



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 28, 2020 – 09:45 AM BST

PDB ID : 1KD1
Title : Co-crystal Structure of Spiramycin bound to the 50S Ribosomal Subunit of *Haloarcula marismortui*
Authors : Hansen, J.L.; Ippolito, J.A.; Ban, N.; Nissen, P.; Moore, P.B.; Steitz, T.A.
Deposited on : 2001-11-12
Resolution : 3.00 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 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 : 2.13
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) : 2.13

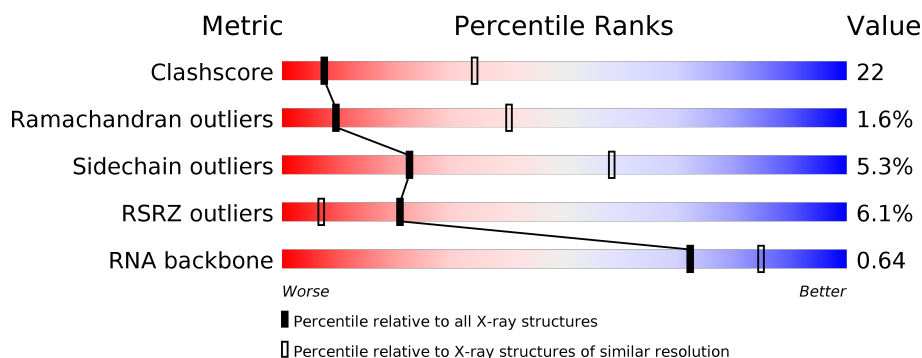
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)
RNA backbone	3102	1173 (3.30-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria 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	A	2922	<div> <div>2%</div> <div> <div>46%</div> <div>39%</div> <div>8%</div> <div>6%</div> </div> </div>
2	B	122	<div> <div>5%</div> <div> <div>46%</div> <div>37%</div> <div>12%</div> <div>5%</div> </div> </div>
3	C	239	<div> <div>4%</div> <div> <div>54%</div> <div>39%</div> <div>6%</div> </div> </div>
4	D	337	<div> <div>%</div> <div> <div>51%</div> <div>43%</div> <div>6%</div> </div> </div>
5	E	246	<div> <div>53%</div> <div>41%</div> <div>6%</div> </div>
6	F	176	<div> <div>28%</div> <div> <div>28%</div> <div>43%</div> <div>6%</div> <div>20%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
7	G	177	
8	H	119	
9	I	348	
10	J	167	
11	K	145	
12	L	132	
13	M	164	
14	N	194	
15	O	186	
16	P	115	
17	Q	148	
18	R	95	
19	S	154	
20	T	84	
21	U	119	
22	V	66	
23	W	70	
24	X	154	
25	Y	91	
26	Z	240	
27	1	73	
28	2	56	
29	3	48	
30	4	92	

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
32	MG	A	8024	-	-	-	X
32	MG	A	8049	-	-	-	X
32	MG	A	8054	-	-	X	-
33	NA	A	8329	-	-	-	X
33	NA	A	8365	-	-	-	X
33	NA	A	8373	-	-	-	X
33	NA	A	8384	-	-	-	X
33	NA	B	8383	-	-	-	X
33	NA	T	8312	-	-	-	X
34	CL	4	8504	-	-	-	X
34	CL	M	8510	-	-	-	X
34	CL	O	8507	-	-	X	-
36	CD	4	8404	-	-	-	X
36	CD	P	8405	-	-	-	X
36	CD	V	8401	-	-	-	X

2 Entry composition

There are 37 unique types of molecules in this entry. The entry contains 98587 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 RRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	2754	Total	C	N	O	P	0	0	0
			59017	26346	10878	19048	2745			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	560	C	U	CONFLICT	? 3377779

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

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

- Molecule 3 is a protein called RIBOSOMAL PROTEIN L2.

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

- Molecule 4 is a protein called RIBOSOMAL PROTEIN L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	337	Total	C	N	O	S	0	0	0
			2624	1616	493	510	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	?	-	PRO	DELETION	UNP P20279
D	310	ARG	PHE	CONFLICT	UNP P20279

- Molecule 5 is a protein called RIBOSOMAL PROTEIN L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	246	Total	C	N	O	S	0	0	0
			1858	1131	344	382	1			

- Molecule 6 is a protein called RIBOSOMAL PROTEIN L5.

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

- Molecule 7 is a protein called RIBOSOMAL PROTEIN L6.

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

- Molecule 8 is a protein called RIBOSOMAL PROTEIN L7AE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	119	Total	C	N	O	S	0	0	0
			885	552	141	191	1			

- Molecule 9 is a protein called RIBOSOMAL PROTEIN L10.

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

- Molecule 10 is a protein called RIBOSOMAL PROTEIN L10E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	156	Total	C	N	O	S	0	0	0
			1215	766	233	212	4			

- Molecule 11 is a protein called RIBOSOMAL PROTEIN L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	142	Total	C	N	O	S	0	0	0
			1119	696	199	221	3			

- Molecule 12 is a protein called RIBOSOMAL PROTEIN L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	132	Total	C	N	O	S	0	0	0
			993	609	189	191	4			

- Molecule 13 is a protein called RIBOSOMAL PROTEIN L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	145	Total	C	N	O		0	0	0
			1114	668	222	224				

- Molecule 14 is a protein called RIBOSOMAL PROTEIN L15E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	194	Total	C	N	O	S	0	0	0
			1605	988	346	266	5			

- Molecule 15 is a protein called RIBOSOMAL PROTEIN L18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	O	186	Total	C	N	O	S	0	0	0
			1444	895	262	285	2			

- Molecule 16 is a protein called RIBOSOMAL PROTEIN L18E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	P	115	Total	C	N	O		0	0	0
			864	529	161	174				

- Molecule 17 is a protein called RIBOSOMAL PROTEIN L19E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Q	143	Total	C	N	O		0	0	0
			1133	680	230	223				

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	71	LYS	TYR	CONFLICT	UNP P14119

- Molecule 18 is a protein called RIBOSOMAL PROTEIN L21E.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	R	95	Total	C	N	O			
			734	450	141	143	0	0	0

- Molecule 19 is a protein called RIBOSOMAL PROTEIN L22.

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

- Molecule 20 is a protein called RIBOSOMAL PROTEIN L23.

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

- Molecule 21 is a protein called RIBOSOMAL PROTEIN L24.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	U	119	Total	C	N	O			
			949	568	180	201		0	0

- Molecule 22 is a protein called RIBOSOMAL PROTEIN L24E.

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

- Molecule 23 is a protein called RIBOSOMAL PROTEIN L29.

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

- Molecule 24 is a protein called RIBOSOMAL PROTEIN L30.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
24	X	154	Total	C	N	O	S		
			1195	737	209	243	6	0	0

- Molecule 25 is a protein called RIBOSOMAL PROTEIN L31E.

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

- Molecule 26 is a protein called RIBOSOMAL PROTEIN L32E.

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

- Molecule 27 is a protein called RIBOSOMAL PROTEIN L37Ae.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	1	73	Total	C	N	O	S	0	0	0
			563	359	111	86	7			

- Molecule 28 is a protein called RIBOSOMAL PROTEIN L37E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	2	56	Total	C	N	O	S	0	0	0
			430	258	86	82	4			

- Molecule 29 is a protein called RIBOSOMAL PROTEIN L39E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	3	46	Total	C	N	O	S	0	0	0
			393	238	86	68	1			

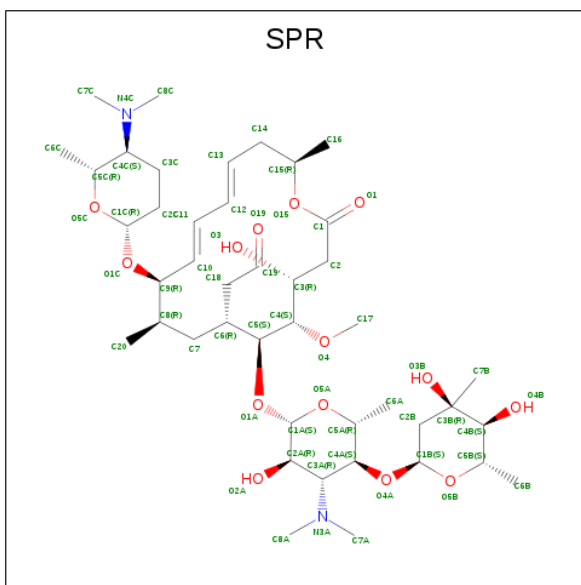
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
3	?	-	ARG	DELETION	UNP P22452

- Molecule 30 is a protein called RIBOSOMAL PROTEIN L44E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	4	92	Total	C	N	O	S	0	0	0
			755	458	153	137	7			

- Molecule 31 is SPIRAMYCIN I (three-letter code: SPR) (formula: C₄₃H₇₄N₂O₁₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	A	1	Total	C	N	O	0	0
			59	43	2	14		

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	1	1	Total 1 Mg 1	0	0
32	B	1	Total 1 Mg 1	0	0
32	C	1	Total 1 Mg 1	0	0
32	Z	1	Total 1 Mg 1	0	0
32	A	112	Total 112 Mg 112	0	0
32	4	1	Total 1 Mg 1	0	0
32	U	1	Total 1 Mg 1	0	0
32	L	1	Total 1 Mg 1	0	0

- Molecule 33 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	J	1	Total Na 1 1	0	0
33	K	1	Total Na 1 1	0	0
33	E	1	Total Na 1 1	0	0
33	B	2	Total Na 2 2	0	0
33	C	1	Total Na 1 1	0	0
33	A	73	Total Na 73 73	0	0
33	T	1	Total Na 1 1	0	0
33	N	1	Total Na 1 1	0	0
33	R	1	Total Na 1 1	0	0
33	S	2	Total Na 2 2	0	0
33	M	1	Total Na 1 1	0	0

- Molecule 34 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	P	1	Total Cl 1 1	0	0
34	D	1	Total Cl 1 1	0	0
34	K	3	Total Cl 3 3	0	0
34	C	1	Total Cl 1 1	0	0
34	Z	1	Total Cl 1 1	0	0
34	A	9	Total Cl 9 9	0	0
34	4	1	Total Cl 1 1	0	0
34	N	1	Total Cl 1 1	0	0
34	O	1	Total Cl 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	R	1	Total 1	Cl 1	0	0
34	S	1	Total 1	Cl 1	0	0
34	M	1	Total 1	Cl 1	0	0

- Molecule 35 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	A	3	Total 3	K 3	0	0

- Molecule 36 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	P	1	Total 1	Cd 1	0	0
36	2	1	Total 1	Cd 1	0	0
36	1	1	Total 1	Cd 1	0	0
36	4	1	Total 1	Cd 1	0	0
36	V	1	Total 1	Cd 1	0	0

- Molecule 37 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	A	5910	Total 5910	O 5910	0	0
37	B	142	Total 142	O 142	0	0
37	C	126	Total 126	O 126	0	0
37	D	150	Total 150	O 150	0	0
37	E	169	Total 169	O 169	0	0
37	F	51	Total 51	O 51	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	G	42	Total 42	O 42	0	0
37	H	26	Total 26	O 26	0	0
37	I	21	Total 21	O 21	0	0
37	J	78	Total 78	O 78	0	0
37	K	54	Total 54	O 54	0	0
37	L	65	Total 65	O 65	0	0
37	M	79	Total 79	O 79	0	0
37	N	132	Total 132	O 132	0	0
37	O	69	Total 69	O 69	0	0
37	P	45	Total 45	O 45	0	0
37	Q	65	Total 65	O 65	0	0
37	R	55	Total 55	O 55	0	0
37	S	83	Total 83	O 83	0	0
37	T	35	Total 35	O 35	0	0
37	U	39	Total 39	O 39	0	0
37	V	25	Total 25	O 25	0	0
37	W	15	Total 15	O 15	0	0
37	X	70	Total 70	O 70	0	0
37	Y	25	Total 25	O 25	0	0
37	Z	94	Total 94	O 94	0	0
37	1	41	Total 41	O 41	0	0

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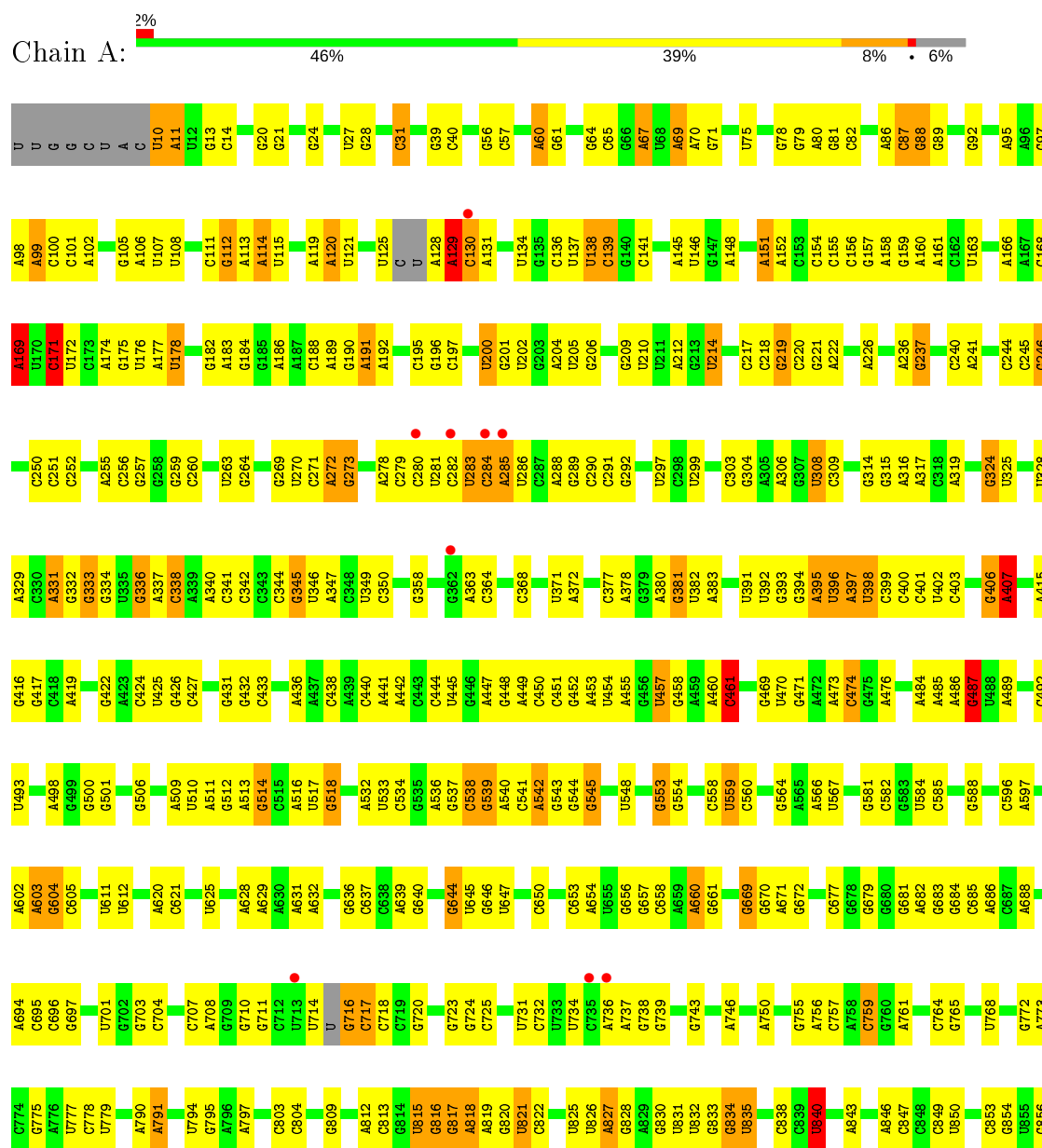
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	2	55	Total 55	O 55	0	0
37	3	42	Total 42	O 42	0	0
37	4	73	Total 73	O 73	0	0

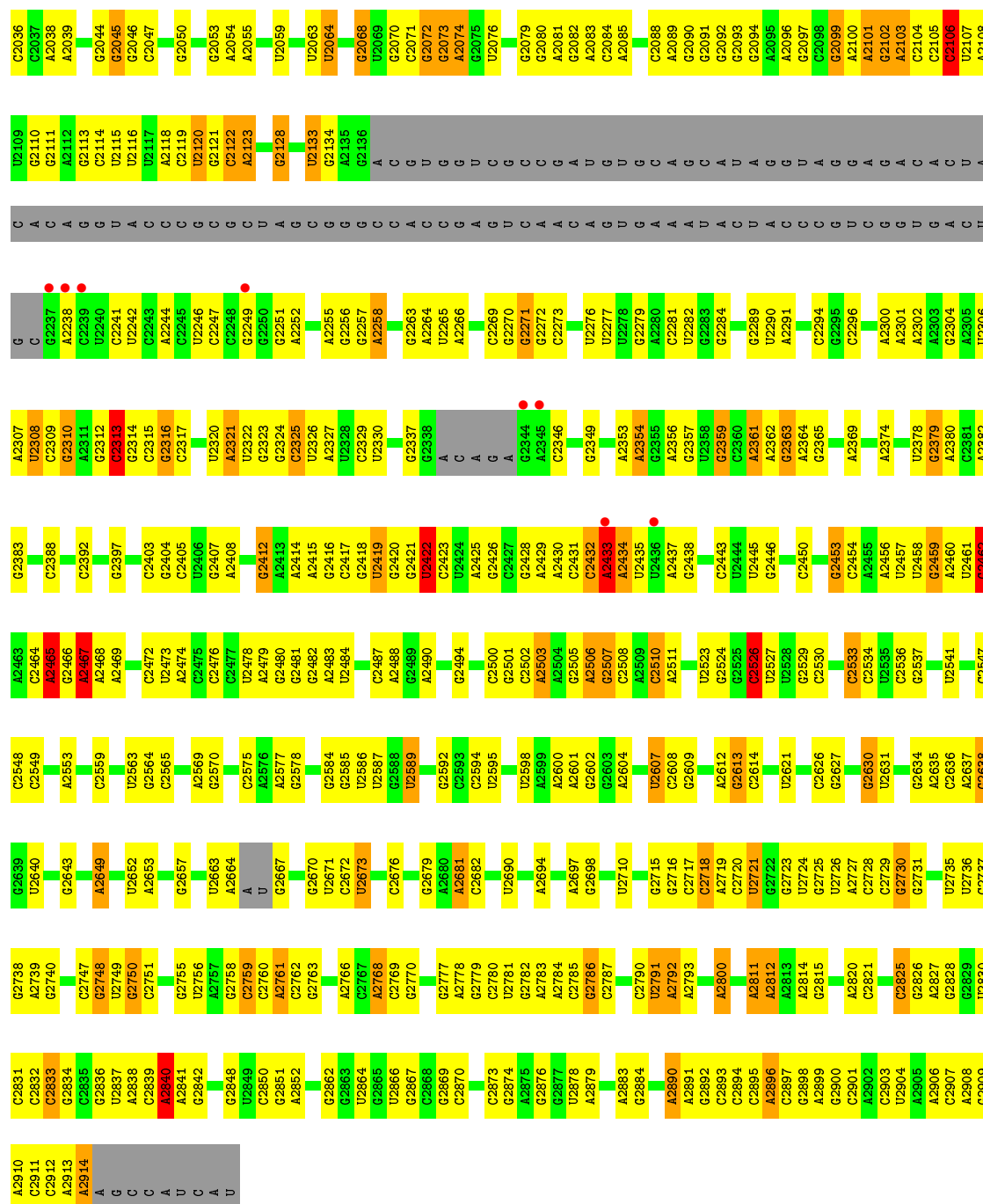
3 Residue-property plots

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.

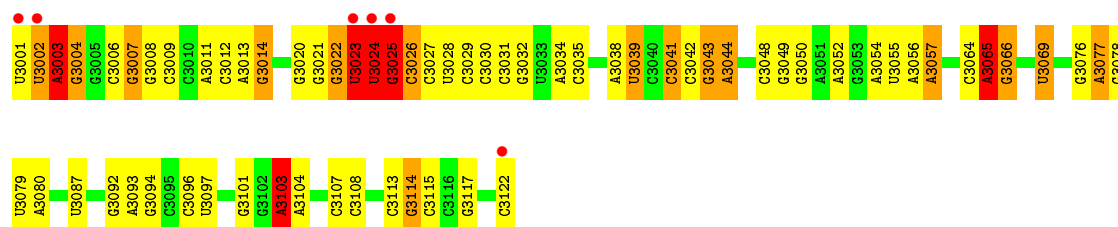
• Molecule 1: 23S rRNA



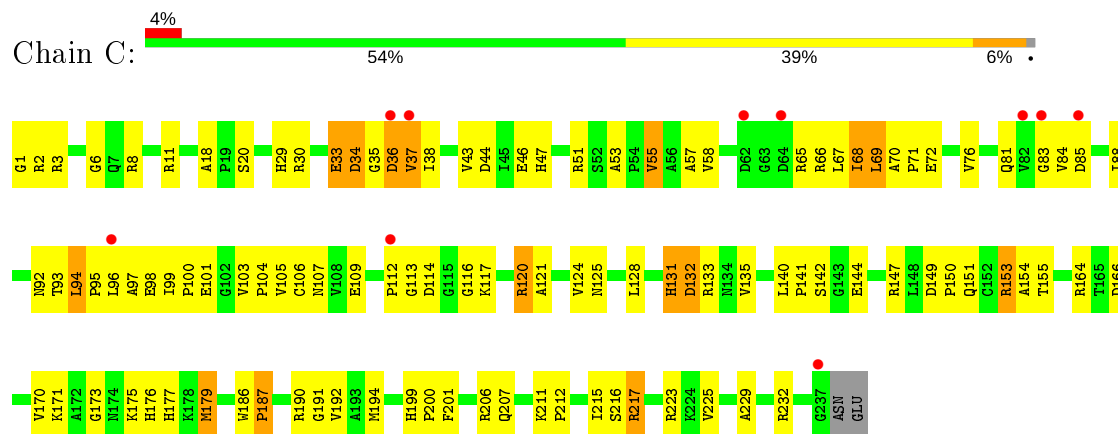
U	A857	A1013	A1097	U1180	U1362	A1528	A1624	C1705	C1798	G1878	U1866	U1964	U2008	U2009	A2010	A2011	U2012	G2013	A2014	A2015	U2016	A2019	G2023	A2030	C2031	U2032	G2033	U2034	C2035
G	U888	A1014	A1099	A1181	G1363	G1529	U1625	G1706	C1798	U1879	U1886	C1965	G2000	G2001	A2010	A2011	U2012	G2013	A2014	A2015	U2016	A2019	G2023	A2030	C2031	U2032	G2033	U2034	C2035
A	C859	C1015	G1099	C1182	U1368	A1533	G1626	G1707	A1804	U1879	U1886	C1966	G2001	G2002	A2010	A2011	U2012	G2013	A2014	A2015	U2016	A2019	G2023	A2030	C2031	U2032	G2033	U2034	C2035
C	U860	U1016	C1103	C1183	U1369	C1534	G1627		G1805	U1881	U1886	C1967	G2002	G2003	A2010	A2011	U2012	G2013	A2014	A2015	U2016	A2019	G2023	A2030	C2031	U2032	G2033	U2034	C2035
C	U861	C946	C1109	U1184	U1370	G1536	G1628	A1710	G1806	C1882	U1887	C1968	G2003	G2004	A2010	A2011	U2012	G2013	A2014	A2015	U2016	A2019	G2023	A2030	C2031	U2032	G2033	U2034	C2035
U1964	U862	U947	U1109	U1185	U1371	U1457	G1629	A1711	G1807	C1883	U1888	C1969	G2004	G2005	A2010	A2011	U2012	G2013	A2014	A2015	U2016	A2019	G2023	A2030	C2031	U2032	G2033	U2034	C2035
C1965	U863	U948	U1110	U1186	U1372	U1458	G1630	A1712	G1808	U1889	U1889	C1970	G2005	G2006	A2010	A2011	U2012	G2013	A2014	A2015	U2016	A2019	G2023	A2030	C2031	U2032	G2033	U2034	C2035
U1966	U864	U949	U1111	U1187	U1373	U1459	A1630	A1713	G1809	U1890	U1890	C1971	G2006	G2007	A2010	A2011	U2012	G2013	A2014	A2015	U2016	A2019	G2023	A2030	C2031	U2032	G2033	U2034	C2035
C1967		U950	A1114	U1188	A1375	U1460	G1631	C1720	G1810	U1891	U1891	C1972	G2007	G2008	A2010	A2011	U2012	G2013	A2014	A2015	U2016	A2019	G2023	A2030	C2031	U2032	G2033	U2034	C2035
U1968	A867	A951	A1115	U1189	A1376	C1462	G1632	U1721	G1811	U1892	U1892	C1973	G2008	G2009	A2010	A2011	U2012	G2013	A2014	A2015	U2016	A2019	G2023	A2030	C2031	U2032	G2033	U2034	C2035
A1969	G868	A952	U1116	U1190	U1376	C1463	G1633	U1722	G1812	U1893	U1893	C1974	G2009	G2010	A2010	A2011	U2012	G2013	A2014	A2015	U2016	A2019	G2023	A2030	C2031	U2032	G2033	U2034	C2035
U1970	G869	G953	U1117	U1191	C1377	U1464	G1634	U1723	G1813	U1894	U1894	C1975	G2010	G2011	A2010	A2011	U2012	G2013	A2014	A2015	U2016	A2019	G2023	A2030	C2031	U2032	G2033	U2034	C2035
G1971	G870	U954	A1118	U1192	C1378	U1465	G1635	U1724	G1814	U1895	U1895	C1976	G2011	G2012	A2010	A2011	U2012	G2013	A2014	A2015	U2016	A2019	G2023	A2030	C2031	U2032	G2033	U2034	C2035
U1972	G871	A955	A1119	U1193	U1380	U1466	G1636	C1725	G1815	U1896	U1896	C1977	G2012	G2013	A2010	A2011	U2012	G2013	A2014	A2015	U2016	A2019	G2023	A2030	C2031	U2032	G2033	U2034	C2035
U1973	U872		U1120	U1194	U1381	U1467	G1637		G1816	U1897	U1897	C1978	G2013	G2014	A2010	A2011	U2012	G2013	A2014	A2015	U2016	A2019	G2023	A2030	C2031	U2032	G2033	U2034	C2035
U1974			U1121	U1195	U1382	U1468	A1641	G1730	G1817	U1898	U1898	C1979	G2014	G2015	A2010	A2011	U2012	G2013	A2014	A2015	U2016	A2019	G2023	A2030	C2031	U2032	G2033	U2034	C2035
	A875	G958	U1122	U1196	U1383	U1469	A1642	G1731	G1818	U1899	U1899	C1980	G2015	G2016	A2010	A2011	U2012	G2013	A2014	A2015	U2016	A2019	G2023	A2030	C2031	U2032	G2033	U2034	C2035
A876	G959	G960	U1123	U1197	U1384	U1470	G1647	G1732	G1819	U1900	U1900	C1981	G2016	G2017	A2010	A2011	U2012	G2013	A2014	A2015	U2016	A2019	G2023	A2030	C2031	U2032	G2033	U2034	C2035
G877	G961	A961	A1124	U1198	U1385	U1471	U1653	A1733	G1820	U1901	U1901	C1982	G2017	G2018	A2010	A2011	U2012	G2013	A2014	A2015	U2016	A2019	G2023	A2030	C2031	U2032	G2033	U2034	C2035
G878	G962	C963	C1125	U1199	U1386	U1472	U1654	G1734	G1821	U1902	U1902	C1983	G2018	G2019	A2010	A2011	U2012	G2013	A2014	A2015	U2016	A2019	G2023	A2030	C2031	U2032	G2033	U2034	C2035
		C964	C1126	U1200	U1387	U1473	U1655	G1735	G1822	U1903	U1903	C1984	G2019	G2020	A2010	A2011	U2012	G2013	A2014	A2015	U2016	A2019	G2023	A2030	C2031	U2032	G2033	U2034	C2035
		C965	C1127	U1201	U1388	U1474	U1656	G1736	G1823	U1904	U1904	C1985	G2020	G2021	A2010	A2011	U2012	G2013	A2014	A2015	U2016	A2019	G2023	A2030	C2031	U2032	G2033	U2034	C2035
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		C973	U1135	U1209	U1396	U1482	U1664	G1744	G1831	U1912	U1912	C1993	G2028	G2029	A2010	A2011	U2012	G2013	A2014	A2015	U2016	A2019	G2023	A2030	C2031	U2032	G2033	U2034	C2035
		C974	U1136	U1210	U1397	U1483	U1665	G1745	G1832	U1913	U1913	C1994	G2029	G2030	A2010	A2011	U2012	G2013	A2014	A2015	U2016	A2019	G2023	A2030	C2031	U2032	G2033	U2034	C2035
		C975	U1137	U1211	U1398	U1484	U1666	G1746	G1833	U1914	U1914	C1995	G2030	G2031	A2010	A2011	U2012	G2013	A2014	A2015	U2016	A2019	G2023	A2030	C2031	U2032	G2033	U2034	C2035
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		C978	U1140	U1214	U1401	U1487	U1669	G1749	G1836	U1917	U1917	C1998	G2033	G2034	A2010	A2011	U2012	G2013	A2014	A2015	U2016	A2019	G2023	A2030	C2031	U2032	G2033	U2034	C2035
		C979	U1141	U1215	U1402	U1488	U1670	G1750	G1837	U1918	U1918	C1999	G2034	G2035	A2010	A2011	U2012	G2013	A2014	A2015	U2016	A2019	G2023	A2030	C2031	U2032	G2033	U2034	C2035
		C980	U1142	U1216	U1403	U1489	U1671	G1751	G1838	U1919	U1919	C2000	G2035	G2036	A2010	A2011	U2012	G2013	A2014	A2015	U2016	A2019	G2023	A2030	C2031	U2032	G2033	U2034	C2035
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		C983	U1145	U1219	U1406	U1492	U1674	G1754	G1841	U1922	U1922	C2003	G2038	G2039	A2010	A2011	U2012	G2013	A2014	A2015	U2016	A2019	G2023	A2030	C2031	U2032	G2033	U2034	C2035
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		C985	U1147	U1221	U1408	U1494	U1676	G1756	G1843	U1924	U1924	C2005	G2040	G2041	A2010	A2011	U2012	G2013	A2014	A2015	U2016	A2019	G2023	A2030	C2031	U2032	G2033	U2034	C2035
		C986	U1148	U1222	U1409	U1495	U1677	G1757	G1844	U1925	U1925	C2006	G2041	G2042	A2010	A2011	U2012	G2013	A2014	A2015	U2016	A2019	G2023	A2030	C2031	U2032	G2033	U2034	C2035
		C987	U1149	U1223	U1410	U1496	U1678	G1758	G1845	U1926	U1926	C2007	G2042	G2043	A2010	A2011	U2012	G2013	A2014	A2015	U2016	A2019	G2023	A2030	C2031	U2032	G2033	U2034	C2035



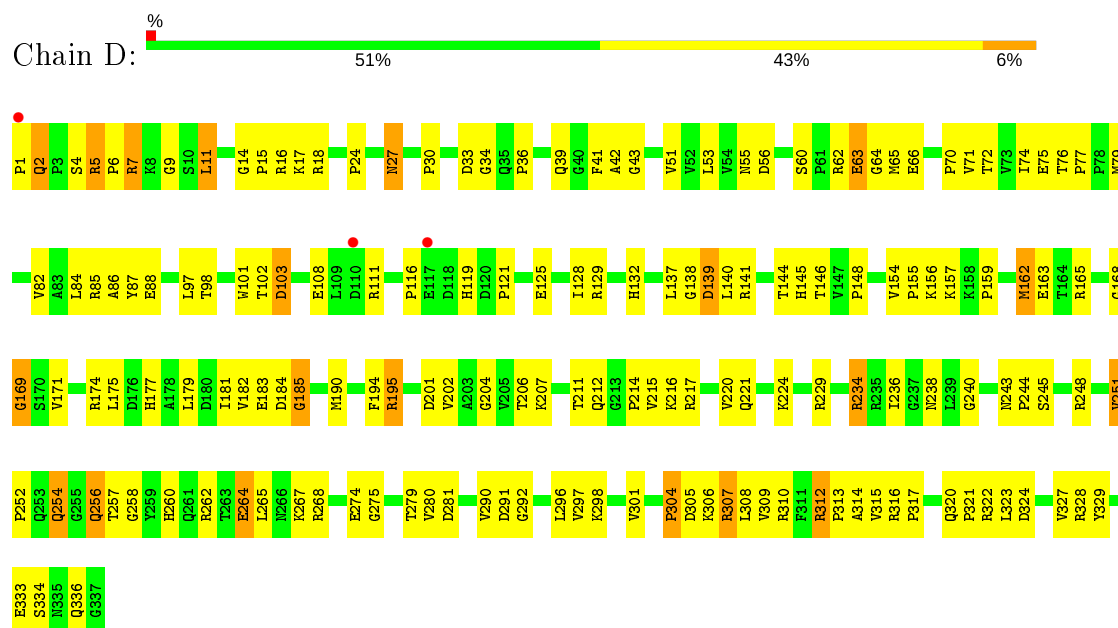
• Molecule 2: 5S rRNA



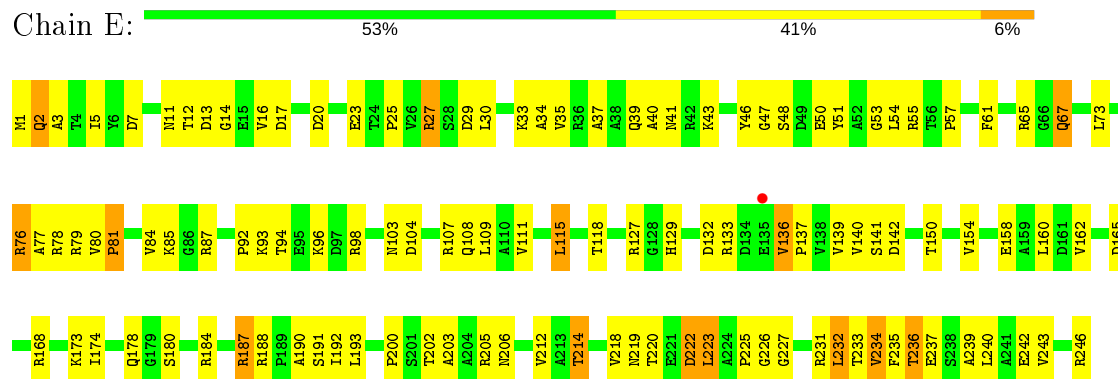
- Molecule 3: RIBOSOMAL PROTEIN L2



- Molecule 4: RIBOSOMAL PROTEIN L3

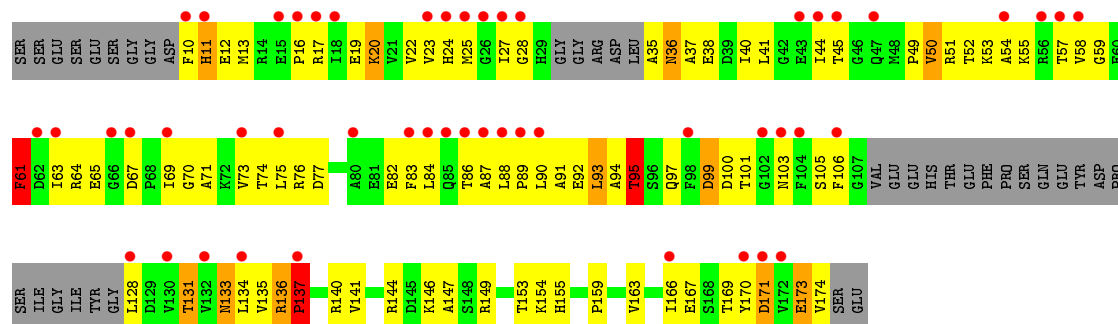


- Molecule 5: RIBOSOMAL PROTEIN L4

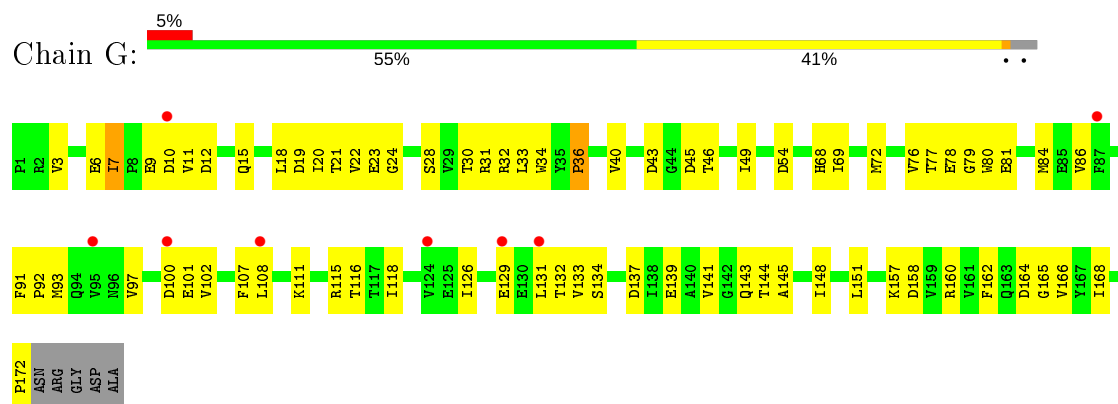


- Molecule 6: RIBOSOMAL PROTEIN L5

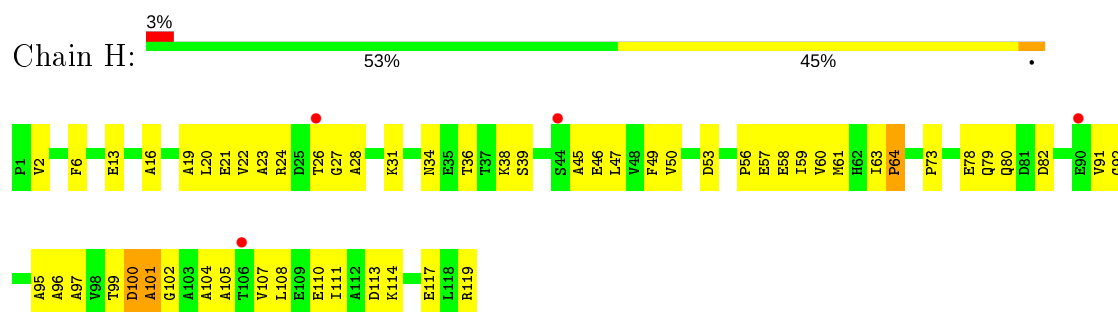




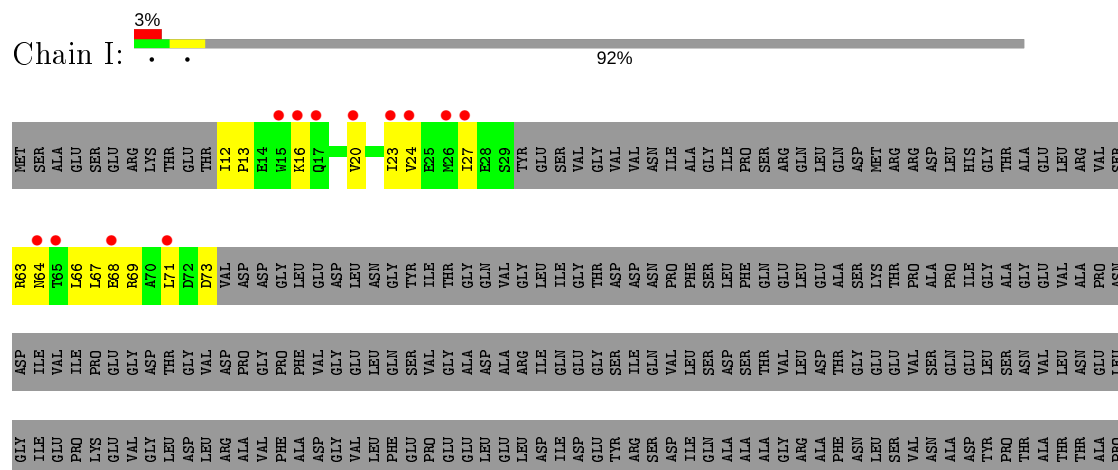
- Molecule 7: RIBOSOMAL PROTEIN L6



- Molecule 8: RIBOSOMAL PROTEIN L7AE

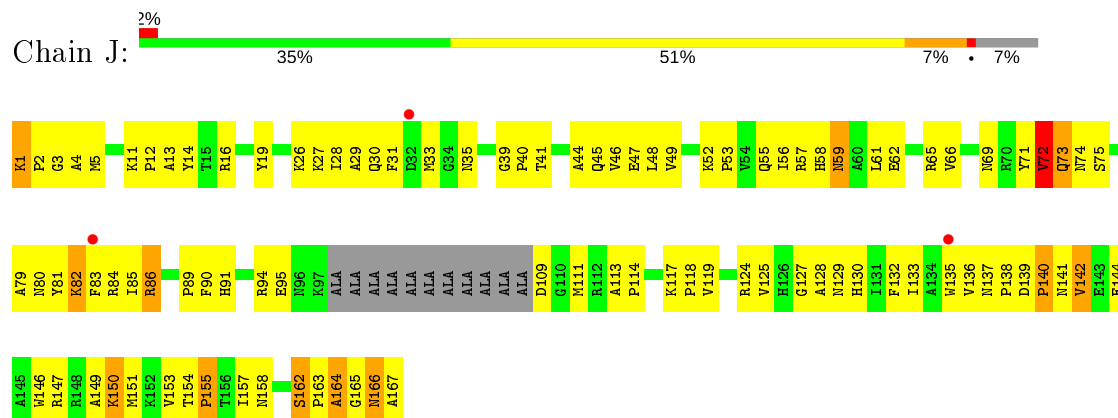


- Molecule 9: RIBOSOMAL PROTEIN L10

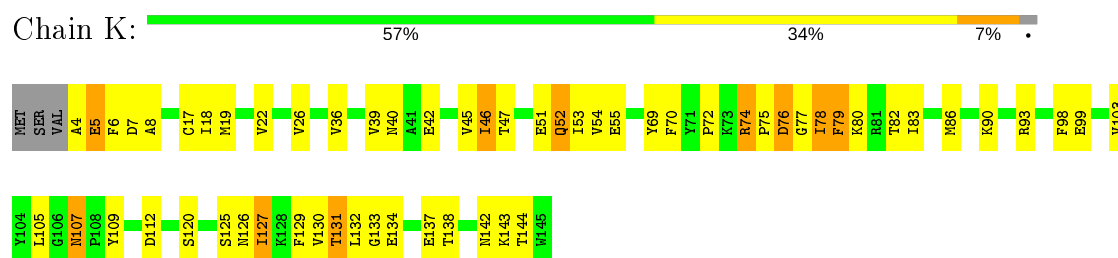


THR	MET	LEU	GLN	SER	ASP	ARG	GLY	ASN	ALA	LYS	SER	LEU	ALA	LEU	GLN	ALA	ALA	TLE	GLU	ASP	PRO	GLU	VAL	ALA	VAL	PRO	ASP	VAL	SER	LYS	ALA	ASP	ALA	ASP	GLN	VAL	ARG	ALA	LEU	ALA	GLY	ASP	ALA	SER	GLN	TLE	ASP	GLU	ALA	ALA	LEU	PRO	GLU	ALA	GLN	VAL	GLU	ASP	VAL
ALA	THR	GLU	GLY	PRO	THR	ASP	ASP	GLN	ASP	ASP	THR	ALA	SER	GLN	ASP	ALA	ASP	ALA	ASP	ALA	ASP	PRO	ASP	ALA	ALA	GLU	GLU	ALA	ASP	VAL	ASP	ASP	ASP	ASP	GLN	VAL	ARG	ALA	ALA	GLY	ASP	ALA	SER	LEU	GLY	ASP	ALA	ALA	GLU	VAL	GLU	ASP	ALA	VAL					

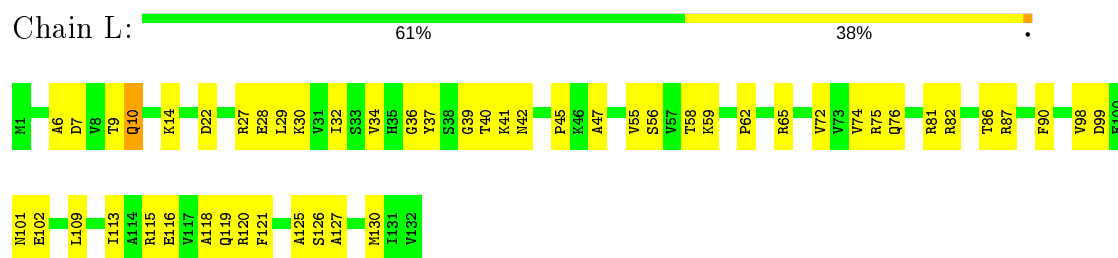
• Molecule 10: RIBOSOMAL PROTEIN L10E



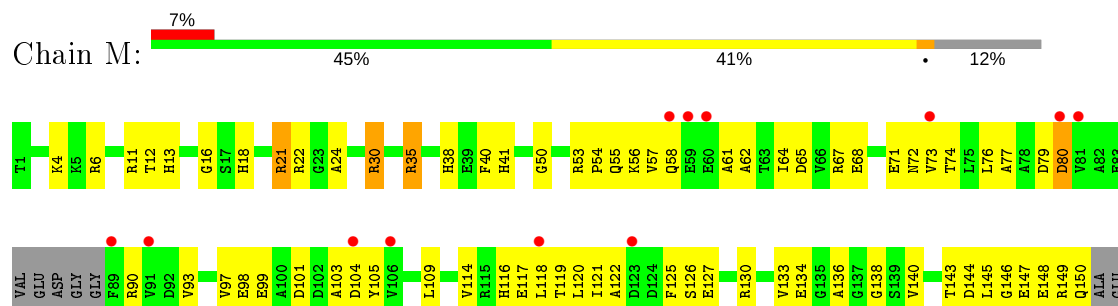
• Molecule 11: RIBOSOMAL PROTEIN L13



• Molecule 12: RIBOSOMAL PROTEIN L14



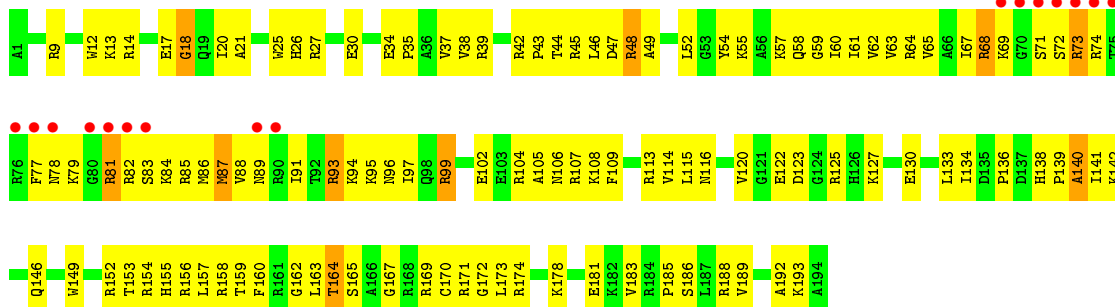
• Molecule 13: RIBOSOMAL PROTEIN L15



ALA
GLU
GLU
THR
GLU
ASP
ALA
ASP
ALA
ASP
GLU
GLU

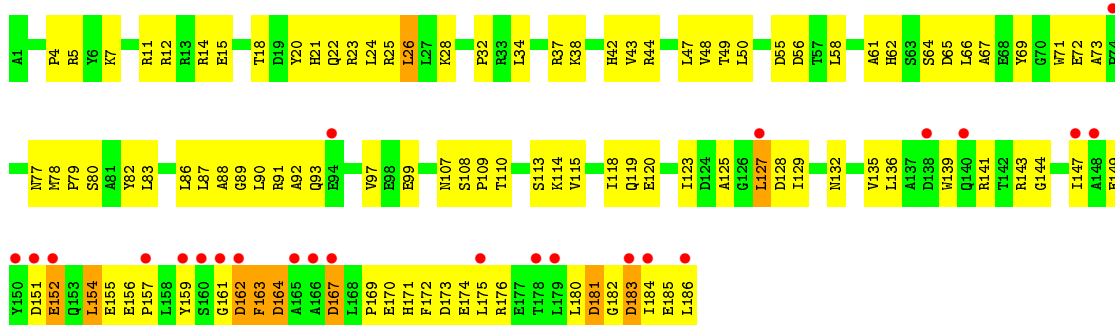
• Molecule 14: RIBOSOMAL PROTEIN L15E

Chain N: 



