type	Atoms
38	0	2924	MYL	CAM-CBC-CBF-CBG-OAR-OAS

1 monomer is involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
38	0	2924	MYL	22	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	0	2749/2923 (94%)	-0.36	3 (0%) 95 92	31, 61, 109, 181	0
2	A	237/240 (98%)	-0.02	5 (2%) 63 43	37, 75, 110, 131	0
3	B	337/338 (99%)	-0.41	0 100 100	37, 65, 93, 103	0
4	C	246/246 (100%)	-0.31	0 100 100	34, 60, 84, 96	0
5	D	140/177 (79%)	0.97	25 (17%) 1 0	80, 118, 140, 148	0
6	E	172/178 (96%)	-0.25	0 100 100	54, 81, 102, 112	0
7	F	119/120 (99%)	0.14	2 (1%) 70 50	65, 93, 121, 135	0
8	G	29/348 (8%)	0.36	1 (3%) 45 24	86, 102, 109, 114	0
9	H	160/174 (91%)	0.10	4 (2%) 57 35	58, 79, 111, 121	0
10	I	70/162 (43%)	1.92	32 (45%) 0 0	137, 154, 180, 181	0
11	J	142/145 (97%)	-0.45	0 100 100	48, 63, 82, 98	0
12	K	132/132 (100%)	-0.30	0 100 100	46, 63, 88, 95	0
13	L	145/165 (87%)	0.18	6 (4%) 37 18	38, 86, 124, 133	0
14	M	194/194 (100%)	0.21	19 (9%) 7 2	38, 60, 136, 151	0
15	N	186/187 (99%)	0.21	5 (2%) 54 31	65, 89, 138, 146	0
16	O	115/116 (99%)	-0.35	0 100 100	51, 70, 84, 91	0
17	P	143/149 (95%)	-0.15	1 (0%) 87 77	52, 69, 87, 93	0
18	Q	95/96 (98%)	-0.17	0 100 100	51, 62, 77, 85	0
19	R	150/155 (96%)	-0.41	0 100 100	42, 56, 77, 89	0
20	S	81/85 (95%)	-0.12	1 (1%) 79 63	57, 76, 99, 111	0
21	T	119/120 (99%)	-0.03	2 (1%) 70 50	55, 73, 106, 125	0
22	U	53/66 (80%)	1.58	18 (33%) 0 0	95, 117, 133, 135	0
23	V	65/71 (91%)	0.79	8 (12%) 4 1	65, 90, 140, 144	0
24	W	154/154 (100%)	-0.25	2 (1%) 77 60	46, 62, 79, 95	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	X	82/92 (89%)	-0.03	3 (3%) 41 21	52, 70, 88, 105	0
26	Y	142/241 (58%)	-0.43	1 (0%) 87 77	39, 58, 80, 99	0
27	Z	73/116 (62%)	4.94	46 (63%) 0 0	107, 143, 170, 176	0
28	1	56/57 (98%)	-0.23	0 100 100	34, 47, 58, 62	0
29	2	46/50 (92%)	0.14	3 (6%) 18 7	47, 80, 113, 121	0
30	3	92/92 (100%)	7.53	90 (97%) 0 0	164, 175, 184, 189	0
31	9	122/122 (100%)	-0.57	1 (0%) 86 74	52, 86, 113, 166	0
32	4	5/8 (62%)	1.30	0 100 100	41, 43, 47, 47	0
All	All	6651/7519 (88%)	-0.01	278 (4%) 36 18	31, 67, 132, 189	0

All (278) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
27	Z	34	SER	24.2
30	3	82	GLY	23.8
27	Z	35	SER	22.6
27	Z	58	ASN	21.8
27	Z	46	SER	20.6
30	3	30	GLN	19.6
30	3	62	THR	18.7
30	3	33	MET	15.5
30	3	38	ARG	15.3
30	3	31	THR	14.4
27	Z	36	GLY	13.9
30	3	32	GLY	13.9
30	3	44	SER	13.3
30	3	58	GLY	13.2
30	3	35	TRP	13.0
27	Z	49	ARG	12.8
30	3	14	CYS	12.7
30	3	39	GLN	12.3
27	Z	50	VAL	11.9
30	3	40	ARG	11.7
30	3	78	HIS	11.0
27	Z	48	ARG	10.8
27	Z	45	VAL	10.8
27	Z	39	GLY	10.6
30	3	72	GLY	10.2
30	3	41	GLU	9.9

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Mol	Chain	Res	Type	RSRZ
30	3	56	PRO	9.8
27	Z	51	ALA	9.8
30	3	77	ALA	9.6
30	3	52	PHE	9.6
30	3	86	GLY	9.6
27	Z	44	ARG	9.6
30	3	57	GLY	9.5
30	3	15	ASN	9.4
27	Z	54	GLU	9.2
30	3	11	CYS	9.2
30	3	13	HIS	9.2
14	M	77	HIS	9.2
27	Z	55	SER	9.1
30	3	36	ILE	9.0
30	3	42	ARG	9.0
30	3	25	VAL	8.9
30	3	71	CYS	8.8
30	3	66	ASP	8.6
30	3	48	ASN	8.6
30	3	34	LYS	8.4
30	3	45	GLY	8.4
27	Z	42	TYR	8.4
30	3	68	LYS	8.1
30	3	37	ASP	8.1
14	M	70	GLY	8.0
27	Z	38	PHE	7.9
30	3	3	MET	7.8
27	Z	57	MET	7.8
30	3	20	HIS	7.8
30	3	83	TRP	7.8
30	3	23	GLU	7.7
27	Z	53	ILE	7.7
30	3	64	LYS	7.7
30	3	22	VAL	7.6
14	M	71	SER	7.4
27	Z	56	GLU	7.4
30	3	43	ASN	7.2
27	Z	47	ARG	7.1
30	3	27	SER	7.1
30	3	70	ARG	7.0
30	3	1	MET	6.9
30	3	74	CYS	6.9

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Mol	Chain	Res	Type	RSRZ
30	3	67	LEU	6.8
27	Z	43	GLY	6.7
30	3	59	ASP	6.6
30	3	53	SER	6.6
27	Z	70	ARG	6.6
30	3	9	THR	6.6
30	3	69	TYR	6.5
30	3	76	LYS	6.5
30	3	84	ARG	6.4
30	3	47	GLY	6.4
30	3	81	GLU	6.3
30	3	8	ASN	6.2
27	Z	52	GLU	6.2
30	3	63	LYS	6.1
30	3	65	THR	6.0
14	M	89	THR	5.9
30	3	29	ARG	5.9
27	Z	63	CYS	5.9
27	Z	80	GLN	5.8
22	U	55	ALA	5.8
30	3	91	GLN	5.7
30	3	21	GLU	5.6
30	3	73	GLU	5.6
20	S	81	ILE	5.6
27	Z	59	GLU	5.6
30	3	19	GLU	5.6
30	3	46	ILE	5.6
27	Z	68	GLU	5.5
5	D	26	GLY	5.4
23	V	1	THR	5.4
14	M	90	ARG	5.3
30	3	16	GLU	5.2
10	I	73	LEU	5.2
10	I	71	ALA	5.2
14	M	80	GLY	5.1
30	3	51	LYS	5.1
27	Z	81	CYS	5.1
30	3	17	HIS	5.1
5	D	40	ILE	5.1
22	U	52	THR	5.1
30	3	80	ARG	5.1
14	M	78	LYS	5.0

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Mol	Chain	Res	Type	RSRZ
14	M	87	GLY	5.0
10	I	70	THR	5.0
30	3	2	GLN	4.9
30	3	18	GLN	4.9
30	3	12	PRO	4.9
30	3	10	TYR	4.9
10	I	72	GLU	4.8
23	V	43	PRO	4.8
27	Z	60	ASP	4.8
27	Z	69	ASP	4.7
31	9	1	U	4.7
10	I	74	ILE	4.7
5	D	57	THR	4.7
14	M	86	GLN	4.6
30	3	85	ALA	4.6
14	M	81	ARG	4.5
30	3	50	GLY	4.5
30	3	61	PRO	4.5
30	3	49	ASP	4.5
23	V	41	GLU	4.5
14	M	76	ARG	4.3
22	U	48	ASN	4.2
30	3	92	GLU	4.2
10	I	66	GLY	4.2
5	D	18	ILE	4.1
22	U	9	CYS	4.1
27	Z	62	ALA	4.0
10	I	76	ASP	4.0
30	3	60	LYS	4.0
27	Z	67	GLY	3.9
23	V	39	ALA	3.9
27	Z	37	ARG	3.9
30	3	55	VAL	3.9
30	3	26	ARG	3.9
22	U	10	GLY	3.8
15	N	95	ALA	3.8
30	3	6	ARG	3.8
27	Z	77	GLY	3.8
27	Z	74	GLN	3.7
10	I	68	PRO	3.7
10	I	97	VAL	3.7
2	A	237	GLY	3.6

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Mol	Chain	Res	Type	RSRZ
10	I	128	THR	3.6
14	M	88	VAL	3.5
30	3	24	LYS	3.4
5	D	44	ILE	3.4
10	I	109	PRO	3.4
30	3	75	GLY	3.4
21	T	116	ASP	3.4
30	3	4	PRO	3.4
30	3	54	LYS	3.3
30	3	87	ARG	3.3
5	D	86	THR	3.3
30	3	5	ARG	3.3
10	I	98	ASP	3.3
30	3	28	GLY	3.3
13	L	80	ASP	3.3
5	D	63	ILE	3.2
9	H	86	TYR	3.2
1	0	1198	U	3.2
10	I	102	GLN	3.2
22	U	53	ASP	3.2
22	U	36	CYS	3.1
14	M	79	ALA	3.1
27	Z	93	TYR	3.1
8	G	23	ILE	3.0
23	V	36	ALA	3.0