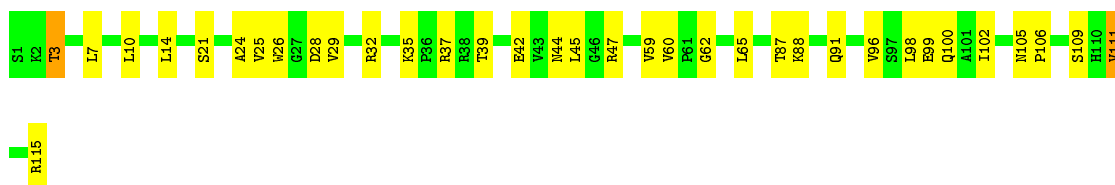
• Molecule 15: RIBOSOMAL PROTEIN L18

Chain O: 



• Molecule 16: RIBOSOMAL PROTEIN L18E

Chain P: 



• Molecule 17: RIBOSOMAL PROTEIN L19E

Chain Q: 

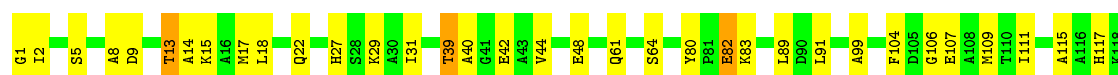




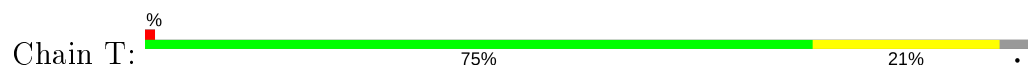
• Molecule 18: RIBOSOMAL PROTEIN L21E



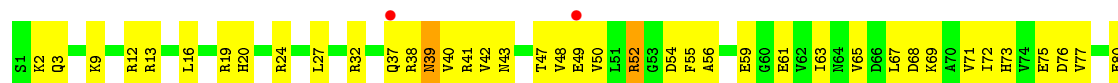
• Molecule 19: RIBOSOMAL PROTEIN L22



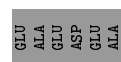
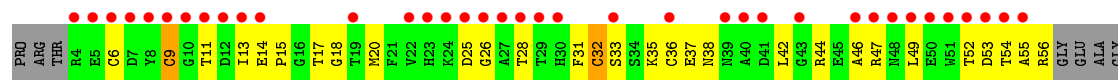
• Molecule 20: RIBOSOMAL PROTEIN L23



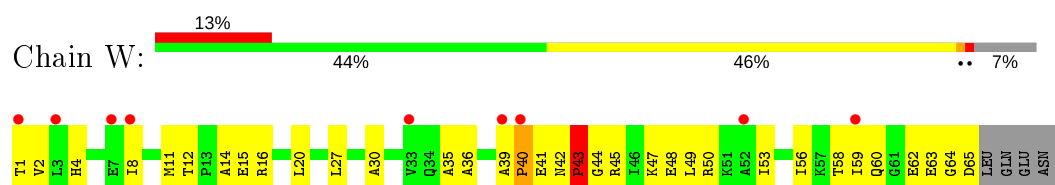
• Molecule 21: RIBOSOMAL PROTEIN L24



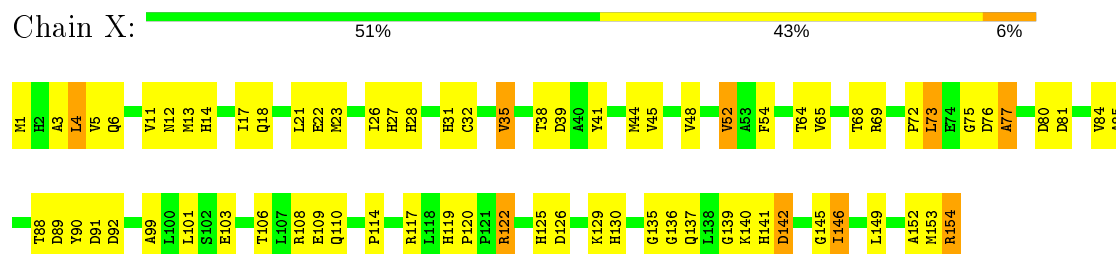
• Molecule 22: RIBOSOMAL PROTEIN L24E



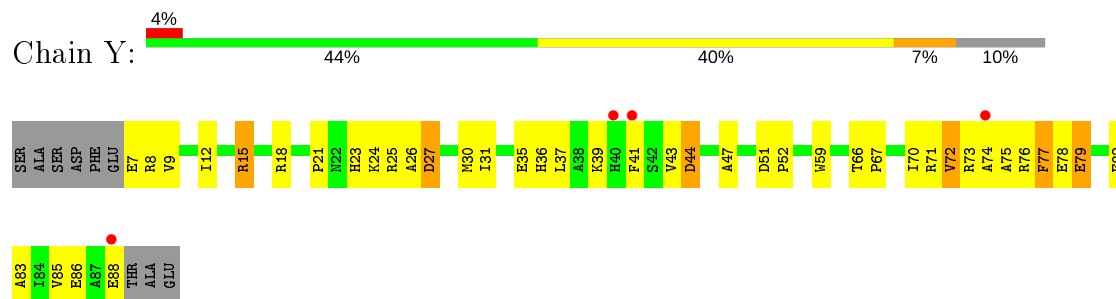
• Molecule 23: RIBOSOMAL PROTEIN L29



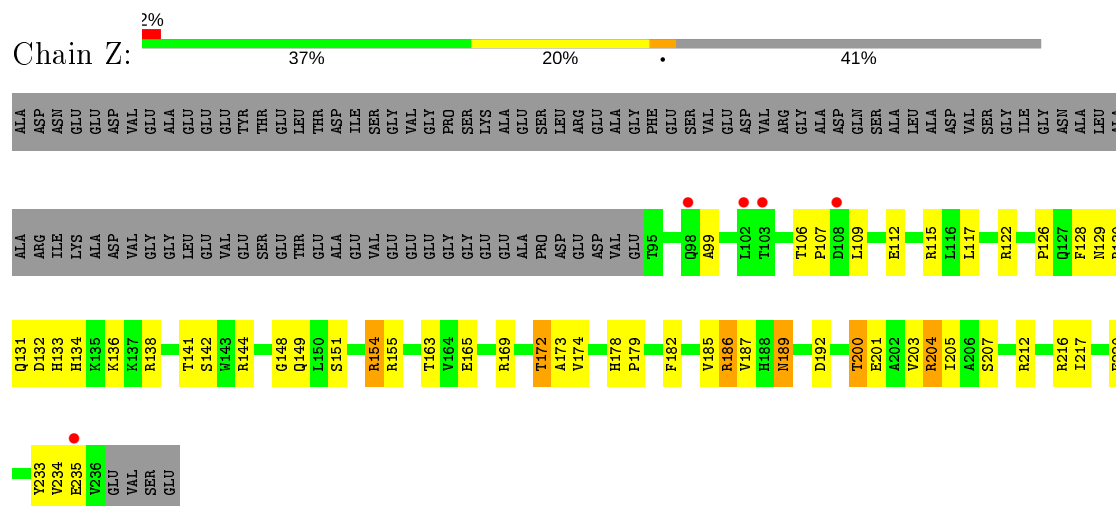
• Molecule 24: RIBOSOMAL PROTEIN L30



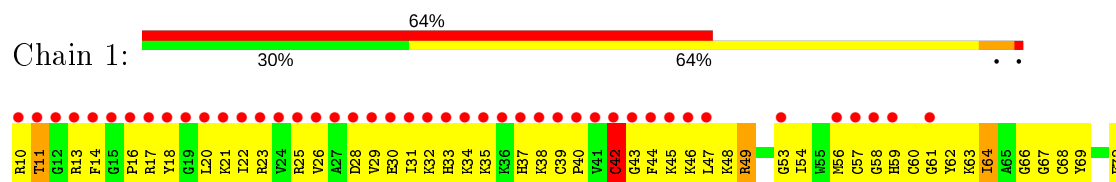
• Molecule 25: RIBOSOMAL PROTEIN L31E

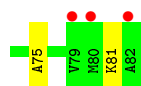


• Molecule 26: RIBOSOMAL PROTEIN L32E



• Molecule 27: RIBOSOMAL PROTEIN L37Ae





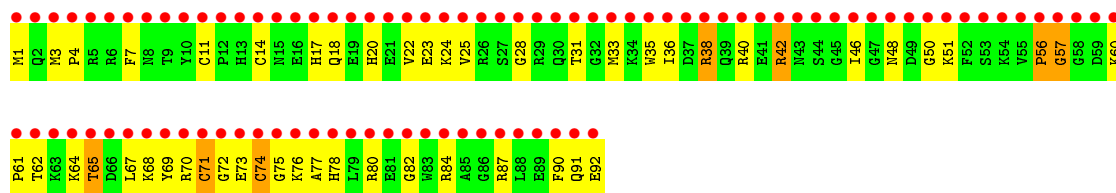
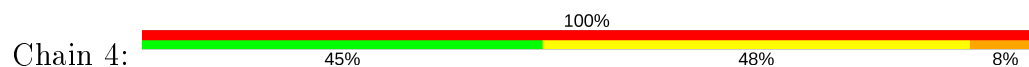
• Molecule 28: RIBOSOMAL PROTEIN L37E



• Molecule 29: RIBOSOMAL PROTEIN L39E



• Molecule 30: RIBOSOMAL PROTEIN L44E



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	212.90Å 300.47Å 575.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.99 – 3.00 50.07 – 2.99	Depositor EDS
% Data completeness (in resolution range)	91.7 (19.99-3.00) 91.1 (50.07-2.99)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	0.15	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.46 (at 3.01Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.220 , 0.269 0.219 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	50.9	Xtriage
Anisotropy	0.399	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 65.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	98587	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.66% 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: MG, CL, NA, SPR, CD, K

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	A	0.62	12/66076 (0.0%)	0.79	45/103052 (0.0%)
2	B	0.90	12/2905 (0.4%)	0.98	17/4528 (0.4%)
3	C	0.53	0/1787	0.79	0/2409
4	D	0.52	0/2689	0.75	0/3652
5	E	0.54	0/1883	0.78	0/2551
6	F	0.43	0/1111	0.65	0/1498
7	G	0.47	0/1382	0.66	0/1880
8	H	0.44	0/896	0.64	0/1219
9	I	0.41	0/241	0.58	0/324
10	J	0.53	0/1246	0.83	1/1686 (0.1%)
11	K	0.52	0/1135	0.70	0/1530
12	L	0.51	0/1003	0.80	0/1351
13	M	0.49	0/1126	0.74	0/1504
14	N	0.67	0/1633	0.86	1/2180 (0.0%)
15	O	0.48	0/1473	0.76	0/1999
16	P	0.53	0/873	0.76	0/1181
17	Q	0.52	0/1143	0.67	0/1521
18	R	0.52	0/748	0.80	1/1005 (0.1%)
19	S	0.66	1/1172 (0.1%)	0.84	2/1578 (0.1%)
20	T	0.45	0/648	0.69	0/875
21	U	0.47	0/957	0.73	1/1289 (0.1%)
22	V	0.77	0/417	0.86	2/562 (0.4%)
23	W	0.42	0/502	0.63	0/675
24	X	0.54	0/1218	0.76	0/1655
25	Y	0.50	0/664	0.72	0/895
26	Z	0.53	0/1146	0.73	0/1536
27	1	0.85	0/575	0.87	1/763 (0.1%)
28	2	0.56	0/437	0.84	0/578
29	3	0.47	0/398	0.64	0/527
30	4	1.04	0/771	0.83	1/1024 (0.1%)
All	All	0.62	25/98255 (0.0%)	0.79	72/147027 (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	A	1	198
2	B	0	6
28	2	0	1
All	All	1	205

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2103	A	C5-C6	13.31	1.53	1.41
2	B	3025	G	O3'-P	11.56	1.75	1.61
2	B	3026	C	P-OP2	-10.89	1.30	1.49
2	B	3026	C	P-O5'	-9.81	1.50	1.59
2	B	3023	U	C2'-O2'	8.99	1.53	1.41
2	B	3025	G	P-OP2	-8.40	1.34	1.49
1	A	2103	A	N7-C5	8.09	1.44	1.39
2	B	3025	G	C4'-O4'	7.84	1.55	1.45
2	B	3023	U	O5'-C5'	7.80	1.56	1.44
1	A	2104	C	O5'-C5'	-6.97	1.31	1.42
1	A	2106	C	O3'-P	-6.78	1.53	1.61
19	S	130	MET	CB-CG	-6.69	1.29	1.51
1	A	2103	A	C5-C4	6.64	1.43	1.38
1	A	2103	A	C3'-C2'	6.43	1.60	1.52
1	A	2103	A	C8-N7	6.38	1.36	1.31
2	B	3025	G	N9-C4	-6.27	1.32	1.38
1	A	2433	A	C5-C6	6.25	1.46	1.41
1	A	2103	A	N9-C4	6.24	1.41	1.37
1	A	2106	C	N1-C2	6.05	1.46	1.40
2	B	3024	U	P-OP2	-5.48	1.39	1.49
1	A	2104	C	P-O5'	5.38	1.65	1.59
2	B	3026	C	O3'-P	5.25	1.67	1.61
2	B	3024	U	C3'-C2'	5.18	1.58	1.52
1	A	2105	C	O3'-P	5.04	1.67	1.61
2	B	3025	G	C2'-C1'	5.01	1.58	1.53

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1164	U	OP2-P-O3'	-18.78	63.89	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1164	U	OP1-P-O3'	-18.34	64.85	105.20
1	A	2104	C	O5'-P-OP1	-14.12	92.99	105.70
2	B	3024	U	O5'-P-OP2	11.53	124.53	110.70
2	B	3026	C	O5'-P-OP2	-11.17	95.65	105.70
1	A	2103	A	C5'-C4'-O4'	11.13	122.46	109.10
1	A	1165	G	O5'-P-OP1	-11.05	95.75	105.70
1	A	2103	A	OP2-P-O3'	9.79	126.73	105.20
2	B	3026	C	O5'-P-OP1	-9.30	97.33	105.70
2	B	3026	C	OP1-P-OP2	9.15	133.32	119.60
1	A	1942	A	C5'-C4'-C3'	9.01	130.41	116.00
1	A	1942	A	C5'-C4'-O4'	9.01	119.91	109.10
1	A	1563	G	C2'-C3'-O3'	8.94	129.18	109.50
1	A	2106	C	N1-C1'-C2'	-8.05	103.14	112.00
2	B	3004	G	O5'-P-OP1	-7.73	98.74	105.70
1	A	2103	A	O4'-C1'-N9	7.48	114.19	108.20
1	A	2099	G	OP2-P-O3'	7.11	120.84	105.20
1	A	1979	G	C2'-C3'-O3'	6.88	124.71	113.70
2	B	3026	C	C5'-C4'-O4'	6.87	117.35	109.10
22	V	36	CYS	CA-CB-SG	-6.58	102.16	114.00
2	B	3027	C	O5'-P-OP1	-6.45	99.89	105.70
1	A	1165	G	O5'-P-OP2	-6.25	100.07	105.70
19	S	130	MET	CB-CG-SD	6.22	131.06	112.40
1	A	171	C	OP2-P-O3'	6.21	118.86	105.20
1	A	1165	G	OP1-P-OP2	6.09	128.74	119.60
2	B	3023	U	P-O5'-C5'	6.08	130.62	120.90
1	A	2465	A	N9-C1'-C2'	-5.91	105.50	112.00
27	1	42	CYS	CA-CB-SG	5.91	124.63	114.00
1	A	2103	A	C4'-C3'-O3'	-5.87	97.08	109.40
1	A	1738	C	C5'-C4'-C3'	5.86	125.38	116.00
1	A	2313	C	C5'-C4'-O4'	5.76	116.02	109.10
2	B	3024	U	OP1-P-O3'	5.76	117.88	105.20
2	B	3103	A	C5'-C4'-O4'	5.74	115.98	109.10
10	J	74	ASN	N-CA-C	-5.74	95.51	111.00
14	N	73	ARG	N-CA-C	-5.67	95.69	111.00
1	A	129	A	C2'-C3'-O3'	5.65	122.74	113.70
2	B	3039	U	N1-C1'-C2'	5.64	121.33	114.00
2	B	3024	U	C5'-C4'-O4'	5.61	115.83	109.10
1	A	2419	U	N1-C1'-C2'	5.59	121.27	114.00
2	B	3025	G	O5'-P-OP2	-5.56	100.70	105.70
1	A	1342	C	N1-C1'-C2'	-5.50	105.95	112.00
1	A	1878	G	O4'-C1'-N9	5.49	112.59	108.20
18	R	68	GLY	N-CA-C	-5.47	99.41	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2122	C	OP2-P-O3'	5.44	117.17	105.20
1	A	2467	A	C1'-O4'-C4'	-5.44	105.55	109.90
1	A	1563	G	C4'-C3'-O3'	5.43	123.86	113.00
1	A	1504	A	C1'-O4'-C4'	-5.41	105.57	109.90
21	U	52	ARG	N-CA-C	5.40	125.59	111.00
19	S	131	GLY	CA-C-O	-5.40	110.88	120.60
1	A	1504	A	N9-C1'-C2'	5.33	120.93	114.00
1	A	2106	C	O5'-P-OP2	-5.33	100.90	105.70
2	B	3023	U	OP2-P-O3'	-5.33	93.48	105.20
2	B	3003	A	C4'-C3'-C2'	-5.32	97.28	102.60
30	4	71	CYS	CA-CB-SG	-5.32	104.43	114.00
22	V	6	CYS	CA-CB-SG	-5.26	104.53	114.00
1	A	1683	G	N9-C1'-C2'	5.26	120.83	114.00
2	B	3025	G	O3'-P-O5'	5.26	113.99	104.00
1	A	2432	C	N1-C1'-C2'	5.25	120.82	114.00
1	A	2102	G	O4'-C1'-N9	5.22	112.38	108.20
1	A	407	A	O4'-C4'-C3'	-5.13	98.87	104.00
1	A	2105	C	OP2-P-O3'	5.11	116.45	105.20
1	A	928	G	N9-C1'-C2'	-5.10	106.39	112.00
2	B	3113	C	N1-C1'-C2'	5.10	120.63	114.00
1	A	324	G	N9-C1'-C2'	-5.08	106.41	112.00
1	A	2316	G	C5'-C4'-C3'	-5.08	107.87	116.00
1	A	2467	A	O5'-P-OP1	-5.07	101.14	105.70
1	A	2607	U	N1-C1'-C2'	5.05	120.57	114.00
1	A	1829	A	N9-C1'-C2'	-5.05	106.44	112.00
1	A	1051	C	N1-C1'-C2'	-5.04	106.45	112.00
1	A	2106	C	N1-C2-O2	5.04	121.92	118.90
1	A	1119	G	N9-C1'-C2'	5.01	120.52	114.00
1	A	2842	G	N9-C1'-C2'	-5.00	106.50	112.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	1563	G	C3'

All (205) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
28	2	48	TYR	Sidechain
1	A	1005	A	Sidechain
1	A	1023	C	Sidechain
1	A	1027	G	Sidechain

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Mol	Chain	Res	Type	Group
1	A	1039	G	Sidechain
1	A	1042	U	Sidechain
1	A	1055	G	Sidechain
1	A	112	G	Sidechain
1	A	1127	C	Sidechain
1	A	1134	G	Sidechain
1	A	1136	U	Sidechain
1	A	1156	C	Sidechain
1	A	1206	U	Sidechain
1	A	1237	U	Sidechain
1	A	1260	G	Sidechain
1	A	1264	U	Sidechain
1	A	1288	U	Sidechain
1	A	1298	U	Sidechain
1	A	1300	G	Sidechain
1	A	1309	U	Sidechain
1	A	1339	G	Sidechain
1	A	1347	U	Sidechain
1	A	1368	U	Sidechain
1	A	1376	G	Sidechain
1	A	1377	C	Sidechain
1	A	138	U	Sidechain
1	A	1389	G	Sidechain
1	A	1402	G	Sidechain
1	A	1408	U	Sidechain
1	A	1417	G	Sidechain
1	A	1418	U	Sidechain
1	A	1421	C	Sidechain
1	A	1430	G	Sidechain
1	A	1433	G	Sidechain
1	A	1447	U	Sidechain
1	A	1458	A	Sidechain
1	A	146	U	Sidechain
1	A	1468	G	Sidechain
1	A	1487	A	Sidechain
1	A	1501	A	Sidechain
1	A	1503	U	Sidechain
1	A	1614	G	Sidechain
1	A	1621	G	Sidechain
1	A	1628	G	Sidechain
1	A	163	U	Sidechain
1	A	1647	G	Sidechain

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Mol	Chain	Res	Type	Group
1	A	1677	U	Sidechain
1	A	1683	G	Sidechain
1	A	1684	A	Sidechain
1	A	1688	G	Sidechain
1	A	1689	A	Sidechain
1	A	169	A	Sidechain
1	A	171	C	Sidechain
1	A	1720	C	Sidechain
1	A	1736	A	Sidechain
1	A	174	A	Sidechain
1	A	1747	A	Sidechain
1	A	1748	U	Sidechain
1	A	176	U	Sidechain
1	A	1761	U	Sidechain
1	A	1771	U	Sidechain
1	A	178	U	Sidechain
1	A	1809	G	Sidechain
1	A	1816	C	Sidechain
1	A	1819	G	Sidechain
1	A	1823	G	Sidechain
1	A	1826	C	Sidechain
1	A	1833	U	Sidechain
1	A	1835	U	Sidechain
1	A	1839	A	Sidechain
1	A	1848	G	Sidechain
1	A	1860	U	Sidechain
1	A	1861	C	Sidechain
1	A	1867	G	Sidechain
1	A	1878	G	Sidechain
1	A	1882	C	Sidechain
1	A	1908	G	Sidechain
1	A	191	A	Sidechain
1	A	1933	G	Sidechain
1	A	197	C	Sidechain
1	A	1972	U	Sidechain
1	A	2000	G	Sidechain
1	A	2001	G	Sidechain
1	A	2002	C	Sidechain
1	A	2035	C	Sidechain
1	A	2045	G	Sidechain
1	A	2053	G	Sidechain
1	A	2063	U	Sidechain

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Mol	Chain	Res	Type	Group
1	A	2068	G	Sidechain
1	A	2070	G	Sidechain
1	A	2076	U	Sidechain
1	A	2092	G	Sidechain
1	A	2101	A	Sidechain
1	A	2106	C	Sidechain
1	A	2120	U	Sidechain
1	A	2123	A	Sidechain
1	A	2128	G	Sidechain
1	A	2133	U	Sidechain
1	A	214	U	Sidechain
1	A	2244	A	Sidechain
1	A	2273	C	Sidechain
1	A	2294	C	Sidechain
1	A	2304	G	Sidechain
1	A	2308	U	Sidechain
1	A	2310	G	Sidechain
1	A	2312	G	Sidechain
1	A	2313	C	Sidechain
1	A	2325	C	Sidechain
1	A	2337	G	Sidechain
1	A	2359	G	Sidechain
1	A	2363	G	Sidechain
1	A	2364	A	Sidechain
1	A	2378	U	Sidechain
1	A	2412	G	Sidechain
1	A	2422	U	Sidechain
1	A	2423	C	Sidechain
1	A	2433	A	Sidechain
1	A	2434	A	Sidechain
1	A	2453	G	Sidechain
1	A	2458	U	Sidechain
1	A	2459	G	Sidechain
1	A	246	G	Sidechain
1	A	2462	G	Sidechain
1	A	2503	A	Sidechain
1	A	2506	A	Sidechain
1	A	2526	C	Sidechain
1	A	2575	C	Sidechain
1	A	2630	G	Sidechain
1	A	2631	U	Sidechain
1	A	264	G	Sidechain

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Mol	Chain	Res	Type	Group
1	A	2640	U	Sidechain
1	A	2643	G	Sidechain
1	A	2663	U	Sidechain
1	A	2673	U	Sidechain
1	A	2720	C	Sidechain
1	A	2721	U	Sidechain
1	A	2727	A	Sidechain
1	A	2730	G	Sidechain
1	A	2759	C	Sidechain
1	A	2790	C	Sidechain
1	A	2793	A	Sidechain
1	A	2800	A	Sidechain
1	A	2811	A	Sidechain
1	A	2833	C	Sidechain
1	A	2840	A	Sidechain
1	A	2864	U	Sidechain
1	A	2891	A	Sidechain
1	A	331	A	Sidechain
1	A	333	G	Sidechain
1	A	395	A	Sidechain
1	A	396	U	Sidechain
1	A	398	U	Sidechain
1	A	406	G	Sidechain
1	A	407	A	Sidechain
1	A	436	A	Sidechain
1	A	458	G	Sidechain
1	A	461	C	Sidechain
1	A	474	C	Sidechain
1	A	476	A	Sidechain
1	A	486	A	Sidechain
1	A	487	G	Sidechain
1	A	518	G	Sidechain
1	A	548	U	Sidechain
1	A	554	G	Sidechain
1	A	650	C	Sidechain
1	A	669	G	Sidechain
1	A	720	G	Sidechain
1	A	723	G	Sidechain
1	A	743	G	Sidechain
1	A	75	U	Sidechain
1	A	750	A	Sidechain
1	A	755	G	Sidechain

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Mol	Chain	Res	Type	Group
1	A	756	A	Sidechain
1	A	757	C	Sidechain
1	A	759	C	Sidechain
1	A	761	A	Sidechain
1	A	768	U	Sidechain
1	A	791	A	Sidechain
1	A	815	U	Sidechain
1	A	816	G	Sidechain
1	A	817	G	Sidechain
1	A	818	A	Sidechain
1	A	827	A	Sidechain
1	A	838	C	Sidechain
1	A	840	U	Sidechain
1	A	864	U	Sidechain
1	A	867	A	Sidechain
1	A	871	G	Sidechain
1	A	878	G	Sidechain
1	A	882	A	Sidechain
1	A	887	G	Sidechain
1	A	888	U	Sidechain
1	A	889	C	Sidechain
1	A	904	U	Sidechain
1	A	916	A	Sidechain
1	A	919	U	Sidechain
1	A	946	C	Sidechain
1	A	954	U	Sidechain
1	A	99	A	Sidechain
2	B	3023	U	Sidechain
2	B	3025	G	Sidechain
2	B	3065	A	Sidechain
2	B	3069	U	Sidechain
2	B	3087	U	Sidechain
2	B	3094	G	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	A	59017	0	29802	1290	0
2	B	2600	0	1326	80	0
3	C	1754	0	1763	132	0
4	D	2624	0	2533	190	0
5	E	1858	0	1816	149	0
6	F	1094	0	1085	135	0
7	G	1357	0	1266	85	0
8	H	885	0	854	63	0
9	I	240	0	231	21	0
10	J	1215	0	1215	175	0
11	K	1119	0	1098	70	0
12	L	993	0	1027	67	0
13	M	1114	0	1072	72	0
14	N	1605	0	1676	194	0
15	O	1444	0	1401	143	0
16	P	864	0	873	37	0
17	Q	1133	0	1127	53	0
18	R	734	0	727	30	0
19	S	1149	0	1122	60	0
20	T	641	0	605	23	0
21	U	949	0	923	59	0
22	V	410	0	368	45	0
23	W	499	0	511	33	0
24	X	1195	0	1137	99	0
25	Y	654	0	653	51	0
26	Z	1130	0	1133	71	0
27	1	563	0	601	80	0
28	2	430	0	426	27	0
29	3	393	0	406	27	0
30	4	755	0	732	58	0
31	A	59	0	73	9	0
32	1	1	0	0	0	0
32	4	1	0	0	0	0
32	A	112	0	0	5	0
32	B	1	0	0	0	0
32	C	1	0	0	0	0
32	L	1	0	0	0	0
32	U	1	0	0	0	0
32	Z	1	0	0	0	0
33	A	73	0	0	1	0
33	B	2	0	0	0	0
33	C	1	0	0	0	0
33	E	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	J	1	0	0	0	0
33	K	1	0	0	0	0
33	M	1	0	0	0	0
33	N	1	0	0	0	0
33	R	1	0	0	0	0
33	S	2	0	0	0	0
33	T	1	0	0	0	0
34	4	1	0	0	0	0
34	A	9	0	0	2	0
34	C	1	0	0	0	0
34	D	1	0	0	0	0
34	K	3	0	0	2	0
34	M	1	0	0	0	0
34	N	1	0	0	1	0
34	O	1	0	0	3	0
34	P	1	0	0	0	0
34	R	1	0	0	0	0
34	S	1	0	0	0	0
34	Z	1	0	0	0	0
35	A	3	0	0	0	0
36	1	1	0	0	0	0
36	2	1	0	0	0	0
36	4	1	0	0	0	0
36	P	1	0	0	0	0
36	V	1	0	0	0	0
37	1	41	0	0	13	0
37	2	55	0	0	5	0
37	3	42	0	0	5	0
37	4	73	0	0	7	0
37	A	5910	0	0	300	0
37	B	142	0	0	16	0
37	C	126	0	0	23	0
37	D	150	0	0	28	0
37	E	169	0	0	40	0
37	F	51	0	0	22	0
37	G	42	0	0	13	0
37	H	26	0	0	9	0
37	I	21	0	0	5	0
37	J	78	0	0	26	0
37	K	54	0	0	8	0
37	L	65	0	0	12	0
37	M	79	0	0	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	N	132	0	0	36	0
37	O	69	0	0	23	0
37	P	45	0	0	9	0
37	Q	65	0	0	4	0
37	R	55	0	0	6	0
37	S	83	0	0	11	0
37	T	35	0	0	3	0
37	U	39	0	0	4	0
37	V	25	0	0	8	0
37	W	15	0	0	2	0
37	X	70	0	0	10	0
37	Y	25	0	0	11	0
37	Z	94	0	0	18	0
All	All	98587	0	59582	3325	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 22.