23	V	40	PRO	3.0
1	0	735	C	3.0
22	U	47	ARG	3.0
27	Z	78	ILE	3.0
10	I	110	ASP	3.0
5	D	83	PHE	2.9
5	D	92	GLU	2.9
27	Z	40	ALA	2.9
13	L	48	LYS	2.9
27	Z	65	ASN	2.9
27	Z	82	SER	2.9
5	D	61	PHE	2.9
2	A	56	ALA	2.9
25	X	80	GLU	2.9
10	I	99	GLN	2.9
5	D	69	ILE	2.8
10	I	113	SER	2.8

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Mol	Chain	Res	Type	RSRZ
7	F	49	PHE	2.8
5	D	87	ALA	2.8
13	L	60	GLU	2.8
5	D	134	LEU	2.8
10	I	106	GLN	2.7
10	I	69	PRO	2.7
27	Z	64	PRO	2.7
22	U	54	THR	2.7
5	D	88	LEU	2.7
21	T	118	SER	2.7
27	Z	41	ARG	2.7
10	I	82	THR	2.6
10	I	78	ALA	2.6
22	U	46	ALA	2.6
1	0	2645	U	2.6
17	P	128	GLY	2.6
5	D	85	GLN	2.6
23	V	46	ILE	2.6
22	U	39	ASN	2.6
2	A	85	SER	2.6
25	X	88	GLU	2.5
5	D	19	GLU	2.5
10	I	79	GLY	2.5
5	D	84	LEU	2.5
5	D	70	GLY	2.5
5	D	142	ALA	2.5
15	N	179	LEU	2.5
14	M	73	ARG	2.5
10	I	111	LEU	2.5
30	3	90	PHE	2.5
25	X	71	ARG	2.5
9	H	174	LEU	2.5
15	N	50	LEU	2.4
10	I	112	LEU	2.4
22	U	32	CYS	2.4
10	I	108	HIS	2.4
14	M	85	ARG	2.4
23	V	37	GLY	2.4
22	U	30	HIS	2.4
5	D	23	VAL	2.4
15	N	166	ALA	2.4
29	2	35	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
24	W	100	LEU	2.3
10	I	91	PHE	2.3
30	3	79	LEU	2.3
10	I	75	LYS	2.3
10	I	104	ALA	2.3
27	Z	61	HIS	2.3
5	D	89	PRO	2.3
29	2	39	ARG	2.3
5	D	73	VAL	2.3
10	I	118	ASN	2.3
13	L	123	ASP	2.3
14	M	82	ARG	2.2
5	D	41	LEU	2.2
14	M	14	ASN	2.2
22	U	51	TRP	2.2
22	U	31	PHE	2.2
14	M	75	ARG	2.2
7	F	75	ILE	2.2
27	Z	88	PHE	2.2
13	L	79	ASP	2.2
22	U	25	ASP	2.2
26	Y	235	GLU	2.2
2	A	88	ILE	2.2
5	D	25	MET	2.2
13	L	75	LEU	2.2
10	I	132	VAL	2.2
29	2	20	ARG	2.2
10	I	100	VAL	2.1
9	H	82	GLU	2.1
14	M	16	GLY	2.1
15	N	160	SER	2.1
24	W	3	ALA	2.1
22	U	12	ASP	2.1
5	D	75	LEU	2.1
9	H	35	LYS	2.1
27	Z	79	TRP	2.1
10	I	103	ILE	2.0
27	Z	66	CYS	2.0
30	3	88	LEU	2.0
10	I	83	GLY	2.0
22	U	45	GLU	2.0
2	A	37	VAL	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. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
32	5AA	4	76	24/25	0.77	0.29	38,44,48,48	0
1	PSU	0	2621	20/21	0.93	0.19	37,39,44,44	0
1	OMU	0	2587	21/22	0.95	0.14	43,46,50,50	0
1	UR3	0	2619	21/22	0.95	0.17	41,44,49,50	0
1	OMG	0	2588	24/25	0.96	0.16	37,42,44,45	0
1	1MA	0	628	23/24	0.96	0.17	38,41,42,43	0

6.3 Carbohydrates [i](#)

There are no monosaccharides 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. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
37	SR	0	8971	1/1	-0.30	0.33	200,200,200,200	0
37	SR	3	8932	1/1	-0.02	0.28	184,184,184,184	0
33	MG	3	8090	1/1	0.04	2.21	86,86,86,86	0
35	NA	0	8544	1/1	0.07	0.45	75,75,75,75	0
37	SR	0	8962	1/1	0.08	0.43	200,200,200,200	0
36	CL	3	8804	1/1	0.10	0.57	121,121,121,121	0
37	SR	0	8983	1/1	0.16	0.28	199,199,199,199	0
37	SR	0	8965	1/1	0.16	0.19	158,158,158,158	0