All (3325) 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)
30:4:33:MET:SD	30:4:33:MET:CE	2.03	1.47
5:E:236:THR:HG22	5:E:239:ALA:H	1.09	1.15
1:A:2121:G:OP2	37:A:3494:HOH:O	1.64	1.15
1:A:2122:C:OP2	37:A:6549:HOH:O	1.64	1.15
1:A:1134:G:H4'	10:J:151:MET:HE1	1.28	1.12
14:N:87:MET:HG2	30:4:46:ILE:HG21	1.23	1.10
10:J:86:ARG:NH1	10:J:133:ILE:HG13	1.64	1.09
27:1:46:LYS:HD3	27:1:59:HIS:HB2	1.37	1.07
10:J:165:GLY:HA3	37:J:8386:HOH:O	1.54	1.07
1:A:1160:G:H5'	1:A:1161:A:H5'	1.31	1.06
1:A:871:G:H5'	1:A:871:G:H8	1.15	1.06
10:J:45:GLN:HB3	10:J:163:PRO:HD2	1.32	1.06
14:N:164:THR:HG22	14:N:167:GLY:H	1.14	1.06
21:U:71:VAL:HG11	21:U:90:PRO:HB3	1.38	1.04
6:F:25:MET:HE2	6:F:41:LEU:HG	1.40	1.04
31:A:9001:SPR:H6A3	31:A:9001:SPR:H2B1	1.32	1.03
10:J:86:ARG:HH11	10:J:133:ILE:HG13	0.89	1.02
6:F:134:LEU:HD11	6:F:166:ILE:HD11	1.38	1.02
12:L:10:GLN:NE2	12:L:10:GLN:H	1.58	1.01
23:W:12:THR:HG22	23:W:15:GLU:HG3	1.41	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:871:G:H5'	1:A:871:G:C8	1.95	1.00
27:1:40:PRO:HD3	27:1:47:LEU:HD11	1.42	1.00
4:D:62:ARG:HA	4:D:65:MET:HE3	1.43	1.00
1:A:856:G:H2'	37:A:5401:HOH:O	1.62	1.00
5:E:127:ARG:NH2	5:E:225:PRO:HG2	1.77	0.99
14:N:87:MET:CG	30:4:46:ILE:HG21	1.92	0.99
1:A:2432:C:O4'	37:A:9718:HOH:O	1.80	0.99
5:E:5:ILE:HD11	5:E:16:VAL:HG23	1.39	0.99
1:A:2717:C:H2'	1:A:2718:C:H5''	1.45	0.99
17:Q:115:SER:H	17:Q:118:GLN:HE21	1.00	0.98
24:X:88:THR:HB	37:X:6679:HOH:O	1.63	0.98
10:J:26:LYS:HD2	10:J:28:ILE:HD12	1.41	0.98
12:L:29:LEU:HB3	12:L:55:VAL:HG11	1.41	0.98
12:L:74:VAL:HG11	12:L:113:ILE:HG12	1.46	0.98
1:A:156:C:H5''	14:N:171:ARG:HD3	1.43	0.97
1:A:2123:A:OP2	37:A:5266:HOH:O	1.81	0.97
1:A:962:C:H1'	15:O:5:ARG:NH1	1.79	0.97
14:N:35:PRO:HG2	14:N:38:VAL:HG23	1.46	0.97
2:B:3023:U:H5''	2:B:3024:U:OP2	1.62	0.97
4:D:86:ALA:HA	37:D:8581:HOH:O	1.63	0.97
10:J:162:SER:HB2	10:J:163:PRO:HD3	1.43	0.97
1:A:542:A:H8	1:A:542:A:H5'	1.29	0.97
2:B:3056:A:H2'	2:B:3057:A:H5''	1.47	0.96
1:A:1474:C:H6	1:A:1474:C:H5'	1.31	0.95
14:N:52:LEU:HD11	37:N:8616:HOH:O	1.65	0.94
27:1:42:CYS:SG	27:1:44:PHE:HB2	2.06	0.94
10:J:29:ALA:HB3	10:J:65:ARG:HH12	1.33	0.94
10:J:86:ARG:HH11	10:J:133:ILE:CG1	1.78	0.94
11:K:76:ASP:HA	37:K:8565:HOH:O	1.66	0.94
24:X:122:ARG:HH21	24:X:154:ARG:HD2	1.28	0.94
27:1:39:CYS:SG	27:1:47:LEU:HD21	2.08	0.94
4:D:264:GLU:HG2	4:D:267:LYS:HE2	1.49	0.93
1:A:870:G:H2'	1:A:871:G:H5''	1.46	0.93
4:D:140:LEU:HA	37:D:8581:HOH:O	1.67	0.93
13:M:68:GLU:HA	37:M:8546:HOH:O	1.67	0.93
26:Z:187:VAL:HG23	26:Z:192:ASP:HB2	1.50	0.93
1:A:1667:A:H5'	1:A:1667:A:H8	1.34	0.92
10:J:55:GLN:HE21	10:J:124:ARG:HE	1.15	0.92
2:B:3006:C:H5''	15:O:37:ARG:NH1	1.83	0.92
4:D:41:PHE:CD1	4:D:79:MET:HE2	2.03	0.92
1:A:1751:G:H2'	1:A:1752:G:H5''	1.52	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:Z:200:THR:HG22	26:Z:201:GLU:HG3	1.51	0.92
14:N:87:MET:HG2	30:4:46:ILE:CG2	2.00	0.92
6:F:105:SER:HB2	6:F:131:THR:HG23	1.50	0.92
1:A:1835:U:H5	1:A:1840:A:N7	1.66	0.91
5:E:140:VAL:HB	37:E:8450:HOH:O	1.69	0.91
10:J:2:PRO:HB2	37:J:8354:HOH:O	1.69	0.91
5:E:78:ARG:HG3	5:E:78:ARG:HH11	1.36	0.91
12:L:10:GLN:HE21	12:L:10:GLN:H	1.08	0.91
13:M:67:ARG:O	13:M:71:GLU:HG3	1.71	0.91
20:T:57:THR:HG22	20:T:59:ASP:H	1.36	0.91
37:A:3764:HOH:O	14:N:189:VAL:HG21	1.72	0.90
4:D:238:ASN:HD22	4:D:240:GLY:H	1.19	0.90
1:A:871:G:C5'	1:A:871:G:H8	1.83	0.90
12:L:81:ARG:HB2	12:L:87:ARG:HH11	1.36	0.90
15:O:47:LEU:HD11	15:O:127:LEU:HD21	1.50	0.90
15:O:87:LEU:HD12	15:O:186:LEU:HD21	1.51	0.90
26:Z:216:ARG:HD3	37:Z:8569:HOH:O	1.70	0.90
1:A:541:C:H2'	1:A:542:A:H5''	1.52	0.90
14:N:102:GLU:OE1	14:N:164:THR:HG21	1.72	0.90
30:4:70:ARG:HG2	30:4:77:ALA:HB2	1.53	0.89
22:V:9:CYS:SG	22:V:11:THR:HG23	2.13	0.89
5:E:2:GLN:HB3	37:E:8337:HOH:O	1.71	0.89
19:S:99:ALA:HB1	19:S:109:MET:HE1	1.53	0.89
10:J:27:LYS:H	10:J:58:HIS:HD2	1.19	0.88
15:O:83:LEU:HD13	15:O:175:LEU:HD23	1.54	0.88
1:A:1205:U:H2'	1:A:1206:U:H5'	1.54	0.88
1:A:2426:G:H1'	37:A:6061:HOH:O	1.73	0.88
2:B:3076:G:H3'	2:B:3077:A:H5''	1.56	0.88
19:S:9:ASP:O	19:S:13:THR:HB	1.74	0.88
1:A:2466:G:OP1	37:A:3625:HOH:O	1.90	0.88
7:G:100:ASP:HB2	37:G:2789:HOH:O	1.74	0.88
1:A:2533:C:H5'	1:A:2533:C:H6	1.39	0.87
1:A:962:C:H1'	15:O:5:ARG:HH12	1.38	0.87
15:O:144:GLY:O	15:O:147:ILE:HG22	1.75	0.87
1:A:1120:U:H6	1:A:1120:U:H5''	1.39	0.87
1:A:2506:A:HO2'	1:A:2507:G:H8	0.91	0.87
1:A:2812:A:H2	1:A:2814:A:H62	1.22	0.87
37:A:6265:HOH:O	6:F:99:ASP:HA	1.73	0.87
13:M:79:ASP:HB3	37:M:8559:HOH:O	1.75	0.87
5:E:236:THR:HG21	37:E:8372:HOH:O	1.74	0.87
1:A:1184:C:H1'	37:A:7445:HOH:O	1.74	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Y:37:LEU:HD13	25:Y:85:VAL:HG21	1.56	0.87
1:A:541:C:C2'	1:A:542:A:H5''	2.05	0.86
6:F:154:LYS:H	6:F:154:LYS:HD2	1.39	0.86
37:A:3703:HOH:O	14:N:157:LEU:HD11	1.74	0.86
14:N:35:PRO:CG	14:N:38:VAL:HG23	2.05	0.86
1:A:1886:A:N3	37:A:4796:HOH:O	2.07	0.86
1:A:1242:A:H5'	11:K:82:THR:HG23	1.55	0.86
2:B:3069:U:OP1	15:O:4:PRO:HG3	1.75	0.86
17:Q:115:SER:H	17:Q:118:GLN:NE2	1.74	0.85
1:A:960:G:H4'	37:A:7406:HOH:O	1.77	0.85
10:J:150:LYS:HE2	37:J:8372:HOH:O	1.75	0.85
15:O:7:LYS:HE3	18:R:21:ARG:O	1.75	0.85
1:A:1116:U:HO2'	1:A:1118:A:H2	0.88	0.85
5:E:5:ILE:HD11	5:E:16:VAL:CG2	2.06	0.85
13:M:133:VAL:HA	37:M:8572:HOH:O	1.74	0.85
24:X:88:THR:HG22	24:X:89:ASP:H	1.41	0.85
14:N:69:LYS:O	14:N:73:ARG:NH2	2.10	0.85
19:S:8:ALA:HB1	19:S:13:THR:HG21	1.56	0.85
23:W:1:THR:HG23	23:W:2:VAL:H	1.41	0.85
37:A:4928:HOH:O	2:B:3103:A:H4'	1.75	0.85
10:J:162:SER:HB2	10:J:163:PRO:CD	2.06	0.85
8:H:91:VAL:HG12	8:H:92:GLY:H	1.42	0.84
17:Q:115:SER:OG	17:Q:118:GLN:HG3	1.76	0.84
24:X:122:ARG:NH2	24:X:154:ARG:HD2	1.91	0.84
1:A:1166:A:H1'	1:A:1192:A:C2	2.12	0.84
16:P:7:LEU:HD22	37:P:5650:HOH:O	1.76	0.84
1:A:2468:A:H61	30:4:48:ASN:HD21	1.26	0.84
7:G:166:VAL:HG12	37:G:3134:HOH:O	1.76	0.84
37:A:3661:HOH:O	14:N:79:LYS:HD3	1.77	0.84
30:4:25:VAL:HG22	30:4:68:LYS:HG3	1.58	0.83
6:F:20:LYS:HA	6:F:75:LEU:O	1.78	0.83
7:G:107:PHE:CE2	7:G:108:LEU:HD13	2.13	0.83
8:H:96:ALA:HA	37:H:3111:HOH:O	1.76	0.83
10:J:47:GLU:HB3	10:J:133:ILE:CD1	2.08	0.83
1:A:2586:U:H3	1:A:2592:G:H22	1.26	0.83
3:C:211:LYS:HB3	3:C:212:PRO:HD2	1.59	0.83
26:Z:141:THR:HG23	37:Z:8589:HOH:O	1.78	0.83
4:D:321:PRO:HA	37:D:8659:HOH:O	1.79	0.83
1:A:544:G:H2'	1:A:545:G:H5''	1.60	0.83
2:B:3023:U:C5'	2:B:3024:U:OP2	2.26	0.83
12:L:10:GLN:HE21	12:L:10:GLN:N	1.77	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:X:88:THR:HG23	24:X:110:GLN:NE2	1.95	0.82
19:S:17:MET:SD	37:S:8548:HOH:O	2.37	0.82
15:O:37:ARG:HD3	34:O:8507:CL:CL	2.17	0.82
1:A:2717:C:C2'	1:A:2718:C:H5''	2.10	0.82
10:J:142:VAL:HG13	37:J:8370:HOH:O	1.80	0.82
26:Z:133:HIS:HD2	37:Z:8583:HOH:O	1.63	0.82
10:J:47:GLU:HB3	10:J:133:ILE:HD13	1.61	0.81
10:J:26:LYS:HG2	10:J:28:ILE:H	1.44	0.81
3:C:199:HIS:HD2	3:C:201:PHE:H	1.28	0.81
12:L:74:VAL:HG13	12:L:113:ILE:HG23	1.61	0.81
24:X:122:ARG:HG2	24:X:122:ARG:HH11	1.44	0.81
5:E:104:ASP:HA	5:E:107:ARG:HH12	1.45	0.81
1:A:338:C:H4'	5:E:174:ILE:CD1	2.09	0.81
2:B:3006:C:OP1	15:O:37:ARG:NH1	2.14	0.81
10:J:139:ASP:HA	37:J:8360:HOH:O	1.79	0.81
1:A:1474:C:C6	1:A:1474:C:H5'	2.16	0.81
1:A:1701:A:H5'	37:A:6253:HOH:O	1.81	0.81
22:V:9:CYS:HA	22:V:52:THR:HG23	1.59	0.81
1:A:2716:G:H5''	4:D:206:THR:HG21	1.63	0.81
30:4:74:CYS:SG	30:4:76:LYS:HB2	2.21	0.81
12:L:14:LYS:HB2	12:L:45:PRO:HG2	1.61	0.81
37:A:6840:HOH:O	14:N:178:LYS:HB2	1.81	0.81
1:A:1120:U:C6	1:A:1120:U:H5''	2.16	0.80
26:Z:187:VAL:HG23	26:Z:192:ASP:CB	2.11	0.80
1:A:2467:A:OP1	37:A:9038:HOH:O	1.98	0.80
27:1:38:LYS:HG2	27:1:45:LYS:HG2	1.61	0.80
1:A:1735:C:O2'	1:A:1736:A:H5'	1.81	0.80
1:A:1372:A:H3'	37:A:7165:HOH:O	1.81	0.80
10:J:139:ASP:N	10:J:140:PRO:HD3	1.97	0.80
4:D:212:GLN:HB2	4:D:257:THR:HG21	1.64	0.80
5:E:236:THR:HG22	5:E:239:ALA:N	1.93	0.80
14:N:164:THR:HG23	14:N:165:SER:N	1.94	0.80
25:Y:78:GLU:HG2	25:Y:79:GLU:H	1.47	0.80
5:E:115:LEU:HD13	5:E:223:LEU:HD21	1.63	0.80
7:G:97:VAL:HG12	37:G:4191:HOH:O	1.80	0.80
25:Y:71:ARG:HB3	25:Y:88:GLU:OE1	1.81	0.80
1:A:288:A:H61	1:A:364:C:H42	1.29	0.80
14:N:164:THR:HG22	14:N:167:GLY:N	1.96	0.80
25:Y:25:ARG:HD2	37:Y:3861:HOH:O	1.80	0.80
4:D:201:ASP:HB2	4:D:312:ARG:HD2	1.65	0.79
1:A:1603:A:H5'	1:A:1605:G:O4'	1.81	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1209:C:H4'	37:A:5257:HOH:O	1.83	0.79
7:G:15:GLN:HG3	7:G:20:ILE:HG12	1.63	0.79
15:O:4:PRO:HD2	37:O:8558:HOH:O	1.80	0.79
1:A:1118:A:H3'	1:A:1118:A:H8	1.47	0.79
1:A:2064:U:H4'	1:A:2653:A:OP1	1.83	0.79
27:1:30:GLU:HA	27:1:33:HIS:HB3	1.64	0.79
1:A:1835:U:C5	1:A:1840:A:N7	2.51	0.79
10:J:163:PRO:HG2	37:J:8325:HOH:O	1.81	0.79
1:A:1116:U:H3	1:A:1246:A:H62	1.31	0.79
1:A:2420:G:O2'	1:A:2421:G:H5'	1.81	0.79
1:A:272:A:H3'	37:A:7510:HOH:O	1.82	0.79
24:X:4:LEU:HD22	24:X:52:VAL:HG21	1.63	0.79
1:A:1119:G:H2'	11:K:52:GLN:NE2	1.97	0.78
1:A:282:C:H1'	1:A:368:C:N4	1.98	0.78
2:B:3014:G:H8	2:B:3014:G:H5'	1.49	0.78
34:K:8501:CL:CL	37:K:8548:HOH:O	2.38	0.78
1:A:1118:A:C8	1:A:1118:A:H3'	2.18	0.78
1:A:1116:U:O2'	1:A:1118:A:H2	1.67	0.78
27:1:39:CYS:HA	27:1:47:LEU:HD11	1.66	0.78
13:M:53:ARG:NH2	13:M:57:VAL:HG12	1.98	0.78
19:S:106:GLY:HA2	19:S:109:MET:HE3	1.65	0.78
27:1:23:ARG:NH1	37:1:8404:HOH:O	2.17	0.78
37:A:7536:HOH:O	30:4:60:LYS:HG3	1.83	0.78
29:3:39:ARG:HG2	37:3:3143:HOH:O	1.82	0.78
3:C:223:ARG:HG3	37:C:8606:HOH:O	1.84	0.78
24:X:88:THR:HG23	24:X:110:GLN:HE21	1.48	0.78
1:A:545:G:H5'	1:A:545:G:H8	1.49	0.77
1:A:711:G:H1'	37:A:7067:HOH:O	1.82	0.77
15:O:49:THR:HG22	15:O:56:ASP:HB2	1.67	0.77
22:V:35:LYS:NZ	37:V:6621:HOH:O	2.17	0.77
1:A:111:C:O2'	28:2:20:ARG:HG2	1.84	0.77
1:A:1165:G:H4'	1:A:1174:A:O2'	1.84	0.77
24:X:6:GLN:HB2	24:X:26:ILE:HD12	1.67	0.77
1:A:2004:U:H4'	37:A:5284:HOH:O	1.82	0.77
6:F:64:ARG:HG2	6:F:67:ASP:HB3	1.66	0.77
10:J:136:VAL:HG23	37:J:8330:HOH:O	1.84	0.77
1:A:559:U:H6	1:A:559:U:H5'	1.49	0.77
37:A:4837:HOH:O	14:N:14:ARG:HG2	1.83	0.77
1:A:645:U:OP2	13:M:4:LYS:HE2	1.85	0.77
1:A:2508:C:H2'	37:A:6723:HOH:O	1.85	0.77
10:J:33:MET:HB2	10:J:83:PHE:HB3	1.67	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:74:ARG:HB3	11:K:74:ARG:HH11	1.49	0.77
15:O:48:VAL:CG1	15:O:55:ASP:HB3	2.14	0.77
3:C:199:HIS:CD2	3:C:201:PHE:H	2.02	0.77
24:X:4:LEU:HD22	24:X:52:VAL:CG2	2.14	0.77
13:M:53:ARG:HH22	13:M:57:VAL:HG12	1.49	0.76
1:A:1187:U:H2'	37:A:6864:HOH:O	1.85	0.76
1:A:542:A:H5'	1:A:542:A:C8	2.19	0.76
14:N:64:ARG:HD2	37:N:8586:HOH:O	1.84	0.76
1:A:1450:C:H4'	1:A:1451:C:OP2	1.86	0.76
1:A:870:G:C2'	1:A:871:G:H5''	2.15	0.76
15:O:86:LEU:HD12	15:O:125:ALA:HB2	1.66	0.76
1:A:797:A:C4'	27:1:10:ARG:N	2.48	0.76
29:3:41:HIS:H	29:3:45:ASN:HD22	1.30	0.76
1:A:289:G:H22	1:A:363:A:H2	1.33	0.76
2:B:3039:U:H1'	2:B:3044:A:H61	1.51	0.76
2:B:3056:A:C2'	2:B:3057:A:H5''	2.15	0.76
3:C:164:ARG:HB2	27:1:68:CYS:SG	2.24	0.76
8:H:91:VAL:HG12	8:H:92:GLY:N	1.99	0.76
14:N:84:LYS:HE2	37:N:8577:HOH:O	1.85	0.76
27:1:38:LYS:HE2	27:1:45:LYS:HE2	1.67	0.76
1:A:1160:G:C5'	1:A:1161:A:H5'	2.11	0.76
1:A:797:A:H4'	27:1:10:ARG:N	2.01	0.76
28:2:21:ARG:HD2	28:2:37:CYS:SG	2.26	0.76
10:J:55:GLN:NE2	10:J:124:ARG:HE	1.84	0.76
1:A:1666:C:O2'	1:A:1667:A:H5''	1.86	0.76
10:J:137:ASN:O	10:J:139:ASP:N	2.19	0.76
21:U:61:GLU:HG3	37:U:3851:HOH:O	1.85	0.76
26:Z:220:GLU:HG2	37:Z:8550:HOH:O	1.85	0.76
9:I:12:ILE:N	9:I:13:PRO:HD3	2.01	0.76
19:S:99:ALA:HB1	19:S:109:MET:CE	2.16	0.76
25:Y:25:ARG:NH1	37:Y:3861:HOH:O	2.19	0.76
1:A:541:C:H2'	1:A:542:A:C5'	2.15	0.75
1:A:1684:A:H1'	29:3:43:ARG:HH22	1.49	0.75
10:J:14:TYR:H	10:J:91:HIS:CE1	2.04	0.75
14:N:87:MET:CB	30:4:46:ILE:HG21	2.16	0.75
14:N:61:ILE:HG13	37:N:8623:HOH:O	1.85	0.75
25:Y:76:ARG:HH11	25:Y:76:ARG:HG3	1.50	0.75
1:A:236:A:H4'	1:A:237:G:H5'	1.69	0.75
1:A:450:C:OP1	5:E:184:ARG:NH2	2.16	0.75
1:A:506:G:H22	1:A:509:A:C5'	1.98	0.75
6:F:27:ILE:HG22	6:F:28:GLY:H	1.51	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2363:G:O3'	18:R:11:ARG:NH1	2.19	0.75
17:Q:143:ALA:HA	37:Q:2178:HOH:O	1.87	0.75
9:I:23:ILE:HD13	9:I:67:LEU:HD23	1.67	0.75
1:A:2506:A:O2'	1:A:2507:G:H8	1.68	0.75
5:E:162:VAL:HG12	5:E:192:ILE:HD11	1.68	0.75
37:A:4432:HOH:O	14:N:146:GLN:HG2	1.86	0.75
4:D:62:ARG:CA	4:D:65:MET:HE3	2.16	0.74
1:A:1594:C:OP2	17:Q:120:ARG:HD2	1.85	0.74
3:C:88:ILE:HD13	3:C:100:PRO:HD3	1.70	0.74
6:F:135:VAL:HG22	6:F:136:ARG:H	1.51	0.74
3:C:35:GLY:O	3:C:36:ASP:HB3	1.86	0.74
16:P:32:ARG:O	16:P:32:ARG:HD3	1.85	0.74
21:U:32:ARG:NH1	21:U:38:ARG:HH12	1.85	0.74
27:I:49:ARG:HD2	37:I:8431:HOH:O	1.87	0.74
1:A:346:U:H4'	37:A:6811:HOH:O	1.87	0.74
5:E:76:ARG:HD2	37:E:8432:HOH:O	1.87	0.74
10:J:41:THR:HA	37:J:8384:HOH:O	1.87	0.74
1:A:1160:G:H5'	1:A:1161:A:C5'	2.15	0.74
1:A:1701:A:H4'	1:A:1702:U:H5''	1.68	0.74
1:A:2466:G:H5''	37:A:3625:HOH:O	1.87	0.74
5:E:178:GLN:OE1	37:E:8465:HOH:O	2.04	0.74
26:Z:185:VAL:HA	37:Z:8564:HOH:O	1.86	0.74
1:A:21:G:H5'	19:S:2:ILE:HA	1.70	0.74
37:A:9110:HOH:O	14:N:82:ARG:HD2	1.88	0.74
15:O:71:TRP:CE3	15:O:175:LEU:HD22	2.23	0.74
1:A:1329:A:H2	37:A:4655:HOH:O	1.69	0.74
10:J:26:LYS:HD2	10:J:28:ILE:CD1	2.15	0.74
13:M:143:THR:HG22	13:M:144:ASP:N	2.02	0.74
1:A:1058:A:H2'	1:A:1060:C:H5''	1.68	0.74
4:D:221:GLN:HE22	12:L:42:ASN:HD22	1.36	0.74
12:L:22:ASP:HB2	37:L:5264:HOH:O	1.88	0.74
14:N:48:ARG:NH2	37:N:8563:HOH:O	2.21	0.74
22:V:13:ILE:HG12	22:V:32:CYS:CB	2.17	0.73
5:E:78:ARG:HG3	5:E:78:ARG:NH1	2.03	0.73
14:N:172:GLY:O	14:N:183:VAL:HG11	1.89	0.73
1:A:2100:A:N1	31:A:9001:SPR:H2A	2.03	0.73
11:K:99:GLU:HA	37:K:8573:HOH:O	1.88	0.73
20:T:51:GLN:HE21	20:T:53:ASN:HD21	1.35	0.73
17:Q:115:SER:N	17:Q:118:GLN:HE21	1.83	0.73
1:A:1130:U:H2'	1:A:1131:G:O4'	1.89	0.73
2:B:3029:C:H2'	2:B:3030:C:H5'	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:59:ASN:HD22	10:J:59:ASN:N	1.87	0.73
19:S:39:THR:HG22	19:S:42:GLU:H	1.54	0.73
25:Y:15:ARG:HH11	25:Y:15:ARG:HB3	1.54	0.73
5:E:132:ASP:HB3	37:E:8361:HOH:O	1.88	0.73
7:G:11:VAL:HG12	7:G:12:ASP:N	2.04	0.73
9:I:12:ILE:HA	37:I:4499:HOH:O	1.89	0.73
17:Q:80:ARG:HG2	17:Q:87:ARG:CZ	2.19	0.73
24:X:130:HIS:O	24:X:136:GLY:HA3	1.89	0.73
1:A:2271:G:OP2	37:A:9415:HOH:O	2.07	0.73
4:D:62:ARG:HA	4:D:65:MET:CE	2.17	0.72
24:X:137:GLN:HE21	24:X:141:HIS:HE1	1.34	0.72
1:A:1667:A:H5'	1:A:1667:A:C8	2.21	0.72
1:A:172:U:OP2	37:A:6180:HOH:O	2.06	0.72
1:A:1743:G:N7	37:A:9244:HOH:O	2.21	0.72
27:1:11:THR:CG2	27:1:23:ARG:HB2	2.19	0.72
7:G:20:ILE:HD11	7:G:40:VAL:HG11	1.71	0.72
1:A:31:C:H4'	37:A:7400:HOH:O	1.89	0.72
14:N:52:LEU:HD13	14:N:116:ASN:HB3	1.71	0.72
5:E:214:THR:HG21	37:E:8399:HOH:O	1.87	0.72
10:J:130:HIS:CD2	10:J:133:ILE:HD11	2.24	0.72
11:K:133:GLY:O	11:K:137:GLU:HG3	1.90	0.72
14:N:35:PRO:O	37:N:8539:HOH:O	2.06	0.72
19:S:132:ARG:NH2	37:S:8582:HOH:O	2.22	0.72
22:V:46:ALA:HB1	22:V:52:THR:HG21	1.71	0.72
1:A:1834:C:H2'	1:A:1840:A:N6	2.04	0.72
13:M:136:ALA:HB3	37:M:8572:HOH:O	1.89	0.72
25:Y:31:ILE:O	25:Y:35:GLU:HG3	1.90	0.72
1:A:1118:A:H62	1:A:1244:U:H3	1.37	0.72
12:L:39:GLY:HA2	37:L:4183:HOH:O	1.89	0.72
14:N:87:MET:HB2	14:N:91:ILE:HD11	1.71	0.72
20:T:57:THR:HG22	20:T:59:ASP:N	2.05	0.72
1:A:1353:C:P	37:A:4650:HOH:O	2.48	0.72
6:F:88:LEU:HB2	6:F:89:PRO:HD3	1.72	0.72
23:W:42:ASN:HB3	37:W:7247:HOH:O	1.90	0.72
24:X:21:LEU:HD22	24:X:26:ILE:HD11	1.71	0.72
26:Z:212:ARG:HD2	37:Z:8600:HOH:O	1.89	0.72
1:A:1164:U:H3	1:A:1192:A:H2	1.35	0.72
8:H:63:ILE:HB	8:H:64:PRO:HD3	1.71	0.72
1:A:506:G:H22	1:A:509:A:H5'	1.53	0.71
3:C:76:VAL:HG23	27:1:63:LYS:HB3	1.72	0.71
1:A:560:C:H42	1:A:597:A:H61	1.38	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:284:C:H4'	1:A:285:A:O5'	1.89	0.71
4:D:7:ARG:NH1	4:D:11:LEU:CD2	2.53	0.71
25:Y:18:ARG:NH1	37:Y:4132:HOH:O	2.13	0.71
1:A:2301:A:H5''	1:A:2302:A:H5'	1.71	0.71
1:A:2467:A:H2'	37:A:5431:HOH:O	1.90	0.71
15:O:113:SER:HB2	37:O:8560:HOH:O	1.89	0.71
2:B:3013:A:O2'	2:B:3014:G:H5''	1.90	0.71
2:B:3020:G:O2'	2:B:3021:G:H5'	1.91	0.71
1:A:1003:U:HO2'	10:J:90:PHE:HE1	1.36	0.71
14:N:152:ARG:HG3	37:N:8557:HOH:O	1.91	0.71
1:A:2421:G:H3'	1:A:2422:U:H5''	1.71	0.71
18:R:25:PRO:HB2	37:R:4350:HOH:O	1.91	0.71
1:A:1771:U:H4'	27:1:20:LEU:HD21	1.71	0.71
1:A:1918:U:OP2	37:A:3997:HOH:O	2.07	0.71
1:A:214:U:H5'	37:A:6109:HOH:O	1.91	0.71
26:Z:186:ARG:HH11	26:Z:186:ARG:HG2	1.56	0.71
27:1:10:ARG:HA	37:1:8416:HOH:O	1.89	0.71
27:1:42:CYS:SG	27:1:44:PHE:N	2.59	0.71
1:A:1209:C:H2'	1:A:1210:G:H8	1.55	0.71
10:J:59:ASN:HD22	10:J:59:ASN:H	1.38	0.71
10:J:56:ILE:HG22	10:J:61:LEU:HD22	1.72	0.71
11:K:131:THR:HG22	11:K:134:GLU:H	1.53	0.71
11:K:19:MET:HE3	11:K:132:LEU:HD11	1.73	0.71
24:X:13:MET:HE3	24:X:17:ILE:HG22	1.73	0.71
1:A:338:C:H4'	5:E:174:ILE:HD11	1.71	0.71
3:C:69:LEU:HD21	3:C:120:ARG:HB3	1.72	0.70
5:E:104:ASP:HA	5:E:107:ARG:NH1	2.06	0.70
12:L:55:VAL:HG12	12:L:56:SER:N	2.06	0.70
4:D:18:ARG:HG3	4:D:256:GLN:HG3	1.72	0.70
18:R:23:THR:HA	37:R:4792:HOH:O	1.91	0.70
1:A:1019:C:OP1	37:A:3922:HOH:O	2.08	0.70
1:A:1119:G:H2'	11:K:52:GLN:HE22	1.54	0.70
3:C:88:ILE:O	3:C:88:ILE:HG22	1.90	0.70
1:A:2119:C:O2'	1:A:2120:U:H5'	1.91	0.70
2:B:3006:C:H5''	15:O:37:ARG:HH12	1.54	0.70
3:C:100:PRO:HG2	3:C:103:VAL:HG21	1.73	0.70
4:D:41:PHE:CD2	4:D:190:MET:HE3	2.25	0.70
5:E:85:LYS:NZ	37:E:8328:HOH:O	2.13	0.70
6:F:23:VAL:HG23	6:F:23:VAL:O	1.91	0.70
1:A:2276:U:H2'	1:A:2277:U:C6	2.26	0.70
1:A:2638:G:H1'	37:A:7742:HOH:O	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2768:A:H2'	1:A:2769:C:O4'	1.90	0.70
5:E:39:GLN:O	5:E:43:LYS:HD3	1.92	0.70
23:W:39:ALA:N	23:W:40:PRO:HD2	2.07	0.70
27:1:37:HIS:HB2	27:1:47:LEU:HB2	1.72	0.70
8:H:50:VAL:HG21	8:H:63:ILE:HG21	1.72	0.70
1:A:544:G:C2'	1:A:545:G:H5''	2.21	0.70
32:A:8054:MG:MG	37:A:7819:HOH:O	1.33	0.70
2:B:3048:C:H4'	15:O:141:ARG:HH21	1.57	0.70
3:C:53:ALA:HB3	37:C:8610:HOH:O	1.91	0.70
12:L:74:VAL:CG1	12:L:113:ILE:HG12	2.20	0.70
18:R:24:SER:O	37:R:2847:HOH:O	2.10	0.70
1:A:877:G:H5'	1:A:878:G:OP1	1.92	0.70
3:C:121:ALA:O	3:C:124:VAL:HG22	1.90	0.70
4:D:179:LEU:O	4:D:183:GLU:HG2	1.92	0.70
8:H:2:VAL:HG22	8:H:57:GLU:OE1	1.92	0.70
15:O:183:ASP:OD2	15:O:186:LEU:HD12	1.91	0.70
19:S:132:ARG:CZ	37:S:8582:HOH:O	2.40	0.70
26:Z:187:VAL:CG2	26:Z:192:ASP:HB2	2.22	0.70
1:A:1191:A:H3'	1:A:1192:A:H5''	1.72	0.69
1:A:2827:A:H2'	1:A:2828:G:O4'	1.91	0.69
6:F:19:GLU:O	6:F:20:LYS:HG2	1.92	0.69
14:N:89:ASN:HA	37:N:8554:HOH:O	1.91	0.69
27:1:30:GLU:HA	27:1:33:HIS:CB	2.22	0.69
1:A:1406:A:N1	37:A:6004:HOH:O	2.25	0.69
1:A:1810:C:OP1	22:V:44:ARG:NE	2.16	0.69
1:A:603:A:H5''	1:A:604:G:OP1	1.92	0.69
3:C:36:ASP:OD2	3:C:85:ASP:HB2	1.91	0.69
1:A:1080:C:H4'	1:A:1081:A:OP1	1.91	0.69
4:D:145:HIS:HD2	4:D:146:THR:O	1.76	0.69
9:I:63:ARG:N	37:I:2569:HOH:O	2.25	0.69
15:O:159:TYR:HB3	15:O:162:ASP:HB2	1.75	0.69
24:X:154:ARG:C	37:X:4276:HOH:O	2.30	0.69
25:Y:72:VAL:HG22	25:Y:85:VAL:HG12	1.75	0.69
5:E:115:LEU:O	5:E:118:THR:HB	1.90	0.69
8:H:99:THR:HA	37:H:3461:HOH:O	1.93	0.69
14:N:59:GLY:HA3	14:N:141:ILE:CD1	2.22	0.69
10:J:57:ARG:HG3	37:J:8341:HOH:O	1.92	0.69
12:L:62:PRO:HG3	12:L:65:ARG:HH21	1.57	0.69
1:A:134:U:C2	1:A:145:A:C2	2.81	0.69
6:F:64:ARG:CG	6:F:67:ASP:HB3	2.22	0.69
7:G:81:GLU:HG2	7:G:134:SER:HB3	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:71:TYR:C	10:J:73:GLN:H	1.96	0.69
23:W:12:THR:HG22	23:W:15:GLU:CG	2.22	0.69
1:A:821:U:H2'	1:A:822:C:H6	1.58	0.69
11:K:45:VAL:HG23	11:K:130:VAL:O	1.93	0.69
1:A:31:C:H2'	37:A:7669:HOH:O	1.92	0.69
4:D:85:ARG:NH1	37:D:8637:HOH:O	2.26	0.69
19:S:18:LEU:HD12	19:S:143:VAL:HG11	1.75	0.69
1:A:1625:U:H4'	37:A:4637:HOH:O	1.90	0.68
1:A:2291:A:C8	1:A:2309:C:H5'	2.28	0.68
6:F:55:LYS:HA	37:F:6752:HOH:O	1.93	0.68
11:K:107:ASN:ND2	11:K:109:TYR:H	1.91	0.68
16:P:47:ARG:HH11	16:P:47:ARG:HG3	1.57	0.68
5:E:1:MET:HG2	5:E:2:GLN:H	1.57	0.68
22:V:9:CYS:CA	22:V:52:THR:HG23	2.22	0.68
1:A:1119:G:H22	1:A:1246:A:H2	1.39	0.68
1:A:281:U:H2'	1:A:282:C:O4'	1.93	0.68
1:A:516:A:OP2	37:A:5618:HOH:O	2.12	0.68
14:N:60:ILE:C	14:N:61:ILE:HD12	2.14	0.68
6:F:69:ILE:O	6:F:69:ILE:HG22	1.92	0.68
11:K:75:PRO:HG2	11:K:105:LEU:HD21	1.73	0.68
12:L:81:ARG:HB2	12:L:87:ARG:NH1	2.05	0.68
1:A:2434:A:O3'	30:4:28:GLY:HA3	1.92	0.68
3:C:101:GLU:OE2	3:C:131:HIS:HB2	1.94	0.68
4:D:138:GLY:O	4:D:139:ASP:O	2.11	0.68
6:F:38:GLU:HB3	6:F:49:PRO:HG2	1.75	0.68
10:J:162:SER:CB	10:J:163:PRO:HD3	2.22	0.68
17:Q:59:ARG:NH2	17:Q:66:GLN:HE22	1.91	0.68
1:A:1086:A:N6	24:X:11:VAL:HG11	2.08	0.68
1:A:2748:G:H2'	37:A:7521:HOH:O	1.94	0.68
1:A:2862:G:H4'	4:D:336:GLN:O	1.93	0.68
14:N:113:ARG:NH2	14:N:156:ARG:HG2	2.09	0.68
37:A:4639:HOH:O	20:T:23:LYS:HE2	1.94	0.68
27:1:18:TYR:HB3	27:1:22:ILE:HG21	1.76	0.68
1:A:1185:U:H2'	1:A:1186:C:C6	2.29	0.68
1:A:2054:A:N3	19:S:128:ARG:NH2	2.42	0.68
4:D:42:ALA:HB1	4:D:308:LEU:HD11	1.75	0.68
30:4:65:THR:HG23	30:4:67:LEU:HG	1.75	0.68
1:A:1422:U:H2'	1:A:1423:C:C6	2.28	0.68
1:A:2533:C:H5'	1:A:2533:C:C6	2.26	0.68
1:A:1151:G:OP1	9:I:16:LYS:NZ	2.25	0.68
1:A:20:G:H21	19:S:117:HIS:HD2	1.41	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:115:ARG:HG3	12:L:116:GLU:N	2.09	0.68
24:X:88:THR:HG22	24:X:89:ASP:N	2.09	0.68
26:Z:189:ASN:ND2	26:Z:192:ASP:H	1.92	0.68
1:A:677:C:H4'	5:E:246:ARG:NH2	2.09	0.67
2:B:3006:C:C5'	15:O:37:ARG:NH1	2.56	0.67
15:O:61:ALA:HB3	15:O:88:ALA:HB2	1.76	0.67
1:A:1170:U:O2'	1:A:1172:G:N7	2.23	0.67
1:A:1666:C:H2'	1:A:1667:A:H5'	1.74	0.67
11:K:107:ASN:HD21	11:K:109:TYR:HB2	1.59	0.67
37:A:3737:HOH:O	21:U:9:LYS:CD	2.42	0.67
1:A:1041:U:H2'	1:A:1042:U:H5'	1.76	0.67
27:1:34:LYS:HE2	37:1:8428:HOH:O	1.94	0.67
1:A:1187:U:HO2'	1:A:1189:A:H2	1.41	0.67
34:A:8514:CL:CL	37:A:7720:HOH:O	2.50	0.67
3:C:190:ARG:NH2	3:C:207:GLN:OE1	2.26	0.67
12:L:62:PRO:HG3	12:L:65:ARG:NH2	2.09	0.67
19:S:29:LYS:HB3	37:S:8532:HOH:O	1.93	0.67
24:X:65:VAL:HA	24:X:68:THR:HG22	1.76	0.67
1:A:1459:A:OP2	37:A:9224:HOH:O	2.12	0.67
37:A:6996:HOH:O	3:C:211:LYS:HG2	1.94	0.67
4:D:7:ARG:NH1	4:D:11:LEU:HD22	2.10	0.67
10:J:84:ARG:NH2	10:J:135:TRP:HH2	1.92	0.67
11:K:75:PRO:HG2	11:K:105:LEU:CD2	2.24	0.67
15:O:169:PRO:O	15:O:172:PHE:HB3	1.94	0.67
21:U:52:ARG:HB2	21:U:95:ASN:HB3	1.77	0.67
6:F:105:SER:CB	6:F:131:THR:HG23	2.24	0.67
10:J:28:ILE:HA	10:J:62:GLU:OE1	1.95	0.67
14:N:173:LEU:HD23	14:N:183:VAL:HG12	1.77	0.67
15:O:89:GLY:O	15:O:92:ALA:HB3	1.95	0.67
37:A:3737:HOH:O	21:U:9:LYS:HD2	1.92	0.67
3:C:135:VAL:HG21	3:C:147:ARG:NH1	2.09	0.67
12:L:81:ARG:HD3	12:L:87:ARG:NH1	2.10	0.67
23:W:4:HIS:HB3	37:W:6622:HOH:O	1.95	0.67
10:J:127:GLY:O	10:J:128:ALA:HB3	1.92	0.67
10:J:46:VAL:HG12	10:J:146:TRP:HZ3	1.59	0.67
11:K:74:ARG:O	11:K:78:ILE:HG12	1.95	0.67
28:2:10:LYS:HG3	37:2:8432:HOH:O	1.93	0.67
1:A:871:G:C5'	1:A:871:G:C8	2.67	0.67
3:C:2:ARG:NH1	37:C:8515:HOH:O	2.08	0.67
1:A:2780:C:H1'	7:G:143:GLN:HE21	1.59	0.67
1:A:447:A:OP1	21:U:2:LYS:HG2	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:A:7400:HOH:O	21:U:9:LYS:HB2	1.94	0.67
27:1:47:LEU:HD23	27:1:57:CYS:HB2	1.76	0.67
4:D:162:MET:CE	4:D:308:LEU:HD21	2.23	0.67
5:E:139:VAL:HG13	37:E:8447:HOH:O	1.94	0.67
1:A:2346:C:O2'	6:F:52:THR:HG21	1.95	0.67
14:N:164:THR:CG2	14:N:165:SER:N	2.57	0.67
1:A:1244:U:OP1	11:K:18:ILE:HD13	1.95	0.66
1:A:1751:G:C2'	1:A:1752:G:H5''	2.25	0.66
4:D:51:VAL:CG2	4:D:327:VAL:HG13	2.25	0.66
1:A:2548:C:OP2	4:D:5:ARG:NH2	2.28	0.66
10:J:5:MET:HG3	37:J:8354:HOH:O	1.94	0.66
13:M:53:ARG:NH2	13:M:57:VAL:CG1	2.58	0.66
21:U:47:THR:HB	21:U:100:ASP:HB3	1.75	0.66
1:A:1160:G:N3	37:A:5605:HOH:O	2.28	0.66
14:N:139:PRO:O	14:N:140:ALA:HB3	1.93	0.66
15:O:107:ASN:OD1	34:O:8507:CL:CL	2.50	0.66
27:1:46:LYS:HB2	27:1:57:CYS:SG	2.34	0.66
2:B:3026:C:OP2	37:B:3472:HOH:O	2.13	0.66
4:D:162:MET:HE3	4:D:308:LEU:HD21	1.76	0.66
11:K:103:VAL:HG12	37:K:8565:HOH:O	1.96	0.66
14:N:87:MET:HB3	30:4:46:ILE:HD13	1.77	0.66
1:A:154:C:H2'	1:A:155:C:H6	1.60	0.66
1:A:157:G:H4'	14:N:95:LYS:HE3	1.78	0.66
1:A:2000:G:O2'	1:A:2001:G:H5'	1.96	0.66
1:A:2578:G:H5'	1:A:2578:G:H8	1.60	0.66
14:N:74:ARG:NH2	37:N:8631:HOH:O	2.27	0.66
17:Q:105:LEU:HD21	17:Q:137:LEU:HD21	1.77	0.66
1:A:2710:U:H1'	37:A:7602:HOH:O	1.96	0.66
2:B:3049:G:H5''	37:B:4707:HOH:O	1.94	0.66
1:A:2890:A:H1'	22:V:56:ARG:NH2	2.11	0.66
8:H:50:VAL:HG13	8:H:60:VAL:HG11	1.77	0.66
10:J:27:LYS:N	10:J:58:HIS:HD2	1.91	0.66
19:S:132:ARG:HG2	19:S:133:ALA:N	2.10	0.66
4:D:329:TYR:CE2	22:V:15:PRO:HG2	2.30	0.66
1:A:400:C:O3'	37:A:5766:HOH:O	2.13	0.66
2:B:3001:U:O3'	2:B:3003:A:H5''	1.96	0.66
2:B:3039:U:H1'	2:B:3044:A:N6	2.09	0.66
11:K:93:ARG:HH11	11:K:93:ARG:HB3	1.58	0.66
1:A:553:G:P	26:Z:204:ARG:HH22	2.19	0.66
1:A:739:G:C5	37:A:7523:HOH:O	2.49	0.66
5:E:12:THR:HB	37:E:8440:HOH:O	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:141:ASN:HA	37:J:8356:HOH:O	1.94	0.66
3:C:94:LEU:N	3:C:94:LEU:HD23	2.10	0.66
1:A:396:U:H4'	37:A:4403:HOH:O	1.96	0.66
6:F:97:GLN:O	6:F:97:GLN:HG2	1.95	0.66
10:J:140:PRO:HB3	37:J:8370:HOH:O	1.95	0.66
29:3:22:PRO:HG2	29:3:25:VAL:HG23	1.78	0.65
24:X:68:THR:HG23	24:X:69:ARG:HG2	1.77	0.65
1:A:1909:A:N1	1:A:2128:G:H1'	2.11	0.65
6:F:25:MET:HE1	6:F:37:ALA:HB1	1.77	0.65
9:I:12:ILE:N	9:I:13:PRO:CD	2.60	0.65
26:Z:155:ARG:NH1	37:Z:8558:HOH:O	2.27	0.65
28:2:25:LYS:O	28:2:25:LYS:HG2	1.96	0.65
1:A:2472:C:O2'	1:A:2634:G:H4'	1.96	0.65
32:A:8034:MG:MG	37:A:4868:HOH:O	1.37	0.65
25:Y:41:PHE:O	25:Y:43:VAL:HG23	1.96	0.65
1:A:2036:C:OP1	37:A:6671:HOH:O	2.14	0.65
5:E:129:HIS:CE1	5:E:231:ARG:HA	2.31	0.65
23:W:64:GLY:O	23:W:65:ASP:HB2	1.96	0.65
2:B:3003:A:H2'	37:B:2430:HOH:O	1.95	0.65
2:B:3023:U:C4'	2:B:3024:U:OP2	2.41	0.65
6:F:174:VAL:HG13	37:F:6555:HOH:O	1.96	0.65
21:U:37:GLN:OE1	21:U:118:SER:HA	1.95	0.65
25:Y:25:ARG:CZ	37:Y:3861:HOH:O	2.42	0.65
1:A:1634:G:H3'	37:A:3869:HOH:O	1.96	0.65
6:F:44:ILE:HG23	6:F:45:THR:HG23	1.79	0.65
1:A:282:C:H1'	1:A:368:C:H42	1.60	0.65
6:F:23:VAL:HG22	6:F:73:VAL:HB	1.78	0.65
1:A:188:C:H5''	14:N:163:LEU:HD21	1.77	0.65
37:A:3754:HOH:O	22:V:17:THR:CG2	2.44	0.65
30:4:69:TYR:HB2	30:4:78:HIS:CE1	2.32	0.65
1:A:2320:U:H4'	1:A:2321:A:O4'	1.96	0.65
2:B:3014:G:H5'	2:B:3014:G:C8	2.30	0.65
6:F:95:THR:O	6:F:97:GLN:N	2.27	0.65
24:X:141:HIS:HB2	24:X:146:ILE:HG12	1.77	0.65
1:A:1477:C:O2'	1:A:1478:U:H5'	1.96	0.65
1:A:2769:C:H2'	1:A:2770:G:O4'	1.97	0.65
1:A:2908:A:H2'	1:A:2909:G:O4'	1.96	0.65
4:D:36:PRO:HA	4:D:168:GLY:HA3	1.79	0.65
24:X:110:GLN:HA	24:X:110:GLN:NE2	2.12	0.65
26:Z:200:THR:HG22	26:Z:201:GLU:CG	2.26	0.65
1:A:1741:U:H5'	1:A:1742:A:OP1	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1878:G:H1'	37:A:6090:HOH:O	1.97	0.65
2:B:3028:U:H2'	2:B:3029:C:C6	2.32	0.65
6:F:135:VAL:HG22	6:F:136:ARG:N	2.11	0.65
6:F:140:ARG:O	6:F:144:ARG:HG2	1.96	0.65
13:M:148:GLU:HA	37:M:8571:HOH:O	1.96	0.65
1:A:338:C:H5''	37:E:8419:HOH:O	1.97	0.64
3:C:33:GLU:O	3:C:34:ASP:HB2	1.96	0.64
5:E:236:THR:H	5:E:239:ALA:HB3	1.62	0.64
14:N:138:HIS:ND1	14:N:139:PRO:O	2.23	0.64
1:A:2323:G:H5'	37:A:6990:HOH:O	1.98	0.64
1:A:485:A:N3	1:A:487:G:H5''	2.12	0.64
4:D:238:ASN:HD22	4:D:240:GLY:N	1.95	0.64
8:H:110:GLU:HG2	37:H:6926:HOH:O	1.96	0.64
11:K:46:ILE:HA	37:K:8528:HOH:O	1.97	0.64
13:M:143:THR:HG22	13:M:145:LEU:H	1.60	0.64
15:O:163:PHE:HA	37:O:8519:HOH:O	1.96	0.64
5:E:103:ASN:HB3	37:E:8309:HOH:O	1.97	0.64
6:F:54:ALA:HB2	6:F:69:ILE:HD12	1.79	0.64
1:A:539:G:H2'	1:A:540:A:C8	2.32	0.64
7:G:79:GLY:HA3	37:G:7046:HOH:O	1.98	0.64
11:K:19:MET:CE	11:K:132:LEU:HD11	2.28	0.64
14:N:74:ARG:HH11	14:N:74:ARG:HG3	1.62	0.64
1:A:1329:A:C2	37:A:4655:HOH:O	2.48	0.64
1:A:282:C:O2'	1:A:283:U:H5'	1.98	0.64
4:D:7:ARG:HG2	4:D:7:ARG:HH11	1.62	0.64
6:F:57:THR:HG23	6:F:63:ILE:HG22	1.79	0.64
1:A:1303:C:OP2	37:A:4492:HOH:O	2.14	0.64
1:A:182:G:H4'	14:N:157:LEU:HD13	1.78	0.64
4:D:24:PRO:CG	4:D:204:GLY:HA2	2.28	0.64
5:E:162:VAL:HG13	5:E:232:LEU:HD21	1.79	0.64
1:A:240:C:H4'	14:N:146:GLN:NE2	2.13	0.64
1:A:2421:G:H3'	1:A:2422:U:C5'	2.28	0.64
14:N:81:ARG:HG3	14:N:85:ARG:HB2	1.80	0.64
15:O:141:ARG:N	37:O:8571:HOH:O	2.31	0.64
22:V:14:GLU:O	22:V:17:THR:HB	1.96	0.64
2:B:3009:C:OP2	37:B:466:HOH:O	2.15	0.64
10:J:27:LYS:H	10:J:58:HIS:CD2	2.09	0.64
14:N:106:ASN:HD22	14:N:114:VAL:HG23	1.63	0.64
37:L:1387:HOH:O	22:V:20:MET:HE3	1.98	0.64
26:Z:189:ASN:HD22	26:Z:189:ASN:C	2.01	0.64
28:2:8:GLN:HE22	28:2:11:LYS:NZ	1.96	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:A:C4	1:A:177:A:C2	2.86	0.63
3:C:131:HIS:O	3:C:132:ASP:HB2	1.96	0.63
11:K:74:ARG:CB	11:K:74:ARG:HH11	2.11	0.63
19:S:104:PHE:HB2	19:S:109:MET:HE1	1.80	0.63
20:T:43:GLU:HB3	37:T:8344:HOH:O	1.98	0.63
1:A:1086:A:C6	24:X:11:VAL:HG11	2.33	0.63
1:A:2050:G:H5''	19:S:80:TYR:O	1.98	0.63
1:A:1857:A:N6	1:A:2247:C:H1'	2.13	0.63
1:A:263:U:O4'	8:H:59:ILE:HD13	1.98	0.63
1:A:926:A:O2'	13:M:41:HIS:HD2	1.81	0.63
3:C:81:GLN:HB2	3:C:92:ASN:ND2	2.13	0.63
6:F:41:LEU:HA	6:F:44:ILE:HG22	1.81	0.63
1:A:2123:A:H5'	14:N:89:ASN:HD21	1.63	0.63
37:A:5493:HOH:O	4:D:298:LYS:HD3	1.98	0.63
30:4:74:CYS:SG	30:4:76:LYS:CB	2.86	0.63
1:A:2432:C:O2'	1:A:2433:A:H5'	1.98	0.63
1:A:558:C:H5'	37:A:5235:HOH:O	1.99	0.63
32:A:8023:MG:MG	37:A:7787:HOH:O	1.41	0.63
12:L:82:ARG:NH2	12:L:115:ARG:HG2	2.13	0.63
26:Z:235:GLU:CD	26:Z:235:GLU:H	2.01	0.63
1:A:2281:C:C2'	1:A:2282:U:H5'	2.27	0.63
1:A:2676:C:H4'	11:K:70:PHE:CE1	2.34	0.63
37:A:6676:HOH:O	26:Z:165:GLU:HB3	1.98	0.63
1:A:1213:C:O2'	1:A:1214:G:H5'	1.98	0.63
14:N:12:TRP:CE2	14:N:20:ILE:HD11	2.33	0.63
15:O:154:LEU:O	15:O:155:GLU:HB3	1.99	0.63
15:O:48:VAL:HG11	15:O:55:ASP:HB3	1.81	0.63
1:A:1766:U:O2	1:A:1778:A:H5'	1.98	0.63
10:J:46:VAL:O	10:J:146:TRP:HH2	1.82	0.63
29:3:41:HIS:N	29:3:45:ASN:HD22	1.94	0.63
1:A:2637:A:H5'	37:A:9260:HOH:O	1.98	0.63
1:A:299:U:H5'	37:A:7314:HOH:O	1.98	0.63
1:A:952:G:H4'	37:A:4003:HOH:O	1.99	0.63
5:E:16:VAL:HG12	5:E:17:ASP:N	2.13	0.63
6:F:99:ASP:CB	6:F:103:ASN:H	2.12	0.63
1:A:2690:U:O2'	7:G:111:LYS:HE3	1.99	0.63
14:N:34:GLU:HB3	14:N:35:PRO:HD2	1.81	0.63
15:O:61:ALA:CB	15:O:88:ALA:HB2	2.28	0.63
18:R:32:GLU:HA	18:R:71:TYR:OH	1.99	0.63
20:T:51:GLN:HE21	20:T:53:ASN:ND2	1.97	0.63
25:Y:25:ARG:HG2	37:Y:5356:HOH:O	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1679:C:H5'	37:A:9311:HOH:O	1.99	0.63
1:A:113:A:H3'	1:A:114:A:H5''	1.82	0.62
4:D:307:ARG:HH11	4:D:307:ARG:HB2	1.63	0.62
5:E:233:THR:HG22	5:E:234:VAL:N	2.12	0.62
13:M:145:LEU:O	13:M:148:GLU:HG3	1.98	0.62
17:Q:120:ARG:NH2	17:Q:123:TYR:CD2	2.67	0.62
19:S:18:LEU:HB2	19:S:143:VAL:HG12	1.79	0.62
37:L:408:HOH:O	22:V:37:GLU:HB3	1.99	0.62
1:A:926:A:O2'	13:M:41:HIS:CD2	2.51	0.62
5:E:25:PRO:HG2	37:E:8325:HOH:O	1.98	0.62
15:O:73:ALA:N	37:O:8568:HOH:O	2.32	0.62
20:T:51:GLN:NE2	20:T:53:ASN:HD21	1.97	0.62
30:4:40:ARG:HD2	37:4:8552:HOH:O	1.99	0.62
1:A:1159:G:P	37:A:4266:HOH:O	2.57	0.62
1:A:1377:C:H5'	1:A:1377:C:H6	1.63	0.62
1:A:21:G:C5'	19:S:2:ILE:HA	2.28	0.62
1:A:2314:G:C2'	1:A:2315:C:H5'	2.29	0.62
1:A:631:A:N3	1:A:2073:G:O2'	2.32	0.62
32:A:8054:MG:MG	37:A:7765:HOH:O	1.42	0.62
27:1:62:TYR:CE2	27:1:64:ILE:HG23	2.34	0.62
37:A:6162:HOH:O	29:3:44:ARG:HG2	2.00	0.62
1:A:1119:G:N2	1:A:1246:A:C2	2.61	0.62
2:B:3003:A:N6	2:B:3022:G:H1'	2.15	0.62
5:E:236:THR:HA	37:E:8450:HOH:O	1.99	0.62
1:A:1293:U:O2'	26:Z:149:GLN:NE2	2.29	0.62
1:A:2346:C:H6	1:A:2346:C:O5'	1.82	0.62
1:A:2635:A:O2'	1:A:2636:C:H5'	2.00	0.62
15:O:164:ASP:CG	15:O:167:ASP:HA	2.20	0.62
16:P:87:THR:O	16:P:91:GLN:HG3	1.99	0.62
19:S:39:THR:HG23	19:S:107:GLU:O	2.00	0.62
4:D:258:GLY:H	4:D:260:HIS:CE1	2.17	0.62
6:F:25:MET:HE1	6:F:37:ALA:O	1.99	0.62
23:W:39:ALA:C	23:W:41:GLU:H	2.03	0.62
24:X:26:ILE:O	24:X:26:ILE:HG13	1.99	0.62
14:N:87:MET:CB	30:4:46:ILE:HD13	2.30	0.62
1:A:2324:G:H4'	1:A:2418:G:O2'	2.00	0.62
4:D:175:LEU:C	4:D:175:LEU:HD23	2.20	0.62
6:F:101:THR:HG22	37:F:7400:HOH:O	1.99	0.62
24:X:4:LEU:HD23	24:X:54:PHE:HB3	1.81	0.62
1:A:2878:U:H2'	1:A:2879:A:O4'	2.00	0.62
3:C:153:ARG:HB2	3:C:153:ARG:HH11	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:A:7432:HOH:O	4:D:211:THR:HG21	1.99	0.62
5:E:107:ARG:NH1	5:E:107:ARG:HB3	2.15	0.62
14:N:91:ILE:HA	37:N:8645:HOH:O	1.98	0.62
37:B:5071:HOH:O	15:O:23:ARG:HD3	1.99	0.62
21:U:55:PHE:HB2	37:U:6384:HOH:O	1.99	0.62
27:1:29:VAL:O	27:1:33:HIS:HB2	2.00	0.62
1:A:251:C:O2'	1:A:252:C:H5'	2.00	0.62
14:N:74:ARG:HG3	14:N:74:ARG:NH1	2.15	0.62
21:U:9:LYS:HE3	21:U:13:ARG:NH1	2.15	0.62
1:A:714:U:H3'	37:A:6912:HOH:O	1.99	0.62
6:F:64:ARG:CD	6:F:67:ASP:HB3	2.30	0.62
1:A:2779:G:H21	7:G:143:GLN:NE2	1.98	0.62
15:O:184:ILE:HG22	15:O:185:GLU:HG3	1.81	0.62
37:B:5071:HOH:O	15:O:20:TYR:CE2	2.50	0.62
18:R:75:ILE:CD1	18:R:84:ILE:HD11	2.29	0.62
5:E:242:GLU:HG3	37:E:8380:HOH:O	1.99	0.61
14:N:72:SER:OG	14:N:74:ARG:HB2	1.99	0.61
1:A:1919:A:H4'	37:A:4823:HOH:O	1.99	0.61
1:A:2094:G:H4'	4:D:245:SER:HB3	1.81	0.61
10:J:75:SER:O	10:J:79:ALA:HB2	2.00	0.61
1:A:1119:G:H8	11:K:52:GLN:NE2	1.98	0.61
17:Q:98:ILE:HD12	17:Q:102:ARG:NE	2.15	0.61
3:C:211:LYS:NZ	37:C:8623:HOH:O	2.32	0.61
3:C:72:GLU:HG3	27:1:66:GLY:HA2	1.82	0.61
4:D:154:VAL:HG12	4:D:156:LYS:HG2	1.82	0.61
14:N:68:ARG:HD3	14:N:68:ARG:O	2.00	0.61
6:F:146:LYS:NZ	15:O:107:ASN:HD21	1.98	0.61
27:1:53:GLY:HA2	27:1:67:GLY:O	2.00	0.61
1:A:1441:G:O2'	1:A:1442:A:H5'	2.00	0.61
1:A:2502:C:C2'	1:A:2503:A:H5'	2.31	0.61
1:A:2729:C:O2'	1:A:2730:G:H5'	2.00	0.61
1:A:2780:C:H2'	1:A:2781:U:C6	2.35	0.61
1:A:56:G:H5''	23:W:50:ARG:NH1	2.15	0.61
23:W:58:THR:O	23:W:62:GLU:HG3	2.01	0.61
1:A:281:U:H3'	37:A:7182:HOH:O	2.00	0.61
13:M:114:VAL:HG11	37:M:8572:HOH:O	2.01	0.61
15:O:80:SER:HB2	37:O:8537:HOH:O	2.00	0.61
24:X:21:LEU:HD21	24:X:48:VAL:HG11	1.80	0.61
27:1:31:ILE:O	27:1:35:LYS:HG3	2.00	0.61
1:A:1151:G:OP1	9:I:63:ARG:NH1	2.34	0.61
1:A:2419:U:H5''	1:A:2420:G:H5'	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2502:C:H2'	1:A:2503:A:H5'	1.82	0.61
4:D:36:PRO:HA	4:D:168:GLY:CA	2.31	0.61
15:O:12:ARG:HD3	15:O:18:THR:OG1	2.01	0.61
4:D:55:ASN:HB3	4:D:63:GLU:HA	1.81	0.61
7:G:6:GLU:HA	7:G:46:THR:HG22	1.82	0.61
27:1:28:ASP:O	27:1:31:ILE:HG22	2.01	0.61
1:A:1505:U:H6	1:A:1505:U:H5'	1.63	0.61
5:E:118:THR:O	5:E:136:VAL:HG13	2.00	0.61
1:A:121:U:OP2	29:3:10:ARG:NH2	2.33	0.61
29:3:35:ARG:HB2	37:3:2691:HOH:O	1.99	0.61
1:A:2281:C:H2'	1:A:2282:U:H5'	1.82	0.61
1:A:820:G:O2'	1:A:856:G:H4'	2.01	0.61
3:C:179:MET:HG2	3:C:186:TRP:CB	2.30	0.61
4:D:248:ARG:HG2	37:K:8541:HOH:O	1.99	0.61
6:F:25:MET:CE	6:F:37:ALA:HB1	2.31	0.61
14:N:59:GLY:HA3	14:N:141:ILE:HD11	1.83	0.61
25:Y:75:ALA:O	25:Y:83:ALA:HA	2.01	0.61
1:A:1393:A:H2'	1:A:1394:C:C6	2.36	0.61
10:J:166:ASN:N	10:J:166:ASN:HD22	1.98	0.61
10:J:86:ARG:HD3	10:J:130:HIS:HD2	1.66	0.61
11:K:90:LYS:HB2	34:K:8502:CL:CL	2.38	0.61
24:X:5:VAL:HG22	24:X:32:CYS:HB2	1.83	0.61
26:Z:99:ALA:HB2	26:Z:233:TYR:CZ	2.36	0.61
1:A:1773:G:C8	27:1:16:PRO:HA	2.35	0.60
2:B:3054:A:O2'	2:B:3055:U:H5'	2.01	0.60
6:F:99:ASP:HB2	6:F:103:ASN:HB2	1.83	0.60
12:L:74:VAL:HG12	12:L:75:ARG:HG3	1.83	0.60
1:A:431:G:P	14:N:48:ARG:HH12	2.24	0.60
24:X:22:GLU:HG2	24:X:27:HIS:CD2	2.35	0.60
1:A:2432:C:C4'	37:A:9718:HOH:O	2.43	0.60
1:A:383:A:H4'	37:A:5304:HOH:O	2.00	0.60
1:A:929:A:O5'	1:A:929:A:H8	1.84	0.60
1:A:1847:A:OP1	3:C:175:LYS:HG3	2.00	0.60
5:E:237:GLU:HB2	37:E:8429:HOH:O	2.00	0.60
6:F:36:ASN:HA	37:F:7500:HOH:O	2.00	0.60
14:N:186:SER:O	14:N:189:VAL:HG12	2.01	0.60
14:N:87:MET:HB3	30:4:46:ILE:HG21	1.84	0.60
29:3:22:PRO:HG2	29:3:25:VAL:CG2	2.30	0.60
1:A:69:A:H5'	1:A:69:A:C8	2.36	0.60
4:D:305:ASP:O	4:D:306:LYS:HB2	2.02	0.60
10:J:3:GLY:HA2	10:J:57:ARG:HH12	1.64	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:37:ARG:CD	34:O:8507:CL:CL	2.86	0.60
17:Q:10:ALA:HA	17:Q:13:VAL:HG12	1.83	0.60
17:Q:13:VAL:HG21	17:Q:41:ARG:HG2	1.83	0.60
19:S:119:VAL:HG21	19:S:142:ASP:CG	2.21	0.60
30:4:73:GLU:HB3	37:4:8564:HOH:O	2.00	0.60
1:A:2241:C:O2'	1:A:2242:U:H5'	2.01	0.60
1:A:2310:G:OP2	10:J:114:PRO:HD2	2.00	0.60
1:A:797:A:O4'	27:1:10:ARG:N	2.33	0.60
6:F:136:ARG:HD2	6:F:155:HIS:O	2.01	0.60
8:H:46:GLU:O	8:H:73:PRO:HD2	2.02	0.60
14:N:30:GLU:O	14:N:34:GLU:HG3	2.01	0.60
19:S:39:THR:HB	19:S:42:GLU:HG3	1.83	0.60
24:X:4:LEU:O	24:X:32:CYS:HA	2.01	0.60
1:A:125:U:H2'	37:A:3747:HOH:O	2.02	0.60
1:A:1311:G:C2	1:A:1312:G:C8	2.90	0.60
1:A:2249:G:OP2	37:A:5416:HOH:O	2.16	0.60
1:A:821:U:O2'	1:A:822:C:H5'	2.01	0.60
6:F:35:ALA:N	37:F:5576:HOH:O	2.35	0.60
1:A:1205:U:H2'	1:A:1206:U:C5'	2.30	0.60
1:A:2388:C:OP1	37:A:4572:HOH:O	2.16	0.60