37	SR	0	8977	1/1	0.23	0.11	200,200,200,200	0
37	SR	0	8974	1/1	0.28	0.20	163,163,163,163	0
33	MG	0	8075	1/1	0.30	0.14	64,64,64,64	0
37	SR	0	8993	1/1	0.36	0.23	186,186,186,186	0
37	SR	0	8941	1/1	0.38	0.30	152,152,152,152	0
35	NA	0	8568	1/1	0.39	0.61	35,35,35,35	0
37	SR	9	8980	1/1	0.39	0.37	192,192,192,192	0
37	SR	0	8959	1/1	0.40	0.36	194,194,194,194	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
35	NA	0	8548	1/1	0.40	0.33	67,67,67,67	0
37	SR	0	9002	1/1	0.42	0.12	169,169,169,169	0
37	SR	0	8949	1/1	0.44	0.43	157,157,157,157	0
35	NA	0	8506	1/1	0.46	0.78	65,65,65,65	0
35	NA	0	8551	1/1	0.48	0.79	86,86,86,86	0
37	SR	A	8930	1/1	0.49	0.15	168,168,168,168	0
39	CD	Z	8703	1/1	0.51	0.38	200,200,200,200	0
37	SR	0	9000	1/1	0.53	1.07	200,200,200,200	0
37	SR	0	8986	1/1	0.53	0.84	200,200,200,200	0
33	MG	0	8088	1/1	0.53	0.18	37,37,37,37	0
37	SR	L	8969	1/1	0.55	1.29	200,200,200,200	0
35	NA	0	8574	1/1	0.56	0.62	72,72,72,72	0
39	CD	3	8704	1/1	0.56	0.62	200,200,200,200	0
37	SR	0	8908	1/1	0.57	0.22	116,116,116,116	0
37	SR	0	8938	1/1	0.57	0.32	200,200,200,200	0
35	NA	0	8522	1/1	0.57	0.27	71,71,71,71	0
35	NA	0	8557	1/1	0.57	0.15	72,72,72,72	0
35	NA	0	8528	1/1	0.57	0.68	91,91,91,91	0
33	MG	0	8010	1/1	0.57	0.14	25,25,25,25	0
33	MG	0	8066	1/1	0.57	0.25	75,75,75,75	0
35	NA	0	8536	1/1	0.58	0.20	72,72,72,72	0
33	MG	0	8093	1/1	0.59	0.11	29,29,29,29	0
35	NA	0	8521	1/1	0.60	0.47	59,59,59,59	0
33	MG	0	8044	1/1	0.60	0.16	51,51,51,51	0
37	SR	F	9005	1/1	0.61	0.07	153,153,153,153	0
37	SR	0	8968	1/1	0.61	0.15	180,180,180,180	0
35	NA	0	8509	1/1	0.62	0.58	90,90,90,90	0
33	MG	0	8081	1/1	0.63	0.58	80,80,80,80	0
33	MG	0	8055	1/1	0.63	0.53	87,87,87,87	0
36	CL	0	8803	1/1	0.63	0.12	68,68,68,68	0
33	MG	0	8069	1/1	0.64	0.43	63,63,63,63	0
37	SR	9	9003	1/1	0.64	0.06	195,195,195,195	0
35	NA	H	8518	1/1	0.65	0.77	92,92,92,92	0
37	SR	0	8944	1/1	0.66	0.17	169,169,169,169	0
37	SR	3	8999	1/1	0.66	0.69	200,200,200,200	0
36	CL	O	8808	1/1	0.67	0.14	109,109,109,109	0
37	SR	0	8991	1/1	0.67	0.14	197,197,197,197	0
37	SR	0	8989	1/1	0.68	0.16	129,129,129,129	0
33	MG	0	8038	1/1	0.68	0.20	92,92,92,92	0
35	NA	J	8538	1/1	0.69	0.14	56,56,56,56	0
35	NA	0	8571	1/1	0.69	0.36	101,101,101,101	0
35	NA	0	8559	1/1	0.69	0.32	99,99,99,99	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
33	MG	0	8092	1/1	0.69	0.47	133,133,133,133	0
35	NA	0	8570	1/1	0.70	0.26	61,61,61,61	0
35	NA	0	8502	1/1	0.70	0.39	53,53,53,53	0
35	NA	0	8558	1/1	0.71	0.58	60,60,60,60	0
35	NA	0	8508	1/1	0.71	0.42	68,68,68,68	0
35	NA	0	8561	1/1	0.71	0.26	66,66,66,66	0
35	NA	0	8554	1/1	0.71	0.46	106,106,106,106	0
34	K	0	8402	1/1	0.71	0.48	88,88,88,88	0
35	NA	0	8556	1/1	0.72	0.46	49,49,49,49	0
33	MG	K	8054	1/1	0.72	0.19	29,29,29,29	0
35	NA	0	8563	1/1	0.72	1.01	85,85,85,85	0
33	MG	2	8060	1/1	0.72	0.11	62,62,62,62	0
37	SR	0	8915	1/1	0.73	0.14	131,131,131,131	0
33	MG	0	8073	1/1	0.73	0.09	70,70,70,70	0
37	SR	0	8992	1/1	0.73	0.29	164,164,164,164	0
35	NA	9	8543	1/1	0.74	0.18	68,68,68,68	0
35	NA	0	8531	1/1	0.74	0.18	45,45,45,45	0
37	SR	0	8916	1/1	0.74	0.17	126,126,126,126	0
37	SR	0	8979	1/1	0.74	0.24	111,111,111,111	0
37	SR	0	8922	1/1	0.74	0.65	182,182,182,182	0
33	MG	0	8071	1/1	0.74	0.30	67,67,67,67	0
33	MG	0	8065	1/1	0.74	0.12	33,33,33,33	0
37	SR	0	8975	1/1	0.75	0.08	158,158,158,158	0
37	SR	0	8960	1/1	0.75	0.09	175,175,175,175	0
35	NA	Q	8540	1/1	0.75	0.30	84,84,84,84	0
37	SR	0	8911	1/1	0.75	0.10	99,99,99,99	0
37	SR	0	8966	1/1	0.76	0.13	117,117,117,117	0
37	SR	0	8957	1/1	0.76	0.29	200,200,200,200	0
33	MG	0	8053	1/1	0.76	0.10	61,61,61,61	0
35	NA	0	8549	1/1	0.76	0.34	124,124,124,124	0
35	NA	0	8513	1/1	0.76	0.67	62,62,62,62	0
37	SR	0	8953	1/1	0.76	1.09	200,200,200,200	0
37	SR	0	8945	1/1	0.77	0.13	131,131,131,131	0
37	SR	0	8976	1/1	0.77	0.38	200,200,200,200	0
37	SR	0	8927	1/1	0.77	0.16	176,176,176,176	0
33	MG	0	8091	1/1	0.78	0.10	111,111,111,111	0
37	SR	0	8988	1/1	0.78	0.17	183,183,183,183	0
33	MG	0	8029	1/1	0.78	0.18	79,79,79,79	0
37	SR	0	9007	1/1	0.78	0.37	200,200,200,200	0
35	NA	0	8567	1/1	0.78	0.82	57,57,57,57	0
37	SR	B	8987	1/1	0.78	0.99	200,200,200,200	0
35	NA	0	8560	1/1	0.78	0.78	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
35	NA	0	8530	1/1	0.79	0.68	68,68,68,68	0
37	SR	0	8926	1/1	0.79	0.16	127,127,127,127	0
36	CL	L	8810	1/1	0.79	0.16	76,76,76,76	0
33	MG	0	8036	1/1	0.79	0.16	59,59,59,59	0
33	MG	0	8024	1/1	0.79	0.24	55,55,55,55	0
37	SR	0	9001	1/1	0.79	0.18	200,200,200,200	0
33	MG	T	8057	1/1	0.80	0.07	68,68,68,68	0
37	SR	0	8964	1/1	0.80	0.08	160,160,160,160	0
33	MG	0	8064	1/1	0.80	0.29	53,53,53,53	0
37	SR	0	9006	1/1	0.80	0.12	190,190,190,190	0
37	SR	0	8997	1/1	0.80	0.73	200,200,200,200	0
35	NA	0	8507	1/1	0.81	0.17	27,27,27,27	0
35	NA	0	8517	1/1	0.81	0.35	62,62,62,62	0
33	MG	0	8031	1/1	0.81	0.63	77,77,77,77	0
35	NA	0	8534	1/1	0.81	0.38	53,53,53,53	0
39	CD	U	8701	1/1	0.81	0.40	200,200,200,200	0
35	NA	0	8569	1/1	0.81	0.36	63,63,63,63	0
33	MG	0	8076	1/1	0.81	0.24	52,52,52,52	0
33	MG	0	8056	1/1	0.82	0.13	44,44,44,44	0
37	SR	0	8924	1/1	0.82	0.20	140,140,140,140	0
33	MG	0	8004	1/1	0.82	0.18	25,25,25,25	0
33	MG	0	8017	1/1	0.82	0.17	26,26,26,26	0
36	CL	0	8813	1/1	0.82	0.10	77,77,77,77	0
36	CL	A	8809	1/1	0.82	0.76	128,128,128,128	0
37	SR	A	8929	1/1	0.82	0.07	124,124,124,124	0
37	SR	0	8943	1/1	0.82	0.14	105,105,105,105	0
35	NA	0	8541	1/1	0.82	0.38	65,65,65,65	0
34	K	0	8401	1/1	0.83	0.36	132,132,132,132	0