1:A:280:C:H2'	1:A:281:U:O4'	2.02	0.60
1:A:941:G:O2'	1:A:942:U:H5'	2.01	0.60
1:A:948:G:N7	37:A:5820:HOH:O	2.31	0.60
37:A:4037:HOH:O	4:D:27:ASN:HB2	2.01	0.60
7:G:11:VAL:HG13	7:G:23:GLU:O	2.01	0.60
27:1:75:ALA:HB3	37:1:8440:HOH:O	2.01	0.60
1:A:886:A:OP1	37:A:3652:HOH:O	2.17	0.60
2:B:3035:C:H5''	37:B:4078:HOH:O	2.00	0.60
4:D:2:GLN:CD	37:D:8622:HOH:O	2.40	0.60
7:G:3:VAL:HG22	7:G:49:ILE:HB	1.84	0.60
15:O:141:ARG:HB3	37:O:8571:HOH:O	2.00	0.60
15:O:71:TRP:HE3	15:O:175:LEU:HD22	1.67	0.60
22:V:49:LEU:HD11	37:V:3805:HOH:O	2.02	0.60
23:W:39:ALA:O	23:W:41:GLU:N	2.35	0.60
24:X:149:LEU:HG	24:X:153:MET:HE2	1.84	0.60
1:A:1982:C:OP2	37:A:4252:HOH:O	2.16	0.60
1:A:1741:U:O2'	1:A:2723:G:H4'	2.01	0.60
15:O:119:GLN:O	15:O:123:ILE:HG13	2.01	0.60
33:A:8313:NA:NA	37:A:5123:HOH:O	1.74	0.60
12:L:32:ILE:HD11	12:L:56:SER:HB3	1.84	0.60
24:X:21:LEU:HD21	24:X:48:VAL:CG1	2.32	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Y:78:GLU:CG	25:Y:79:GLU:H	2.13	0.60
26:Z:216:ARG:CD	37:Z:8569:HOH:O	2.39	0.60
1:A:1165:G:H3'	1:A:1165:G:OP1	2.02	0.59
4:D:195:ARG:HD2	4:D:324:ASP:OD1	2.01	0.59
5:E:246:ARG:NH1	5:E:246:ARG:HB3	2.16	0.59
11:K:26:VAL:HG13	11:K:36:VAL:HG11	1.82	0.59
14:N:139:PRO:O	14:N:140:ALA:CB	2.50	0.59
14:N:185:PRO:HG2	14:N:189:VAL:HG11	1.84	0.59
26:Z:115:ARG:NE	37:Z:8556:HOH:O	2.34	0.59
15:O:164:ASP:OD2	15:O:167:ASP:HA	2.02	0.59
22:V:47:ARG:HG3	37:V:4381:HOH:O	2.01	0.59
24:X:38:THR:HG22	37:X:3580:HOH:O	2.01	0.59
1:A:558:C:C2'	1:A:559:U:H5''	2.33	0.59
10:J:111:MET:O	10:J:114:PRO:HD3	2.02	0.59
1:A:182:G:H5'	37:A:5135:HOH:O	2.02	0.59
1:A:2505:G:O2'	1:A:2506:A:H5'	2.01	0.59
1:A:349:U:O2'	1:A:350:C:H5'	2.02	0.59
2:B:3055:U:H4'	2:B:3056:A:C8	2.38	0.59
4:D:312:ARG:HD3	4:D:315:VAL:HG13	1.84	0.59
6:F:95:THR:C	6:F:97:GLN:H	2.05	0.59
24:X:21:LEU:HD22	24:X:26:ILE:CD1	2.31	0.59
1:A:1119:G:H8	11:K:52:GLN:HE22	1.49	0.59
1:A:1523:G:H2'	1:A:1524:U:C6	2.38	0.59
1:A:703:G:O2'	1:A:704:C:H5'	2.02	0.59
3:C:166:ASP:OD1	37:C:8621:HOH:O	2.16	0.59
29:3:1:GLY:HA3	37:3:5969:HOH:O	2.02	0.59
1:A:1187:U:O2'	1:A:1189:A:H2	1.85	0.59
1:A:1669:A:H2'	1:A:1670:G:C8	2.38	0.59
1:A:1134:G:C4'	10:J:151:MET:HE1	2.17	0.59
25:Y:15:ARG:NH1	25:Y:15:ARG:HB3	2.16	0.59
3:C:94:LEU:HG	3:C:99:ILE:HD11	1.84	0.59
37:A:9678:HOH:O	4:D:254:GLN:HG3	2.02	0.59
1:A:1972:U:H2'	1:A:1973:A:H5'	1.85	0.59
1:A:2001:G:O2'	1:A:2002:C:H5'	2.03	0.59
1:A:2783:A:H3'	37:A:5210:HOH:O	2.00	0.59
1:A:820:G:OP1	27:1:17:ARG:NH2	2.31	0.59
2:B:3002:U:H4'	2:B:3002:U:OP2	2.01	0.59
4:D:207:LYS:HG2	4:D:304:PRO:HB3	1.83	0.59
5:E:84:VAL:O	5:E:85:LYS:HB2	2.02	0.59
15:O:151:ASP:O	15:O:154:LEU:HB2	2.03	0.59
26:Z:144:ARG:NE	37:Z:8610:HOH:O	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:4:7:PHE:HE2	30:4:22:VAL:HG21	1.67	0.59
1:A:2382:A:OP1	30:4:80:ARG:HG2	2.03	0.59
1:A:2064:U:OP1	37:A:3329:HOH:O	2.17	0.59
1:A:681:G:N3	1:A:681:G:H5'	2.18	0.59
7:G:69:ILE:HA	7:G:72:MET:CE	2.33	0.59
8:H:58:GLU:HA	8:H:61:MET:HG3	1.85	0.59
1:A:962:C:C1'	15:O:5:ARG:NH1	2.63	0.59
1:A:960:G:N3	1:A:960:G:H2'	2.18	0.59
4:D:217:ARG:HG3	4:D:257:THR:HG22	1.84	0.59
6:F:54:ALA:CB	6:F:69:ILE:HD12	2.32	0.59
16:P:26:TRP:N	37:P:3062:HOH:O	2.34	0.59
27:1:11:THR:OG1	27:1:23:ARG:HB2	2.04	0.58
32:A:8011:MG:MG	37:A:3953:HOH:O	1.45	0.58
2:B:3041:C:O4'	6:F:50:VAL:HG23	2.03	0.58
4:D:190:MET:HE2	4:D:194:PHE:CD1	2.38	0.58
1:A:1053:G:OP1	10:J:12:PRO:HG3	2.02	0.58
21:U:49:GLU:OE2	21:U:97:ARG:HD2	2.03	0.58
1:A:2064:U:H5'	1:A:2652:U:H4'	1.85	0.58
6:F:166:ILE:HD12	37:F:6326:HOH:O	2.03	0.58
19:S:14:ALA:HB3	19:S:147:LEU:HB2	1.86	0.58
1:A:1923:G:H4'	30:4:31:THR:O	2.03	0.58
1:A:2748:G:H5'	37:A:7521:HOH:O	2.03	0.58
1:A:2851:G:O2'	1:A:2852:A:H5'	2.03	0.58
4:D:141:ARG:HG2	4:D:165:ARG:HA	1.85	0.58
5:E:168:ARG:NH2	5:E:190:ALA:O	2.36	0.58
5:E:219:ASN:O	5:E:222:ASP:OD1	2.21	0.58
12:L:27:ARG:HD2	37:L:4747:HOH:O	2.03	0.58
16:P:39:THR:O	16:P:115:ARG:NH2	2.36	0.58
26:Z:189:ASN:HA	26:Z:217:ILE:HD11	1.84	0.58
1:A:1183:C:N4	37:A:4371:HOH:O	2.32	0.58
1:A:131:A:OP2	37:A:3142:HOH:O	2.17	0.58
1:A:2121:G:O2'	1:A:2122:C:H5'	2.04	0.58
1:A:2279:G:N3	37:A:9807:HOH:O	2.32	0.58
1:A:2507:G:H2'	1:A:2510:C:H42	1.68	0.58
3:C:11:ARG:HD3	37:C:8518:HOH:O	2.02	0.58
3:C:211:LYS:NZ	37:C:8575:HOH:O	2.37	0.58
6:F:37:ALA:O	6:F:40:ILE:HG12	2.03	0.58
10:J:48:LEU:HG	10:J:157:ILE:HG21	1.85	0.58
27:1:25:ARG:O	27:1:29:VAL:HG23	2.03	0.58
1:A:113:A:OP2	1:A:114:A:H2'	2.02	0.58
8:H:110:GLU:O	8:H:114:LYS:HG3	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:163:PRO:O	10:J:164:ALA:HB2	2.03	0.58
13:M:143:THR:CG2	13:M:144:ASP:N	2.66	0.58
15:O:43:VAL:HG13	15:O:118:ILE:HD11	1.83	0.58
19:S:44:VAL:O	19:S:48:GLU:HG3	2.03	0.58
26:Z:112:GLU:HA	26:Z:112:GLU:OE1	2.04	0.58
1:A:407:A:H5'	37:A:5994:HOH:O	2.03	0.58
3:C:95:PRO:HG2	3:C:98:GLU:HG2	1.86	0.58
10:J:65:ARG:CZ	37:J:8374:HOH:O	2.50	0.58
10:J:13:ALA:HA	10:J:91:HIS:CE1	2.39	0.58
1:A:1134:G:H4'	10:J:151:MET:CE	2.19	0.58
1:A:285:A:H2'	1:A:286:U:O4'	2.04	0.58
1:A:371:U:H2'	1:A:372:A:H8	1.68	0.58
4:D:74:ILE:HG13	37:D:8606:HOH:O	2.03	0.58
14:N:154:ARG:CZ	37:N:8643:HOH:O	2.51	0.58
25:Y:43:VAL:CG1	25:Y:47:ALA:HB3	2.33	0.58
1:A:1127:C:H2'	1:A:1128:U:H5'	1.85	0.58
1:A:2081:A:H4'	11:K:69:TYR:CE1	2.38	0.58
2:B:3055:U:H4'	2:B:3056:A:H8	1.68	0.58
5:E:43:LYS:NZ	37:E:8387:HOH:O	2.36	0.58
6:F:99:ASP:HB3	6:F:103:ASN:H	1.68	0.58
10:J:150:LYS:HA	10:J:153:VAL:HG22	1.86	0.58
10:J:3:GLY:HA2	10:J:57:ARG:NH1	2.19	0.58
14:N:59:GLY:HA3	14:N:141:ILE:HD12	1.85	0.58
17:Q:105:LEU:CD2	17:Q:137:LEU:HD21	2.34	0.58
1:A:2329:C:O2'	1:A:2330:U:H5'	2.04	0.58
1:A:2359:G:N7	37:A:3681:HOH:O	2.32	0.58
1:A:2594:C:O2'	1:A:2595:U:H5'	2.03	0.58
1:A:2718:C:H6	1:A:2718:C:H5'	1.69	0.58
5:E:27:ARG:HG3	5:E:29:ASP:OD1	2.03	0.58
10:J:147:ARG:HA	10:J:150:LYS:NZ	2.19	0.58
37:A:9380:HOH:O	14:N:94:LYS:HE2	2.03	0.58
22:V:9:CYS:HA	22:V:52:THR:CG2	2.30	0.58
1:A:1829:A:H5''	37:A:3062:HOH:O	2.02	0.58
1:A:2694:A:H4'	7:G:91:PHE:CE1	2.39	0.58
1:A:469:G:O2'	37:A:3035:HOH:O	2.16	0.58
1:A:489:A:C8	21:U:82:THR:HG22	2.39	0.58
13:M:143:THR:HG22	13:M:144:ASP:H	1.69	0.58
37:A:4491:HOH:O	14:N:94:LYS:HE3	2.03	0.58
26:Z:107:PRO:HB3	26:Z:182:PHE:CE2	2.39	0.58
1:A:1474:C:H6	1:A:1474:C:C5'	2.11	0.57
1:A:1535:G:H2'	1:A:1536:C:C6	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1559:A:H1'	37:A:5836:HOH:O	2.03	0.57
1:A:815:U:OP1	37:A:3037:HOH:O	2.17	0.57
2:B:3026:C:P	37:B:3472:HOH:O	2.62	0.57
2:B:3107:C:H5	37:B:3167:HOH:O	1.87	0.57
4:D:30:PRO:HB2	4:D:39:GLN:NE2	2.18	0.57
6:F:86:THR:O	6:F:90:LEU:HG	2.04	0.57
8:H:46:GLU:N	37:H:3461:HOH:O	2.37	0.57
8:H:53:ASP:OD1	8:H:80:GLN:HB2	2.03	0.57
1:A:558:C:O2'	1:A:559:U:H5''	2.05	0.57
4:D:125:GLU:O	4:D:129:ARG:HG3	2.03	0.57
37:A:7435:HOH:O	5:E:188:ARG:CD	2.51	0.57
10:J:49:VAL:O	10:J:157:ILE:HG23	2.04	0.57
10:J:58:HIS:HA	10:J:61:LEU:HD23	1.86	0.57
24:X:72:PRO:HG2	24:X:77:ALA:HB3	1.85	0.57
1:A:2729:C:H2'	1:A:2730:G:H8	1.68	0.57
1:A:474:C:O3'	5:E:73:LEU:HD21	2.04	0.57
15:O:157:PRO:HA	37:O:8526:HOH:O	2.03	0.57
1:A:1422:U:H2'	1:A:1423:C:H6	1.67	0.57
1:A:272:A:H5'	1:A:273:G:OP2	2.04	0.57
1:A:920:C:H5'	1:A:921:G:C4	2.40	0.57
7:G:31:ARG:NH1	37:G:5919:HOH:O	2.36	0.57
9:I:64:ASN:N	9:I:64:ASN:HD22	2.01	0.57
10:J:127:GLY:O	10:J:128:ALA:CB	2.52	0.57
14:N:114:VAL:HG21	14:N:159:THR:HG21	1.87	0.57
14:N:165:SER:HB3	37:N:8534:HOH:O	2.04	0.57
15:O:143:ARG:HA	15:O:172:PHE:CD2	2.39	0.57
30:4:18:GLN:OE1	30:4:73:GLU:HB3	2.05	0.57
30:4:74:CYS:SG	30:4:76:LYS:CG	2.93	0.57
1:A:1819:G:H2'	1:A:1820:G:H4'	1.85	0.57
1:A:183:A:H5'	14:N:157:LEU:HD12	1.85	0.57
1:A:2433:A:H2'	1:A:2434:A:C8	2.40	0.57
4:D:221:GLN:HE22	12:L:42:ASN:ND2	2.02	0.57
4:D:238:ASN:ND2	4:D:240:GLY:H	1.96	0.57
6:F:25:MET:CE	6:F:41:LEU:HG	2.26	0.57
22:V:52:THR:HG22	22:V:54:THR:HB	1.87	0.57
25:Y:15:ARG:HH11	25:Y:15:ARG:CB	2.16	0.57
1:A:1351:G:OP1	5:E:96:LYS:NZ	2.37	0.57
1:A:2577:A:O2'	37:A:5373:HOH:O	2.18	0.57
17:Q:13:VAL:HG11	17:Q:40:VAL:CG1	2.34	0.57
19:S:18:LEU:HD12	19:S:143:VAL:CG1	2.35	0.57
25:Y:78:GLU:HG2	25:Y:79:GLU:N	2.16	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2015:A:H2'	1:A:2016:U:O4'	2.04	0.57
1:A:2382:A:H5'	37:A:4715:HOH:O	2.04	0.57
1:A:2769:C:C2'	1:A:2770:G:H5'	2.35	0.57
1:A:951:A:C2'	1:A:952:G:H5'	2.35	0.57
23:W:39:ALA:N	23:W:40:PRO:CD	2.67	0.57
1:A:1126:C:OP2	37:A:3619:HOH:O	2.18	0.57
1:A:2256:G:H2'	1:A:2257:G:H5'	1.87	0.57
1:A:2766:A:O2'	4:D:265:LEU:O	2.22	0.57
5:E:7:ASP:OD1	5:E:11:ASN:O	2.22	0.57
8:H:19:ALA:O	8:H:22:VAL:HG22	2.04	0.57
37:A:4810:HOH:O	11:K:47:THR:HB	2.04	0.57
14:N:172:GLY:C	14:N:183:VAL:HG11	2.25	0.57
1:A:1118:A:C8	1:A:1118:A:C3'	2.83	0.57
1:A:1192:A:O2'	1:A:1193:A:OP1	2.22	0.57
1:A:2506:A:O2'	1:A:2507:G:O5'	2.23	0.57
1:A:69:A:H8	1:A:69:A:H5'	1.70	0.57
1:A:816:G:H5'	1:A:1598:A:H4'	1.87	0.57
4:D:7:ARG:NH1	4:D:11:LEU:HD21	2.20	0.57
6:F:38:GLU:OE2	6:F:51:ARG:CZ	2.53	0.57
7:G:7:ILE:HD11	7:G:11:VAL:C	2.25	0.57
8:H:28:ALA:HB3	8:H:99:THR:O	2.03	0.57
10:J:86:ARG:NH1	10:J:130:HIS:CD2	2.73	0.57
37:A:5504:HOH:O	14:N:58:GLN:HG3	2.03	0.57
20:T:29:ASP:OD1	20:T:31:ARG:HG3	2.04	0.57
21:U:38:ARG:HG3	21:U:38:ARG:HH11	1.69	0.57
1:A:1687:C:O2	28:2:9:GLY:HA2	2.05	0.57
29:3:41:HIS:H	29:3:45:ASN:ND2	2.03	0.57
1:A:1060:C:H6	1:A:1060:C:H5'	1.70	0.57
8:H:107:VAL:O	8:H:111:ILE:HG13	2.04	0.57
1:A:21:G:H4'	19:S:2:ILE:HG22	1.87	0.57
29:3:22:PRO:HB2	29:3:24:TRP:CD1	2.40	0.56
1:A:1677:U:OP2	29:3:8:LYS:NZ	2.35	0.56
1:A:1528:A:H2'	1:A:1529:G:O4'	2.05	0.56
1:A:1820:G:C6	1:A:2030:A:C2	2.93	0.56
1:A:2270:G:H4'	3:C:223:ARG:HH12	1.70	0.56
3:C:192:VAL:O	3:C:207:GLN:HG2	2.05	0.56
10:J:14:TYR:N	10:J:91:HIS:CE1	2.72	0.56
13:M:149:ARG:O	13:M:150:GLN:HB2	2.05	0.56
14:N:169:ARG:HD2	37:N:8590:HOH:O	2.05	0.56
19:S:106:GLY:HA2	19:S:109:MET:CE	2.35	0.56
1:A:315:G:C6	1:A:316:A:C6	2.93	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:559:U:C6	1:A:559:U:H5'	2.37	0.56
3:C:109:GLU:HG2	3:C:116:GLY:H	1.70	0.56
12:L:74:VAL:O	12:L:74:VAL:HG12	2.05	0.56
14:N:18:GLY:O	14:N:21:ALA:HB3	2.05	0.56
15:O:58:LEU:HD12	15:O:58:LEU:N	2.20	0.56
20:T:6:LYS:HB2	20:T:27:ALA:O	2.03	0.56
21:U:63:ILE:HD11	21:U:75:GLU:HB2	1.85	0.56
22:V:13:ILE:HG12	22:V:32:CYS:HB3	1.86	0.56
1:A:184:G:H5''	14:N:153:THR:HG22	1.87	0.56
1:A:1925:G:O2'	1:A:1926:G:H5'	2.05	0.56
1:A:2570:G:H5''	37:A:4890:HOH:O	2.06	0.56
3:C:217:ARG:HG2	3:C:229:ALA:HB2	1.87	0.56
8:H:50:VAL:CG1	8:H:60:VAL:HG11	2.34	0.56
10:J:48:LEU:CD1	10:J:157:ILE:HG21	2.34	0.56
10:J:26:LYS:HD3	10:J:89:PRO:HG3	1.87	0.56
1:A:1887:U:OP1	27:I:21:LYS:HE3	2.05	0.56
1:A:1056:U:H2'	1:A:1057:A:O4'	2.06	0.56
1:A:1595:G:O2'	1:A:1596:U:H5'	2.05	0.56
1:A:2276:U:H2'	1:A:2277:U:H6	1.69	0.56
2:B:3103:A:O2'	2:B:3104:A:H5'	2.04	0.56
4:D:168:GLY:N	4:D:174:ARG:HD3	2.20	0.56
4:D:24:PRO:HG3	4:D:204:GLY:HA2	1.87	0.56
4:D:214:PRO:HD2	37:D:8521:HOH:O	2.05	0.56
4:D:27:ASN:HB3	37:D:8630:HOH:O	2.05	0.56
7:G:20:ILE:CD1	7:G:33:LEU:HD12	2.36	0.56
2:B:3006:C:P	15:O:37:ARG:NH1	2.79	0.56
15:O:49:THR:CG2	15:O:56:ASP:HB2	2.35	0.56
1:A:1450:C:O2'	1:A:1494:A:H5'	2.06	0.56
1:A:1641:A:H2'	1:A:1642:A:H5'	1.87	0.56
1:A:816:G:C6	1:A:817:G:N1	2.73	0.56
2:B:3064:C:H2'	2:B:3065:A:H5'	1.87	0.56
3:C:105:VAL:CG1	3:C:154:ALA:HB1	2.35	0.56
5:E:47:GLY:HA2	5:E:92:PRO:HB2	1.88	0.56
37:A:3822:HOH:O	10:J:11:LYS:HE2	2.04	0.56
10:J:85:ILE:HB	10:J:132:PHE:CE2	2.40	0.56
1:A:2502:C:H4'	10:J:151:MET:HG2	1.88	0.56
10:J:56:ILE:HG22	10:J:61:LEU:CD2	2.33	0.56
14:N:104:ARG:O	14:N:108:LYS:HG2	2.04	0.56
14:N:87:MET:CE	37:N:8531:HOH:O	2.53	0.56
15:O:34:LEU:HA	15:O:47:LEU:HD23	1.87	0.56
24:X:13:MET:CE	24:X:17:ILE:HG22	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1483:C:O2'	1:A:1484:G:H5'	2.05	0.56
1:A:484:A:N1	1:A:506:G:H4'	2.21	0.56
1:A:558:C:H2'	1:A:559:U:C5'	2.35	0.56
4:D:148:PRO:HD2	37:D:8582:HOH:O	2.05	0.56
4:D:240:GLY:HA3	37:D:8528:HOH:O	2.05	0.56
4:D:333:GLU:HB2	22:V:14:GLU:OE2	2.06	0.56
4:D:41:PHE:CG	4:D:190:MET:HE3	2.41	0.56
37:A:4513:HOH:O	10:J:151:MET:HE2	2.05	0.56
14:N:74:ARG:O	14:N:88:VAL:HG13	2.04	0.56
21:U:48:VAL:HG22	21:U:97:ARG:C	2.25	0.56
30:4:3:MET:O	30:4:90:PHE:HA	2.06	0.56
1:A:1116:U:O2'	1:A:1118:A:C2	2.50	0.56
1:A:1701:A:H4'	1:A:1702:U:C5'	2.35	0.56
1:A:2587:U:H2'	1:A:2589:U:H5''	1.86	0.56
1:A:289:G:N2	1:A:363:A:H2	2.01	0.56
1:A:778:C:C4	1:A:779:U:C4	2.94	0.56
4:D:304:PRO:HD2	4:D:307:ARG:HD2	1.86	0.56
8:H:100:ASP:O	8:H:101:ALA:O	2.24	0.56
1:A:710:G:OP1	16:P:24:ALA:HB3	2.04	0.56
26:Z:112:GLU:OE1	26:Z:115:ARG:NH1	2.38	0.56
1:A:88:G:N7	29:3:28:LYS:HD2	2.20	0.56
30:4:71:CYS:SG	30:4:72:GLY:N	2.78	0.56
1:A:134:U:O2	1:A:145:A:C2	2.58	0.56
1:A:2361:A:H2'	1:A:2362:A:C8	2.40	0.56
1:A:2547:C:OP2	4:D:5:ARG:NH1	2.39	0.56
1:A:1174:A:C5	1:A:1201:C:H4'	2.40	0.56
1:A:1711:A:O2'	1:A:1712:A:H5'	2.05	0.56
1:A:2064:U:H5'	1:A:2652:U:O3'	2.06	0.56
1:A:2432:C:H4'	30:4:36:ILE:HG12	1.86	0.56
8:H:107:VAL:HG23	37:H:6617:HOH:O	2.06	0.56
9:I:12:ILE:HG22	9:I:12:ILE:O	2.05	0.56
11:K:52:GLN:HG3	11:K:53:ILE:N	2.21	0.56
24:X:81:ASP:OD1	24:X:92:ASP:HB2	2.04	0.56
24:X:80:ASP:O	24:X:84:VAL:HG23	2.05	0.56
1:A:1362:U:H5'	37:E:8342:HOH:O	2.06	0.56
1:A:1730:G:H5'	1:A:1731:C:C5	2.41	0.56
1:A:2011:A:P	37:A:5928:HOH:O	2.64	0.56
4:D:16:ARG:NH2	37:D:8556:HOH:O	2.28	0.56
1:A:1234:U:N3	4:D:244:PRO:HB3	2.21	0.56
2:B:3044:A:O4'	6:F:76:ARG:NE	2.39	0.56
10:J:53:PRO:HA	10:J:125:VAL:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:C:H2'	1:A:137:U:O4'	2.04	0.56
1:A:1733:A:H4'	4:D:212:GLN:HA	1.87	0.56
1:A:1874:U:H2'	3:C:120:ARG:HG3	1.88	0.56
1:A:2433:A:H2'	1:A:2434:A:H8	1.70	0.56
1:A:2526:C:O2'	1:A:2527:U:H5'	2.05	0.56
4:D:141:ARG:HD2	4:D:163:GLU:OE2	2.05	0.56
5:E:133:ARG:HD2	37:E:8408:HOH:O	2.06	0.56
10:J:83:PHE:HZ	10:J:146:TRP:HE1	1.50	0.56
12:L:101:ASN:O	12:L:102:GLU:HB2	2.06	0.56
14:N:39:ARG:NH2	37:N:8623:HOH:O	2.38	0.56
14:N:52:LEU:HD21	37:N:8616:HOH:O	2.06	0.56
21:U:24:ARG:HH21	21:U:39:ASN:HD22	1.53	0.56
1:A:1654:U:H2'	3:C:47:HIS:HD2	1.71	0.55
1:A:1688:G:H4'	28:2:8:GLN:HG3	1.87	0.55
1:A:2256:G:C2'	1:A:2257:G:H5'	2.36	0.55
1:A:2314:G:H2'	1:A:2315:C:H5'	1.87	0.55
1:A:2791:U:H1'	1:A:2792:A:H5''	1.88	0.55
1:A:821:U:H2'	1:A:822:C:C6	2.39	0.55
4:D:195:ARG:HG2	4:D:323:LEU:HD22	1.88	0.55
7:G:23:GLU:HG2	7:G:28:SER:HB3	1.88	0.55
10:J:44:ALA:HA	10:J:163:PRO:O	2.07	0.55
14:N:91:ILE:HG23	37:N:8645:HOH:O	2.05	0.55
18:R:75:ILE:HD13	18:R:84:ILE:HD11	1.88	0.55
26:Z:117:LEU:HD12	26:Z:174:VAL:HG11	1.88	0.55
1:A:1168:C:H2'	1:A:1169:U:O4'	2.05	0.55
1:A:542:A:H2'	1:A:543:G:O4'	2.05	0.55
3:C:96:LEU:HD22	3:C:128:LEU:HD13	1.88	0.55
13:M:54:PRO:HG2	13:M:57:VAL:CG2	2.37	0.55
23:W:56:ILE:O	23:W:60:GLN:HG3	2.05	0.55
1:A:111:C:H2'	1:A:112:G:O4'	2.06	0.55
1:A:1181:A:H2'	1:A:1182:C:O4'	2.05	0.55
1:A:1123:A:C6	1:A:1238:C:H5'	2.42	0.55
2:B:3042:C:O2	6:F:76:ARG:NH1	2.38	0.55
1:A:820:G:C6	3:C:171:LYS:HB2	2.41	0.55
10:J:69:ASN:O	10:J:72:VAL:HG12	2.07	0.55
24:X:106:THR:OG1	24:X:109:GLU:HG3	2.06	0.55
1:A:2316:G:H8	37:A:5626:HOH:O	1.89	0.55
1:A:2464:C:P	37:A:9912:HOH:O	2.64	0.55
1:A:639:A:H2'	1:A:640:G:C8	2.40	0.55
7:G:20:ILE:CD1	7:G:40:VAL:HG11	2.35	0.55
12:L:30:LYS:O	12:L:55:VAL:HG13	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:155:HIS:CE1	14:N:158:ARG:HE	2.24	0.55
15:O:86:LEU:O	15:O:90:LEU:HG	2.06	0.55
23:W:44:GLY:O	23:W:48:GLU:HG2	2.06	0.55
1:A:1182:C:H1'	1:A:1192:A:H8	1.72	0.55
1:A:283:U:H5''	1:A:284:C:P	2.47	0.55
2:B:3029:C:C2'	2:B:3030:C:H5'	2.36	0.55
4:D:7:ARG:HD3	4:D:9:GLY:O	2.06	0.55
5:E:16:VAL:HG12	5:E:17:ASP:H	1.71	0.55
6:F:140:ARG:O	6:F:140:ARG:HG2	2.06	0.55
7:G:81:GLU:HG2	7:G:134:SER:CB	2.37	0.55
15:O:159:TYR:HE2	15:O:163:PHE:HE2	1.55	0.55
24:X:108:ARG:HE	24:X:114:PRO:HG3	1.70	0.55
25:Y:76:ARG:HG3	25:Y:76:ARG:NH1	2.21	0.55
1:A:2271:G:P	37:A:9415:HOH:O	2.65	0.55
1:A:2349:G:OP1	6:F:20:LYS:NZ	2.39	0.55
1:A:2897:C:H2'	1:A:2898:G:H8	1.71	0.55
1:A:57:C:H5''	37:A:6728:HOH:O	2.06	0.55
13:M:57:VAL:HG12	13:M:57:VAL:O	2.05	0.55
15:O:152:GLU:C	15:O:154:LEU:H	2.08	0.55
26:Z:126:PRO:HG2	26:Z:128:PHE:CE1	2.42	0.55
1:A:2649:A:H8	1:A:2649:A:H5'	1.71	0.55
1:A:506:G:H22	1:A:509:A:H5''	1.68	0.55
1:A:516:A:P	37:A:5618:HOH:O	2.64	0.55
1:A:545:G:C8	1:A:545:G:H5'	2.37	0.55
1:A:671:A:O2'	1:A:672:G:H2'	2.07	0.55
37:A:6996:HOH:O	3:C:211:LYS:CG	2.52	0.55
4:D:24:PRO:HG2	4:D:204:GLY:HA2	1.88	0.55
4:D:280:VAL:CG1	4:D:334:SER:HA	2.36	0.55
10:J:75:SER:C	10:J:79:ALA:HB2	2.27	0.55
14:N:149:TRP:O	14:N:152:ARG:HG2	2.06	0.55
15:O:82:TYR:CD2	15:O:82:TYR:C	2.80	0.55
23:W:64:GLY:O	23:W:65:ASP:CB	2.55	0.55
25:Y:43:VAL:HG12	25:Y:44:ASP:N	2.22	0.55
26:Z:99:ALA:HB2	26:Z:233:TYR:CE2	2.42	0.55
28:2:25:LYS:HE2	37:3:7213:HOH:O	2.06	0.55
1:A:1825:U:O4'	1:A:1999:C:H5''	2.06	0.55
1:A:1862:C:H1'	37:A:7195:HOH:O	2.07	0.55
1:A:2897:C:O2'	1:A:2898:G:H5'	2.07	0.55
4:D:320:GLN:HG3	4:D:321:PRO:HD2	1.88	0.55
10:J:71:TYR:C	10:J:73:GLN:N	2.58	0.55
15:O:22:GLN:HG2	15:O:26:LEU:HD22	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:44:ASN:OD1	16:P:65:LEU:HB2	2.07	0.55
37:A:3051:HOH:O	19:S:83:LYS:HB3	2.06	0.55
26:Z:144:ARG:CZ	37:Z:8610:HOH:O	2.54	0.55
1:A:2326:U:H4'	1:A:2412:G:C4'	2.37	0.55
4:D:140:LEU:HD23	37:D:8581:HOH:O	2.07	0.55
8:H:100:ASP:HB3	37:H:5691:HOH:O	2.07	0.55
1:A:2365:G:H4'	18:R:45:PRO:O	2.06	0.55
1:A:1205:U:C2'	1:A:1206:U:H5'	2.32	0.55
1:A:1653:A:N6	37:A:4237:HOH:O	2.40	0.55
1:A:694:A:H2'	1:A:695:C:H5'	1.89	0.55
4:D:190:MET:HE2	4:D:194:PHE:HD1	1.72	0.55
4:D:1:PRO:O	4:D:2:GLN:HB2	2.07	0.55
7:G:11:VAL:CG1	7:G:12:ASP:N	2.69	0.55
1:A:2404:G:O3'	37:A:6569:HOH:O	2.18	0.54
1:A:2679:G:H2'	1:A:2681:A:OP2	2.07	0.54
3:C:105:VAL:HG12	3:C:106:CYS:N	2.22	0.54
4:D:314:ALA:HB3	4:D:317:PRO:HG3	1.89	0.54
4:D:66:GLU:OE1	4:D:328:ARG:HD2	2.07	0.54
12:L:37:TYR:CD2	37:L:7169:HOH:O	2.53	0.54
1:A:902:G:N7	13:M:18:HIS:HD2	2.05	0.54
17:Q:13:VAL:HG11	17:Q:40:VAL:HG11	1.87	0.54
26:Z:107:PRO:HB3	26:Z:182:PHE:CD2	2.43	0.54
29:3:18:ASN:HD21	29:3:40:ARG:H	1.53	0.54
1:A:2760:C:H5''	37:A:5303:HOH:O	2.07	0.54
1:A:2821:C:H4'	4:D:116:PRO:HB3	1.88	0.54
8:H:91:VAL:CG1	8:H:92:GLY:H	2.17	0.54
14:N:154:ARG:HG3	37:N:8613:HOH:O	2.07	0.54
1:A:1159:G:H21	1:A:1189:A:H8	1.53	0.54
1:A:1269:G:H2'	1:A:1270:U:C6	2.43	0.54
1:A:1562:C:O2	1:A:1562:C:H2'	2.07	0.54
1:A:1882:C:O2'	1:A:2012:U:OP2	2.23	0.54
1:A:281:U:O2'	1:A:282:C:H5'	2.08	0.54
1:A:401:C:P	37:A:5766:HOH:O	2.66	0.54
1:A:739:G:N7	37:A:7523:HOH:O	2.38	0.54
31:A:9001:SPR:H6A3	31:A:9001:SPR:C2B	2.22	0.54
5:E:115:LEU:HD21	5:E:243:VAL:HG13	1.88	0.54
6:F:50:VAL:O	6:F:71:ALA:HA	2.07	0.54
8:H:21:GLU:O	8:H:24:ARG:HG3	2.06	0.54
21:U:106:GLU:HG3	37:U:4913:HOH:O	2.06	0.54
23:W:49:LEU:O	23:W:53:ILE:HG13	2.06	0.54
1:A:1164:U:O4'	1:A:1165:G:OP1	2.25	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:G:H2'	14:N:192:ALA:HB3	1.88	0.54
5:E:235:PHE:HE2	5:E:243:VAL:HG21	1.72	0.54
1:A:1470:A:OP1	14:N:93:ARG:HD2	2.08	0.54
15:O:91:ARG:HG3	15:O:186:LEU:HD23	1.89	0.54
27:1:39:CYS:HA	27:1:47:LEU:CD1	2.34	0.54
1:A:2359:G:H3'	37:A:5662:HOH:O	2.08	0.54
4:D:305:ASP:O	4:D:306:LYS:CB	2.55	0.54
5:E:129:HIS:HE1	5:E:231:ARG:HA	1.72	0.54
6:F:170:TYR:O	6:F:171:ASP:HB3	2.06	0.54
10:J:147:ARG:HA	10:J:150:LYS:HZ2	1.73	0.54
10:J:71:TYR:O	10:J:73:GLN:N	2.40	0.54
14:N:37:VAL:HG13	14:N:63:VAL:HG11	1.90	0.54
1:A:2894:C:O2'	1:A:2895:C:H5'	2.07	0.54
7:G:69:ILE:HA	7:G:72:MET:HE3	1.90	0.54
10:J:136:VAL:HG22	10:J:137:ASN:O	2.07	0.54
13:M:104:ASP:O	13:M:105:TYR:HB3	2.05	0.54
15:O:155:GLU:O	15:O:156:GLU:HG3	2.08	0.54
24:X:6:GLN:HB2	24:X:26:ILE:CD1	2.36	0.54
28:2:8:GLN:HE22	28:2:11:LYS:HZ2	1.56	0.54
1:A:1330:A:H5''	1:A:1331:A:OP2	2.08	0.54
1:A:1847:A:OP1	3:C:175:LYS:NZ	2.41	0.54
1:A:204:A:H2'	1:A:205:U:H5'	1.89	0.54
1:A:661:G:C5	1:A:686:A:C2	2.95	0.54
4:D:75:GLU:C	4:D:77:PRO:HD3	2.28	0.54
5:E:154:VAL:O	5:E:158:GLU:HG3	2.07	0.54
7:G:32:ARG:O	7:G:33:LEU:HD23	2.07	0.54
10:J:13:ALA:HA	10:J:91:HIS:HE1	1.72	0.54
19:S:111:ILE:HG23	19:S:145:LEU:HD11	1.90	0.54
22:V:13:ILE:HG12	22:V:32:CYS:HB2	1.89	0.54
22:V:52:THR:CG2	22:V:54:THR:HB	2.38	0.54
26:Z:112:GLU:CD	26:Z:115:ARG:NH1	2.61	0.54
1:A:1887:U:OP1	27:1:21:LYS:HG3	2.07	0.54
1:A:470:U:O2'	28:2:16:HIS:HD2	1.90	0.54
1:A:1878:G:C1'	37:A:6090:HOH:O	2.54	0.54
1:A:2082:G:O2'	1:A:2083:A:H5'	2.07	0.54
1:A:541:C:O2'	1:A:542:A:H5''	2.07	0.54
1:A:775:G:OP1	28:2:16:HIS:HE1	1.91	0.54
3:C:175:LYS:HE2	37:C:8579:HOH:O	2.07	0.54
4:D:56:ASP:OD1	4:D:322:ARG:HB3	2.07	0.54
1:A:338:C:H4'	5:E:174:ILE:HD12	1.86	0.54
6:F:163:VAL:HA	37:F:6326:HOH:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:139:ASP:N	10:J:140:PRO:CD	2.69	0.54
14:N:123:ASP:C	14:N:123:ASP:OD1	2.46	0.54
1:A:1268:C:H2'	1:A:1269:G:H8	1.73	0.54
6:F:10:PHE:CG	6:F:11:HIS:N	2.76	0.54
10:J:26:LYS:HD3	10:J:89:PRO:CG	2.38	0.54
14:N:154:ARG:HD3	37:N:8643:HOH:O	2.07	0.54
37:A:5766:HOH:O	14:N:170:CYS:SG	2.59	0.54
15:O:182:GLY:N	37:O:8572:HOH:O	2.39	0.54
1:A:1266:U:H4'	26:Z:115:ARG:HH21	1.71	0.54
30:4:48:ASN:ND2	30:4:50:GLY:H	2.06	0.54
1:A:1695:G:C6	1:A:1696:U:C4	2.96	0.54
1:A:921:G:H4'	1:A:924:G:N1	2.23	0.54
1:A:963:C:O5'	1:A:963:C:H6	1.91	0.54
3:C:105:VAL:HG11	3:C:154:ALA:HB1	1.88	0.54
3:C:171:LYS:NZ	37:C:8526:HOH:O	2.23	0.54
4:D:251:VAL:HG23	4:D:252:PRO:HD2	1.89	0.54
4:D:55:ASN:HB3	4:D:64:GLY:H	1.73	0.54
6:F:154:LYS:H	6:F:154:LYS:CD	2.15	0.54
11:K:22:VAL:O	11:K:26:VAL:HG23	2.08	0.54
22:V:11:THR:HG22	22:V:53:ASP:OD2	2.08	0.54
8:H:47:LEU:HB2	8:H:108:LEU:HD11	1.91	0.53
10:J:139:ASP:H	10:J:140:PRO:HD3	1.68	0.53
13:M:104:ASP:HB3	37:M:8564:HOH:O	2.08	0.53
14:N:122:GLU:OE2	14:N:127:LYS:HE2	2.08	0.53
24:X:26:ILE:O	24:X:26:ILE:CG1	2.56	0.53
26:Z:187:VAL:HB	37:Z:8570:HOH:O	2.08	0.53
1:A:1007:A:H2'	10:J:19:TYR:CZ	2.44	0.53
1:A:119:A:H2'	1:A:120:A:H5''	1.89	0.53
1:A:558:C:H2'	1:A:559:U:H5'	1.90	0.53
1:A:922:A:N7	1:A:2281:C:H5'	2.23	0.53
8:H:99:THR:O	8:H:99:THR:HG23	2.07	0.53
10:J:130:HIS:CG	10:J:133:ILE:HD11	2.43	0.53
10:J:26:LYS:HD2	10:J:28:ILE:CG1	2.37	0.53
11:K:107:ASN:C	11:K:107:ASN:HD22	2.11	0.53
13:M:133:VAL:HB	37:M:8558:HOH:O	2.08	0.53
22:V:49:LEU:CD1	37:V:3805:HOH:O	2.56	0.53
27:1:39:CYS:CB	27:1:47:LEU:HD21	2.37	0.53
1:A:1176:C:H1'	37:A:3905:HOH:O	2.08	0.53
1:A:1636:G:O2'	1:A:1637:A:H5'	2.08	0.53
1:A:39:G:N2	1:A:444:C:C2	2.77	0.53
2:B:3041:C:C6	6:F:50:VAL:HG21	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:117:LYS:HB2	37:J:8326:HOH:O	2.08	0.53
11:K:4:ALA:N	37:K:8572:HOH:O	2.41	0.53
16:P:59:VAL:HG23	16:P:111:VAL:HG23	1.89	0.53
22:V:47:ARG:CG	37:V:4381:HOH:O	2.55	0.53
27:1:46:LYS:O	27:1:57:CYS:HA	2.08	0.53
1:A:1308:A:H5'	37:A:6904:HOH:O	2.08	0.53
1:A:154:C:H2'	1:A:155:C:C6	2.42	0.53
1:A:2073:G:OP2	1:A:2490:A:H5'	2.08	0.53
1:A:553:G:O4'	1:A:1325:G:H5'	2.08	0.53
4:D:275:GLY:O	4:D:291:ASP:HA	2.08	0.53
6:F:93:LEU:HB3	6:F:97:GLN:OE1	2.09	0.53
1:A:2055:A:H5'	19:S:134:SER:HB2	1.90	0.53
20:T:81:ILE:HG23	37:T:8336:HOH:O	2.07	0.53
21:U:38:ARG:HG3	21:U:38:ARG:NH1	2.23	0.53
24:X:122:ARG:HH22	24:X:154:ARG:C	2.12	0.53
1:A:2459:G:OP2	30:4:64:LYS:HD2	2.07	0.53
1:A:657:G:OP1	5:E:27:ARG:NH2	2.29	0.53
37:A:9544:HOH:O	4:D:267:LYS:HD3	2.07	0.53
37:A:6290:HOH:O	6:F:55:LYS:HB2	2.08	0.53
7:G:21:THR:HG23	7:G:30:THR:OG1	2.09	0.53
8:H:39:SER:HB3	8:H:45:ALA:HB2	1.89	0.53
8:H:13:GLU:OE2	8:H:78:GLU:HG2	2.09	0.53
10:J:45:GLN:HG3	10:J:135:TRP:NE1	2.23	0.53
11:K:107:ASN:HD22	11:K:109:TYR:H	1.54	0.53
14:N:154:ARG:NE	37:N:8643:HOH:O	2.42	0.53
14:N:87:MET:SD	37:N:8533:HOH:O	2.58	0.53
1:A:396:U:OP2	30:4:38:ARG:NH1	2.42	0.53
1:A:1189:A:H1'	1:A:1209:C:C1'	2.39	0.53
1:A:1209:C:H2'	1:A:1210:G:C8	2.40	0.53
1:A:1250:C:O2'	1:A:1251:C:H5'	2.08	0.53
1:A:2121:G:C2'	1:A:2122:C:H5'	2.38	0.53
1:A:2414:A:H2'	1:A:2415:A:C8	2.43	0.53
3:C:217:ARG:CG	3:C:217:ARG:HH11	2.21	0.53
6:F:23:VAL:CG2	6:F:23:VAL:O	2.55	0.53
14:N:87:MET:HB2	14:N:91:ILE:CD1	2.39	0.53
17:Q:103:THR:O	17:Q:107:GLU:HG3	2.09	0.53
17:Q:115:SER:O	17:Q:117:SER:N	2.42	0.53
1:A:1527:A:H1'	1:A:1528:A:C8	2.43	0.53
1:A:2613:G:O2'	1:A:2614:C:H5'	2.08	0.53
1:A:2676:C:H4'	11:K:70:PHE:HE1	1.71	0.53
3:C:109:GLU:HG2	3:C:116:GLY:N	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:140:LEU:HB3	3:C:141:PRO:HD2	1.91	0.53
3:C:200:PRO:HG2	3:C:225:VAL:HG21	1.90	0.53
8:H:50:VAL:CG2	8:H:63:ILE:HG21	2.39	0.53
1:A:1164:U:C4'	1:A:1165:G:OP1	2.50	0.53
1:A:1166:A:H1'	1:A:1192:A:N1	2.23	0.53
1:A:1947:G:N2	1:A:1966:U:C2	2.77	0.53
1:A:329:A:OP1	5:E:205:ARG:NE	2.37	0.53
5:E:236:THR:O	5:E:237:GLU:C	2.47	0.53
7:G:20:ILE:HD12	7:G:33:LEU:HD12	1.90	0.53
14:N:61:ILE:N	14:N:61:ILE:HD12	2.24	0.53
22:V:14:GLU:OE1	22:V:15:PRO:HD2	2.09	0.53
25:Y:73:ARG:O	25:Y:85:VAL:HG13	2.09	0.53
1:A:2634:G:O2'	1:A:2635:A:H5'	2.09	0.53
3:C:191:GLY:HA2	3:C:194:MET:HE3	1.90	0.53
37:A:7435:HOH:O	5:E:188:ARG:HD2	2.09	0.53
1:A:449:A:N7	5:E:43:LYS:HG2	2.23	0.53
19:S:115:ALA:O	19:S:143:VAL:HG23	2.09	0.53
19:S:18:LEU:HG	19:S:91:LEU:HD13	1.90	0.53
21:U:48:VAL:HG22	21:U:97:ARG:O	2.09	0.53
1:A:1185:U:H5'	37:A:7445:HOH:O	2.08	0.53
1:A:1525:G:H5'	1:A:1526:A:OP2	2.09	0.53
1:A:2405:C:P	37:A:6569:HOH:O	2.66	0.53
4:D:82:VAL:HG12	4:D:82:VAL:O	2.09	0.53
4:D:7:ARG:CD	4:D:9:GLY:O	2.57	0.53
7:G:15:GLN:HG2	7:G:19:ASP:O	2.09	0.53
15:O:47:LEU:HD13	15:O:97:VAL:HG11	1.91	0.53
17:Q:58:SER:HB3	37:Q:4744:HOH:O	2.08	0.53
24:X:90:TYR:CE2	24:X:99:ALA:HB2	2.44	0.53
1:A:1667:A:H2'	1:A:1668:U:C6	2.44	0.52
1:A:2326:U:H4'	1:A:2412:G:H4'	1.90	0.52
3:C:164:ARG:NE	37:C:8593:HOH:O	2.41	0.52
7:G:43:ASP:HA	37:G:5864:HOH:O	2.08	0.52
1:A:1733:A:C6	1:A:1734:C:C2	2.97	0.52
1:A:88:G:H8	1:A:88:G:H5'	1.74	0.52
3:C:37:VAL:HG22	37:C:8600:HOH:O	2.09	0.52
14:N:115:LEU:C	14:N:115:LEU:HD13	2.30	0.52
1:A:656:G:OP2	16:P:37:ARG:HD2	2.09	0.52
17:Q:18:LYS:O	17:Q:21:VAL:HG22	2.08	0.52
17:Q:38:GLU:HA	17:Q:41:ARG:HH11	1.73	0.52
24:X:38:THR:HG22	24:X:39:ASP:N	2.25	0.52
30:4:11:CYS:HB2	30:4:20:HIS:CE1	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1041:U:C2'	1:A:1042:U:H5'	2.39	0.52
1:A:1200:A:C4'	37:A:7318:HOH:O	2.57	0.52
1:A:1375:A:O2'	1:A:1376:G:H5'	2.10	0.52
1:A:1490:G:OP2	37:A:3628:HOH:O	2.18	0.52
1:A:2735:U:H2'	1:A:2736:U:C6	2.45	0.52
1:A:820:G:H5'	1:A:821:U:H5'	1.91	0.52
2:B:3020:G:H3'	37:B:2984:HOH:O	2.09	0.52
2:B:3092:G:H2'	2:B:3093:A:C8	2.45	0.52
5:E:1:MET:HG2	5:E:2:GLN:N	2.23	0.52
6:F:64:ARG:O	6:F:67:ASP:OD2	2.26	0.52
10:J:117:LYS:O	10:J:119:VAL:HG13	2.09	0.52
14:N:39:ARG:HA	14:N:63:VAL:HG22	1.92	0.52
15:O:170:GLU:O	15:O:174:GLU:HG3	2.09	0.52
15:O:5:ARG:HG3	18:R:18:PRO:CB	2.39	0.52
37:A:3737:HOH:O	21:U:9:LYS:HD3	2.09	0.52
24:X:137:GLN:HE21	24:X:141:HIS:CE1	2.20	0.52
28:2:37:CYS:SG	28:2:39:PHE:HB2	2.49	0.52
1:A:1197:G:N2	37:A:6202:HOH:O	2.42	0.52
1:A:628:A:C8	1:A:2071:C:N4	2.78	0.52
1:A:256:C:H2'	1:A:257:G:O4'	2.09	0.52
1:A:2787:C:H5	37:A:4602:HOH:O	1.91	0.52
1:A:738:G:H3'	37:A:7019:HOH:O	2.08	0.52
4:D:307:ARG:HH11	4:D:307:ARG:CG	2.22	0.52
10:J:65:ARG:NH1	37:J:8374:HOH:O	2.42	0.52
12:L:34:VAL:HG22	12:L:47:ALA:HB2	1.90	0.52
27:1:30:GLU:HB3	27:1:34:LYS:HE3	1.92	0.52
1:A:1079:A:N1	1:A:2068:G:O2'	2.39	0.52
1:A:1127:C:C5	1:A:1128:U:C4	2.97	0.52
1:A:1166:A:H61	1:A:1180:U:H3	1.55	0.52
2:B:3044:A:H1'	6:F:76:ARG:NH2	2.24	0.52
1:A:2780:C:H1'	7:G:143:GLN:NE2	2.24	0.52
7:G:23:GLU:HG2	7:G:28:SER:CB	2.40	0.52
7:G:7:ILE:HD11	7:G:11:VAL:O	2.09	0.52
13:M:143:THR:CG2	13:M:144:ASP:H	2.22	0.52
37:A:9079:HOH:O	14:N:172:GLY:HA2	2.09	0.52
27:1:59:HIS:HA	37:1:8444:HOH:O	2.10	0.52
1:A:381:G:H5''	37:A:4291:HOH:O	2.08	0.52
1:A:82:C:OP1	21:U:67:LEU:HB2	2.09	0.52
1:A:1861:C:H4'	3:C:6:GLY:O	2.10	0.52
6:F:19:GLU:HG3	37:F:6165:HOH:O	2.09	0.52
7:G:11:VAL:HG12	7:G:12:ASP:H	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:101:ASN:O	12:L:102:GLU:CB	2.58	0.52
13:M:24:ALA:HB2	13:M:30:ARG:HD2	1.91	0.52
14:N:38:VAL:C	14:N:63:VAL:HG13	2.30	0.52
37:A:4332:HOH:O	16:P:37:ARG:HG3	2.10	0.52
1:A:2768:A:O2'	1:A:2769:C:H5'	2.10	0.52
1:A:432:G:O2'	1:A:433:C:H5'	2.09	0.52
1:A:921:G:H4'	1:A:924:G:C6	2.45	0.52
6:F:91:ALA:HB1	37:F:5198:HOH:O	2.10	0.52
8:H:28:ALA:CB	8:H:99:THR:HG23	2.40	0.52
10:J:132:PHE:O	10:J:133:ILE:HD13	2.10	0.52
10:J:46:VAL:HG12	10:J:146:TRP:CZ3	2.43	0.52
24:X:13:MET:HE1	24:X:18:GLN:HA	1.90	0.52
29:3:48:ASP:O	29:3:49:GLU:HB2	2.10	0.52
30:4:51:LYS:NZ	37:4:8531:HOH:O	2.41	0.52
1:A:1180:U:H2'	1:A:1181:A:O4'	2.10	0.52
1:A:1205:U:C2'	1:A:1206:U:C5'	2.88	0.52
1:A:2123:A:H5'	14:N:89:ASN:ND2	2.25	0.52
1:A:2435:U:H1'	37:A:5404:HOH:O	2.09	0.52
1:A:316:A:N3	1:A:336:G:O2'	2.41	0.52
2:B:3006:C:C5'	15:O:37:ARG:HH12	2.19	0.52
5:E:104:ASP:O	5:E:108:GLN:HG3	2.09	0.52
6:F:49:PRO:HG3	37:F:5828:HOH:O	2.08	0.52
8:H:91:VAL:CG1	8:H:92:GLY:N	2.70	0.52
10:J:53:PRO:HG3	10:J:127:GLY:H	1.75	0.52
14:N:115:LEU:HD13	14:N:116:ASN:HB2	1.91	0.52
15:O:110:THR:HB	15:O:113:SER:OG	2.10	0.52
17:Q:98:ILE:HD13	17:Q:98:ILE:O	2.10	0.52
27:1:47:LEU:CD2	27:1:57:CYS:HB2	2.40	0.52
1:A:1398:G:H2'	1:A:1399:A:C8	2.45	0.52
1:A:564:G:H1'	37:A:6280:HOH:O	2.10	0.52
4:D:27:ASN:HD22	4:D:27:ASN:H	1.57	0.52
6:F:23:VAL:HG21	6:F:45:THR:HG21	1.91	0.52
14:N:59:GLY:CA	14:N:141:ILE:HD11	2.39	0.52
1:A:105:G:O2'	1:A:106:A:H5'	2.10	0.52
1:A:1189:A:O2'	1:A:1208:C:H2'	2.10	0.52
1:A:2256:G:H2'	1:A:2257:G:C5'	2.40	0.52
1:A:151:A:C2	1:A:442:A:C8	2.98	0.52
1:A:820:G:C5	3:C:171:LYS:HB2	2.45	0.52
3:C:88:ILE:HD13	3:C:100:PRO:CD	2.40	0.52
10:J:47:GLU:CB	10:J:133:ILE:HD13	2.34	0.52
10:J:56:ILE:HG21	10:J:61:LEU:HD13	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:A:4675:HOH:O	27:1:54:ILE:HD12	2.09	0.51
1:A:2638:G:H5'	37:A:4906:HOH:O	2.09	0.51
1:A:283:U:H5''	1:A:284:C:OP2	2.11	0.51
4:D:14:GLY:HA2	4:D:15:PRO:C	2.30	0.51
5:E:109:LEU:HD12	5:E:109:LEU:O	2.10	0.51
9:I:16:LYS:O	9:I:20:VAL:HG23	2.10	0.51
12:L:10:GLN:NE2	12:L:10:GLN:N	2.40	0.51
15:O:87:LEU:CD1	15:O:186:LEU:HD21	2.34	0.51
17:Q:143:ALA:HA	37:Q:5521:HOH:O	2.08	0.51
18:R:40:HIS:HD2	18:R:60:THR:OG1	1.93	0.51
24:X:28:HIS:HD2	24:X:31:HIS:CE1	2.27	0.51
1:A:2468:A:H61	30:4:48:ASN:ND2	2.03	0.51
1:A:2672:C:H1'	37:D:8637:HOH:O	2.10	0.51
1:A:2812:A:C2	1:A:2814:A:N6	2.74	0.51
10:J:150:LYS:HE2	37:J:8368:HOH:O	2.09	0.51
10:J:39:GLY:O	10:J:41:THR:N	2.44	0.51
12:L:55:VAL:CG1	12:L:56:SER:N	2.74	0.51
14:N:59:GLY:C	14:N:141:ILE:HD11	2.31	0.51
14:N:67:ILE:HG21	14:N:97:ILE:HG23	1.93	0.51
16:P:42:GLU:HB2	37:P:2176:HOH:O	2.09	0.51
1:A:2429:A:H2'	1:A:2430:A:C8	2.45	0.51
1:A:514:G:OP1	1:A:514:G:H2'	2.10	0.51
3:C:8:ARG:NH1	37:C:8554:HOH:O	2.30	0.51
4:D:79:MET:HE3	4:D:144:THR:HG21	1.93	0.51
5:E:246:ARG:HH11	5:E:246:ARG:HB3	1.73	0.51
5:E:85:LYS:CE	37:E:8328:HOH:O	2.55	0.51
21:U:69:LYS:O	21:U:71:VAL:HG23	2.11	0.51
25:Y:9:VAL:HG13	25:Y:88:GLU:OE2	2.10	0.51
37:A:4163:HOH:O	26:Z:186:ARG:HD2	2.10	0.51
26:Z:186:ARG:NH1	26:Z:186:ARG:HG2	2.22	0.51
1:A:371:U:H2'	1:A:372:A:C8	2.44	0.51
1:A:603:A:H4'	1:A:604:G:O5'	2.09	0.51
3:C:132:ASP:OD1	3:C:133:ARG:N	2.42	0.51
4:D:307:ARG:HH11	4:D:307:ARG:CB	2.23	0.51
5:E:162:VAL:HG12	5:E:162:VAL:O	2.09	0.51
22:V:9:CYS:SG	37:V:6796:HOH:O	2.59	0.51
24:X:119:HIS:HD2	24:X:120:PRO:O	1.92	0.51
26:Z:142:SER:OG	37:Z:8610:HOH:O	2.18	0.51
27:1:61:GLY:HA3	37:1:8429:HOH:O	2.09	0.51
37:A:7116:HOH:O	28:2:1:THR:HB	2.09	0.51
1:A:1450:C:C4'	1:A:1451:C:OP2	2.58	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1654:U:H2'	3:C:47:HIS:CD2	2.46	0.51
1:A:2284:G:H5'	37:A:9437:HOH:O	2.11	0.51
1:A:2392:C:N3	37:A:4825:HOH:O	2.34	0.51
1:A:2408:A:H2	37:A:3080:HOH:O	1.92	0.51
1:A:2466:G:C5'	37:A:3625:HOH:O	2.50	0.51
1:A:2478:U:O2'	1:A:2479:A:H5'	2.10	0.51
1:A:2724:U:H2'	1:A:2725:G:O4'	2.10	0.51
1:A:424:C:H2'	1:A:425:U:C6	2.44	0.51
3:C:36:ASP:HA	3:C:83:GLY:HA3	1.93	0.51
4:D:63:GLU:HG3	4:D:63:GLU:O	2.11	0.51
6:F:11:HIS:C	6:F:13:MET:H	2.13	0.51
37:A:4543:HOH:O	14:N:83:SER:HA	2.10	0.51
16:P:96:VAL:HA	37:P:4258:HOH:O	2.10	0.51
20:T:29:ASP:OD1	20:T:31:ARG:NH1	2.44	0.51
21:U:48:VAL:CG1	21:U:96:VAL:HG13	2.41	0.51
25:Y:25:ARG:CD	37:Y:3861:HOH:O	2.50	0.51
1:A:1850:U:H2'	1:A:1851:G:H8	1.75	0.51
1:A:2269:C:H2'	1:A:2270:G:H5'	1.92	0.51
4:D:119:HIS:O	4:D:121:PRO:HD3	2.10	0.51
4:D:144:THR:HG22	4:D:145:HIS:N	2.25	0.51
6:F:65:GLU:HG3	37:F:6752:HOH:O	2.10	0.51
12:L:75:ARG:CZ	37:L:4172:HOH:O	2.58	0.51
14:N:114:VAL:HB	14:N:159:THR:HG23	1.93	0.51
14:N:55:LYS:HB2	14:N:60:ILE:CD1	2.41	0.51
17:Q:7:LYS:CD	17:Q:21:VAL:CG2	2.89	0.51
1:A:538:C:OP2	26:Z:134:HIS:HE1	1.93	0.51
1:A:1669:A:H2'	1:A:1670:G:H8	1.75	0.51
1:A:2315:C:H4'	1:A:2425:A:C6	2.46	0.51
4:D:43:GLY:O	4:D:308:LEU:HD12	2.11	0.51
8:H:101:ALA:HB2	8:H:108:LEU:HD22	1.92	0.51
17:Q:115:SER:HG	17:Q:118:GLN:HG3	1.74	0.51
1:A:56:G:H5''	23:W:50:ARG:HH12	1.74	0.51
27:1:26:VAL:O	27:1:30:GLU:HG3	2.10	0.51
27:1:42:CYS:SG	27:1:43:GLY:N	2.84	0.51
1:A:1189:A:H1'	1:A:1209:C:O4'	2.11	0.51
1:A:1299:G:O6	13:M:6:ARG:HD3	2.11	0.51
1:A:1329:A:N1	34:A:8513:CL:CL	2.81	0.51
4:D:103:ASP:HB2	37:D:8593:HOH:O	2.10	0.51
4:D:146:THR:O	4:D:159:PRO:HB3	2.10	0.51
6:F:59:GLY:C	6:F:61:PHE:H	2.14	0.51
11:K:6:PHE:O	11:K:8:ALA:N	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:13:HIS:NE2	37:M:8522:HOH:O	2.35	0.51
17:Q:21:VAL:O	17:Q:21:VAL:HG23	2.09	0.51
1:A:2247:C:H5''	37:A:7322:HOH:O	2.11	0.51
1:A:2769:C:O2'	1:A:2770:G:H5'	2.11	0.51
1:A:2756:U:H3	1:A:2896:A:H2	1.55	0.51
1:A:382:U:C5	1:A:406:G:N2	2.78	0.51
1:A:489:A:C8	21:U:82:THR:CG2	2.94	0.51
4:D:2:GLN:NE2	37:D:8622:HOH:O	2.44	0.51
5:E:212:VAL:HG23	5:E:212:VAL:O	2.11	0.51
6:F:57:THR:HG23	6:F:63:ILE:CB	2.41	0.51
7:G:68:HIS:O	7:G:72:MET:HG3	2.11	0.51
13:M:21:ARG:N	37:M:8535:HOH:O	2.44	0.51
24:X:122:ARG:HH11	24:X:122:ARG:CG	2.15	0.51
26:Z:154:ARG:NH1	26:Z:155:ARG:HG3	2.26	0.51
1:A:113:A:H3'	1:A:114:A:C5'	2.41	0.51
1:A:1192:A:H3'	1:A:1193:A:H5'	1.92	0.51
1:A:461:C:H2'	37:A:3974:HOH:O	2.11	0.51
4:D:297:VAL:HB	37:D:8606:HOH:O	2.11	0.51
7:G:157:LYS:NZ	37:G:2401:HOH:O	2.44	0.51
10:J:57:ARG:HG3	10:J:57:ARG:HH11	1.76	0.51
10:J:35:ASN:ND2	10:J:80:ASN:HA	2.26	0.51
1:A:1119:G:C8	11:K:52:GLN:NE2	2.79	0.51
12:L:29:LEU:HB3	12:L:55:VAL:CG1	2.28	0.51
12:L:45:PRO:HB2	37:L:7169:HOH:O	2.11	0.51
29:3:40:ARG:HH11	29:3:40:ARG:HG2	1.76	0.50
1:A:1209:C:C2	1:A:1210:G:C8	2.99	0.50
1:A:154:C:P	14:N:188:ARG:HH12	2.34	0.50
1:A:2321:A:O2'	1:A:2322:U:H3'	2.11	0.50
1:A:639:A:C2	1:A:1363:G:C2	2.99	0.50
3:C:191:GLY:HA2	3:C:194:MET:CE	2.41	0.50
4:D:16:ARG:NE	37:D:8556:HOH:O	2.28	0.50
4:D:162:MET:CE	4:D:310:ARG:HD3	2.41	0.50
6:F:44:ILE:HG12	6:F:83:PHE:HE1	1.74	0.50
8:H:47:LEU:HD22	8:H:108:LEU:CD1	2.41	0.50
12:L:109:LEU:HD13	12:L:113:ILE:HD11	1.93	0.50
12:L:34:VAL:HB	37:L:7169:HOH:O	2.11	0.50
16:P:98:LEU:O	16:P:102:ILE:HG13	2.11	0.50
21:U:75:GLU:O	21:U:76:ASP:HB2	2.10	0.50
24:X:48:VAL:O	24:X:48:VAL:CG1	2.58	0.50
1:A:1041:U:H2'	1:A:1042:U:C5'	2.41	0.50
1:A:1200:A:H4'	37:A:7318:HOH:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1189:A:H1'	1:A:1209:C:H1'	1.93	0.50
1:A:790:A:H1'	1:A:1710:A:H2'	1.92	0.50
1:A:2912:C:OP2	37:A:5528:HOH:O	2.20	0.50
1:A:344:C:H2'	1:A:345:G:O4'	2.10	0.50
1:A:445:U:H1'	37:A:7314:HOH:O	2.12	0.50
8:H:58:GLU:OE1	14:N:27:ARG:NH2	2.41	0.50
11:K:130:VAL:HG12	11:K:131:THR:N	2.24	0.50
24:X:38:THR:HG22	24:X:39:ASP:H	1.77	0.50
1:A:1353:C:OP2	37:A:4516:HOH:O	2.19	0.50
1:A:1690:C:C5	1:A:1692:C:C4	2.99	0.50
1:A:1700:C:OP2	37:A:6004:HOH:O	2.19	0.50
1:A:204:A:C2'	1:A:205:U:H5'	2.41	0.50
1:A:2064:U:H4'	1:A:2653:A:P	2.51	0.50
3:C:211:LYS:HB3	3:C:212:PRO:CD	2.35	0.50
5:E:46:TYR:CE2	5:E:98:ARG:NH1	2.79	0.50
7:G:84:MET:HE1	7:G:148:ILE:HD12	1.93	0.50
7:G:15:GLN:NE2	7:G:40:VAL:O	2.44	0.50
1:A:244:C:OP2	8:H:38:LYS:HE3	2.12	0.50
37:A:3641:HOH:O	14:N:79:LYS:HD2	2.11	0.50
21:U:20:HIS:ND1	21:U:41:ARG:NE	2.54	0.50
25:Y:71:ARG:CD	37:Y:2171:HOH:O	2.59	0.50
30:4:57:GLY:HA2	37:4:8528:HOH:O	2.10	0.50
1:A:1370:G:OP1	19:S:64:SER:OG	2.29	0.50
1:A:1787:C:H4'	1:A:2883:A:O4'	2.11	0.50
1:A:2271:G:H2'	1:A:2271:G:N3	2.27	0.50
1:A:2314:G:O2'	1:A:2315:C:H5'	2.10	0.50
1:A:2361:A:H5''	37:A:9002:HOH:O	2.11	0.50
1:A:454:U:O4	37:A:9151:HOH:O	2.19	0.50
1:A:778:C:OP1	37:A:5516:HOH:O	2.20	0.50
3:C:51:ARG:HB2	37:C:8610:HOH:O	2.11	0.50
5:E:234:VAL:HG22	5:E:234:VAL:O	2.11	0.50
6:F:58:VAL:HG12	6:F:59:GLY:N	2.26	0.50
10:J:47:GLU:CB	10:J:133:ILE:CD1	2.86	0.50
10:J:166:ASN:N	10:J:166:ASN:ND2	2.59	0.50
14:N:84:LYS:O	14:N:87:MET:HG2	2.10	0.50
15:O:37:ARG:NH2	37:O:8534:HOH:O	2.44	0.50
28:2:28:HIS:CE1	28:2:31:LYS:HE2	2.47	0.50
1:A:2464:C:H5''	1:A:2465:A:OP1	2.11	0.50
1:A:2694:A:H4'	7:G:91:PHE:HE1	1.76	0.50
5:E:118:THR:CG2	5:E:137:PRO:HB3	2.42	0.50
6:F:40:ILE:HG23	37:F:5583:HOH:O	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:134:GLU:HA	13:M:138:GLY:O	2.12	0.50
14:N:134:ILE:O	14:N:136:PRO:HD3	2.12	0.50
15:O:34:LEU:HD22	15:O:129:ILE:HD13	1.93	0.50
15:O:64:SER:C	15:O:66:LEU:H	2.15	0.50
27:1:59:HIS:CE1	37:1:8441:HOH:O	2.64	0.50
1:A:88:G:C8	29:3:28:LYS:HB2	2.46	0.50
1:A:1666:C:C2'	1:A:1667:A:C5'	2.90	0.50
3:C:36:ASP:O	3:C:38:ILE:N	2.45	0.50
6:F:11:HIS:O	6:F:12:GLU:HB3	2.10	0.50
6:F:27:ILE:HD11	6:F:37:ALA:CB	2.41	0.50
17:Q:38:GLU:HA	17:Q:41:ARG:NH1	2.27	0.50
26:Z:106:THR:HG23	26:Z:107:PRO:HD2	1.93	0.50
1:A:1834:C:H2'	1:A:1840:A:H62	1.75	0.50
1:A:424:C:H2'	1:A:425:U:H6	1.77	0.50
1:A:559:U:H2'	1:A:560:C:O4'	2.12	0.50
3:C:149:ASP:OD1	3:C:151:GLN:HB2	2.11	0.50
4:D:248:ARG:NH2	37:D:8525:HOH:O	2.44	0.50
10:J:118:PRO:HD2	37:J:8326:HOH:O	2.10	0.50
10:J:72:VAL:HG11	10:J:81:TYR:CZ	2.47	0.50
19:S:29:LYS:NZ	37:S:8541:HOH:O	2.44	0.50
24:X:88:THR:CG2	24:X:110:GLN:NE2	2.70	0.50
1:A:1845:A:OP2	3:C:190:ARG:NH1	2.43	0.50
1:A:2099:G:H1	31:A:9001:SPR:HO2A	1.54	0.50
1:A:2265:U:H2'	1:A:2266:A:C8	2.47	0.50
1:A:2505:G:C2'	1:A:2506:A:H5'	2.41	0.50
1:A:415:A:O2'	1:A:416:G:H5'	2.12	0.50
5:E:192:ILE:CG2	5:E:234:VAL:HG12	2.42	0.50
8:H:99:THR:O	8:H:100:ASP:HB2	2.11	0.50
14:N:85:ARG:NE	37:N:8519:HOH:O	2.14	0.50
21:U:19:ARG:NH1	21:U:68:ASP:O	2.44	0.50
1:A:402:U:H2'	1:A:403:C:C6	2.47	0.50
3:C:199:HIS:CD2	3:C:201:PHE:HB2	2.46	0.50
3:C:199:HIS:HD2	3:C:201:PHE:HB2	1.77	0.50
4:D:217:ARG:HG3	4:D:257:THR:CG2	2.42	0.50
7:G:80:TRP:O	7:G:134:SER:HA	2.11	0.50
10:J:62:GLU:O	10:J:66:VAL:HG23	2.11	0.50
14:N:157:LEU:HB3	14:N:160:PHE:HD1	1.77	0.50
20:T:29:ASP:CG	20:T:31:ARG:NH1	2.65	0.50
21:U:48:VAL:HG23	21:U:98:VAL:HA	1.93	0.50
21:U:9:LYS:HE3	21:U:13:ARG:HH11	1.77	0.50
1:A:1008:C:H5''	10:J:16:ARG:HH12	1.75	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1123:A:C2	1:A:1129:C:H4'	2.47	0.49
1:A:1589:G:N2	1:A:1605:G:H1'	2.27	0.49
1:A:1682:A:H5''	37:A:9436:HOH:O	2.11	0.49
1:A:2763:G:OP1	12:L:9:THR:OG1	2.16	0.49
5:E:133:ARG:NH2	37:E:8424:HOH:O	2.45	0.49
10:J:95:GLU:HB3	10:J:119:VAL:HG11	1.93	0.49
1:A:1003:U:O2	10:J:90:PHE:CZ	2.65	0.49
16:P:25:VAL:HG23	16:P:26:TRP:N	2.27	0.49
20:T:80:ARG:HG2	37:T:8336:HOH:O	2.11	0.49
37:L:7438:HOH:O	22:V:20:MET:HE1	2.12	0.49
30:4:74:CYS:SG	30:4:76:LYS:HG3	2.51	0.49
1:A:1804:A:H2'	1:A:1805:G:C8	2.46	0.49
1:A:2506:A:H1'	37:A:6024:HOH:O	2.13	0.49
1:A:2563:U:H2'	1:A:2565:C:O5'	2.11	0.49
1:A:2094:G:C2	1:A:2652:U:O2	2.65	0.49
1:A:2906:A:H5'	1:A:2907:C:O4'	2.12	0.49
1:A:453:A:H4'	1:A:455:A:N7	2.27	0.49
1:A:2719:A:C2	4:D:70:PRO:HG3	2.48	0.49
8:H:57:GLU:O	8:H:61:MET:HG3	2.12	0.49
11:K:80:LYS:HE2	11:K:98:PHE:CZ	2.47	0.49
14:N:107:ARG:NH1	37:N:8579:HOH:O	2.45	0.49
14:N:25:TRP:HE3	14:N:26:HIS:HD2	1.59	0.49
14:N:39:ARG:NE	37:N:8623:HOH:O	2.45	0.49
18:R:33:PHE:N	18:R:71:TYR:OH	2.38	0.49
20:T:57:THR:HG22	20:T:59:ASP:HB2	1.94	0.49
24:X:88:THR:CG2	24:X:89:ASP:H	2.21	0.49
26:Z:148:GLY:O	26:Z:154:ARG:HD3	2.12	0.49
29:3:18:ASN:ND2	29:3:40:ARG:H	2.10	0.49
1:A:221:G:H2'	1:A:222:A:C8	2.46	0.49
1:A:241:A:C2	1:A:378:A:H4'	2.47	0.49
1:A:92:G:H4'	23:W:44:GLY:HA3	1.93	0.49
4:D:248:ARG:O	4:D:251:VAL:CG1	2.60	0.49
4:D:88:GLU:HG3	4:D:88:GLU:O	2.11	0.49
5:E:184:ARG:HB3	37:E:8362:HOH:O	2.12	0.49
13:M:73:VAL:HG21	13:M:116:HIS:CD2	2.47	0.49
15:O:67:ALA:C	15:O:69:TYR:H	2.15	0.49
17:Q:103:THR:HA	17:Q:106:ARG:NH1	2.27	0.49
19:S:27:HIS:O	19:S:31:ILE:HG13	2.11	0.49
4:D:329:TYR:HE2	22:V:15:PRO:HG2	1.75	0.49
24:X:11:VAL:O	24:X:12:ASN:HB2	2.12	0.49
25:Y:71:ARG:HD3	37:Y:2171:HOH:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:G:H2'	1:A:175:G:N2	2.27	0.49
1:A:2559:C:H4'	37:A:7232:HOH:O	2.12	0.49
1:A:539:G:H2'	1:A:540:A:H8	1.76	0.49
2:B:3031:C:H2'	2:B:3032:G:O4'	2.12	0.49
4:D:4:SER:O	4:D:5:ARG:HB2	2.13	0.49
7:G:132:THR:HB	37:G:2227:HOH:O	2.11	0.49
7:G:31:ARG:HH12	7:G:68:HIS:CE1	2.30	0.49
10:J:144:GLU:HA	10:J:144:GLU:OE1	2.12	0.49
12:L:99:ASP:OD1	12:L:101:ASN:N	2.44	0.49
13:M:122:ALA:HB3	13:M:125:PHE:CZ	2.48	0.49
21:U:19:ARG:HD3	21:U:67:LEU:O	2.12	0.49
24:X:65:VAL:HA	24:X:68:THR:CG2	2.41	0.49
1:A:1699:C:H4'	37:A:6415:HOH:O	2.12	0.49
1:A:1768:C:H2'	1:A:1769:C:O4'	2.12	0.49
1:A:1827:G:C6	1:A:1828:G:C6	3.01	0.49
1:A:2251:G:H2'	1:A:2252:A:C8	2.48	0.49
4:D:16:ARG:NH1	37:D:8617:HOH:O	2.45	0.49
5:E:127:ARG:HG2	5:E:127:ARG:HH11	1.77	0.49
12:L:125:ALA:C	12:L:127:ALA:H	2.15	0.49
37:A:6218:HOH:O	22:V:56:ARG:HB3	2.11	0.49
1:A:1840:A:H4'	1:A:1841:C:O5'	2.13	0.49
1:A:2353:A:H4'	1:A:2354:A:O5'	2.12	0.49
6:F:86:THR:C	6:F:89:PRO:HD2	2.32	0.49
8:H:113:ASP:O	8:H:117:GLU:HG3	2.12	0.49
12:L:74:VAL:O	12:L:74:VAL:CG1	2.60	0.49
13:M:72:ASN:HB2	37:M:8580:HOH:O	2.12	0.49
37:A:7661:HOH:O	14:N:154:ARG:HB2	2.12	0.49
17:Q:27:ARG:O	17:Q:31:ILE:HG13	2.12	0.49
24:X:122:ARG:HG2	24:X:122:ARG:NH1	2.21	0.49
1:A:2577:A:H5'	37:A:7734:HOH:O	2.13	0.49
1:A:333:G:O2'	1:A:334:G:H5'	2.12	0.49
13:M:120:LEU:HD12	13:M:133:VAL:HG21	1.93	0.49
13:M:125:PHE:CZ	13:M:140:VAL:HG13	2.47	0.49
1:A:710:G:P	16:P:24:ALA:HB3	2.53	0.49
19:S:39:THR:HB	19:S:42:GLU:CG	2.41	0.49
24:X:28:HIS:CD2	24:X:31:HIS:CE1	3.01	0.49
24:X:69:ARG:HD2	24:X:117:ARG:O	2.12	0.49
1:A:470:U:H2'	1:A:471:G:O4'	2.13	0.49
1:A:536:A:H3'	37:A:5025:HOH:O	2.13	0.49
2:B:3064:C:C2'	2:B:3065:A:H5'	2.43	0.49
4:D:315:VAL:HG23	4:D:316:ARG:HG2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:110:GLU:HA	8:H:113:ASP:OD2	2.13	0.49
9:I:64:ASN:O	9:I:68:GLU:HG3	2.13	0.49
10:J:59:ASN:ND2	10:J:59:ASN:H	2.10	0.49
1:A:926:A:H1'	13:M:38:HIS:O	2.13	0.49
13:M:65:ASP:HA	13:M:109:LEU:O	2.12	0.49
16:P:10:LEU:HD13	16:P:99:GLU:HG3	1.95	0.49
18:R:28:ARG:NH1	37:R:6206:HOH:O	2.39	0.49
19:S:39:THR:CG2	19:S:42:GLU:HG3	2.42	0.49
1:A:107:U:H2'	1:A:108:U:H5'	1.95	0.49
1:A:1609:C:H2'	1:A:1610:G:H8	1.77	0.49
1:A:2780:C:H2'	1:A:2781:U:H6	1.76	0.49
1:A:660:A:H4'	1:A:661:G:O5'	2.13	0.49
1:A:669:G:O2'	1:A:670:G:H5'	2.13	0.49
5:E:111:VAL:HB	37:E:8324:HOH:O	2.13	0.49
6:F:94:ALA:HB3	6:F:174:VAL:HA	1.95	0.49
7:G:20:ILE:HD12	7:G:33:LEU:CD1	2.43	0.49
7:G:18:LEU:HD13	7:G:34:TRP:CG	2.47	0.49
8:H:28:ALA:HB3	8:H:99:THR:HG23	1.95	0.49
10:J:129:ASN:N	10:J:129:ASN:HD22	2.10	0.49
14:N:78:ASN:ND2	37:N:8647:HOH:O	2.40	0.49
15:O:38:LYS:HD2	15:O:114:LYS:HE3	1.95	0.49
17:Q:16:VAL:HG12	17:Q:17:GLY:N	2.27	0.49
19:S:18:LEU:HB2	19:S:143:VAL:CG1	2.41	0.49
27:1:38:LYS:HE2	27:1:45:LYS:CE	2.39	0.49
1:A:1477:C:H5'	1:A:1868:G:C5'	2.43	0.49
1:A:1593:C:O2'	1:A:1594:C:H5'	2.13	0.49
1:A:159:G:H2'	1:A:175:G:H22	1.77	0.49
1:A:2649:A:C8	1:A:2649:A:H5'	2.48	0.49
1:A:2896:A:H2'	1:A:2896:A:N3	2.28	0.49
1:A:538:C:H5''	1:A:539:G:C8	2.48	0.49
1:A:737:A:H2'	1:A:738:G:O4'	2.13	0.49
4:D:279:THR:CG2	4:D:280:VAL:N	2.75	0.49
4:D:202:VAL:HG11	4:D:301:VAL:HG13	1.95	0.49
4:D:41:PHE:CB	4:D:190:MET:HE3	2.43	0.49
6:F:57:THR:HG23	6:F:63:ILE:CG2	2.42	0.49
10:J:75:SER:HB3	10:J:79:ALA:HB1	1.95	0.49
1:A:380:A:C2	14:N:13:LYS:HB3	2.48	0.49
27:1:11:THR:HG21	27:1:23:ARG:HB2	1.94	0.48
27:1:57:CYS:O	27:1:61:GLY:N	2.44	0.48
1:A:1209:C:O2	1:A:1210:G:C8	2.66	0.48
1:A:13:G:H2'	1:A:14:C:H6	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1787:C:OP1	17:Q:68:LYS:HE2	2.13	0.48
1:A:2004:U:H1'	37:A:3178:HOH:O	2.12	0.48
1:A:2421:G:HO2'	1:A:2422:U:P	2.36	0.48
1:A:2502:C:C4'	10:J:151:MET:HG2	2.42	0.48
4:D:243:ASN:HA	4:D:244:PRO:C	2.32	0.48
6:F:27:ILE:HG22	6:F:28:GLY:N	2.22	0.48
10:J:154:THR:HB	10:J:155:PRO:HD3	1.95	0.48
13:M:72:ASN:O	13:M:76:LEU:HG	2.13	0.48
1:A:182:G:O3'	14:N:157:LEU:HD13	2.13	0.48
15:O:77:ASN:OD1	15:O:80:SER:HB2	2.13	0.48
20:T:29:ASP:OD2	20:T:31:ARG:NH1	2.45	0.48
1:A:584:U:H3'	37:A:6064:HOH:O	2.12	0.48
1:A:734:U:O2'	1:A:737:A:N6	2.45	0.48
1:A:2781:U:H1'	7:G:139:GLU:OE2	2.13	0.48
7:G:18:LEU:HD13	7:G:34:TRP:CD1	2.49	0.48
10:J:31:PHE:HA	10:J:85:ILE:CG2	2.43	0.48
13:M:73:VAL:HG23	13:M:74:THR:H	1.76	0.48
16:P:47:ARG:NH1	16:P:47:ARG:HG3	2.27	0.48
1:A:101:C:H2'	1:A:102:A:H8	1.78	0.48
1:A:1044:C:H5''	37:A:9022:HOH:O	2.13	0.48
1:A:625:U:H5''	1:A:1044:C:N4	2.28	0.48
1:A:1268:C:O2'	1:A:1269:G:H5'	2.13	0.48
1:A:1383:U:H5''	37:A:6631:HOH:O	2.12	0.48
1:A:2584:G:C2	1:A:2585:G:N7	2.81	0.48
1:A:81:G:N3	1:A:98:A:C2	2.81	0.48
3:C:18:ALA:O	3:C:20:SER:N	2.43	0.48
3:C:93:THR:C	3:C:94:LEU:HD23	2.33	0.48
5:E:214:THR:HG23	37:E:8436:HOH:O	2.12	0.48
7:G:31:ARG:NH1	7:G:68:HIS:CG	2.82	0.48
10:J:84:ARG:CZ	10:J:135:TRP:HH2	2.25	0.48
14:N:52:LEU:HD13	14:N:116:ASN:CB	2.42	0.48
15:O:62:HIS:HB3	15:O:65:ASP:OD1	2.12	0.48
17:Q:83:LYS:O	17:Q:86:ALA:HB3	2.12	0.48
24:X:90:TYR:N	24:X:90:TYR:CD1	2.80	0.48
1:A:1743:G:H1'	37:A:4867:HOH:O	2.12	0.48
1:A:2256:G:O2'	1:A:2257:G:H5'	2.12	0.48
1:A:581:G:H5'	37:A:7664:HOH:O	2.13	0.48
2:B:3042:C:H5'	2:B:3043:G:OP2	2.13	0.48
1:A:2657:G:OP1	4:D:17:LYS:HB2	2.13	0.48
4:D:76:THR:N	4:D:77:PRO:HD3	2.29	0.48
5:E:218:VAL:HG12	37:E:8422:HOH:O	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:101:GLU:HB2	7:G:116:THR:O	2.13	0.48
15:O:139:TRP:HA	15:O:139:TRP:CE3	2.47	0.48
24:X:110:GLN:HE21	24:X:110:GLN:HA	1.78	0.48
30:4:62:THR:HB	37:4:8554:HOH:O	2.12	0.48
30:4:69:TYR:CB	30:4:78:HIS:CE1	2.96	0.48
1:A:1333:U:H2'	1:A:1334:C:C6	2.48	0.48
1:A:1850:U:H2'	1:A:1851:G:C8	2.48	0.48
1:A:2019:A:H5'	37:A:4508:HOH:O	2.13	0.48
1:A:2459:G:P	30:4:64:LYS:HB2	2.54	0.48
1:A:2866:U:H4'	1:A:2867:G:H5'	1.95	0.48
1:A:485:A:O2'	1:A:487:G:H5'	2.13	0.48
1:A:832:U:H2'	1:A:833:G:C8	2.49	0.48
5:E:184:ARG:NE	37:E:8409:HOH:O	2.41	0.48
5:E:236:THR:CG2	5:E:239:ALA:H	2.00	0.48
6:F:84:LEU:C	6:F:86:THR:H	2.16	0.48
6:F:84:LEU:HA	6:F:87:ALA:HB3	1.96	0.48
8:H:117:GLU:C	8:H:119:ARG:H	2.16	0.48
10:J:35:ASN:ND2	10:J:79:ALA:O	2.46	0.48
10:J:48:LEU:CG	10:J:157:ILE:HG21	2.43	0.48
17:Q:10:ALA:HA	17:Q:13:VAL:CG1	2.43	0.48
19:S:82:GLU:HG3	19:S:83:LYS:N	2.28	0.48
37:A:7382:HOH:O	21:U:2:LYS:HE2	2.13	0.48
21:U:41:ARG:HG2	21:U:41:ARG:HH11	1.79	0.48
24:X:122:ARG:CG	24:X:122:ARG:NH1	2.74	0.48
24:X:4:LEU:HD22	24:X:52:VAL:HG22	1.93	0.48
26:Z:151:SER:HB3	26:Z:154:ARG:HB3	1.96	0.48
26:Z:187:VAL:HG23	26:Z:192:ASP:HB3	1.94	0.48
1:A:2251:G:H4'	37:A:7385:HOH:O	2.14	0.48
2:B:3038:A:H2	2:B:3043:G:H5''	1.78	0.48
2:B:3080:A:C2	2:B:3103:A:C4	3.02	0.48
1:A:1361:C:O3'	5:E:77:ALA:HB3	2.14	0.48
6:F:51:ARG:HD3	37:F:7636:HOH:O	2.14	0.48
10:J:59:ASN:ND2	10:J:59:ASN:N	2.59	0.48
1:A:2730:G:O2'	1:A:2731:G:H5'	2.14	0.48
1:A:288:A:H2'	1:A:289:G:C8	2.49	0.48
1:A:380:A:H5''	14:N:48:ARG:NH2	2.29	0.48
10:J:157:ILE:CG2	10:J:158:ASN:N	2.76	0.48
10:J:26:LYS:HG2	10:J:28:ILE:N	2.23	0.48
37:A:4700:HOH:O	15:O:21:HIS:HD2	1.96	0.48
17:Q:7:LYS:HD2	17:Q:21:VAL:CG2	2.43	0.48
23:W:1:THR:HG23	23:W:2:VAL:N	2.20	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:X:75:GLY:HA3	37:X:5763:HOH:O	2.13	0.48
25:Y:27:ASP:OD2	25:Y:27:ASP:N	2.47	0.48
1:A:1380:U:H5'	37:A:9206:HOH:O	2.14	0.48
1:A:639:A:H2'	1:A:640:G:H8	1.79	0.48
1:A:2837:U:H1'	4:D:307:ARG:HH12	1.78	0.48
5:E:79:ARG:O	5:E:87:ARG:N	2.42	0.48
11:K:19:MET:HE1	11:K:132:LEU:HD21	1.94	0.48
11:K:19:MET:HE1	11:K:132:LEU:CD2	2.43	0.48
11:K:93:ARG:HB3	11:K:93:ARG:NH1	2.27	0.48
1:A:1075:G:C2	1:A:1085:C:C2	3.02	0.48
1:A:1316:G:H1'	1:A:1340:G:N2	2.29	0.48
1:A:1666:C:H2'	1:A:1667:A:C5'	2.44	0.48
1:A:2073:G:C6	1:A:2607:U:C2	3.01	0.48
1:A:2269:C:C2'	1:A:2270:G:H5'	2.44	0.48
1:A:2755:G:H1'	37:A:4654:HOH:O	2.13	0.48
3:C:212:PRO:HB2	37:C:8562:HOH:O	2.14	0.48
4:D:84:LEU:HD13	4:D:84:LEU:O	2.13	0.48
10:J:45:GLN:HE21	10:J:135:TRP:HE1	1.62	0.48
14:N:154:ARG:CD	37:N:8643:HOH:O	2.62	0.48
37:A:4849:HOH:O	14:N:174:ARG:HG2	2.13	0.48
25:Y:66:THR:HG23	25:Y:67:PRO:HD2	1.95	0.48
1:A:1377:C:C6	1:A:1377:C:H5'	2.45	0.48
1:A:138:U:H5''	1:A:139:C:OP2	2.14	0.48
1:A:244:C:O5'	1:A:244:C:H6	1.96	0.48
1:A:2781:U:C2'	1:A:2782:G:H5'	2.44	0.48
2:B:3092:G:H22	10:J:52:LYS:NZ	2.12	0.48
7:G:92:PRO:HB2	37:G:4917:HOH:O	2.13	0.48
10:J:57:ARG:C	10:J:59:ASN:N	2.65	0.48
11:K:131:THR:HG22	11:K:133:GLY:N	2.29	0.48
37:A:3147:HOH:O	14:N:87:MET:HE3	2.13	0.48
1:A:1052:G:H2'	1:A:1052:G:N3	2.28	0.47
1:A:1249:U:H2'	1:A:1250:C:C6	2.49	0.47
1:A:1407:A:O2'	1:A:1408:U:H3'	2.14	0.47
1:A:182:G:O3'	14:N:157:LEU:CD1	2.62	0.47
1:A:2001:G:C2'	1:A:2002:C:H5'	2.44	0.47
1:A:212:A:O4'	1:A:214:U:C6	2.67	0.47
1:A:861:A:H2'	1:A:862:U:C6	2.48	0.47
1:A:894:A:C2	5:E:87:ARG:NH2	2.82	0.47
31:A:9001:SPR:C7C	31:A:9001:SPR:H6C3	2.43	0.47
5:E:107:ARG:HH11	5:E:107:ARG:HB3	1.77	0.47
1:A:1352:A:N1	5:E:48:SER:HB3	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:41:LEU:HA	6:F:44:ILE:CG2	2.44	0.47
14:N:104:ARG:O	14:N:108:LYS:HE2	2.14	0.47
1:A:2055:A:H4'	19:S:132:ARG:NH2	2.29	0.47
1:A:1164:U:C1'	1:A:1165:G:OP1	2.62	0.47
1:A:1934:A:C8	1:A:1935:C:C5	3.01	0.47
1:A:2670:G:O2'	1:A:2671:U:H5'	2.14	0.47
1:A:682:A:H2'	1:A:683:G:O4'	2.14	0.47
4:D:168:GLY:O	4:D:169:GLY:O	2.32	0.47
37:A:7435:HOH:O	5:E:188:ARG:HD3	2.12	0.47
6:F:22:VAL:HG22	6:F:74:THR:HG22	1.96	0.47
11:K:77:GLY:O	11:K:78:ILE:C	2.52	0.47
15:O:34:LEU:HD13	15:O:47:LEU:HD21	1.96	0.47
19:S:39:THR:HB	19:S:42:GLU:CD	2.34	0.47
21:U:32:ARG:NH1	21:U:38:ARG:NH1	2.56	0.47
22:V:44:ARG:HB3	37:V:3805:HOH:O	2.13	0.47
1:A:2443:C:H3'	37:A:3456:HOH:O	2.14	0.47
1:A:558:C:C2'	1:A:559:U:C5'	2.92	0.47
1:A:920:C:H4'	1:A:921:G:C2	2.49	0.47
4:D:279:THR:OG1	4:D:290:VAL:HB	2.14	0.47
5:E:65:ARG:HG3	5:E:67:GLN:HB2	1.97	0.47
7:G:93:MET:HE1	7:G:165:GLY:N	2.29	0.47
9:I:23:ILE:O	9:I:27:ILE:HG13	2.13	0.47
11:K:142:ASN:O	11:K:144:THR:N	2.47	0.47
12:L:55:VAL:HG12	12:L:56:SER:H	1.77	0.47
15:O:154:LEU:HG	15:O:155:GLU:H	1.78	0.47
1:A:952:G:OP1	18:R:42:LYS:HE2	2.14	0.47
23:W:16:ARG:NH2	23:W:63:GLU:HG3	2.28	0.47
1:A:1097:A:H5''	24:X:125:HIS:NE2	2.30	0.47
1:A:1119:G:N2	1:A:1246:A:H2	2.08	0.47
1:A:1504:A:H5'	37:A:4384:HOH:O	2.14	0.47
1:A:1659:A:H2'	1:A:1660:G:O4'	2.15	0.47
4:D:177:HIS:O	4:D:181:ILE:HG13	2.15	0.47
4:D:82:VAL:HG12	4:D:101:TRP:CE3	2.50	0.47
5:E:127:ARG:CZ	5:E:225:PRO:HG2	2.44	0.47
6:F:10:PHE:CD1	6:F:11:HIS:N	2.82	0.47
6:F:86:THR:HG23	37:F:7477:HOH:O	2.14	0.47
6:F:99:ASP:HB2	6:F:103:ASN:H	1.80	0.47
10:J:150:LYS:HB2	10:J:157:ILE:HD12	1.95	0.47
37:A:9776:HOH:O	12:L:39:GLY:HA3	2.13	0.47
14:N:35:PRO:HD2	14:N:38:VAL:HG21	1.96	0.47
17:Q:71:LYS:O	17:Q:71:LYS:HG3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:39:THR:O	19:S:40:ALA:C	2.51	0.47
26:Z:187:VAL:O	26:Z:187:VAL:HG13	2.14	0.47
27:1:58:GLY:HA3	37:1:8442:HOH:O	2.13	0.47
1:A:1503:U:H2'	1:A:1504:A:O4'	2.14	0.47
1:A:2430:A:H8	1:A:2430:A:O5'	1.97	0.47
1:A:2524:G:H21	1:A:2526:C:N4	2.12	0.47
1:A:2830:U:H3'	37:A:5206:HOH:O	2.13	0.47
1:A:2883:A:H2'	1:A:2884:G:O4'	2.15	0.47
1:A:625:U:H5'	37:A:3169:HOH:O	2.14	0.47
1:A:637:C:OP1	26:Z:136:LYS:NZ	2.33	0.47
5:E:118:THR:HG22	5:E:137:PRO:HB3	1.96	0.47
5:E:223:LEU:HD12	5:E:223:LEU:HA	1.77	0.47
6:F:128:LEU:HD23	6:F:128:LEU:C	2.35	0.47
6:F:99:ASP:CB	6:F:103:ASN:HB2	2.43	0.47
37:A:3180:HOH:O	13:M:4:LYS:HG3	2.13	0.47
14:N:113:ARG:HH21	14:N:156:ARG:HG2	1.77	0.47
15:O:113:SER:C	37:O:8560:HOH:O	2.53	0.47
12:L:130:MET:SD	22:V:26:GLY:HA3	2.54	0.47
24:X:149:LEU:HG	24:X:153:MET:CE	2.45	0.47
27:1:13:ARG:NH1	27:1:14:PHE:CZ	2.82	0.47
1:A:1127:C:C2'	1:A:1128:U:H5'	2.44	0.47
1:A:151:A:H2'	1:A:152:A:O4'	2.14	0.47
1:A:2093:G:H5''	37:A:9462:HOH:O	2.13	0.47
1:A:2133:U:H4'	1:A:2134:G:H5'	1.97	0.47
1:A:2416:G:H2'	1:A:2417:C:C6	2.50	0.47
1:A:2488:A:H61	1:A:2534:C:H42	1.62	0.47
1:A:2812:A:H1'	37:A:5763:HOH:O	2.14	0.47
3:C:192:VAL:O	3:C:192:VAL:HG12	2.13	0.47
10:J:48:LEU:HD13	10:J:146:TRP:HB3	1.96	0.47
15:O:182:GLY:O	15:O:183:ASP:O	2.32	0.47
18:R:21:ARG:NH2	37:R:5853:HOH:O	2.29	0.47
24:X:65:VAL:CA	24:X:68:THR:HG22	2.44	0.47
1:A:1019:C:P	37:A:3922:HOH:O	2.73	0.47
1:A:1023:C:H2'	1:A:1024:G:O4'	2.14	0.47
1:A:1463:A:C6	1:A:1464:U:O4	2.68	0.47
1:A:1694:G:H1'	37:A:9177:HOH:O	2.14	0.47
1:A:1858:A:H2'	1:A:1859:A:C8	2.50	0.47
1:A:1878:G:O2'	1:A:1879:U:C6	2.65	0.47
1:A:2089:A:O2'	1:A:2090:G:H5'	2.15	0.47
1:A:2456:A:H5'	37:A:5666:HOH:O	2.14	0.47
1:A:2781:U:O2'	1:A:2782:G:H5'	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:470:U:O2'	28:2:16:HIS:CD2	2.67	0.47
1:A:790:A:H2'	1:A:791:A:O4'	2.14	0.47
3:C:217:ARG:NH1	3:C:217:ARG:CG	2.76	0.47
4:D:139:ASP:HB2	4:D:165:ARG:HE	1.80	0.47
4:D:51:VAL:HG23	4:D:329:TYR:O	2.14	0.47
11:K:42:GLU:O	11:K:131:THR:HG23	2.14	0.47
13:M:73:VAL:HG23	13:M:74:THR:N	2.29	0.47
15:O:11:ARG:O	15:O:15:GLU:HG3	2.14	0.47
15:O:154:LEU:O	15:O:155:GLU:CB	2.63	0.47
15:O:67:ALA:C	15:O:69:TYR:N	2.68	0.47
20:T:32:ALA:HA	20:T:36:GLU:OE1	2.14	0.47
27:1:13:ARG:NH1	27:1:14:PHE:CE2	2.83	0.47
1:A:1555:G:H4'	1:A:1630:A:H2	1.80	0.47
1:A:2005:G:O2'	1:A:2008:U:OP2	2.25	0.47
1:A:2533:C:H6	1:A:2533:C:C5'	2.20	0.47
2:B:3031:C:O2'	2:B:3032:G:H5'	2.14	0.47
2:B:3049:G:O2'	2:B:3050:G:H5'	2.15	0.47
6:F:76:ARG:O	6:F:77:ASP:HB2	2.15	0.47
8:H:20:LEU:O	8:H:23:ALA:HB3	2.15	0.47
14:N:37:VAL:HG21	14:N:108:LYS:HG3	1.97	0.47
15:O:37:ARG:NE	37:O:8534:HOH:O	2.47	0.47
24:X:129:LYS:HG2	37:X:1990:HOH:O	2.15	0.47
1:A:2834:G:OP1	25:Y:39:LYS:HE2	2.15	0.47
1:A:168:C:O2'	1:A:169:A:H5'	2.15	0.47
1:A:2383:G:N3	37:A:6675:HOH:O	2.35	0.47
1:A:2723:G:H1'	37:A:4815:HOH:O	2.14	0.47
1:A:646:G:H2'	1:A:647:U:C6	2.50	0.47
5:E:1:MET:HG2	5:E:2:GLN:NE2	2.30	0.47
37:A:7202:HOH:O	14:N:13:LYS:HE2	2.14	0.47
14:N:65:VAL:HG21	14:N:105:ALA:HB2	1.96	0.47
37:A:5324:HOH:O	21:U:3:GLN:HG2	2.14	0.47
26:Z:172:THR:HG22	26:Z:173:ALA:N	2.29	0.47
29:3:40:ARG:NH1	29:3:40:ARG:HG2	2.30	0.47
1:A:1702:U:H5''	37:A:7193:HOH:O	2.14	0.47
1:A:1759:A:N3	1:A:1818:C:H2'	2.30	0.47
1:A:2421:G:H4'	37:A:4754:HOH:O	2.15	0.47
1:A:2431:C:O2'	1:A:2432:C:H5'	2.15	0.47
1:A:2481:G:C3'	1:A:2482:G:H5''	2.44	0.47
1:A:825:U:H5''	1:A:826:U:OP1	2.15	0.47
1:A:843:A:C2	1:A:846:A:C8	3.03	0.47
3:C:217:ARG:HG3	3:C:217:ARG:HH11	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:73:VAL:HG11	13:M:118:LEU:HD21	1.97	0.47
2:B:3008:G:O6	15:O:11:ARG:NH1	2.47	0.47
15:O:154:LEU:HD12	15:O:156:GLU:O	2.15	0.47
37:A:5995:HOH:O	18:R:50:GLY:HA2	2.15	0.47
24:X:76:ASP:O	24:X:77:ALA:C	2.53	0.47
1:A:1268:C:H2'	1:A:1269:G:C8	2.49	0.47
1:A:128:A:H3'	1:A:128:A:C8	2.50	0.47
1:A:13:G:H2'	1:A:14:C:C6	2.50	0.47
1:A:1609:C:H2'	1:A:1610:G:C8	2.50	0.47
1:A:2072:G:C6	1:A:2533:C:H1'	2.50	0.47
1:A:2840:A:OP1	4:D:211:THR:HG23	2.15	0.47
1:A:283:U:H5	1:A:284:C:N4	2.13	0.47
1:A:426:G:H2'	1:A:427:C:O4'	2.14	0.47
1:A:512:G:O3'	1:A:513:A:H8	1.98	0.47
1:A:581:G:O2'	1:A:582:C:H5'	2.15	0.47
3:C:192:VAL:HB	37:C:8598:HOH:O	2.14	0.47
8:H:34:ASN:O	8:H:38:LYS:HG3	2.15	0.47
10:J:84:ARG:CZ	10:J:135:TRP:CH2	2.98	0.47
7:G:34:TRP:O	11:K:127:ILE:HD11	2.14	0.47
15:O:67:ALA:HA	15:O:71:TRP:H	1.80	0.47
16:P:32:ARG:HE	16:P:35:LYS:HD2	1.80	0.47
22:V:33:SER:O	22:V:37:GLU:HG3	2.15	0.47
24:X:1:MET:HB2	24:X:103:GLU:HG2	1.97	0.47
24:X:126:ASP:HB3	24:X:135:GLY:O	2.15	0.47
1:A:1114:A:H2'	1:A:1115:U:H6	1.80	0.46
1:A:1130:U:H5'	37:A:7653:HOH:O	2.15	0.46
3:C:153:ARG:CB	3:C:153:ARG:HH11	2.27	0.46
4:D:162:MET:HE1	4:D:308:LEU:HD21	1.94	0.46
4:D:74:ILE:HD13	4:D:309:VAL:HG21	1.97	0.46
5:E:107:ARG:CB	5:E:107:ARG:HH11	2.28	0.46
6:F:19:GLU:O	6:F:133:ASN:HB3	2.15	0.46
10:J:29:ALA:N	10:J:62:GLU:OE1	2.45	0.46
11:K:131:THR:HB	11:K:134:GLU:HG3	1.97	0.46
1:A:2598:U:H5''	12:L:36:GLY:HA2	1.96	0.46
1:A:869:G:OP1	14:N:79:LYS:HE2	2.13	0.46
20:T:57:THR:C	20:T:59:ASP:H	2.17	0.46
21:U:41:ARG:NH1	21:U:42:VAL:O	2.49	0.46
1:A:317:A:H5''	21:U:52:ARG:HD2	1.97	0.46
24:X:122:ARG:CG	24:X:152:ALA:O	2.63	0.46
25:Y:72:VAL:HG22	25:Y:85:VAL:CG1	2.44	0.46
26:Z:189:ASN:HD22	26:Z:192:ASP:H	1.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1334:C:H2'	1:A:1335:C:H6	1.79	0.46
1:A:1506:U:H6	1:A:1506:U:H5'	1.80	0.46
1:A:2010:A:H5''	37:A:4144:HOH:O	2.14	0.46
1:A:2089:A:C2'	1:A:2090:G:H5'	2.45	0.46
1:A:308:U:C4	1:A:342:C:H1'	2.50	0.46
1:A:514:G:O5'	1:A:514:G:H8	1.98	0.46
1:A:832:U:H2'	1:A:833:G:H8	1.80	0.46
7:G:158:ASP:OD1	7:G:160:ARG:HB2	2.14	0.46
8:H:60:VAL:O	8:H:61:MET:C	2.53	0.46
37:A:9966:HOH:O	13:M:22:ARG:HG2	2.14	0.46
14:N:138:HIS:C	14:N:139:PRO:O	2.47	0.46
37:E:8355:HOH:O	16:P:3:THR:HG21	2.14	0.46
19:S:22:GLN:HA	19:S:139:PRO:O	2.15	0.46
21:U:48:VAL:CG2	21:U:98:VAL:HA	2.44	0.46
22:V:9:CYS:HG	22:V:11:THR:HG23	1.79	0.46
30:4:23:GLU:HG2	30:4:24:LYS:O	2.15	0.46
1:A:1162:G:H2'	37:A:6556:HOH:O	2.15	0.46
1:A:200:U:H2'	37:A:3428:HOH:O	2.14	0.46
1:A:2090:G:H2'	1:A:2091:G:C8	2.49	0.46
1:A:2494:G:H4'	10:J:5:MET:SD	2.55	0.46
1:A:2898:G:O2'	1:A:2899:A:H5'	2.16	0.46
1:A:447:A:O2'	1:A:448:G:H5'	2.16	0.46
1:A:60:A:C2	1:A:61:G:C8	3.04	0.46
3:C:97:ALA:HB2	3:C:150:PRO:HB2	1.97	0.46
4:D:234:ARG:NH1	37:D:8620:HOH:O	2.37	0.46
4:D:41:PHE:CZ	4:D:79:MET:HG3	2.50	0.46
5:E:33:LYS:HE2	37:E:8358:HOH:O	2.14	0.46
11:K:45:VAL:HG22	11:K:46:ILE:N	2.30	0.46
15:O:180:LEU:O	15:O:181:ASP:HB3	2.15	0.46
16:P:25:VAL:O	16:P:29:VAL:HG23	2.14	0.46
17:Q:41:ARG:O	17:Q:44:VAL:HB	2.15	0.46
18:R:50:GLY:HA3	18:R:87:THR:OG1	2.15	0.46
27:1:30:GLU:CA	27:1:33:HIS:HB3	2.41	0.46
27:1:39:CYS:SG	27:1:40:PRO:HD2	2.55	0.46
1:A:1513:C:O2'	1:A:1514:C:H5'	2.15	0.46
1:A:160:A:C5	1:A:177:A:C2	3.03	0.46
1:A:2010:A:H2'	37:A:5928:HOH:O	2.15	0.46
1:A:2445:U:H2'	1:A:2446:G:C8	2.50	0.46
1:A:2506:A:C1'	37:A:6024:HOH:O	2.62	0.46
1:A:396:U:H1'	37:A:7610:HOH:O	2.14	0.46
1:A:500:G:O2'	1:A:501:G:H5'	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2630:G:O6	3:C:206:ARG:NH2	2.49	0.46
3:C:29:HIS:CE1	3:C:107:ASN:ND2	2.84	0.46
4:D:204:GLY:HA3	37:D:8655:HOH:O	2.15	0.46
5:E:115:LEU:HA	5:E:115:LEU:HD12	1.80	0.46
6:F:59:GLY:O	6:F:61:PHE:N	2.37	0.46
10:J:157:ILE:HG22	10:J:158:ASN:N	2.30	0.46
4:D:221:GLN:NE2	12:L:42:ASN:HD22	2.09	0.46
13:M:12:THR:HG21	13:M:16:GLY:O	2.16	0.46
14:N:169:ARG:NH1	37:N:8573:HOH:O	2.49	0.46
14:N:57:LYS:HE2	14:N:140:ALA:O	2.15	0.46
14:N:95:LYS:HG2	14:N:99:ARG:HB3	1.97	0.46
24:X:88:THR:O	37:X:2374:HOH:O	2.21	0.46
25:Y:43:VAL:CG1	25:Y:44:ASP:N	2.78	0.46
28:2:10:LYS:CG	37:2:8432:HOH:O	2.58	0.46
1:A:1064:U:H2'	1:A:1065:G:C8	2.51	0.46
1:A:2099:G:O6	31:A:9001:SPR:H8A2	2.16	0.46
1:A:858:U:H2'	1:A:859:C:C6	2.49	0.46
2:B:3065:A:O2'	2:B:3066:G:P	2.72	0.46
3:C:186:TRP:CG	3:C:187:PRO:HA	2.51	0.46
3:C:8:ARG:HG2	37:C:8554:HOH:O	2.14	0.46
7:G:7:ILE:HG22	7:G:45:ASP:O	2.15	0.46
14:N:69:LYS:O	14:N:73:ARG:CZ	2.64	0.46
21:U:9:LYS:CE	21:U:13:ARG:NH1	2.79	0.46
27:1:38:LYS:HG3	37:1:8432:HOH:O	2.14	0.46
1:A:1218:U:H2'	1:A:1219:U:C6	2.50	0.46
1:A:278:A:H2'	1:A:279:C:O4'	2.16	0.46
1:A:79:G:H22	1:A:97:G:H1'	1.80	0.46
1:A:820:G:H5'	1:A:821:U:C5'	2.45	0.46
1:A:849:C:O2'	1:A:850:U:H5'	2.16	0.46
5:E:61:PHE:HD1	37:E:8377:HOH:O	1.98	0.46
21:U:48:VAL:HG13	21:U:49:GLU:N	2.30	0.46
25:Y:12:ILE:HG23	25:Y:36:HIS:CG	2.50	0.46
26:Z:130:ARG:HB2	26:Z:142:SER:O	2.16	0.46
1:A:1015:C:H2'	1:A:1016:U:C6	2.51	0.46
1:A:101:C:O2'	1:A:102:A:H5'	2.15	0.46
1:A:1855:G:H8	3:C:144:GLU:OE2	1.99	0.46
1:A:319:A:H4'	1:A:338:C:C4	2.51	0.46
1:A:679:G:OP2	37:A:4409:HOH:O	2.20	0.46
3:C:192:VAL:O	3:C:192:VAL:CG1	2.63	0.46
6:F:167:GLU:OE2	6:F:173:GLU:HG2	2.15	0.46
7:G:86:VAL:CG1	7:G:129:GLU:HA	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:A:4055:HOH:O	8:H:31:LYS:HE3	2.16	0.46
12:L:37:TYR:HD2	37:L:7169:HOH:O	1.96	0.46
13:M:146:GLY:C	13:M:148:GLU:H	2.19	0.46
13:M:77:ALA:HB3	37:M:8534:HOH:O	2.15	0.46
15:O:115:VAL:O	15:O:118:ILE:HB	2.14	0.46
19:S:111:ILE:HG23	19:S:145:LEU:CD1	2.46	0.46
24:X:14:HIS:HB2	24:X:17:ILE:HG13	1.98	0.46
26:Z:187:VAL:HG12	26:Z:205:ILE:HA	1.97	0.46
1:A:1534:C:N3	37:A:9465:HOH:O	2.36	0.46
1:A:1613:C:H2'	1:A:1614:G:O4'	2.15	0.46
1:A:190:G:OP2	37:A:3713:HOH:O	2.21	0.46
1:A:2016:U:H6	1:A:2016:U:O5'	1.99	0.46
1:A:331:A:C6	1:A:332:G:C4	3.03	0.46
2:B:3057:A:C8	6:F:141:VAL:HG21	2.51	0.46
10:J:141:ASN:CA	37:J:8356:HOH:O	2.59	0.46
14:N:133:LEU:O	14:N:134:ILE:HD13	2.16	0.46
14:N:68:ARG:O	14:N:68:ARG:CG	2.61	0.46
16:P:105:ASN:HD21	16:P:109:SER:H	1.62	0.46
19:S:15:LYS:HE3	37:S:8578:HOH:O	2.16	0.46
1:A:2873:C:N4	1:A:2874:G:C6	2.84	0.46
1:A:450:C:H4'	5:E:46:TYR:CE1	2.51	0.46
2:B:3078:G:O2'	2:B:3079:U:P	2.74	0.46
4:D:154:VAL:CG1	4:D:156:LYS:HG2	2.46	0.46
7:G:11:VAL:CG1	7:G:12:ASP:H	2.29	0.46
1:A:1003:U:O2	10:J:90:PHE:HZ	1.99	0.46
1:A:2453:G:H4'	13:M:50:GLY:C	2.36	0.46
37:A:7400:HOH:O	21:U:9:LYS:HD2	2.16	0.46
25:Y:76:ARG:O	25:Y:77:PHE:HB3	2.16	0.46
28:2:25:LYS:NZ	37:2:8433:HOH:O	2.45	0.46
37:A:9939:HOH:O	30:4:84:ARG:HB2	2.16	0.46
1:A:1497:G:H4'	1:A:1627:G:O2'	2.16	0.46
1:A:1603:A:H5'	1:A:1605:G:C4'	2.46	0.46
1:A:1657:A:H2'	1:A:1658:A:C8	2.51	0.46
1:A:1909:A:H2'	1:A:1910:A:C8	2.51	0.46
1:A:2045:G:H2'	1:A:2046:G:O4'	2.16	0.46
1:A:2604:A:H5'	37:A:5764:HOH:O	2.16	0.46
1:A:289:G:O2'	1:A:290:C:H5'	2.15	0.46
4:D:132:HIS:CE1	4:D:171:VAL:HG21	2.50	0.46
4:D:41:PHE:HB3	4:D:190:MET:CE	2.46	0.46
5:E:191:SER:OG	5:E:192:ILE:N	2.49	0.46
5:E:142:ASP:OD1	5:E:236:THR:HG23	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:35:ALA:HB1	37:F:3279:HOH:O	2.15	0.46
6:F:94:ALA:O	6:F:95:THR:O	2.33	0.46
10:J:4:ALA:HB3	37:J:8354:HOH:O	2.16	0.46
12:L:118:ALA:C	12:L:120:ARG:H	2.19	0.46
14:N:155:HIS:O	14:N:158:ARG:HG2	2.16	0.46
1:A:392:U:C5'	14:N:193:LYS:HB3	2.46	0.46
15:O:50:LEU:HB2	37:O:8523:HOH:O	2.16	0.46
15:O:78:MET:HB2	15:O:79:PRO:HD3	1.98	0.46
1:A:1004:C:O2'	1:A:1005:A:H5'	2.16	0.45
1:A:1191:A:C3'	1:A:1192:A:H5''	2.42	0.45
1:A:1420:C:C2	1:A:1445:G:N2	2.84	0.45
1:A:1603:A:C5'	1:A:1605:G:H5'	2.46	0.45
1:A:1624:A:H5'	1:A:1626:A:O4'	2.17	0.45
1:A:2460:A:OP1	30:4:60:LYS:N	2.46	0.45
1:A:2697:A:H2'	1:A:2698:G:O4'	2.15	0.45
1:A:1562:C:H42	1:A:2738:G:H1	1.63	0.45
1:A:2833:C:C2	1:A:2848:G:N2	2.84	0.45
1:A:566:A:H2'	1:A:567:U:O4'	2.16	0.45
2:B:3042:C:H2'	37:B:6700:HOH:O	2.14	0.45
3:C:57:ALA:HA	3:C:67:LEU:HD23	1.97	0.45
4:D:320:GLN:HG3	4:D:321:PRO:CD	2.46	0.45
5:E:142:ASP:OD1	5:E:237:GLU:HB3	2.16	0.45
6:F:93:LEU:HG	37:F:3862:HOH:O	2.16	0.45
7:G:101:GLU:OE2	7:G:115:ARG:NH1	2.49	0.45
7:G:145:ALA:HB1	7:G:168:ILE:CD1	2.46	0.45
13:M:35:ARG:O	13:M:35:ARG:NH1	2.49	0.45
28:2:28:HIS:CD2	28:2:30:LYS:HB2	2.51	0.45
29:3:49:GLU:CD	37:3:719:HOH:O	2.54	0.45
1:A:1057:A:C6	1:A:1058:A:C6	3.04	0.45
1:A:1753:C:O2	4:D:229:ARG:NH2	2.47	0.45
1:A:2478:U:H2'	1:A:2479:A:C8	2.51	0.45
1:A:2821:C:H4'	4:D:116:PRO:CB	2.46	0.45
1:A:960:G:N3	1:A:960:G:C2'	2.78	0.45
3:C:94:LEU:N	3:C:94:LEU:CD2	2.79	0.45
5:E:200:PRO:HB3	5:E:212:VAL:HG23	1.98	0.45
25:Y:30:MET:HE3	25:Y:59:TRP:HE1	1.81	0.45
37:N:8533:HOH:O	30:4:46:ILE:HB	2.16	0.45
1:A:1552:G:H2'	1:A:1553:C:C6	2.50	0.45
1:A:1603:A:H5''	1:A:1605:G:H5'	1.97	0.45
1:A:1730:G:C5'	1:A:1731:C:C6	2.99	0.45
1:A:2004:U:H2'	1:A:2004:U:O2	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2467:A:P	37:A:9038:HOH:O	2.73	0.45
1:A:316:A:H5'	21:U:54:ASP:OD2	2.16	0.45
1:A:920:C:N4	1:A:2467:A:C8	2.84	0.45
1:A:949:U:O2'	18:R:40:HIS:HE1	1.99	0.45
1:A:970:U:H2'	37:A:6298:HOH:O	2.16	0.45
4:D:53:LEU:HD11	4:D:327:VAL:HG22	1.99	0.45
5:E:233:THR:CG2	5:E:234:VAL:N	2.77	0.45
5:E:34:ALA:HB3	5:E:220:THR:HG21	1.99	0.45
13:M:30:ARG:NH2	37:M:8524:HOH:O	2.37	0.45
1:A:1172:G:H1'	37:A:4951:HOH:O	2.15	0.45
1:A:2107:U:O2'	1:A:2108:A:H5'	2.16	0.45
1:A:2300:A:C2	1:A:2306:U:C5	3.03	0.45
1:A:2450:C:O5'	1:A:2450:C:H6	2.00	0.45
1:A:2487:C:H5	37:A:4863:HOH:O	2.00	0.45
1:A:2533:C:O2'	1:A:2534:C:H5'	2.17	0.45
1:A:558:C:H2'	1:A:559:U:H5''	1.97	0.45
1:A:695:C:H2'	1:A:696:C:C6	2.51	0.45
1:A:716:G:H2'	1:A:717:C:O5'	2.17	0.45
2:B:3006:C:P	15:O:37:ARG:HH11	2.40	0.45
8:H:46:GLU:OE1	8:H:100:ASP:HA	2.15	0.45
11:K:39:VAL:CG1	11:K:107:ASN:HB2	2.47	0.45
37:A:3444:HOH:O	11:K:46:ILE:HD12	2.16	0.45
13:M:101:ASP:C	13:M:103:ALA:H	2.18	0.45
1:A:1500:U:P	17:Q:41:ARG:HH22	2.38	0.45
18:R:25:PRO:HA	18:R:26:PRO:HD3	1.80	0.45
24:X:88:THR:CG2	24:X:89:ASP:N	2.79	0.45
26:Z:109:LEU:HA	37:Z:8571:HOH:O	2.16	0.45
1:A:1328:A:OP1	26:Z:169:ARG:HD2	2.17	0.45
1:A:1593:C:OP1	17:Q:117:SER:CB	2.65	0.45
1:A:1778:A:H2'	1:A:1779:A:H5'	1.98	0.45
1:A:1805:G:H2'	1:A:1806:G:H8	1.81	0.45
1:A:1896:G:H1'	37:A:4232:HOH:O	2.15	0.45
1:A:2437:A:H2'	1:A:2438:G:C8	2.52	0.45
1:A:2769:C:H2'	1:A:2770:G:C5'	2.46	0.45
1:A:711:G:C2	1:A:718:C:C2	3.04	0.45
2:B:3057:A:N6	37:B:3535:HOH:O	2.44	0.45
4:D:274:GLU:HA	4:D:292:GLY:O	2.16	0.45
6:F:65:GLU:HA	37:F:6752:HOH:O	2.16	0.45
10:J:109:ASP:HB2	37:J:8333:HOH:O	2.15	0.45
10:J:58:HIS:CE1	10:J:59:ASN:ND2	2.84	0.45
12:L:14:LYS:HD2	12:L:45:PRO:HG3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:143:THR:HG21	37:M:8542:HOH:O	2.17	0.45
15:O:154:LEU:HG	15:O:155:GLU:N	2.30	0.45
15:O:5:ARG:HG3	18:R:18:PRO:HB3	1.98	0.45
1:A:21:G:H5'	19:S:1:GLY:O	2.17	0.45
1:A:1008:C:OP1	10:J:16:ARG:NH2	2.47	0.45
1:A:1161:A:O5'	1:A:1161:A:H8	2.00	0.45
1:A:2038:A:OP2	4:D:224:LYS:NZ	2.43	0.45
1:A:328:U:O4'	5:E:202:THR:HG22	2.17	0.45
2:B:3049:G:H2'	2:B:3050:G:O4'	2.16	0.45
3:C:211:LYS:HD3	37:C:8615:HOH:O	2.16	0.45
4:D:72:THR:HB	37:D:8606:HOH:O	2.15	0.45
5:E:85:LYS:HE2	37:E:8328:HOH:O	2.16	0.45
6:F:25:MET:SD	6:F:40:ILE:HD11	2.57	0.45
7:G:69:ILE:HA	7:G:72:MET:HE2	1.97	0.45
10:J:46:VAL:O	10:J:146:TRP:CH2	2.66	0.45
14:N:77:PHE:CD2	14:N:86:MET:HA	2.52	0.45
37:A:5657:HOH:O	15:O:21:HIS:HE1	1.99	0.45
30:4:7:PHE:HE2	30:4:22:VAL:CG2	2.27	0.45
1:A:1188:A:C5	1:A:1189:A:C2	3.05	0.45
1:A:1745:G:H5'	37:A:4303:HOH:O	2.17	0.45
1:A:1827:G:H2'	1:A:1828:G:C8	2.51	0.45
1:A:1862:C:O2'	1:A:1863:G:H5'	2.16	0.45
1:A:2428:G:O6	1:A:2464:C:H1'	2.17	0.45
1:A:422:G:C6	1:A:2446:G:C6	3.04	0.45
1:A:2909:G:H2'	1:A:2910:A:H8	1.82	0.45
1:A:457:U:H5	1:A:460:A:OP2	2.00	0.45
1:A:920:C:H5'	1:A:921:G:N3	2.31	0.45
2:B:3008:G:C6	2:B:3009:C:C4	3.04	0.45
4:D:55:ASN:HB3	4:D:64:GLY:N	2.31	0.45
4:D:7:ARG:HH12	4:D:11:LEU:HD21	1.81	0.45
5:E:187:ARG:O	5:E:187:ARG:HG3	2.15	0.45
5:E:80:VAL:HA	5:E:81:PRO:HD3	1.82	0.45
11:K:126:ASN:O	11:K:129:PHE:HE2	1.99	0.45
14:N:173:LEU:HD23	14:N:183:VAL:CG1	2.46	0.45
14:N:38:VAL:O	14:N:63:VAL:HG13	2.17	0.45
23:W:42:ASN:O	23:W:44:GLY:N	2.49	0.45
25:Y:21:PRO:HD3	37:Y:6179:HOH:O	2.16	0.45
26:Z:126:PRO:HG2	26:Z:128:PHE:CZ	2.50	0.45
5:E:51:TYR:CE2	28:2:53:LYS:HB3	2.52	0.45
1:A:1301:C:O2'	1:A:1331:A:H4'	2.17	0.45
1:A:158:A:O2'	1:A:159:G:H5'	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1614:G:H2'	37:A:4597:HOH:O	2.16	0.45
1:A:168:C:C2'	1:A:169:A:H5'	2.46	0.45
1:A:2032:U:O2'	1:A:2033:G:H5''	2.15	0.45
1:A:2290:U:H4'	1:A:2291:A:OP1	2.17	0.45
1:A:2379:G:H4'	1:A:2380:A:H5''	1.99	0.45
1:A:2420:G:H4'	37:A:4068:HOH:O	2.17	0.45
1:A:2667:G:H1'	1:A:2914:A:N3	2.31	0.45
1:A:426:G:C2	1:A:427:C:C2	3.05	0.45
1:A:958:G:H2'	1:A:959:C:C6	2.51	0.45
3:C:164:ARG:HA	27:1:69:TYR:CE1	2.52	0.45
7:G:12:ASP:HA	37:G:1750:HOH:O	2.17	0.45
8:H:58:GLU:HA	8:H:61:MET:HE2	1.99	0.45
16:P:60:VAL:O	16:P:62:GLY:N	2.39	0.45
17:Q:28:GLN:N	37:Q:6051:HOH:O	2.50	0.45
19:S:89:LEU:HD23	19:S:89:LEU:HA	1.82	0.45
24:X:122:ARG:HG2	24:X:152:ALA:O	2.15	0.45
24:X:142:ASP:HB3	24:X:145:GLY:H	1.81	0.45
24:X:64:THR:O	24:X:68:THR:HG22	2.16	0.45
1:A:2904:U:H4'	25:Y:8:ARG:NH1	2.32	0.45
26:Z:129:ASN:OD1	26:Z:141:THR:OG1	2.35	0.45
1:A:1335:C:OP2	26:Z:207:SER:CB	2.64	0.45
27:1:47:LEU:HD23	27:1:57:CYS:CB	2.45	0.45
1:A:1656:A:H2'	1:A:1657:A:O4'	2.17	0.45
1:A:1706:G:C5	1:A:1707:G:C6	3.05	0.45
1:A:2547:C:H2'	1:A:2548:C:H6	1.81	0.45
1:A:2569:A:O5'	1:A:2569:A:H8	2.00	0.45
1:A:2761:A:C4	1:A:2763:G:C8	3.05	0.45
1:A:644:G:H5'	1:A:644:G:N3	2.32	0.45
1:A:653:C:H2'	1:A:654:A:C8	2.51	0.45
3:C:109:GLU:CD	3:C:113:GLY:H	2.20	0.45
7:G:126:ILE:HB	7:G:131:LEU:CD2	2.46	0.45
7:G:162:PHE:CD1	7:G:162:PHE:N	2.84	0.45
15:O:58:LEU:CD1	15:O:58:LEU:N	2.80	0.45
15:O:71:TRP:N	37:O:8540:HOH:O	2.49	0.45
22:V:31:PHE:CG	22:V:37:GLU:HG2	2.52	0.45
27:1:11:THR:O	27:1:14:PHE:HB2	2.17	0.45
1:A:1477:C:H5'	1:A:1868:G:H5''	1.98	0.45
1:A:1880:C:C2	1:A:1881:A:C8	3.05	0.45
1:A:2011:A:H4'	1:A:2012:U:O5'	2.17	0.45
1:A:2434:A:O3'	30:4:28:GLY:CA	2.65	0.45
1:A:2909:G:O2'	1:A:2910:A:H5'	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:846:A:O2'	1:A:847:C:H5'	2.17	0.45
2:B:3114:G:H2'	2:B:3115:C:C6	2.52	0.45
3:C:125:ASN:ND2	37:C:8538:HOH:O	2.41	0.45
3:C:105:VAL:HG13	3:C:155:THR:O	2.16	0.45
5:E:27:ARG:HD2	5:E:29:ASP:OD1	2.16	0.45
6:F:58:VAL:CG1	6:F:59:GLY:N	2.78	0.45
10:J:30:GLN:H	10:J:65:ARG:NH1	2.15	0.45
10:J:81:TYR:CD1	10:J:81:TYR:C	2.89	0.45
11:K:70:PHE:O	11:K:70:PHE:CD2	2.70	0.45
12:L:14:LYS:CB	12:L:45:PRO:HG2	2.41	0.45
15:O:11:ARG:HG3	15:O:14:ARG:NH1	2.32	0.45
15:O:25:ARG:HA	15:O:28:LYS:HG3	1.98	0.45
25:Y:51:ASP:OD2	25:Y:52:PRO:HD2	2.17	0.45
26:Z:144:ARG:NH2	37:Z:8610:HOH:O	2.50	0.45
1:A:2435:U:P	30:4:28:GLY:HA3	2.56	0.44
1:A:2325:C:H1'	37:A:4120:HOH:O	2.18	0.44
1:A:2362:A:H2'	1:A:2363:G:C8	2.52	0.44
1:A:401:C:H2'	1:A:402:U:C6	2.52	0.44
1:A:596:C:H2'	1:A:597:A:C8	2.52	0.44
1:A:711:G:N2	1:A:718:C:C2	2.85	0.44
4:D:316:ARG:N	4:D:317:PRO:HD3	2.33	0.44
5:E:173:LYS:NZ	37:E:8319:HOH:O	2.49	0.44
10:J:1:LYS:HA	10:J:2:PRO:HD3	1.68	0.44
14:N:37:VAL:HG21	14:N:108:LYS:CG	2.47	0.44
15:O:143:ARG:NH1	15:O:173:ASP:OD2	2.40	0.44
19:S:29:LYS:HD3	37:S:8532:HOH:O	2.15	0.44
24:X:48:VAL:O	24:X:48:VAL:HG12	2.16	0.44
26:Z:117:LEU:HD12	26:Z:174:VAL:CG1	2.46	0.44
1:A:1886:A:O2'	27:1:20:LEU:HB2	2.17	0.44
1:A:1384:C:H5'	25:Y:30:MET:HG2	1.99	0.44
1:A:1434:A:H2'	1:A:1436:C:C5	2.51	0.44
1:A:1592:G:O2'	1:A:1593:C:O5'	2.35	0.44
1:A:1596:U:H2'	1:A:1598:A:OP2	2.16	0.44
1:A:1543:G:N1	1:A:1641:A:OP2	2.39	0.44
1:A:1701:A:H5''	1:A:1702:U:H3'	1.99	0.44
1:A:1771:U:O2'	27:1:23:ARG:NH2	2.49	0.44
1:A:2044:G:OP1	25:Y:23:HIS:HE1	1.99	0.44
1:A:2467:A:O2'	1:A:2468:A:H2'	2.17	0.44
1:A:2598:U:O2	1:A:2600:A:H8	2.00	0.44
1:A:746:A:C6	16:P:65:LEU:HD13	2.52	0.44
2:B:3076:G:C3'	2:B:3077:A:H5''	2.38	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:105:VAL:CG1	3:C:106:CYS:N	2.80	0.44
5:E:13:ASP:N	37:E:8440:HOH:O	2.51	0.44
5:E:173:LYS:HB3	5:E:187:ARG:HG3	1.98	0.44
5:E:20:ASP:O	5:E:23:GLU:HB2	2.17	0.44
7:G:77:THR:OG1	7:G:78:GLU:N	2.49	0.44
15:O:113:SER:CB	37:O:8560:HOH:O	2.58	0.44
15:O:120:GLU:HG3	15:O:136:LEU:HD13	1.99	0.44
17:Q:59:ARG:HH22	17:Q:66:GLN:HE22	1.62	0.44
23:W:12:THR:HG23	23:W:14:ALA:H	1.81	0.44
27:1:10:ARG:HG3	27:1:11:THR:N	2.33	0.44
28:2:28:HIS:HD2	28:2:30:LYS:H	1.64	0.44
1:A:1114:A:H2'	1:A:1115:U:C6	2.53	0.44
1:A:1269:G:O2'	1:A:1270:U:H5'	2.17	0.44
1:A:240:C:H2'	1:A:240:C:O2	2.17	0.44
1:A:2715:G:N2	4:D:264:GLU:OE1	2.51	0.44
1:A:2791:U:C1'	1:A:2792:A:H5''	2.47	0.44
1:A:533:U:C5	1:A:2084:C:H5'	2.53	0.44
1:A:818:A:C2	27:1:13:ARG:HA	2.52	0.44
1:A:920:C:H5''	1:A:921:G:O5'	2.17	0.44
1:A:958:G:O2'	1:A:959:C:H5'	2.17	0.44
5:E:55:ARG:HB2	37:E:8311:HOH:O	2.16	0.44
6:F:101:THR:HG22	6:F:101:THR:O	2.17	0.44
6:F:41:LEU:CA	6:F:44:ILE:HG22	2.46	0.44
7:G:81:GLU:HA	7:G:133:VAL:O	2.17	0.44
37:A:3671:HOH:O	7:G:143:GLN:HG2	2.17	0.44
10:J:82:LYS:HB2	10:J:82:LYS:NZ	2.32	0.44
20:T:37:VAL:O	20:T:41:VAL:HG23	2.18	0.44
25:Y:74:ALA:CB	25:Y:85:VAL:HG22	2.47	0.44
30:4:38:ARG:O	30:4:42:ARG:HB2	2.17	0.44
1:A:10:U:H5'	37:A:6007:HOH:O	2.17	0.44
1:A:1236:A:H2'	1:A:1237:U:O4'	2.17	0.44
1:A:1353:C:O5'	37:A:4650:HOH:O	2.19	0.44
1:A:1423:C:O2'	1:A:1424:A:H5'	2.17	0.44
1:A:1440:U:OP2	37:A:4435:HOH:O	2.21	0.44
1:A:157:G:H4'	14:N:95:LYS:CE	2.44	0.44
1:A:1685:A:H4'	1:A:1686:C:OP2	2.17	0.44
1:A:195:C:H2'	1:A:196:G:H5'	1.99	0.44
1:A:1979:G:O2'	1:A:1980:U:OP1	2.32	0.44
1:A:2284:G:H1'	37:A:9552:HOH:O	2.18	0.44
1:A:2851:G:C2'	1:A:2852:A:H5'	2.48	0.44
1:A:226:A:H1'	1:A:393:G:C5	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:602:A:O2'	1:A:605:C:H4'	2.17	0.44
4:D:41:PHE:CE1	4:D:79:MET:HG3	2.51	0.44
7:G:126:ILE:HB	7:G:131:LEU:HD23	1.98	0.44
10:J:72:VAL:CG1	10:J:81:TYR:CZ	3.01	0.44
18:R:64:GLU:HG3	18:R:74:ASP:OD2	2.18	0.44
21:U:50:VAL:HG12	21:U:56:ALA:HA	1.99	0.44
26:Z:136:LYS:HE2	26:Z:138:ARG:NH1	2.31	0.44
27:1:22:ILE:O	27:1:26:VAL:HG23	2.18	0.44