37	SR	0	8933	1/1	0.83	0.06	122,122,122,122	0
37	SR	0	8917	1/1	0.83	0.23	157,157,157,157	0
33	MG	0	8039	1/1	0.83	0.19	55,55,55,55	0
33	MG	0	8020	1/1	0.83	0.15	56,56,56,56	0
33	MG	9	8074	1/1	0.83	0.11	87,87,87,87	0
35	NA	R	8533	1/1	0.84	0.20	62,62,62,62	0
37	SR	0	8951	1/1	0.84	0.06	144,144,144,144	0
35	NA	S	8510	1/1	0.84	0.12	56,56,56,56	0
35	NA	0	8564	1/1	0.84	0.21	94,94,94,94	0
35	NA	0	8529	1/1	0.84	0.09	45,45,45,45	0
35	NA	0	8523	1/1	0.84	0.20	52,52,52,52	0
35	NA	0	8537	1/1	0.84	0.09	40,40,40,40	0
35	NA	M	8539	1/1	0.84	0.26	51,51,51,51	0
38	MYL	0	2924	35/35	0.84	0.26	80,83,86,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
37	SR	0	8984	1/1	0.84	0.07	118,118,118,118	0
33	MG	0	8083	1/1	0.84	0.18	50,50,50,50	0
37	SR	0	8947	1/1	0.84	0.76	200,200,200,200	0
35	NA	0	8525	1/1	0.85	0.25	67,67,67,67	0
35	NA	0	8546	1/1	0.85	0.62	65,65,65,65	0
37	SR	0	8918	1/1	0.85	0.14	92,92,92,92	0
33	MG	0	8046	1/1	0.85	0.13	46,46,46,46	0
37	SR	0	8995	1/1	0.85	0.45	191,191,191,191	0
37	SR	0	8973	1/1	0.85	0.12	162,162,162,162	0
33	MG	0	8047	1/1	0.85	0.55	68,68,68,68	0
37	SR	0	8942	1/1	0.85	0.21	139,139,139,139	0
35	NA	0	8550	1/1	0.87	0.27	76,76,76,76	0
36	CL	Y	8820	1/1	0.87	0.21	58,58,58,58	0
33	MG	0	8045	1/1	0.87	0.10	64,64,64,64	0
35	NA	0	8520	1/1	0.87	0.18	63,63,63,63	0
33	MG	0	8019	1/1	0.87	0.16	11,11,11,11	0
33	MG	0	8079	1/1	0.87	0.41	76,76,76,76	0
33	MG	Y	8086	1/1	0.87	0.25	53,53,53,53	0
37	SR	0	8982	1/1	0.87	1.35	200,200,200,200	0
33	MG	0	8026	1/1	0.87	0.20	39,39,39,39	0
33	MG	0	8018	1/1	0.88	0.15	32,32,32,32	0
36	CL	0	8805	1/1	0.88	0.24	101,101,101,101	0
33	MG	0	8070	1/1	0.88	0.09	58,58,58,58	0
37	SR	0	8914	1/1	0.88	0.15	109,109,109,109	0
36	CL	0	8822	1/1	0.88	0.88	123,123,123,123	0
33	MG	0	8089	1/1	0.88	0.21	42,42,42,42	0
36	CL	B	8819	1/1	0.88	0.23	80,80,80,80	0
36	CL	J	8802	1/1	0.88	0.25	84,84,84,84	0
37	SR	0	8919	1/1	0.88	0.09	81,81,81,81	0
35	NA	0	8505	1/1	0.88	0.49	58,58,58,58	0
36	CL	N	8807	1/1	0.88	0.29	98,98,98,98	0
37	SR	0	8956	1/1	0.88	0.09	154,154,154,154	0
35	NA	C	8503	1/1	0.88	0.17	32,32,32,32	0
33	MG	0	8082	1/1	0.88	0.23	61,61,61,61	0
37	SR	0	8931	1/1	0.89	0.09	147,147,147,147	0
33	MG	0	8077	1/1	0.89	0.63	60,60,60,60	0
37	SR	0	8934	1/1	0.89	0.31	168,168,168,168	0
37	SR	0	8910	1/1	0.89	0.13	107,107,107,107	0
37	SR	0	8955	1/1	0.89	0.13	200,200,200,200	0
35	NA	0	8516	1/1	0.89	0.20	39,39,39,39	0
37	SR	0	8913	1/1	0.89	0.78	181,181,181,181	0
33	MG	0	8063	1/1	0.89	0.16	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
35	NA	0	8565	1/1	0.89	1.65	80,80,80,80	0
35	NA	0	8501	1/1	0.89	0.24	41,41,41,41	0
37	SR	B	8950	1/1	0.90	0.15	125,125,125,125	0
35	NA	0	8553	1/1	0.90	0.36	98,98,98,98	0