1:A:1517:U:C2	1:A:1670:G:N2	2.85	0.44
1:A:2428:G:C6	1:A:2464:C:H1'	2.53	0.44
1:A:2503:A:OP1	10:J:147:ARG:NH2	2.44	0.44
1:A:2777:G:O2'	1:A:2778:A:H5'	2.17	0.44
4:D:195:ARG:NH1	4:D:324:ASP:OD1	2.48	0.44
5:E:84:VAL:O	5:E:85:LYS:CB	2.65	0.44
6:F:36:ASN:CA	37:F:7500:HOH:O	2.62	0.44
7:G:22:VAL:O	7:G:28:SER:HA	2.18	0.44
9:I:12:ILE:HD12	37:I:692:HOH:O	2.16	0.44
10:J:150:LYS:HG2	37:J:8372:HOH:O	2.17	0.44
13:M:62:ALA:HB2	13:M:103:ALA:CB	2.48	0.44
13:M:93:VAL:HG12	13:M:97:VAL:HG23	2.00	0.44
15:O:132:ASN:O	15:O:135:VAL:HG12	2.18	0.44
24:X:54:PHE:CZ	24:X:140:LYS:HB2	2.53	0.44
30:4:69:TYR:O	30:4:77:ALA:HA	2.17	0.44
1:A:1414:A:H2'	1:A:1415:G:O4'	2.17	0.44
1:A:160:A:C8	1:A:177:A:C6	3.05	0.44
1:A:2443:C:O3'	13:M:56:LYS:HE3	2.17	0.44
1:A:534:C:N4	37:A:7556:HOH:O	2.47	0.44
1:A:818:A:H2	27:1:13:ARG:HA	1.81	0.44
1:A:920:C:C4	1:A:2467:A:C5	3.05	0.44
4:D:248:ARG:NH1	37:D:8616:HOH:O	2.49	0.44
7:G:36:PRO:HD3	11:K:127:ILE:HD12	1.99	0.44
17:Q:2:ASP:OD1	17:Q:2:ASP:C	2.55	0.44
1:A:2363:G:O2'	18:R:11:ARG:HG3	2.18	0.44
1:A:100:C:H4'	21:U:16:LEU:HB2	2.00	0.44
23:W:39:ALA:C	23:W:41:GLU:N	2.71	0.44
37:A:6516:HOH:O	27:1:22:ILE:HG13	2.16	0.44
1:A:1137:G:H1'	37:A:3854:HOH:O	2.18	0.44
1:A:1158:G:O2'	1:A:1159:G:H5'	2.17	0.44
1:A:1992:U:H2'	1:A:1994:A:OP2	2.17	0.44
1:A:236:A:O5'	1:A:236:A:H2'	2.17	0.44
4:D:2:GLN:HA	37:D:8622:HOH:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:304:PRO:HD2	4:D:307:ARG:CD	2.48	0.44
8:H:101:ALA:HB2	8:H:108:LEU:CD2	2.48	0.44
9:I:64:ASN:ND2	9:I:64:ASN:N	2.65	0.44
10:J:85:ILE:O	10:J:85:ILE:HG23	2.18	0.44
12:L:22:ASP:OD1	12:L:22:ASP:C	2.56	0.44
12:L:28:GLU:OE2	12:L:58:THR:HG21	2.17	0.44
24:X:4:LEU:HD21	24:X:52:VAL:HG11	1.99	0.44
1:A:1135:G:H5'	37:A:5898:HOH:O	2.17	0.44
1:A:2265:U:H2'	1:A:2266:A:H8	1.83	0.44
1:A:236:A:H4'	1:A:237:G:OP1	2.18	0.44
1:A:2547:C:C2	1:A:2548:C:C5	3.05	0.44
1:A:628:A:C4	1:A:2071:C:C4	3.06	0.44
1:A:731:U:O2'	1:A:732:C:H5'	2.18	0.44
1:A:920:C:H4'	1:A:921:G:N2	2.32	0.44
5:E:150:THR:HA	5:E:203:ALA:O	2.17	0.44
5:E:35:VAL:HG21	5:E:227:GLY:HA2	1.99	0.44
9:I:63:ARG:O	9:I:67:LEU:HG	2.18	0.44
12:L:40:THR:O	12:L:41:LYS:C	2.55	0.44
1:A:2721:U:H4'	12:L:87:ARG:HG3	1.99	0.44
13:M:54:PRO:HG2	13:M:57:VAL:HG21	1.99	0.44
18:R:93:ARG:HH11	18:R:93:ARG:HG3	1.82	0.44
24:X:5:VAL:O	24:X:52:VAL:HG22	2.17	0.44
24:X:6:GLN:HA	24:X:52:VAL:HG23	1.98	0.44
24:X:85:ALA:HB2	24:X:91:ASP:O	2.18	0.44
1:A:797:A:H5'	27:1:10:ARG:HG2	2.00	0.44
37:A:7559:HOH:O	27:1:31:ILE:HG13	2.18	0.44
1:A:148:A:H5''	28:2:44:LYS:HG2	2.00	0.44
30:4:17:HIS:O	30:4:18:GLN:HG3	2.18	0.44
1:A:1819:G:H2'	1:A:1820:G:C5'	2.48	0.44
1:A:1855:G:O6	3:C:142:SER:HB3	2.18	0.44
1:A:2010:A:C2'	37:A:5928:HOH:O	2.66	0.44
1:A:513:A:N3	37:A:3639:HOH:O	2.36	0.44
1:A:716:G:C2'	1:A:717:C:O5'	2.66	0.44
1:A:834:G:H5''	1:A:835:U:O5'	2.18	0.44
3:C:99:ILE:O	3:C:131:HIS:CE1	2.71	0.44
6:F:23:VAL:CG2	6:F:73:VAL:HB	2.47	0.44
13:M:126:SER:O	13:M:127:GLU:C	2.54	0.44
14:N:114:VAL:HG21	14:N:159:THR:CG2	2.47	0.44
14:N:61:ILE:HA	37:N:8623:HOH:O	2.18	0.44
15:O:171:HIS:CE1	37:O:8568:HOH:O	2.70	0.44
19:S:39:THR:CB	19:S:42:GLU:HG3	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:V:49:LEU:O	22:V:55:ALA:CB	2.66	0.44
24:X:154:ARG:HE	24:X:154:ARG:HB3	1.59	0.44
1:A:1348:A:N3	37:A:9951:HOH:O	2.36	0.43
1:A:1375:A:C2'	1:A:1376:G:H5'	2.48	0.43
1:A:1594:C:O2'	1:A:1607:A:H4'	2.18	0.43
1:A:1730:G:C5'	1:A:1731:C:H6	2.30	0.43
1:A:1878:G:C4'	37:A:6090:HOH:O	2.65	0.43
1:A:1881:A:OP1	3:C:199:HIS:HE1	2.01	0.43
1:A:2453:G:H5'	37:A:4663:HOH:O	2.17	0.43
1:A:2715:G:O2'	4:D:262:ARG:HD2	2.18	0.43
1:A:585:C:H6	37:A:6064:HOH:O	1.99	0.43
3:C:103:VAL:HA	3:C:104:PRO:HD3	1.85	0.43
3:C:81:GLN:CB	3:C:92:ASN:ND2	2.80	0.43
4:D:132:HIS:HB2	4:D:137:LEU:HD22	2.00	0.43
4:D:314:ALA:CB	4:D:317:PRO:HG3	2.48	0.43
5:E:165:ASP:O	5:E:168:ARG:HB3	2.18	0.43
6:F:99:ASP:O	6:F:159:PRO:HG3	2.17	0.43
7:G:107:PHE:CZ	7:G:108:LEU:HD13	2.52	0.43
9:I:71:LEU:C	9:I:73:ASP:H	2.21	0.43
10:J:113:ALA:N	10:J:114:PRO:CD	2.81	0.43
10:J:65:ARG:HD3	37:J:8374:HOH:O	2.17	0.43
15:O:24:LEU:HD13	18:R:26:PRO:HB3	2.00	0.43
19:S:125:ARG:HG2	37:S:8543:HOH:O	2.18	0.43
20:T:10:VAL:HG11	23:W:36:ALA:HA	1.99	0.43
27:1:56:MET:HA	27:1:62:TYR:O	2.18	0.43
30:4:3:MET:HG3	30:4:4:PRO:HD2	2.00	0.43
1:A:1185:U:C5'	37:A:7445:HOH:O	2.65	0.43
1:A:1545:C:O2'	1:A:1546:G:H5'	2.18	0.43
1:A:177:A:H2'	1:A:178:U:O4'	2.18	0.43
1:A:1819:G:H2'	1:A:1820:G:C4'	2.48	0.43
1:A:920:C:N4	1:A:2467:A:C4	2.86	0.43
1:A:707:C:H2'	1:A:708:A:H8	1.82	0.43
3:C:199:HIS:HD2	3:C:201:PHE:N	2.06	0.43
5:E:140:VAL:HG12	5:E:141:SER:N	2.33	0.43
5:E:180:SER:HB2	37:E:8444:HOH:O	2.18	0.43
7:G:139:GLU:CG	37:G:5919:HOH:O	2.65	0.43
7:G:20:ILE:O	7:G:30:THR:HA	2.18	0.43
8:H:79:GLN:HG3	8:H:82:ASP:OD2	2.17	0.43
11:K:130:VAL:CG1	11:K:131:THR:N	2.81	0.43
11:K:39:VAL:HG12	11:K:40:ASN:ND2	2.33	0.43
12:L:14:LYS:HB2	12:L:45:PRO:CG	2.41	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:148:GLU:HB2	37:M:8587:HOH:O	2.17	0.43
17:Q:10:ALA:CA	17:Q:13:VAL:HG12	2.45	0.43
20:T:57:THR:CG2	20:T:59:ASP:HB2	2.49	0.43
22:V:17:THR:HG22	22:V:18:GLY:N	2.33	0.43
26:Z:189:ASN:ND2	26:Z:189:ASN:C	2.71	0.43
27:1:47:LEU:HA	27:1:56:MET:O	2.18	0.43
29:3:36:ASN:HB3	29:3:39:ARG:NE	2.33	0.43
1:A:1215:A:O3'	1:A:1216:G:C4'	2.66	0.43
1:A:1973:A:H2'	1:A:1974:G:O4'	2.18	0.43
1:A:2004:U:H5''	1:A:2005:G:C8	2.53	0.43
1:A:2084:C:O2'	1:A:2085:A:H5'	2.18	0.43
1:A:255:A:H2'	1:A:256:C:C6	2.53	0.43
1:A:303:C:H2'	1:A:304:G:O4'	2.19	0.43
1:A:340:A:C2	1:A:341:C:C6	3.06	0.43
1:A:394:G:H1	14:N:181:GLU:CD	2.22	0.43
1:A:694:A:C2'	1:A:695:C:H5'	2.48	0.43
1:A:827:A:H2'	1:A:828:G:O4'	2.17	0.43
2:B:3007:G:OP1	15:O:23:ARG:HD2	2.18	0.43
3:C:179:MET:HG2	3:C:186:TRP:HB3	1.99	0.43
3:C:58:VAL:O	3:C:65:ARG:HD2	2.18	0.43
5:E:5:ILE:CD1	5:E:16:VAL:HG23	2.28	0.43
6:F:52:THR:N	6:F:70:GLY:O	2.51	0.43
11:K:45:VAL:HG21	11:K:129:PHE:CD1	2.54	0.43
12:L:72:VAL:HG11	12:L:121:PHE:CD1	2.53	0.43
13:M:98:GLU:O	13:M:99:GLU:CB	2.66	0.43
14:N:139:PRO:HA	14:N:142:LYS:HB2	2.00	0.43
14:N:158:ARG:N	34:N:8518:CL:CL	2.88	0.43
15:O:184:ILE:HG22	15:O:185:GLU:N	2.33	0.43
17:Q:141:ILE:C	17:Q:143:ALA:H	2.22	0.43
26:Z:107:PRO:HD3	26:Z:182:PHE:CE1	2.54	0.43
30:4:1:MET:N	30:4:87:ARG:O	2.47	0.43
1:A:1069:C:H4'	1:A:1081:A:O2'	2.18	0.43
1:A:10:U:HO2'	1:A:11:A:P	2.42	0.43
1:A:907:A:H4'	1:A:1328:A:C2	2.53	0.43
1:A:2419:U:H5''	1:A:2420:G:C5'	2.48	0.43
1:A:392:U:H4'	14:N:193:LYS:HB3	2.00	0.43
1:A:621:C:H5'	26:Z:132:ASP:OD2	2.19	0.43
1:A:629:A:N7	37:A:9835:HOH:O	2.37	0.43
1:A:911:G:H5'	1:A:932:U:OP1	2.18	0.43
1:A:95:A:H5''	1:A:97:G:O4'	2.18	0.43
3:C:93:THR:HG23	3:C:154:ALA:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:108:GLU:HB3	4:D:111:ARG:HD2	2.00	0.43
5:E:136:VAL:HG22	5:E:137:PRO:HA	1.99	0.43
7:G:107:PHE:CD2	7:G:108:LEU:HD13	2.51	0.43
8:H:105:ALA:HB2	37:H:5522:HOH:O	2.19	0.43
11:K:72:PRO:O	11:K:78:ILE:CD1	2.67	0.43
37:B:4707:HOH:O	15:O:147:ILE:HB	2.19	0.43
16:P:96:VAL:HG13	16:P:100:GLN:HB2	2.01	0.43
17:Q:115:SER:C	17:Q:117:SER:H	2.22	0.43
20:T:23:LYS:HD3	20:T:65:VAL:HG12	2.00	0.43
21:U:96:VAL:HG13	21:U:97:ARG:N	2.33	0.43
23:W:20:LEU:HD22	23:W:60:GLN:HE22	1.82	0.43
24:X:35:VAL:HG23	24:X:41:TYR:CD2	2.53	0.43
27:1:48:LYS:HG2	37:1:8434:HOH:O	2.18	0.43
1:A:1894:C:C2	1:A:1939:U:C4	3.05	0.43
1:A:2478:U:H2'	1:A:2479:A:H8	1.83	0.43
1:A:2484:U:C2	37:A:9600:HOH:O	2.57	0.43
1:A:2783:A:O2'	1:A:2784:A:H5'	2.18	0.43
1:A:297:U:H1'	37:A:3911:HOH:O	2.17	0.43
1:A:299:U:C5'	37:A:7314:HOH:O	2.62	0.43
1:A:440:C:C4	1:A:441:A:C6	3.06	0.43
1:A:899:C:OP2	13:M:22:ARG:NH1	2.51	0.43
3:C:94:LEU:HG	3:C:99:ILE:CD1	2.48	0.43
6:F:92:GLU:O	6:F:93:LEU:O	2.36	0.43
1:A:1003:U:O2'	10:J:90:PHE:HE1	1.97	0.43
1:A:183:A:C5'	14:N:157:LEU:HD12	2.48	0.43
14:N:186:SER:OG	14:N:189:VAL:HG12	2.19	0.43
16:P:14:LEU:CD2	16:P:102:ILE:HD11	2.48	0.43
20:T:10:VAL:HG13	23:W:35:ALA:O	2.18	0.43
1:A:1098:A:H2'	1:A:1099:G:O4'	2.19	0.43
1:A:1730:G:H5'	1:A:1731:C:C6	2.54	0.43
1:A:2769:C:H2'	1:A:2770:G:H5'	2.01	0.43
1:A:282:C:H2'	1:A:283:U:O4'	2.17	0.43
1:A:628:A:C4	1:A:2071:C:N4	2.86	0.43
1:A:772:G:H2'	1:A:773:A:O4'	2.19	0.43
4:D:185:GLY:HA2	37:D:8636:HOH:O	2.19	0.43
37:A:5056:HOH:O	4:D:216:LYS:HA	2.18	0.43
4:D:280:VAL:HG13	4:D:334:SER:HA	1.99	0.43
4:D:86:ALA:HB2	4:D:128:ILE:HD13	2.01	0.43
5:E:218:VAL:CG1	37:E:8422:HOH:O	2.67	0.43
5:E:54:LEU:HD21	5:E:87:ARG:HD2	1.99	0.43
7:G:9:GLU:HG3	7:G:10:ASP:N	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:104:ALA:HA	37:H:6617:HOH:O	2.18	0.43
8:H:27:GLY:HA3	37:H:5413:HOH:O	2.18	0.43
8:H:36:THR:HG23	8:H:97:ALA:HB2	2.00	0.43
13:M:90:ARG:NH1	13:M:119:THR:HG21	2.34	0.43
14:N:115:LEU:O	14:N:115:LEU:HD13	2.19	0.43
14:N:47:ASP:CG	14:N:48:ARG:N	2.72	0.43
15:O:73:ALA:CB	37:O:8568:HOH:O	2.66	0.43
21:U:48:VAL:HG11	21:U:96:VAL:CG1	2.48	0.43
26:Z:115:ARG:CZ	37:Z:8556:HOH:O	2.67	0.43
29:3:19:SER:O	29:3:36:ASN:ND2	2.52	0.43
1:A:1066:U:H2'	1:A:1067:A:C8	2.53	0.43
1:A:1159:G:H1	1:A:1208:C:H42	1.67	0.43
1:A:1495:C:H1'	1:A:1573:A:H1'	2.01	0.43
1:A:1545:C:H2'	1:A:1546:G:O4'	2.18	0.43
1:A:1666:C:C2'	1:A:1667:A:H5'	2.46	0.43
1:A:1732:A:O5'	1:A:1732:A:H8	2.02	0.43
1:A:1790:C:H2'	1:A:1791:U:H6	1.83	0.43
1:A:2269:C:H2'	1:A:2270:G:C5'	2.49	0.43
1:A:2403:C:H5'	37:A:5995:HOH:O	2.19	0.43
1:A:2405:C:H5'	37:A:6569:HOH:O	2.19	0.43
1:A:245:C:H2'	1:A:246:G:H5'	1.99	0.43
1:A:2728:C:O5'	1:A:2728:C:H6	2.01	0.43
1:A:1815:A:H4'	1:A:2751:C:O4'	2.18	0.43
1:A:2781:U:H2'	1:A:2782:G:H5'	2.00	0.43
4:D:258:GLY:N	4:D:260:HIS:CE1	2.86	0.43
37:A:9185:HOH:O	5:E:107:ARG:NH2	2.51	0.43
1:A:1308:A:O4'	5:E:226:GLY:HA3	2.19	0.43
6:F:23:VAL:HG23	6:F:41:LEU:HD22	2.00	0.43
10:J:149:ALA:C	10:J:151:MET:H	2.21	0.43
10:J:26:LYS:HG3	10:J:58:HIS:HB2	2.01	0.43
10:J:62:GLU:OE2	10:J:66:VAL:CG2	2.67	0.43
12:L:37:TYR:CE2	12:L:45:PRO:HA	2.54	0.43
14:N:68:ARG:CD	14:N:68:ARG:O	2.65	0.43
15:O:67:ALA:HA	15:O:71:TRP:HB3	2.01	0.43
1:A:2737:C:OP2	17:Q:58:SER:HB2	2.19	0.43
22:V:52:THR:HG22	22:V:54:THR:H	1.84	0.43
28:2:52:SER:HA	37:2:8442:HOH:O	2.19	0.43
1:A:1187:U:C2'	37:A:6864:HOH:O	2.55	0.43
1:A:1221:G:C8	37:A:5958:HOH:O	2.69	0.43
1:A:1332:C:O2'	1:A:1333:U:H5'	2.19	0.43
1:A:1773:G:H2'	1:A:1774:G:H5'	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1862:C:C2'	1:A:1863:G:H5'	2.49	0.43
1:A:2246:U:N3	1:A:2256:G:C2	2.87	0.43
1:A:2300:A:H4'	1:A:2301:A:O5'	2.19	0.43
1:A:2456:A:H2'	1:A:2457:U:C6	2.54	0.43
1:A:2911:C:H2'	1:A:2912:C:C6	2.54	0.43
1:A:377:C:H5	37:A:3291:HOH:O	2.01	0.43
1:A:830:G:O2'	1:A:831:U:H5'	2.19	0.43
1:A:962:C:H5''	37:A:4892:HOH:O	2.18	0.43
3:C:1:GLY:N	37:C:8612:HOH:O	2.29	0.43
1:A:890:C:OP1	5:E:57:PRO:HG3	2.18	0.43
6:F:94:ALA:HB3	6:F:174:VAL:CA	2.48	0.43
10:J:14:TYR:N	10:J:91:HIS:HE1	2.15	0.43
13:M:130:ARG:NH2	37:M:8547:HOH:O	2.51	0.43
14:N:84:LYS:O	14:N:87:MET:CG	2.67	0.43
19:S:141:VAL:HG12	19:S:142:ASP:O	2.19	0.43
19:S:40:ALA:O	19:S:44:VAL:HG23	2.18	0.43
19:S:82:GLU:HG3	19:S:83:LYS:H	1.84	0.43
21:U:105:ASP:OD1	21:U:107:LYS:N	2.51	0.43
21:U:12:ARG:NH1	37:U:3035:HOH:O	2.51	0.43
24:X:41:TYR:CD2	24:X:44:MET:HE3	2.53	0.43
1:A:101:C:H2'	1:A:102:A:C8	2.53	0.43
1:A:1262:C:H1'	24:X:120:PRO:HG3	2.00	0.43
1:A:1299:G:N2	37:A:4655:HOH:O	2.51	0.43
1:A:1463:A:C6	1:A:1464:U:C4	3.07	0.43
1:A:1940:C:H4'	37:A:7324:HOH:O	2.18	0.43
1:A:201:G:N2	1:A:202:U:C2	2.87	0.43
1:A:2296:C:H5	37:R:5998:HOH:O	2.02	0.43
1:A:2415:A:N3	15:O:26:LEU:HD13	2.33	0.43
1:A:2672:C:O2'	1:A:2673:U:H5'	2.19	0.43
1:A:451:C:N4	1:A:452:G:C6	2.87	0.43
1:A:684:G:H2'	1:A:685:C:C6	2.53	0.43
1:A:696:C:O2'	1:A:697:G:H5'	2.18	0.43
2:B:3056:A:C3'	2:B:3057:A:H5''	2.49	0.43
3:C:55:VAL:HG22	3:C:68:ILE:O	2.19	0.43
4:D:279:THR:HG22	4:D:280:VAL:N	2.32	0.43
5:E:193:LEU:O	5:E:233:THR:HG23	2.18	0.43
5:E:78:ARG:HG2	37:E:8307:HOH:O	2.19	0.43
7:G:132:THR:HG23	7:G:132:THR:O	2.19	0.43
10:J:136:VAL:CG2	37:J:8330:HOH:O	2.56	0.43
12:L:90:PHE:CD1	12:L:90:PHE:N	2.87	0.43
14:N:69:LYS:HG2	14:N:127:LYS:HG3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:41:LEU:HD12	18:R:41:LEU:N	2.33	0.43
25:Y:76:ARG:HA	25:Y:82:GLU:O	2.19	0.43
27:1:38:LYS:HA	27:1:45:LYS:HA	2.01	0.43
1:A:1044:C:C5'	37:A:9022:HOH:O	2.66	0.43
1:A:1634:G:H2'	1:A:1635:U:C6	2.53	0.43
1:A:217:C:OP1	1:A:395:A:O2'	2.25	0.43
1:A:794:U:H3	1:A:819:A:H61	1.66	0.43
1:A:812:A:H2'	1:A:813:C:O4'	2.18	0.43
5:E:127:ARG:HG2	5:E:127:ARG:NH1	2.33	0.43
6:F:23:VAL:HG21	6:F:45:THR:CG2	2.49	0.43
11:K:17:CYS:O	11:K:45:VAL:HG12	2.18	0.43
1:A:1103:C:O2'	11:K:86:MET:HB3	2.19	0.43
14:N:42:ARG:HA	14:N:43:PRO:HD3	1.75	0.43
18:R:40:HIS:CE1	18:R:94:GLN:HA	2.54	0.43
21:U:48:VAL:HG13	21:U:96:VAL:HG13	2.01	0.43
1:A:2460:A:OP1	30:4:60:LYS:HB2	2.19	0.42
1:A:1279:U:H5''	37:A:9572:HOH:O	2.19	0.42
1:A:1391:G:H2'	1:A:1392:A:H5'	2.01	0.42
1:A:2500:C:O2'	1:A:2501:G:H5'	2.18	0.42
1:A:2621:U:H5	37:A:9961:HOH:O	2.01	0.42
1:A:290:C:H2'	1:A:291:C:O4'	2.19	0.42
1:A:445:U:C1'	37:A:7314:HOH:O	2.66	0.42
1:A:517:U:H1'	37:A:7554:HOH:O	2.19	0.42
1:A:80:A:H3'	21:U:43:ASN:OD1	2.19	0.42
2:B:3048:C:H4'	15:O:141:ARG:NH2	2.29	0.42
5:E:77:ALA:O	5:E:78:ARG:HG3	2.19	0.42
6:F:166:ILE:O	6:F:169:THR:N	2.52	0.42
6:F:173:GLU:HG3	6:F:174:VAL:N	2.34	0.42
6:F:35:ALA:C	6:F:37:ALA:N	2.72	0.42
12:L:130:MET:SD	22:V:25:ASP:O	2.77	0.42
12:L:86:THR:HG22	12:L:87:ARG:N	2.34	0.42
14:N:88:VAL:O	14:N:88:VAL:HG12	2.19	0.42
15:O:143:ARG:NH1	15:O:173:ASP:OD1	2.52	0.42
15:O:24:LEU:O	15:O:28:LYS:HG2	2.19	0.42
15:O:32:PRO:HD2	15:O:99:GLU:O	2.19	0.42
21:U:55:PHE:CD2	21:U:77:VAL:HG13	2.54	0.42
25:Y:21:PRO:HG2	25:Y:24:LYS:HD3	2.01	0.42
1:A:1706:G:C6	1:A:1707:G:C6	3.07	0.42
1:A:1968:A:H2'	1:A:1969:A:C8	2.54	0.42
1:A:636:G:H5'	1:A:2059:U:OP2	2.19	0.42
1:A:2526:C:H5'	1:A:2526:C:C6	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:291:C:H2'	1:A:292:G:O4'	2.19	0.42
1:A:567:U:H5''	37:A:6375:HOH:O	2.19	0.42
1:A:724:G:O2'	1:A:725:C:H5'	2.19	0.42
2:B:3034:A:H2'	2:B:3035:C:O4'	2.19	0.42
3:C:70:ALA:HA	3:C:71:PRO:HD3	1.80	0.42
5:E:13:ASP:O	5:E:13:ASP:OD1	2.37	0.42
5:E:79:ARG:O	5:E:87:ARG:HG2	2.19	0.42
13:M:148:GLU:HG2	37:M:8553:HOH:O	2.20	0.42
13:M:35:ARG:O	13:M:40:PHE:HA	2.18	0.42
14:N:27:ARG:O	14:N:30:GLU:N	2.51	0.42
14:N:35:PRO:HD2	14:N:38:VAL:CG2	2.49	0.42
14:N:63:VAL:HG21	14:N:109:PHE:CE1	2.54	0.42
16:P:47:ARG:NH2	37:P:510:HOH:O	2.51	0.42
1:A:1789:G:O6	17:Q:73:HIS:HE1	2.03	0.42
19:S:132:ARG:NH1	37:S:8582:HOH:O	2.51	0.42
24:X:73:LEU:HD12	24:X:73:LEU:HA	1.86	0.42
30:4:73:GLU:HB2	37:4:8529:HOH:O	2.18	0.42
1:A:1117:A:C2	1:A:1244:U:C2	3.07	0.42
1:A:1166:A:H2'	1:A:1166:A:N3	2.34	0.42
1:A:1215:A:O3'	1:A:1216:G:H4'	2.19	0.42
1:A:1611:G:O2'	1:A:1612:A:H5'	2.20	0.42
1:A:1902:G:H2'	1:A:1903:U:O4'	2.19	0.42
1:A:2247:C:C5'	37:A:7322:HOH:O	2.67	0.42
37:A:7336:HOH:O	3:C:177:HIS:HE1	2.01	0.42
6:F:144:ARG:NH2	37:F:3839:HOH:O	2.49	0.42
6:F:169:THR:O	6:F:170:TYR:HB2	2.19	0.42
6:F:59:GLY:C	6:F:61:PHE:N	2.73	0.42
13:M:55:GLN:HA	13:M:58:GLN:NE2	2.33	0.42
14:N:87:MET:HG3	14:N:87:MET:H	1.42	0.42
14:N:74:ARG:HD3	14:N:91:ILE:HD12	2.00	0.42
15:O:47:LEU:CD1	15:O:97:VAL:HG11	2.49	0.42
19:S:119:VAL:O	19:S:119:VAL:HG12	2.18	0.42
30:4:75:GLY:HA2	37:4:8563:HOH:O	2.19	0.42
1:A:120:A:H5'	28:2:20:ARG:HH21	1.84	0.42
1:A:1681:G:H5''	1:A:1682:A:H5'	2.00	0.42
1:A:2241:C:H2'	1:A:2242:U:C6	2.54	0.42
1:A:259:G:H21	14:N:58:GLN:NE2	2.17	0.42
1:A:2088:C:H1'	1:A:2841:A:N1	2.34	0.42
1:A:553:G:P	26:Z:204:ARG:NH2	2.91	0.42
1:A:707:C:C2	1:A:708:A:C8	3.06	0.42
1:A:795:G:N3	1:A:817:G:C2	2.88	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:876:A:H2'	1:A:876:A:N3	2.35	0.42
2:B:3030:C:OP1	6:F:137:PRO:O	2.37	0.42
6:F:53:LYS:HA	6:F:67:ASP:O	2.20	0.42
10:J:57:ARG:C	10:J:59:ASN:H	2.21	0.42
10:J:65:ARG:NH2	10:J:66:VAL:HG22	2.35	0.42
17:Q:7:LYS:CD	17:Q:21:VAL:HG21	2.49	0.42
37:A:9535:HOH:O	24:X:119:HIS:HE1	2.02	0.42
1:A:1586:G:O2'	1:A:1587:U:H5'	2.19	0.42
1:A:1886:A:H4'	37:1:8405:HOH:O	2.19	0.42
1:A:2270:G:H4'	3:C:223:ARG:NH1	2.34	0.42
1:A:2307:A:C2	1:A:2308:U:N3	2.87	0.42
1:A:473:A:O2'	1:A:474:C:H5'	2.19	0.42
3:C:211:LYS:HB2	37:C:8622:HOH:O	2.18	0.42
4:D:84:LEU:HD13	4:D:84:LEU:C	2.40	0.42
5:E:27:ARG:HG2	5:E:30:LEU:HG	2.02	0.42
5:E:78:ARG:CG	5:E:78:ARG:NH1	2.76	0.42
6:F:153:THR:HG22	37:F:5234:HOH:O	2.19	0.42
8:H:49:PHE:O	8:H:95:ALA:HA	2.19	0.42
10:J:58:HIS:CE1	10:J:59:ASN:HD21	2.37	0.42
14:N:71:SER:O	14:N:73:ARG:NH1	2.51	0.42
18:R:10:THR:O	18:R:11:ARG:C	2.58	0.42
18:R:41:LEU:HB3	18:R:52:PHE:CZ	2.55	0.42
26:Z:133:HIS:CD2	37:Z:8583:HOH:O	2.52	0.42
28:2:5:THR:HB	28:2:6:PRO:CD	2.50	0.42
1:A:1450:C:O2'	1:A:1493:A:H2'	2.19	0.42
1:A:1616:A:H5''	1:A:1617:C:OP1	2.20	0.42
1:A:161:A:OP1	14:N:82:ARG:HG2	2.20	0.42
1:A:1666:C:H2'	1:A:1667:A:H8	1.84	0.42
1:A:1972:U:C2'	1:A:1973:A:H5'	2.48	0.42
1:A:2134:G:C6	1:A:2258:A:C8	3.08	0.42
1:A:269:G:C2	1:A:270:U:O4	2.72	0.42
1:A:2900:G:H2'	1:A:2901:C:O4'	2.20	0.42
1:A:2911:C:H3'	37:A:5528:HOH:O	2.19	0.42
1:A:657:G:H2'	1:A:658:C:C6	2.55	0.42
5:E:53:GLY:O	5:E:79:ARG:HA	2.19	0.42
11:K:54:VAL:HG11	11:K:138:THR:HG21	2.01	0.42
13:M:90:ARG:NH2	13:M:121:ILE:HD11	2.34	0.42
8:H:56:PRO:CG	14:N:44:THR:HA	2.49	0.42
37:B:4707:HOH:O	15:O:147:ILE:HD12	2.20	0.42
16:P:14:LEU:HD23	16:P:102:ILE:HD11	2.01	0.42
17:Q:115:SER:C	17:Q:117:SER:N	2.73	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:5:SER:OG	19:S:144:GLU:OE1	2.33	0.42
21:U:96:VAL:CG1	21:U:97:ARG:N	2.80	0.42
26:Z:122:ARG:NH2	37:Z:8535:HOH:O	2.52	0.42
3:C:72:GLU:OE1	27:1:72:GLU:HA	2.19	0.42
30:4:91:GLN:O	30:4:92:GLU:HB2	2.19	0.42
1:A:1139:U:H2'	1:A:1140:C:C6	2.54	0.42
1:A:1185:U:O4'	37:A:7445:HOH:O	2.22	0.42
1:A:1456:C:H2'	1:A:1457:U:C6	2.55	0.42
1:A:1593:C:OP1	17:Q:117:SER:HB3	2.20	0.42
1:A:219:G:O5'	1:A:220:C:H5''	2.20	0.42
1:A:2820:A:H2'	1:A:2821:C:C6	2.55	0.42
1:A:2836:G:C6	1:A:2838:A:C2	3.07	0.42
1:A:324:G:O2'	1:A:325:U:H5'	2.19	0.42
1:A:88:G:H2'	1:A:89:G:C8	2.53	0.42
4:D:312:ARG:HG2	4:D:313:PRO:N	2.33	0.42
12:L:34:VAL:CG2	12:L:47:ALA:HB2	2.48	0.42
15:O:181:ASP:HA	37:O:8572:HOH:O	2.19	0.42
15:O:90:LEU:HB2	15:O:186:LEU:HD22	2.00	0.42
16:P:21:SER:OG	16:P:106:PRO:HB2	2.20	0.42
20:T:10:VAL:CG1	23:W:35:ALA:O	2.68	0.42
1:A:97:G:C2	21:U:107:LYS:HD2	2.54	0.42
24:X:139:GLY:O	24:X:141:HIS:HD2	2.01	0.42
25:Y:79:GLU:OE2	37:Y:5564:HOH:O	2.21	0.42
1:A:1829:A:N6	27:1:18:TYR:HA	2.34	0.42
1:A:1741:U:HO2'	1:A:2723:G:H4'	1.84	0.42
1:A:24:G:N2	1:A:518:G:H1'	2.34	0.42
1:A:736:A:H2'	1:A:737:A:O4'	2.19	0.42
1:A:87:C:H2'	29:3:28:LYS:O	2.19	0.42
3:C:43:VAL:O	3:C:44:ASP:HB2	2.20	0.42
4:D:71:VAL:HG11	4:D:296:LEU:HB3	2.01	0.42
4:D:87:TYR:O	4:D:138:GLY:N	2.39	0.42
6:F:35:ALA:O	6:F:37:ALA:N	2.53	0.42
6:F:95:THR:C	6:F:97:GLN:N	2.70	0.42
14:N:39:ARG:CZ	37:N:8623:HOH:O	2.66	0.42
14:N:87:MET:SD	37:N:8531:HOH:O	2.62	0.42
17:Q:91:LYS:O	17:Q:95:GLU:HG3	2.19	0.42
21:U:65:VAL:HG22	21:U:72:ILE:HG22	2.02	0.42
24:X:101:LEU:HA	24:X:101:LEU:HD23	1.89	0.42
25:Y:76:ARG:NH1	25:Y:76:ARG:CG	2.82	0.42
1:A:86:A:C2	29:3:25:VAL:HG13	2.55	0.42
1:A:1089:G:C8	1:A:1290:G:C2	3.07	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1559:A:C1'	37:A:5836:HOH:O	2.67	0.42
1:A:1890:U:H4'	1:A:2010:A:C6	2.55	0.42
1:A:629:A:C2	1:A:2074:A:C2	3.08	0.42
1:A:2785:C:H4'	1:A:2786:G:OP2	2.20	0.42
1:A:2852:A:OP1	4:D:157:LYS:HE2	2.19	0.42
1:A:391:U:OP2	14:N:84:LYS:NZ	2.48	0.42
1:A:67:A:H5''	1:A:69:A:C8	2.55	0.42
11:K:51:GLU:O	11:K:55:GLU:HG3	2.20	0.42
14:N:162:GLY:HA2	37:N:8520:HOH:O	2.20	0.42
15:O:176:ARG:O	15:O:180:LEU:HG	2.19	0.42
23:W:27:LEU:O	23:W:30:ALA:N	2.52	0.42
24:X:31:HIS:HB3	37:X:5420:HOH:O	2.20	0.42
24:X:84:VAL:HG12	37:X:6679:HOH:O	2.20	0.42
24:X:90:TYR:N	37:X:6679:HOH:O	2.53	0.42
1:A:99:A:H3'	1:A:100:C:C6	2.55	0.42
1:A:1051:C:H2'	1:A:1052:G:O4'	2.20	0.42
1:A:10:U:H1'	1:A:532:A:H62	1.85	0.42
1:A:1187:U:C3'	37:A:6864:HOH:O	2.67	0.42
1:A:1132:A:N6	1:A:1229:C:H2'	2.35	0.42
1:A:1444:G:O2'	1:A:1445:G:H5'	2.20	0.42
1:A:2453:G:H2'	1:A:2454:C:C6	2.55	0.42
1:A:245:C:C2'	1:A:246:G:H5'	2.50	0.42
1:A:2529:G:O2'	1:A:2530:C:H5'	2.20	0.42
1:A:1705:C:O2	1:A:2735:U:H5''	2.20	0.42
1:A:803:C:O2'	1:A:804:C:H5'	2.20	0.42
1:A:870:G:C3'	1:A:871:G:H5''	2.50	0.42
4:D:264:GLU:HG2	4:D:267:LYS:CE	2.34	0.42
5:E:160:LEU:O	5:E:162:VAL:HG23	2.19	0.42
6:F:41:LEU:O	6:F:44:ILE:HG22	2.20	0.42
7:G:84:MET:HB2	7:G:131:LEU:HB2	2.01	0.42
10:J:57:ARG:HG3	10:J:57:ARG:NH1	2.35	0.42
11:K:72:PRO:O	11:K:78:ILE:HD11	2.20	0.42
11:K:79:PHE:O	11:K:83:ILE:HG13	2.19	0.42
12:L:58:THR:HG22	12:L:59:LYS:HG3	2.00	0.42
14:N:45:ARG:CZ	14:N:48:ARG:HG3	2.50	0.42
15:O:80:SER:CB	37:O:8537:HOH:O	2.63	0.42
28:2:21:ARG:HD2	28:2:39:PHE:HB2	2.02	0.41
1:A:940:G:C5	1:A:1027:G:C2	3.07	0.41
1:A:1947:G:N2	1:A:1966:U:O2	2.52	0.41
1:A:236:A:O5'	1:A:236:A:C2'	2.68	0.41
1:A:250:C:O2'	1:A:251:C:H5'	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:259:G:O2'	1:A:260:C:H5'	2.20	0.41
1:A:2758:G:H2'	1:A:2759:C:C6	2.55	0.41
1:A:2815:G:N7	11:K:80:LYS:NZ	2.66	0.41
1:A:314:G:N2	1:A:316:A:H3'	2.35	0.41
3:C:192:VAL:HG12	3:C:207:GLN:HB3	2.02	0.41
3:C:30:ARG:HB3	3:C:30:ARG:HE	1.65	0.41
3:C:46:GLU:O	3:C:55:VAL:N	2.49	0.41
4:D:102:THR:HG23	4:D:182:VAL:CG1	2.50	0.41
6:F:140:ARG:HG3	6:F:140:ARG:HH11	1.85	0.41
37:A:3671:HOH:O	7:G:143:GLN:CG	2.68	0.41
14:N:77:PHE:HD2	37:N:8527:HOH:O	2.02	0.41
16:P:32:ARG:HG2	37:P:2336:HOH:O	2.20	0.41
16:P:44:ASN:HA	16:P:65:LEU:O	2.19	0.41
17:Q:131:PHE:CD1	17:Q:137:LEU:HD13	2.55	0.41
18:R:31:GLU:CD	18:R:93:ARG:HH12	2.24	0.41
22:V:52:THR:HG22	22:V:54:THR:N	2.35	0.41
25:Y:7:GLU:HA	25:Y:74:ALA:O	2.20	0.41
26:Z:154:ARG:HH12	26:Z:155:ARG:HG3	1.84	0.41
26:Z:178:HIS:CG	26:Z:179:PRO:HD2	2.55	0.41
27:1:42:CYS:SG	27:1:44:PHE:CB	2.94	0.41
1:A:1921:A:C6	1:A:1922:A:C2	3.07	0.41
1:A:1985:U:C5	1:A:1996:U:C2	3.07	0.41
1:A:2047:C:H5'	37:A:9799:HOH:O	2.19	0.41
1:A:2523:U:O2'	1:A:2524:G:H5'	2.20	0.41
1:A:2549:C:H1'	4:D:248:ARG:NH2	2.34	0.41
1:A:2739:A:N6	1:A:2740:G:C6	2.88	0.41
1:A:951:A:H2'	1:A:952:G:H5'	2.00	0.41
2:B:3057:A:H8	6:F:141:VAL:HG21	1.85	0.41
2:B:3096:C:H2'	2:B:3097:U:C6	2.55	0.41
3:C:100:PRO:HG2	3:C:103:VAL:CG2	2.48	0.41
3:C:101:GLU:HG2	3:C:131:HIS:ND1	2.34	0.41
3:C:36:ASP:CB	3:C:85:ASP:H	2.32	0.41
5:E:3:ALA:HA	37:E:8451:HOH:O	2.20	0.41
37:A:4537:HOH:O	5:E:50:GLU:HG2	2.20	0.41
6:F:101:THR:CG2	37:F:7400:HOH:O	2.65	0.41
8:H:21:GLU:HA	8:H:24:ARG:HE	1.84	0.41
10:J:48:LEU:HD11	10:J:157:ILE:HG21	2.01	0.41
10:J:56:ILE:HG21	10:J:61:LEU:CD1	2.50	0.41
11:K:4:ALA:O	11:K:5:GLU:O	2.38	0.41
11:K:46:ILE:HG12	11:K:53:ILE:HD13	2.02	0.41
14:N:49:ALA:C	14:N:54:TYR:HB3	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:96:ASN:ND2	37:N:8541:HOH:O	2.48	0.41
15:O:127:LEU:HA	15:O:127:LEU:HD12	1.84	0.41
15:O:159:TYR:CE2	15:O:163:PHE:HE2	2.34	0.41
16:P:26:TRP:HB2	37:P:3062:HOH:O	2.21	0.41
22:V:20:MET:CG	22:V:28:THR:HG23	2.50	0.41
22:V:31:PHE:CE2	22:V:37:GLU:HA	2.54	0.41
28:2:10:LYS:CB	37:2:8432:HOH:O	2.68	0.41
1:A:1014:A:H5''	2:B:3101:G:O2'	2.20	0.41
1:A:1865:A:H2'	1:A:1866:A:C8	2.55	0.41
1:A:2255:A:C6	1:A:2256:G:C5	3.08	0.41
1:A:2626:C:H2'	1:A:2627:G:C8	2.55	0.41
1:A:382:U:C5	1:A:406:G:C2	3.07	0.41
1:A:645:U:H2'	1:A:646:G:C8	2.55	0.41
1:A:883:U:O2	1:A:883:U:C2'	2.68	0.41
3:C:194:MET:HE1	37:C:8517:HOH:O	2.20	0.41
4:D:132:HIS:CE1	4:D:171:VAL:CG2	3.03	0.41
6:F:95:THR:HG21	6:F:174:VAL:HG22	2.02	0.41
10:J:154:THR:HB	10:J:155:PRO:CD	2.50	0.41
10:J:73:GLN:OE1	10:J:73:GLN:CA	2.68	0.41
15:O:143:ARG:HH12	15:O:173:ASP:CG	2.21	0.41
15:O:163:PHE:O	15:O:164:ASP:O	2.38	0.41
16:P:25:VAL:HG23	16:P:26:TRP:H	1.85	0.41
1:A:1265:G:H1'	37:A:4979:HOH:O	2.19	0.41
1:A:1653:A:N7	37:A:6918:HOH:O	2.37	0.41
1:A:1825:U:O2'	1:A:1826:C:H5'	2.21	0.41
1:A:419:A:H1'	1:A:1921:A:C2	2.56	0.41
1:A:306:A:H2'	1:A:341:C:O2'	2.20	0.41
1:A:764:C:H2'	1:A:765:G:O4'	2.20	0.41
4:D:60:SER:C	4:D:62:ARG:H	2.23	0.41
5:E:200:PRO:HB3	5:E:212:VAL:CG2	2.50	0.41
5:E:40:ALA:O	5:E:43:LYS:HB2	2.20	0.41
6:F:95:THR:OG1	6:F:174:VAL:HG22	2.20	0.41
7:G:49:ILE:HD11	7:G:69:ILE:HD12	2.02	0.41
10:J:136:VAL:HG22	10:J:137:ASN:N	2.36	0.41
23:W:11:MET:HB3	23:W:15:GLU:HB2	2.02	0.41
1:A:130:C:H5'	37:A:5192:HOH:O	2.19	0.41
3:C:232:ARG:NE	37:C:8586:HOH:O	2.54	0.41
3:C:66:ARG:HB2	3:C:66:ARG:HH11	1.85	0.41
3:C:36:ASP:HB2	3:C:84:VAL:N	2.36	0.41
4:D:154:VAL:HA	4:D:155:PRO:HD3	1.89	0.41
5:E:93:LYS:O	5:E:98:ARG:NH2	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:12:ILE:O	9:I:13:PRO:C	2.58	0.41
15:O:34:LEU:HD22	15:O:129:ILE:CD1	2.51	0.41
17:Q:13:VAL:HG11	17:Q:40:VAL:HG12	2.02	0.41
24:X:122:ARG:NH2	37:X:4276:HOH:O	2.53	0.41
24:X:122:ARG:NH1	24:X:152:ALA:O	2.53	0.41
25:Y:25:ARG:NE	37:Y:3861:HOH:O	2.52	0.41
1:A:1025:C:H5'	24:X:23:MET:O	2.20	0.41
1:A:1278:A:H4'	1:A:1279:U:C4	2.56	0.41
1:A:1462:C:H2'	1:A:1463:A:C8	2.56	0.41
1:A:1751:G:C3'	1:A:1752:G:H5''	2.50	0.41
1:A:155:C:H4'	1:A:188:C:H4'	2.03	0.41
1:A:2079:G:H2'	1:A:2080:G:O4'	2.20	0.41
1:A:2505:G:H8	37:A:5611:HOH:O	2.04	0.41
1:A:2607:U:O5'	1:A:2609:G:H4'	2.20	0.41
1:A:2739:A:C6	1:A:2740:G:C5	3.08	0.41
1:A:40:C:O5'	1:A:40:C:H6	2.04	0.41
1:A:492:C:O2'	1:A:493:U:H5'	2.21	0.41
1:A:661:G:C4	1:A:686:A:C2	3.09	0.41
1:A:849:C:C2'	1:A:850:U:H5'	2.51	0.41
3:C:29:HIS:HB2	3:C:153:ARG:HH12	1.86	0.41
4:D:5:ARG:HA	4:D:6:PRO:HD3	1.94	0.41
6:F:170:TYR:N	6:F:170:TYR:CD1	2.88	0.41
6:F:17:ARG:NH2	37:F:3723:HOH:O	2.43	0.41
8:H:16:ALA:HA	8:H:111:ILE:HD13	2.01	0.41
10:J:26:LYS:HD2	10:J:28:ILE:HB	2.02	0.41
12:L:9:THR:O	12:L:10:GLN:C	2.59	0.41
14:N:94:LYS:CE	37:N:8646:HOH:O	2.69	0.41
15:O:108:SER:HA	15:O:109:PRO:HD3	1.79	0.41
22:V:38:ASN:O	22:V:42:LEU:HG	2.21	0.41
22:V:44:ARG:CB	37:V:3805:HOH:O	2.67	0.41
24:X:21:LEU:HB3	24:X:26:ILE:HG12	2.02	0.41
26:Z:189:ASN:ND2	26:Z:192:ASP:N	2.65	0.41
1:A:1116:U:H3	1:A:1246:A:N6	2.09	0.41
1:A:1167:G:O2'	1:A:1168:C:H5'	2.21	0.41
1:A:1377:C:C5'	1:A:1377:C:H6	2.33	0.41
1:A:1515:A:H2'	1:A:1516:C:C6	2.56	0.41
1:A:1888:C:N4	1:A:1889:C:C4	2.89	0.41
1:A:1912:A:O5'	1:A:1912:A:H8	2.03	0.41
1:A:209:G:C6	1:A:210:U:N3	2.89	0.41
1:A:2327:A:C2	1:A:2374:A:C2	3.08	0.41
1:A:329:A:OP2	5:E:206:ASN:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:304:G:H1'	1:A:347:A:N6	2.35	0.41
1:A:398:U:H2'	1:A:399:C:C6	2.56	0.41
1:A:542:A:H1'	37:A:4648:HOH:O	2.21	0.41
1:A:812:A:H2'	1:A:813:C:C6	2.55	0.41
4:D:138:GLY:O	4:D:139:ASP:C	2.58	0.41
4:D:268:ARG:NE	37:D:8608:HOH:O	2.53	0.41
4:D:280:VAL:CG1	4:D:281:ASP:N	2.83	0.41
6:F:57:THR:HA	6:F:63:ILE:HA	2.01	0.41
8:H:26:THR:HB	8:H:102:GLY:HA3	2.03	0.41
9:I:12:ILE:HB	37:I:4714:HOH:O	2.19	0.41
10:J:113:ALA:N	10:J:114:PRO:HD3	2.36	0.41
12:L:99:ASP:OD1	12:L:99:ASP:C	2.58	0.41
14:N:63:VAL:O	14:N:130:GLU:HA	2.21	0.41
15:O:149:GLU:O	15:O:152:GLU:HB2	2.20	0.41
15:O:37:ARG:CZ	37:O:8534:HOH:O	2.69	0.41
15:O:37:ARG:HD3	15:O:37:ARG:HA	1.84	0.41
16:P:47:ARG:NH1	37:P:4564:HOH:O	2.53	0.41
19:S:132:ARG:NH1	37:S:8558:HOH:O	2.53	0.41
21:U:27:LEU:HD21	21:U:40:VAL:CG1	2.51	0.41
21:U:80:GLU:OE2	21:U:84:GLY:HA2	2.20	0.41
25:Y:12:ILE:HD12	25:Y:36:HIS:ND1	2.36	0.41
1:A:1471:A:H2'	1:A:1472:C:C6	2.56	0.41
1:A:1490:G:H4'	1:A:1533:A:OP1	2.20	0.41
1:A:1666:C:O2'	1:A:1667:A:C5'	2.65	0.41
1:A:183:A:O2'	1:A:184:G:H5'	2.21	0.41
1:A:1871:U:O4'	1:A:1873:G:C8	2.74	0.41
1:A:2118:A:H2'	1:A:2119:C:H6	1.85	0.41
1:A:2456:A:H2'	1:A:2457:U:H6	1.86	0.41
1:A:2481:G:H3'	1:A:2482:G:H5''	2.02	0.41
1:A:542:A:C8	1:A:542:A:C5'	2.99	0.41
1:A:955:A:C2	1:A:1013:A:C4	3.08	0.41
2:B:3107:C:H2'	2:B:3108:C:C6	2.55	0.41
4:D:168:GLY:H	4:D:174:ARG:HD3	1.84	0.41
4:D:236:ILE:HG21	4:D:236:ILE:HD13	1.80	0.41
4:D:307:ARG:CG	4:D:307:ARG:NH1	2.84	0.41
5:E:14:GLY:N	37:E:8440:HOH:O	2.54	0.41
7:G:34:TRP:HA	37:G:4572:HOH:O	2.20	0.41
10:J:47:GLU:HG2	10:J:133:ILE:HD12	2.02	0.41
10:J:57:ARG:O	10:J:61:LEU:HD22	2.21	0.41
1:A:171:C:OP2	14:N:84:LYS:HG3	2.20	0.41
1:A:2123:A:P	14:N:89:ASN:HD22	2.44	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:37:ARG:O	17:Q:41:ARG:HG3	2.20	0.41
1:A:1021:G:O2'	1:A:1022:A:H5'	2.20	0.41
1:A:1589:G:H4'	37:A:6824:HOH:O	2.21	0.41
1:A:2246:U:C2	1:A:2256:G:N2	2.89	0.41
1:A:858:U:H2'	1:A:859:C:H6	1.85	0.41
1:A:903:U:OP2	13:M:11:ARG:NH1	2.50	0.41
2:B:3011:A:O2'	2:B:3012:C:H3'	2.21	0.41
2:B:3042:C:N4	2:B:3044:A:N1	2.68	0.41
3:C:170:VAL:HG13	27:1:22:ILE:HG21	2.02	0.41
4:D:102:THR:HG23	4:D:182:VAL:HG12	2.03	0.41
4:D:240:GLY:HA3	37:D:8657:HOH:O	2.21	0.41
7:G:116:THR:HG22	7:G:151:LEU:HD22	2.03	0.41
7:G:172:PRO:HB3	37:G:6931:HOH:O	2.20	0.41
8:H:59:ILE:HG22	8:H:59:ILE:O	2.20	0.41
11:K:6:PHE:HB3	11:K:109:TYR:OH	2.21	0.41
15:O:72:GLU:H	15:O:171:HIS:CE1	2.38	0.41
25:Y:85:VAL:HG12	25:Y:86:GLU:N	2.36	0.41
26:Z:136:LYS:HG3	26:Z:138:ARG:HG2	2.02	0.41
27:1:13:ARG:NH1	37:1:8422:HOH:O	2.54	0.41
29:3:11:LEU:HD23	29:3:11:LEU:HA	1.78	0.41
30:4:35:TRP:HA	30:4:38:ARG:NH1	2.36	0.41
1:A:1744:G:N7	1:A:1745:G:C5	2.89	0.41
1:A:2111:G:H1'	37:A:9042:HOH:O	2.20	0.41
1:A:2122:C:H3'	37:A:5266:HOH:O	2.20	0.41
1:A:2263:G:C6	1:A:2264:A:C5	3.09	0.41
1:A:2473:U:O3'	1:A:2474:A:H3'	2.20	0.41
1:A:2825:C:H4'	1:A:2826:G:O5'	2.21	0.41
1:A:396:U:HO2'	1:A:397:A:P	2.44	0.41
1:A:64:G:H2'	1:A:65:C:O4'	2.21	0.41
1:A:834:G:H4'	1:A:835:U:OP2	2.20	0.41
1:A:853:C:H2'	1:A:854:G:O4'	2.20	0.41
3:C:192:VAL:CG1	3:C:207:GLN:HB3	2.51	0.41
37:A:7107:HOH:O	5:E:107:ARG:NE	2.46	0.41
8:H:6:PHE:CD1	8:H:6:PHE:O	2.74	0.41
10:J:65:ARG:HB3	37:J:8374:HOH:O	2.21	0.41
13:M:64:ILE:O	13:M:64:ILE:HG23	2.20	0.41
13:M:98:GLU:O	13:M:99:GLU:HB2	2.21	0.41
14:N:69:LYS:HD3	14:N:125:ARG:HA	2.02	0.41
14:N:87:MET:HE1	37:N:8531:HOH:O	2.20	0.41
15:O:93:GLN:HG2	37:O:8557:HOH:O	2.21	0.41
16:P:35:LYS:HD3	37:P:3360:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:U:49:GLU:HB3	21:U:59:GLU:CG	2.51	0.41
23:W:45:ARG:C	23:W:47:LYS:N	2.74	0.41
25:Y:26:ALA:HB1	25:Y:59:TRP:CE2	2.56	0.41
26:Z:234:VAL:HG12	26:Z:235:GLU:N	2.36	0.41
30:4:22:VAL:HG11	30:4:67:LEU:HD13	2.02	0.41
1:A:1421:C:O2'	1:A:1422:U:H5'	2.20	0.41
1:A:1440:U:P	37:A:4435:HOH:O	2.79	0.41
1:A:1447:U:OP2	1:A:1503:U:O2'	2.35	0.41
1:A:1896:G:C6	1:A:1897:U:C4	3.08	0.41
1:A:1942:A:H3'	37:A:7324:HOH:O	2.21	0.41
1:A:1969:A:O2'	1:A:1970:G:H5'	2.21	0.41
1:A:2113:G:C6	1:A:2114:C:C4	3.09	0.41
1:A:2289:G:H21	1:A:2291:A:H2	1.65	0.41
1:A:2428:G:C4	1:A:2461:U:C5	3.09	0.41
1:A:2781:U:H2'	1:A:2782:G:C5'	2.51	0.41
1:A:2831:C:H2'	1:A:2832:C:H5'	2.03	0.41
1:A:2826:G:C6	1:A:2913:A:N6	2.89	0.41
1:A:431:G:OP1	14:N:48:ARG:NH1	2.53	0.41
1:A:902:G:N7	13:M:18:HIS:CD2	2.87	0.41
3:C:190:ARG:NH2	37:C:8598:HOH:O	2.53	0.41
4:D:215:VAL:HA	4:D:220:VAL:HG22	2.02	0.41
5:E:236:THR:C	37:E:8447:HOH:O	2.59	0.41
7:G:137:ASP:O	7:G:141:VAL:HG23	2.21	0.41
8:H:21:GLU:O	8:H:24:ARG:CG	2.68	0.41
9:I:66:LEU:O	9:I:69:ARG:HB3	2.21	0.41
10:J:45:GLN:NE2	10:J:135:TRP:HE1	2.19	0.41
12:L:6:ALA:HB3	12:L:116:GLU:HG2	2.02	0.41
12:L:76:GLN:HB2	37:L:1433:HOH:O	2.21	0.41
1:A:1299:G:N7	13:M:6:ARG:NH1	2.68	0.41
14:N:108:LYS:N	14:N:108:LYS:HD3	2.36	0.41
15:O:139:TRP:HA	15:O:139:TRP:HE3	1.86	0.41
16:P:45:LEU:HD12	16:P:88:LYS:HD2	2.02	0.41
19:S:119:VAL:CG2	19:S:142:ASP:HB2	2.51	0.41
24:X:41:TYR:O	24:X:45:VAL:HG13	2.21	0.41
25:Y:78:GLU:CG	25:Y:79:GLU:N	2.76	0.41
1:A:1044:C:H3'	1:A:1045:G:H5''	2.03	0.40
1:A:1161:A:O5'	1:A:1161:A:C8	2.74	0.40
1:A:1790:C:H2'	1:A:1791:U:C6	2.55	0.40
1:A:1804:A:H2'	1:A:1805:G:H8	1.86	0.40
1:A:1992:U:C2	1:A:1994:A:OP2	2.75	0.40
1:A:1827:G:C2	1:A:2023:G:C6	3.09	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:218:C:C5	1:A:220:C:C4	3.09	0.40
1:A:2116:U:C4	1:A:2271:G:C6	3.09	0.40
1:A:2356:A:H2'	1:A:2357:G:O4'	2.20	0.40
1:A:2780:C:C4	1:A:2781:U:C4	3.10	0.40
1:A:27:U:H2'	1:A:28:G:O4'	2.20	0.40
1:A:2869:G:H2'	1:A:2870:C:C6	2.56	0.40
1:A:78:G:C6	1:A:79:G:C6	3.10	0.40
1:A:941:G:C2'	1:A:942:U:H5'	2.51	0.40
3:C:114:ASP:HB2	3:C:117:LYS:HE2	2.02	0.40
5:E:76:ARG:HD3	37:E:8365:HOH:O	2.21	0.40
7:G:118:ILE:HG23	7:G:144:THR:HG21	2.03	0.40
10:J:150:LYS:CG	37:J:8372:HOH:O	2.69	0.40
11:K:80:LYS:NZ	37:K:8573:HOH:O	2.50	0.40
12:L:30:LYS:C	12:L:55:VAL:HG13	2.42	0.40
12:L:6:ALA:CB	12:L:116:GLU:HG2	2.51	0.40
1:A:240:C:C5'	14:N:146:GLN:NE2	2.84	0.40
14:N:14:ARG:HB3	14:N:17:GLU:HG3	2.02	0.40
14:N:12:TRP:CZ2	14:N:20:ILE:HD11	2.56	0.40
15:O:141:ARG:CB	37:O:8571:HOH:O	2.66	0.40
15:O:175:LEU:HD12	15:O:175:LEU:HA	1.91	0.40
15:O:48:VAL:HG12	37:O:8555:HOH:O	2.21	0.40
16:P:26:TRP:HA	16:P:26:TRP:CE3	2.55	0.40
22:V:9:CYS:O	22:V:52:THR:HG23	2.20	0.40
24:X:3:ALA:O	24:X:54:PHE:HA	2.22	0.40
1:A:2106:C:H2'	1:A:2107:U:C6	2.57	0.40
1:A:2407:G:O2'	1:A:2408:A:H5'	2.21	0.40
1:A:2415:A:H2'	1:A:2416:G:H5'	2.02	0.40
1:A:2690:U:H4'	7:G:111:LYS:CE	2.51	0.40
1:A:2750:G:H8	1:A:2750:G:O5'	2.05	0.40
1:A:380:A:OP2	14:N:9:ARG:HD2	2.22	0.40
2:B:3117:G:C2'	37:B:2118:HOH:O	2.69	0.40
3:C:36:ASP:HB2	3:C:83:GLY:HA3	2.03	0.40
6:F:159:PRO:O	6:F:163:VAL:HG23	2.20	0.40
7:G:24:GLY:HA3	7:G:76:VAL:HB	2.03	0.40
15:O:43:VAL:CG1	15:O:118:ILE:HD11	2.50	0.40
15:O:50:LEU:HA	15:O:50:LEU:HD12	1.87	0.40
23:W:42:ASN:N	23:W:43:PRO:HD3	2.36	0.40
23:W:4:HIS:O	23:W:8:ILE:HG13	2.21	0.40
30:4:65:THR:O	30:4:82:GLY:HA3	2.22	0.40
1:A:1206:U:H2'	1:A:1207:A:O4'	2.22	0.40
1:A:1213:C:C2'	1:A:1214:G:H5'	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:A:O2'	1:A:129:A:H5'	2.21	0.40
1:A:189:A:OP1	14:N:171:ARG:NH2	2.55	0.40
1:A:2115:U:H2'	1:A:2116:U:C6	2.57	0.40
1:A:2123:A:P	14:N:89:ASN:ND2	2.94	0.40
1:A:2838:A:H2'	1:A:2839:C:O4'	2.21	0.40
1:A:2892:G:C6	1:A:2893:C:N3	2.90	0.40
1:A:397:A:P	37:A:4317:HOH:O	2.79	0.40
1:A:2099:G:N1	31:A:9001:SPR:O2A	2.47	0.40
2:B:3008:G:P	37:B:5071:HOH:O	2.79	0.40
3:C:173:GLY:O	3:C:176:HIS:HB3	2.20	0.40
3:C:215:ILE:HG13	3:C:216:SER:N	2.37	0.40
8:H:22:VAL:HG21	8:H:104:ALA:HB2	2.02	0.40
9:I:20:VAL:O	9:I:24:VAL:HG23	2.21	0.40
11:K:79:PHE:HB3	11:K:103:VAL:HG11	2.02	0.40
13:M:61:ALA:HA	37:M:8564:HOH:O	2.21	0.40
14:N:61:ILE:CG2	14:N:62:VAL:N	2.84	0.40
15:O:161:GLY:O	15:O:162:ASP:C	2.59	0.40
19:S:61:GLN:CD	37:S:8541:HOH:O	2.59	0.40
23:W:8:ILE:HG21	23:W:59:ILE:HG13	2.03	0.40
26:Z:131:GLN:O	26:Z:132:ASP:HB2	2.21	0.40
29:3:18:ASN:HD22	29:3:18:ASN:HA	1.64	0.40
1:A:1164:U:H6	1:A:1164:U:O5'	2.05	0.40
1:A:1494:A:C4	1:A:1495:C:C5	3.10	0.40
1:A:1562:C:C2'	1:A:1562:C:O2	2.69	0.40
1:A:1592:G:C5	1:A:1593:C:C4	3.09	0.40
1:A:2034:U:H2'	1:A:2035:C:H6	1.87	0.40
1:A:2038:A:O2'	1:A:2039:A:H5'	2.21	0.40
1:A:2502:C:H2'	1:A:2503:A:C5'	2.50	0.40
1:A:611:U:H2'	1:A:612:U:C6	2.57	0.40
31:A:9001:SPR:H6	31:A:9001:SPR:H3	1.84	0.40
31:A:9001:SPR:C8A	31:A:9001:SPR:O2A	2.70	0.40
3:C:36:ASP:HB2	3:C:85:ASP:H	1.86	0.40
4:D:41:PHE:HB3	4:D:190:MET:HE3	2.03	0.40
6:F:95:THR:CG2	6:F:174:VAL:HG22	2.51	0.40
6:F:91:ALA:HB2	6:F:106:PHE:CD2	2.56	0.40
7:G:11:VAL:HG11	7:G:22:VAL:HG13	2.04	0.40
7:G:91:PHE:HA	7:G:92:PRO:HD3	1.91	0.40
9:I:12:ILE:HG13	37:I:6833:HOH:O	2.21	0.40
10:J:167:ALA:HA	37:J:8362:HOH:O	2.20	0.40
10:J:26:LYS:CG	10:J:28:ILE:H	2.25	0.40
10:J:82:LYS:CB	10:J:82:LYS:NZ	2.84	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:38:LYS:HE2	15:O:107:ASN:ND2	2.36	0.40
15:O:163:PHE:CZ	15:O:164:ASP:OD2	2.73	0.40
15:O:42:HIS:CG	15:O:62:HIS:HE1	2.40	0.40
2:B:3004:G:O2'	15:O:44:ARG:NH2	2.55	0.40
22:V:14:GLU:HA	22:V:15:PRO:HD2	1.93	0.40
27:1:30:GLU:O	27:1:33:HIS:HB3	2.21	0.40
28:2:28:HIS:O	28:2:32:LYS:N	2.48	0.40
1:A:2462:G:O6	30:4:61:PRO:HG3	2.21	0.40
1:A:2397:G:C5	1:A:2465:A:C6	3.10	0.40
1:A:255:A:C5	1:A:256:C:C4	3.10	0.40
1:A:2612:A:H2'	1:A:2649:A:N6	2.37	0.40
1:A:206:G:O2'	1:A:438:C:N3	2.48	0.40
2:B:3065:A:C2'	2:B:3066:G:OP2	2.69	0.40
3:C:149:ASP:OD1	3:C:151:GLN:CB	2.69	0.40
3:C:51:ARG:NH1	3:C:51:ARG:HB3	2.36	0.40
4:D:156:LYS:HE3	37:D:8633:HOH:O	2.21	0.40
5:E:37:ALA:O	5:E:41:ASN:ND2	2.54	0.40
6:F:103:ASN:ND2	6:F:134:LEU:H	2.19	0.40
1:A:263:U:C2	8:H:59:ILE:HD12	2.57	0.40
11:K:39:VAL:HG11	11:K:107:ASN:HB2	2.04	0.40
14:N:69:LYS:O	14:N:73:ARG:NH1	2.55	0.40
18:R:53:HIS:O	18:R:55:ARG:N	2.55	0.40
1:A:840:U:H2'	19:S:128:ARG:NH1	2.37	0.40
21:U:113:GLU:O	21:U:114:SER:C	2.59	0.40
25:Y:73:ARG:C	25:Y:85:VAL:HG13	2.42	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	C	235/239 (98%)	205 (87%)	26 (11%)	4 (2%)	9 39

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	D	335/337 (99%)	307 (92%)	21 (6%)	7 (2%)	7	33
5	E	244/246 (99%)	225 (92%)	18 (7%)	1 (0%)	34	72
6	F	134/176 (76%)	95 (71%)	27 (20%)	12 (9%)	1	3
7	G	170/177 (96%)	158 (93%)	12 (7%)	0	100	100
8	H	117/119 (98%)	103 (88%)	12 (10%)	2 (2%)	9	39
9	I	25/348 (7%)	24 (96%)	1 (4%)	0	100	100
10	J	152/167 (91%)	129 (85%)	17 (11%)	6 (4%)	3	17
11	K	140/145 (97%)	131 (94%)	5 (4%)	4 (3%)	4	24
12	L	130/132 (98%)	117 (90%)	11 (8%)	2 (2%)	10	42
13	M	141/164 (86%)	118 (84%)	20 (14%)	3 (2%)	7	33
14	N	192/194 (99%)	172 (90%)	18 (9%)	2 (1%)	15	53
15	O	184/186 (99%)	165 (90%)	13 (7%)	6 (3%)	4	21
16	P	113/115 (98%)	110 (97%)	3 (3%)	0	100	100
17	Q	141/148 (95%)	138 (98%)	2 (1%)	1 (1%)	22	60
18	R	93/95 (98%)	87 (94%)	5 (5%)	1 (1%)	14	50
19	S	148/154 (96%)	138 (93%)	10 (7%)	0	100	100
20	T	79/84 (94%)	72 (91%)	7 (9%)	0	100	100
21	U	117/119 (98%)	108 (92%)	9 (8%)	0	100	100
22	V	51/66 (77%)	47 (92%)	4 (8%)	0	100	100
23	W	63/70 (90%)	57 (90%)	4 (6%)	2 (3%)	4	22
24	X	152/154 (99%)	145 (95%)	6 (4%)	1 (1%)	22	60
25	Y	80/91 (88%)	71 (89%)	7 (9%)	2 (2%)	5	28
26	Z	140/240 (58%)	138 (99%)	2 (1%)	0	100	100
27	1	71/73 (97%)	63 (89%)	7 (10%)	1 (1%)	11	43
28	2	54/56 (96%)	50 (93%)	4 (7%)	0	100	100
29	3	42/48 (88%)	41 (98%)	1 (2%)	0	100	100
30	4	90/92 (98%)	85 (94%)	3 (3%)	2 (2%)	6	31
All	All	3633/4235 (86%)	3299 (91%)	275 (8%)	59 (2%)	9	40