35	NA	0	8545	1/1	0.90	0.26	25,25,25,25	0
35	NA	0	8555	1/1	0.90	0.76	61,61,61,61	0
33	MG	0	8011	1/1	0.90	0.16	14,14,14,14	0
33	MG	0	8013	1/1	0.90	0.08	24,24,24,24	0
35	NA	0	8512	1/1	0.90	0.44	54,54,54,54	0
37	SR	0	8985	1/1	0.90	0.12	150,150,150,150	0
37	SR	0	8939	1/1	0.90	0.15	166,166,166,166	0
33	MG	0	8059	1/1	0.90	0.15	56,56,56,56	0
33	MG	0	8005	1/1	0.90	0.31	46,46,46,46	0
36	CL	J	8801	1/1	0.90	0.33	88,88,88,88	0
37	SR	0	8901	1/1	0.91	0.15	78,78,78,78	0
37	SR	S	8961	1/1	0.91	0.12	150,150,150,150	0
35	NA	0	8511	1/1	0.91	0.26	54,54,54,54	0
33	MG	A	8050	1/1	0.91	0.18	68,68,68,68	0
35	NA	0	8566	1/1	0.91	0.37	64,64,64,64	0
37	SR	0	8921	1/1	0.91	0.16	98,98,98,98	0
33	MG	0	8080	1/1	0.91	2.93	126,126,126,126	0
37	SR	0	8923	1/1	0.91	0.17	108,108,108,108	0
33	MG	0	8025	1/1	0.91	0.14	30,30,30,30	0
33	MG	0	8048	1/1	0.91	0.29	41,41,41,41	0
37	SR	0	8963	1/1	0.92	0.12	146,146,146,146	0
35	NA	0	8535	1/1	0.92	0.76	72,72,72,72	0
33	MG	B	8042	1/1	0.92	0.47	121,121,121,121	0
37	SR	0	8946	1/1	0.92	0.14	127,127,127,127	0
37	SR	0	8967	1/1	0.92	0.07	164,164,164,164	0
33	MG	0	8028	1/1	0.92	0.15	13,13,13,13	0
37	SR	0	8928	1/1	0.92	0.11	148,148,148,148	0
33	MG	0	8058	1/1	0.92	0.12	22,22,22,22	0
35	NA	0	8562	1/1	0.92	0.21	49,49,49,49	0
35	NA	0	8573	1/1	0.92	0.15	78,78,78,78	0
35	NA	0	8519	1/1	0.92	0.35	69,69,69,69	0
36	CL	0	8811	1/1	0.92	0.21	87,87,87,87	0
33	MG	0	8052	1/1	0.92	0.13	60,60,60,60	0
33	MG	0	8043	1/1	0.92	0.21	48,48,48,48	0
33	MG	0	8032	1/1	0.92	0.15	66,66,66,66	0
33	MG	0	8003	1/1	0.93	0.17	32,32,32,32	0
37	SR	0	9008	1/1	0.93	0.16	107,107,107,107	0
35	NA	B	8552	1/1	0.93	0.23	111,111,111,111	0

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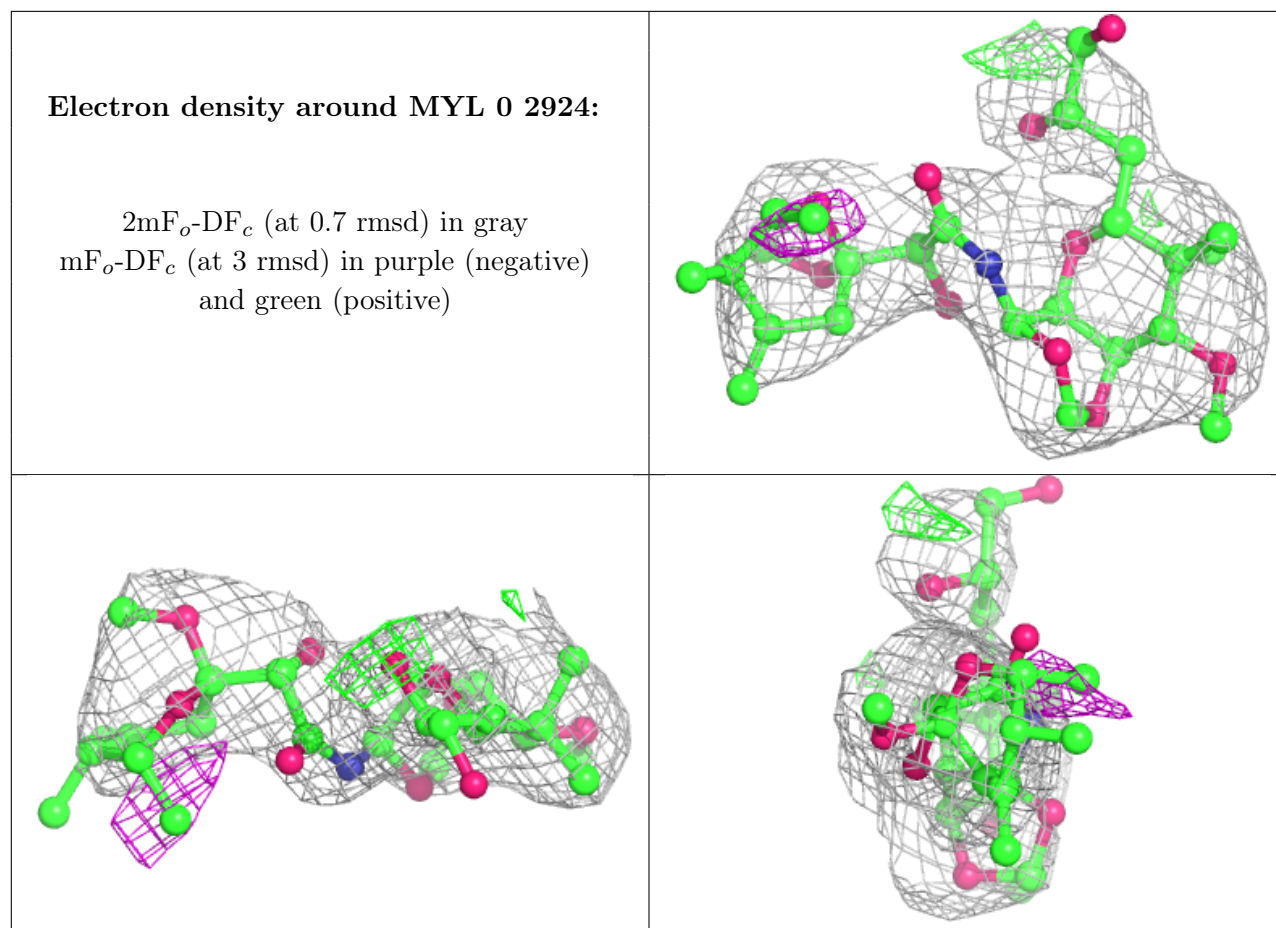
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
36	CL	J	8821	1/1	0.93	0.19	90,90,90,90	0
35	NA	9	8572	1/1	0.93	0.04	78,78,78,78	0
33	MG	0	8008	1/1	0.93	0.15	23,23,23,23	0
37	SR	0	8948	1/1	0.93	0.12	113,113,113,113	0
33	MG	9	8040	1/1	0.93	0.23	89,89,89,89	0
33	MG	0	8034	1/1	0.93	0.19	57,57,57,57	0
37	SR	0	8935	1/1	0.93	0.09	91,91,91,91	0
37	SR	0	8954	1/1	0.93	0.15	108,108,108,108	0
37	SR	0	8937	1/1	0.93	0.10	116,116,116,116	0
35	NA	0	8515	1/1	0.93	0.17	39,39,39,39	0
33	MG	0	8061	1/1	0.93	0.41	48,48,48,48	0
35	NA	R	8532	1/1	0.93	0.08	52,52,52,52	0
37	SR	0	9004	1/1	0.93	0.25	172,172,172,172	0
33	MG	0	8085	1/1	0.93	0.13	73,73,73,73	0
36	CL	M	8818	1/1	0.94	0.18	62,62,62,62	0
33	MG	0	8041	1/1	0.94	0.21	29,29,29,29	0
37	SR	0	8970	1/1	0.94	0.13	148,148,148,148	0
33	MG	0	8049	1/1	0.94	0.35	82,82,82,82	0
35	NA	0	8547	1/1	0.94	0.60	82,82,82,82	0
36	CL	0	8815	1/1	0.94	0.21	83,83,83,83	0
36	CL	0	8816	1/1	0.94	0.80	89,89,89,89	0
37	SR	1	8952	1/1	0.94	0.16	81,81,81,81	0
33	MG	0	8022	1/1	0.94	0.07	56,56,56,56	0
33	MG	0	8035	1/1	0.94	0.25	52,52,52,52	0
33	MG	0	8030	1/1	0.94	0.39	88,88,88,88	0
37	SR	0	8981	1/1	0.94	0.28	198,198,198,198	0
35	NA	0	8526	1/1	0.94	0.12	40,40,40,40	0
33	MG	0	8023	1/1	0.94	0.18	41,41,41,41	0
35	NA	0	8542	1/1	0.94	0.34	51,51,51,51	0
39	CD	1	8702	1/1	0.94	0.11	78,78,78,78	0
33	MG	0	8014	1/1	0.94	0.20	24,24,24,24	0
33	MG	0	8087	1/1	0.95	0.11	29,29,29,29	0
36	CL	R	8806	1/1	0.95	0.08	56,56,56,56	0
33	MG	0	8072	1/1	0.95	0.40	60,60,60,60	0
37	SR	9	8978	1/1	0.95	0.10	154,154,154,154	0
36	CL	0	8817	1/1	0.95	0.34	80,80,80,80	0
33	MG	0	8078	1/1	0.95	0.84	91,91,91,91	0
37	SR	0	8998	1/1	0.95	0.20	196,196,196,196	0
39	CD	O	8705	1/1	0.95	0.07	117,117,117,117	0
37	SR	0	8906	1/1	0.95	0.21	64,64,64,64	0
36	CL	0	8812	1/1	0.95	0.12	66,66,66,66	0
35	NA	0	8514	1/1	0.95	0.56	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
37	SR	0	8920	1/1	0.95	0.14	130,130,130,130	0
37	SR	0	8907	1/1	0.96	0.14	59,59,59,59	0
35	NA	0	8524	1/1	0.96	0.12	67,67,67,67	0
37	SR	0	8936	1/1	0.96	0.13	125,125,125,125	0
33	MG	0	8007	1/1	0.96	0.12	27,27,27,27	0
37	SR	0	8996	1/1	0.96	0.22	200,200,200,200	0
37	SR	0	8958	1/1	0.96	0.16	120,120,120,120	0
33	MG	0	8012	1/1	0.96	0.17	23,23,23,23	0
37	SR	0	8903	1/1	0.96	0.15	62,62,62,62	0
37	SR	0	8940	1/1	0.96	0.16	110,110,110,110	0
37	SR	0	8905	1/1	0.96	0.27	78,78,78,78	0
33	MG	0	8033	1/1	0.96	0.20	79,79,79,79	0
37	SR	R	8912	1/1	0.97	0.16	93,93,93,93	0
33	MG	0	8067	1/1	0.97	0.17	33,33,33,33	0
33	MG	0	8021	1/1	0.97	0.10	53,53,53,53	0
33	MG	0	8015	1/1	0.97	0.17	26,26,26,26	0
35	NA	R	8575	1/1	0.97	0.18	92,92,92,92	0
37	SR	0	8925	1/1	0.97	0.10	99,99,99,99	0
36	CL	0	8814	1/1	0.97	0.17	55,55,55,55	0
37	SR	0	8994	1/1	0.97	0.61	200,200,200,200	0
33	MG	0	8016	1/1	0.97	0.19	34,34,34,34	0
35	NA	0	8527	1/1	0.97	0.34	75,75,75,75	0
33	MG	0	8002	1/1	0.97	0.17	40,40,40,40	0
33	MG	0	8084	1/1	0.97	0.11	31,31,31,31	0
37	SR	H	8972	1/1	0.97	0.11	139,139,139,139	0
37	SR	0	8909	1/1	0.97	0.18	105,105,105,105	0
33	MG	0	8062	1/1	0.98	0.20	53,53,53,53	0
33	MG	0	8006	1/1	0.98	0.16	44,44,44,44	0
33	MG	0	8027	1/1	0.98	0.08	47,47,47,47	0
33	MG	0	8009	1/1	0.98	0.13	22,22,22,22	0
33	MG	0	8001	1/1	0.98	0.17	24,24,24,24	0
37	SR	0	8990	1/1	0.98	0.19	108,108,108,108	0
33	MG	A	8051	1/1	0.99	0.20	81,81,81,81	0
37	SR	0	8902	1/1	0.99	0.20	44,44,44,44	0
35	NA	0	8504	1/1	0.99	0.13	32,32,32,32	0
37	SR	0	8904	1/1	0.99	0.23	65,65,65,65	0
33	MG	0	8068	1/1	0.99	0.12	64,64,64,64	0
33	MG	0	8037	1/1	0.99	0.10	67,67,67,67	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers [i](#)

There are no such residues in this entry.