All (59) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	139	ASP

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Mol	Chain	Res	Type
6	F	93	LEU
6	F	95	THR
6	F	137	PRO
6	F	173	GLU
8	H	101	ALA
10	J	162	SER
10	J	164	ALA
13	M	80	ASP
15	O	154	LEU
15	O	164	ASP
15	O	183	ASP
3	C	34	ASP
3	C	37	VAL
4	D	34	GLY
4	D	169	GLY
6	F	11	HIS
6	F	16	PRO
10	J	138	PRO
11	K	5	GLU
11	K	7	ASP
11	K	143	LYS
12	L	119	GLN
17	Q	116	SER
23	W	43	PRO
30	4	57	GLY
3	C	132	ASP
4	D	184	ASP
6	F	20	LYS
6	F	171	ASP
8	H	64	PRO
10	J	40	PRO
10	J	72	VAL
14	N	140	ALA
15	O	162	ASP
15	O	181	ASP
24	X	77	ALA
25	Y	77	PHE
30	4	56	PRO
6	F	36	ASN
6	F	147	ALA
12	L	126	SER
13	M	21	ARG

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Mol	Chain	Res	Type
15	O	167	ASP
27	I	81	LYS
4	D	2	GLN
4	D	185	GLY
5	E	232	LEU
6	F	61	PHE
14	N	18	GLY
18	R	54	PRO
6	F	82	GLU
10	J	140	PRO
13	M	147	GLU
23	W	40	PRO
4	D	5	ARG
11	K	78	ILE
25	Y	70	ILE
3	C	112	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	179/181 (99%)	166 (93%)	13 (7%)	14	44
4	D	282/282 (100%)	264 (94%)	18 (6%)	17	51
5	E	193/193 (100%)	178 (92%)	15 (8%)	12	42
6	F	117/147 (80%)	106 (91%)	11 (9%)	8	32
7	G	152/155 (98%)	147 (97%)	5 (3%)	38	73
8	H	92/92 (100%)	91 (99%)	1 (1%)	73	90
9	I	27/283 (10%)	27 (100%)	0	100	100
10	J	122/122 (100%)	111 (91%)	11 (9%)	9	35
11	K	118/121 (98%)	107 (91%)	11 (9%)	9	33
12	L	106/106 (100%)	103 (97%)	3 (3%)	43	77
13	M	112/126 (89%)	108 (96%)	4 (4%)	35	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	N	166/166 (100%)	157 (95%)	9 (5%)	22	57
15	O	149/149 (100%)	144 (97%)	5 (3%)	37	72
16	P	93/93 (100%)	90 (97%)	3 (3%)	39	74
17	Q	113/116 (97%)	110 (97%)	3 (3%)	44	77
18	R	79/79 (100%)	75 (95%)	4 (5%)	24	60
19	S	117/121 (97%)	112 (96%)	5 (4%)	29	66
20	T	71/73 (97%)	71 (100%)	0	100	100
21	U	105/105 (100%)	103 (98%)	2 (2%)	57	84
22	V	44/52 (85%)	42 (96%)	2 (4%)	27	64
23	W	51/56 (91%)	50 (98%)	1 (2%)	55	83
24	X	130/130 (100%)	122 (94%)	8 (6%)	18	52
25	Y	66/73 (90%)	61 (92%)	5 (8%)	13	43
26	Z	120/195 (62%)	112 (93%)	8 (7%)	16	49
27	1	56/56 (100%)	50 (89%)	6 (11%)	6	26
28	2	46/46 (100%)	46 (100%)	0	100	100
29	3	42/44 (96%)	41 (98%)	1 (2%)	49	79
30	4	79/79 (100%)	73 (92%)	6 (8%)	13	43
All	All	3027/3441 (88%)	2867 (95%)	160 (5%)	22	58

All (160) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	3	ARG
3	C	33	GLU
3	C	36	ASP
3	C	55	VAL
3	C	68	ILE
3	C	69	LEU
3	C	94	LEU
3	C	120	ARG
3	C	131	HIS
3	C	153	ARG
3	C	179	MET
3	C	187	PRO
3	C	217	ARG
4	D	7	ARG

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Mol	Chain	Res	Type
4	D	11	LEU
4	D	27	ASN
4	D	33	ASP
4	D	63	GLU
4	D	97	LEU
4	D	98	THR
4	D	103	ASP
4	D	162	MET
4	D	195	ARG
4	D	234	ARG
4	D	251	VAL
4	D	254	GLN
4	D	256	GLN
4	D	264	GLU
4	D	304	PRO
4	D	307	ARG
4	D	312	ARG
5	E	2	GLN
5	E	27	ARG
5	E	67	GLN
5	E	76	ARG
5	E	81	PRO
5	E	94	THR
5	E	115	LEU
5	E	136	VAL
5	E	187	ARG
5	E	214	THR
5	E	222	ASP
5	E	223	LEU
5	E	234	VAL
5	E	236	THR
5	E	240	LEU
6	F	24	HIS
6	F	50	VAL
6	F	61	PHE
6	F	95	THR
6	F	99	ASP
6	F	100	ASP
6	F	131	THR
6	F	133	ASN
6	F	136	ARG
6	F	137	PRO

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Mol	Chain	Res	Type
6	F	149	ARG
7	G	7	ILE
7	G	36	PRO
7	G	54	ASP
7	G	102	VAL
7	G	164	ASP
8	H	100	ASP
10	J	1	LYS
10	J	59	ASN
10	J	72	VAL
10	J	73	GLN
10	J	82	LYS
10	J	86	ARG
10	J	94	ARG
10	J	142	VAL
10	J	150	LYS
10	J	155	PRO
10	J	166	ASN
11	K	46	ILE
11	K	52	GLN
11	K	74	ARG
11	K	76	ASP
11	K	79	PHE
11	K	107	ASN
11	K	112	ASP
11	K	120	SER
11	K	125	SER
11	K	127	ILE
11	K	131	THR
12	L	7	ASP
12	L	10	GLN
12	L	98	VAL
13	M	30	ARG
13	M	35	ARG
13	M	80	ASP
13	M	117	GLU
14	N	46	LEU
14	N	48	ARG
14	N	68	ARG
14	N	81	ARG
14	N	87	MET
14	N	93	ARG

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Mol	Chain	Res	Type
14	N	99	ARG
14	N	120	VAL
14	N	164	THR
15	O	26	LEU
15	O	127	LEU
15	O	128	ASP
15	O	152	GLU
15	O	163	PHE
16	P	3	THR
16	P	28	ASP
16	P	111	VAL
17	Q	52	LYS
17	Q	91	LYS
17	Q	98	ILE
18	R	11	ARG
18	R	16	ASN
18	R	57	ASP
18	R	95	GLU
19	S	13	THR
19	S	39	THR
19	S	82	GLU
19	S	130	MET
19	S	132	ARG
21	U	39	ASN
21	U	73	HIS
22	V	9	CYS
22	V	32	CYS
23	W	43	PRO
24	X	4	LEU
24	X	35	VAL
24	X	52	VAL
24	X	73	LEU
24	X	122	ARG
24	X	142	ASP
24	X	146	ILE
24	X	154	ARG
25	Y	15	ARG
25	Y	27	ASP
25	Y	44	ASP
25	Y	72	VAL
25	Y	79	GLU
26	Z	154	ARG

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Mol	Chain	Res	Type
26	Z	163	THR
26	Z	172	THR
26	Z	186	ARG
26	Z	189	ASN
26	Z	200	THR
26	Z	203	VAL
26	Z	204	ARG
27	1	11	THR
27	1	32	LYS
27	1	42	CYS
27	1	49	ARG
27	1	60	CYS
27	1	64	ILE
29	3	18	ASN
30	4	14	CYS
30	4	38	ARG
30	4	42	ARG
30	4	56	PRO
30	4	65	THR
30	4	74	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (84) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	47	HIS
3	C	92	ASN
3	C	127	GLN
3	C	199	HIS
4	D	27	ASN
4	D	145	HIS
4	D	238	ASN
4	D	260	HIS
4	D	318	ASN
4	D	332	ASN
5	E	2	GLN
5	E	39	GLN
5	E	129	HIS
6	F	103	ASN
6	F	133	ASN
7	G	106	ASN
7	G	143	GLN
9	I	17	GLN

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Mol	Chain	Res	Type
9	I	64	ASN
10	J	8	ASN
10	J	35	ASN
10	J	55	GLN
10	J	58	HIS
10	J	59	ASN
10	J	69	ASN
10	J	74	ASN
10	J	91	HIS
10	J	129	ASN
10	J	130	HIS
10	J	166	ASN
11	K	52	GLN
11	K	107	ASN
12	L	10	GLN
12	L	42	ASN
13	M	18	HIS
13	M	41	HIS
13	M	58	GLN
13	M	116	HIS
14	N	26	HIS
14	N	58	GLN
14	N	89	ASN
14	N	106	ASN
14	N	176	GLN
15	O	107	ASN
15	O	140	GLN
17	Q	50	GLN
17	Q	66	GLN
17	Q	73	HIS
17	Q	118	GLN
18	R	16	ASN
18	R	40	HIS
19	S	61	GLN
19	S	94	ASN
19	S	98	ASN
19	S	113	HIS
19	S	117	HIS
19	S	122	GLN
19	S	123	GLN
20	T	53	ASN
21	U	39	ASN

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Mol	Chain	Res	Type
22	V	39	ASN
23	W	60	GLN
24	X	27	HIS
24	X	28	HIS
24	X	31	HIS
24	X	87	HIS
24	X	110	GLN
24	X	119	HIS
24	X	125	HIS
24	X	141	HIS
25	Y	23	HIS
26	Z	134	HIS
26	Z	149	GLN
26	Z	189	ASN
27	1	33	HIS
27	1	70	GLN
28	2	8	GLN
28	2	16	HIS
28	2	28	HIS
29	3	16	ASN
29	3	18	ASN
29	3	41	HIS
29	3	45	ASN
30	4	48	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2747/2922 (94%)	248 (9%)	40 (1%)
2	B	121/122 (99%)	15 (12%)	5 (4%)
All	All	2868/3044 (94%)	263 (9%)	45 (1%)

All (263) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	11	A
1	A	31	C
1	A	60	A
1	A	67	A
1	A	69	A
1	A	70	A

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Mol	Chain	Res	Type
1	A	71	G
1	A	87	C
1	A	88	G
1	A	114	A
1	A	115	U
1	A	120	A
1	A	130	C
1	A	139	C
1	A	141	C
1	A	151	A
1	A	166	A
1	A	169	A
1	A	186	A
1	A	191	A
1	A	192	A
1	A	200	U
1	A	219	G
1	A	237	G
1	A	271	C
1	A	272	A
1	A	273	G
1	A	283	U
1	A	284	C
1	A	285	A
1	A	308	U
1	A	309	C
1	A	336	G
1	A	337	A
1	A	345	G
1	A	358	G
1	A	381	G
1	A	397	A
1	A	417	G
1	A	457	U
1	A	461	C
1	A	487	G
1	A	498	A
1	A	510	U
1	A	511	A
1	A	514	G
1	A	537	G
1	A	538	C

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Mol	Chain	Res	Type
1	A	539	G
1	A	542	A
1	A	545	G
1	A	553	G
1	A	559	U
1	A	588	G
1	A	604	G
1	A	620	A
1	A	632	A
1	A	644	G
1	A	660	A
1	A	688	A
1	A	701	U
1	A	717	C
1	A	759	C
1	A	777	U
1	A	809	G
1	A	821	U
1	A	835	U
1	A	840	U
1	A	858	U
1	A	868	G
1	A	869	G
1	A	871	G
1	A	872	U
1	A	875	A
1	A	877	G
1	A	878	G
1	A	884	C
1	A	885	G
1	A	898	G
1	A	905	C
1	A	921	G
1	A	923	A
1	A	953	G
1	A	960	G
1	A	961	A
1	A	1006	A
1	A	1008	C
1	A	1029	U
1	A	1045	G
1	A	1059	G

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Mol	Chain	Res	Type
1	A	1060	C
1	A	1072	G
1	A	1081	A
1	A	1083	C
1	A	1088	A
1	A	1109	U
1	A	1110	G
1	A	1119	G
1	A	1127	C
1	A	1130	U
1	A	1137	G
1	A	1151	G
1	A	1162	G
1	A	1164	U
1	A	1165	G
1	A	1166	A
1	A	1171	A
1	A	1174	A
1	A	1175	G
1	A	1177	A
1	A	1185	U
1	A	1192	A
1	A	1193	A
1	A	1206	U
1	A	1208	C
1	A	1216	G
1	A	1234	U
1	A	1238	C
1	A	1239	G
1	A	1279	U
1	A	1289	C
1	A	1331	A
1	A	1342	C
1	A	1353	C
1	A	1360	C
1	A	1377	C
1	A	1407	A
1	A	1451	C
1	A	1474	C
1	A	1485	A
1	A	1488	U
1	A	1505	U

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Mol	Chain	Res	Type
1	A	1506	U
1	A	1507	C
1	A	1524	U
1	A	1525	G
1	A	1526	A
1	A	1562	C
1	A	1564	C
1	A	1580	A
1	A	1592	G
1	A	1625	U
1	A	1626	A
1	A	1633	C
1	A	1634	G
1	A	1656	A
1	A	1667	A
1	A	1682	A
1	A	1684	A
1	A	1685	A
1	A	1692	C
1	A	1701	A
1	A	1710	A
1	A	1722	U
1	A	1723	G
1	A	1725	C
1	A	1731	C
1	A	1752	G
1	A	1778	A
1	A	1798	C
1	A	1820	G
1	A	1829	A
1	A	1856	C
1	A	1879	U
1	A	1904	A
1	A	1919	A
1	A	1942	A
1	A	1943	C
1	A	1971	G
1	A	1973	A
1	A	1974	G
1	A	1978	A
1	A	1979	G
1	A	1980	U

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Mol	Chain	Res	Type
1	A	1996	U
1	A	2004	U
1	A	2008	U
1	A	2011	A
1	A	2012	U
1	A	2013	G
1	A	2033	G
1	A	2034	U
1	A	2064	U
1	A	2072	G
1	A	2073	G
1	A	2074	A
1	A	2096	A
1	A	2097	G
1	A	2101	A
1	A	2102	G
1	A	2103	A
1	A	2110	G
1	A	2238	A
1	A	2258	A
1	A	2271	G
1	A	2272	G
1	A	2317	C
1	A	2321	A
1	A	2354	A
1	A	2361	A
1	A	2369	A
1	A	2379	G
1	A	2422	U
1	A	2462	G
1	A	2465	A
1	A	2467	A
1	A	2469	A
1	A	2476	C
1	A	2480	G
1	A	2483	A
1	A	2507	G
1	A	2510	C
1	A	2511	A
1	A	2533	C
1	A	2537	G
1	A	2541	U

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Mol	Chain	Res	Type
1	A	2553	A
1	A	2564	G
1	A	2589	U
1	A	2601	A
1	A	2602	G
1	A	2608	C
1	A	2613	G
1	A	2638	G
1	A	2649	A
1	A	2664	A
1	A	2681	A
1	A	2682	C
1	A	2726	U
1	A	2747	C
1	A	2748	G
1	A	2749	U
1	A	2750	G
1	A	2762	C
1	A	2768	A
1	A	2786	G
1	A	2792	A
1	A	2800	A
1	A	2811	A
1	A	2812	A
1	A	2825	C
1	A	2840	A
1	A	2850	C
1	A	2876	G
1	A	2890	A
1	A	2896	A
1	A	2903	C
1	A	2914	A
2	B	3002	U
2	B	3003	A
2	B	3007	G
2	B	3014	G
2	B	3022	G
2	B	3024	U
2	B	3041	C
2	B	3043	G
2	B	3044	A
2	B	3052	A

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Mol	Chain	Res	Type
2	B	3057	A
2	B	3066	G
2	B	3077	A
2	B	3114	G
2	B	3122	C

All (45) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	10	U
1	A	69	A
1	A	129	A
1	A	284	C
1	A	338	C
1	A	407	A
1	A	603	A
1	A	644	G
1	A	716	G
1	A	834	G
1	A	857	A
1	A	871	G
1	A	877	G
1	A	898	G
1	A	1080	C
1	A	1164	U
1	A	1232	A
1	A	1237	U
1	A	1246	A
1	A	1352	A
1	A	1377	C
1	A	1450	C
1	A	1506	U
1	A	1563	G
1	A	1667	A
1	A	1692	C
1	A	1856	C
1	A	1942	A
1	A	1979	G
1	A	2011	A
1	A	2103	A
1	A	2313	C
1	A	2379	G

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Mol	Chain	Res	Type
1	A	2467	A
1	A	2526	C
1	A	2536	C
1	A	2649	A
1	A	2718	C
1	A	2761	A
1	A	2791	U
2	B	3002	U
2	B	3023	U
2	B	3025	G
2	B	3065	A
2	B	3103	A

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 235 ligands modelled in this entry, 234 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	$\# Z > 2$
31	SPR	A	9001	1	61,62,62	3.01	28 (45%)	74,89,89	3.09	31 (41%)

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
31	SPR	A	9001	1	-	11/61/113/113	0/3/4/4

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	A	9001	SPR	C14-C15	9.02	1.60	1.52
31	A	9001	SPR	C3C-C4C	6.98	1.68	1.52
31	A	9001	SPR	C4C-N4C	6.52	1.63	1.48
31	A	9001	SPR	C4A-C5A	6.34	1.64	1.52
31	A	9001	SPR	C7-C6	5.69	1.65	1.53
31	A	9001	SPR	O1A-C5	5.47	1.58	1.43
31	A	9001	SPR	C6-C5	-5.40	1.42	1.52
31	A	9001	SPR	O5A-C5A	-4.86	1.33	1.44
31	A	9001	SPR	C2A-C3A	4.82	1.61	1.53
31	A	9001	SPR	O15-C1	-4.62	1.21	1.34
31	A	9001	SPR	O4A-C1B	-4.13	1.31	1.41
31	A	9001	SPR	C2C-C1C	3.99	1.63	1.50
31	A	9001	SPR	O1C-C1C	-3.92	1.31	1.41
31	A	9001	SPR	O1C-C9	3.81	1.52	1.44
31	A	9001	SPR	C6B-C5B	3.39	1.59	1.51
31	A	9001	SPR	C12-C13	2.87	1.43	1.33
31	A	9001	SPR	O19-C19	2.86	1.36	1.19
31	A	9001	SPR	C14-C13	2.47	1.57	1.50
31	A	9001	SPR	O3B-C3B	-2.39	1.40	1.44
31	A	9001	SPR	C3-C4	2.36	1.57	1.52
31	A	9001	SPR	C2B-C3B	2.35	1.58	1.53
31	A	9001	SPR	O5B-C5B	2.33	1.50	1.44
31	A	9001	SPR	O15-C15	2.30	1.51	1.47
31	A	9001	SPR	C2B-C1B	2.18	1.56	1.51
31	A	9001	SPR	C9-C10	2.17	1.57	1.50
31	A	9001	SPR	C3C-C2C	-2.16	1.47	1.52
31	A	9001	SPR	C7C-N4C	2.08	1.53	1.46
31	A	9001	SPR	C5B-C4B	2.02	1.57	1.53

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	A	9001	SPR	C8A-N3A-C7A	-9.47	82.41	110.38
31	A	9001	SPR	O19-C19-C18	-7.97	102.19	125.43
31	A	9001	SPR	O1C-C9-C8	7.62	124.98	108.09
31	A	9001	SPR	C16-C15-C14	7.40	123.58	113.26
31	A	9001	SPR	C7C-N4C-C4C	7.29	135.04	113.11
31	A	9001	SPR	O1C-C1C-O5C	-6.00	90.45	109.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	A	9001	SPR	C15-C14-C13	-6.00	102.86	113.92
31	A	9001	SPR	C4A-C3A-N3A	-5.49	98.69	111.68
31	A	9001	SPR	C7A-N3A-C3A	-4.48	102.98	113.59
31	A	9001	SPR	C6A-C5A-C4A	-4.40	106.71	113.41
31	A	9001	SPR	O5A-C5A-C4A	4.22	117.00	109.13
31	A	9001	SPR	O4A-C4A-C5A	3.99	117.19	106.79
31	A	9001	SPR	C14-C13-C12	-3.99	120.26	125.41
31	A	9001	SPR	C17-O4-C4	-3.86	104.40	114.52
31	A	9001	SPR	C3C-C4C-C5C	3.83	117.89	110.11
31	A	9001	SPR	O15-C15-C14	3.66	113.83	107.33
31	A	9001	SPR	C1C-O5C-C5C	-2.98	105.82	113.84
31	A	9001	SPR	O4A-C1B-C2B	2.93	114.06	109.01
31	A	9001	SPR	C15-O15-C1	2.89	121.59	117.88
31	A	9001	SPR	O2A-C2A-C1A	-2.84	103.15	110.05
31	A	9001	SPR	O5B-C1B-C2B	2.68	117.21	112.12
31	A	9001	SPR	C3C-C4C-N4C	2.65	121.20	114.97
31	A	9001	SPR	O5C-C1C-C2C	2.56	116.75	111.25
31	A	9001	SPR	C1A-C2A-C3A	-2.55	105.06	109.24
31	A	9001	SPR	C1A-O1A-C5	2.52	124.20	117.96
31	A	9001	SPR	O15-C15-C16	-2.44	102.36	107.93
31	A	9001	SPR	O1-C1-C2	-2.38	119.46	124.73
31	A	9001	SPR	C1C-O1C-C9	-2.33	109.86	113.78
31	A	9001	SPR	C3C-C2C-C1C	-2.17	105.90	110.85
31	A	9001	SPR	C20-C8-C9	-2.14	107.46	111.02
31	A	9001	SPR	O15-C1-C2	2.04	115.21	111.46

There are no chirality outliers.

All (11) torsion outliers are listed below:

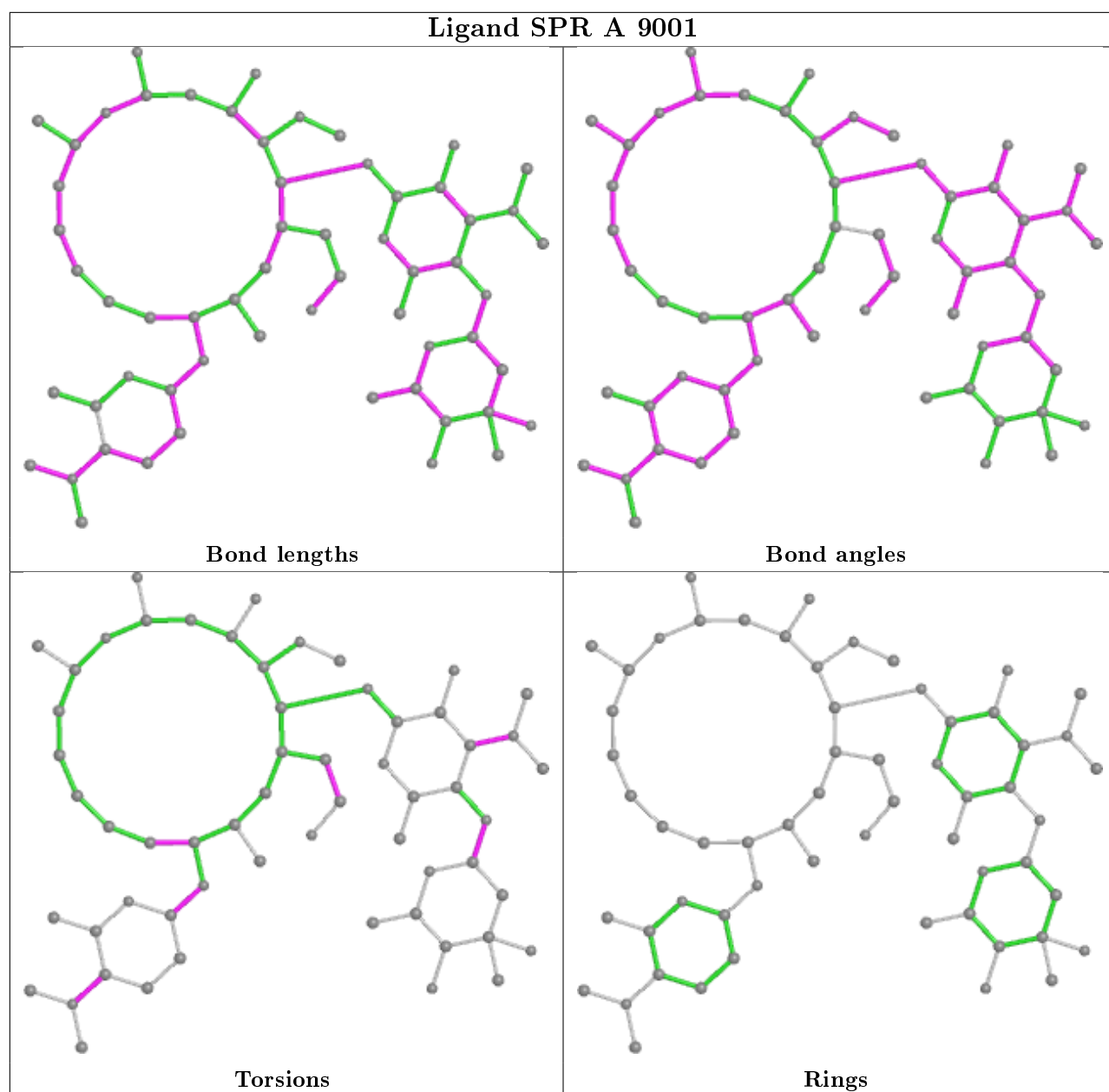
Mol	Chain	Res	Type	Atoms
31	A	9001	SPR	C2A-C3A-N3A-C7A
31	A	9001	SPR	C4A-C3A-N3A-C7A
31	A	9001	SPR	C2B-C1B-O4A-C4A
31	A	9001	SPR	O5B-C1B-O4A-C4A
31	A	9001	SPR	C2C-C1C-O1C-C9
31	A	9001	SPR	C5C-C4C-N4C-C7C
31	A	9001	SPR	C5C-C4C-N4C-C8C
31	A	9001	SPR	O5C-C1C-O1C-C9
31	A	9001	SPR	C3C-C4C-N4C-C8C
31	A	9001	SPR	C11-C10-C9-O1C
31	A	9001	SPR	C6-C18-C19-O19

There are no ring outliers.

1 monomer is involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	A	9001	SPR	9	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	A	2754/2922 (94%)	-0.07	47 (1%) 70 41	23, 51, 96, 143	0
2	B	122/122 (100%)	0.25	6 (4%) 29 11	37, 70, 100, 150	0
3	C	237/239 (99%)	0.12	10 (4%) 36 14	32, 63, 96, 110	0
4	D	337/337 (100%)	-0.13	3 (0%) 84 63	28, 57, 84, 95	0
5	E	246/246 (100%)	-0.18	1 (0%) 92 79	24, 50, 74, 85	0
6	F	140/176 (79%)	1.55	50 (35%) 0 0	60, 103, 122, 127	0
7	G	172/177 (97%)	0.48	8 (4%) 31 11	43, 68, 92, 98	0
8	H	119/119 (100%)	0.43	4 (3%) 45 19	59, 79, 102, 107	0
9	I	29/348 (8%)	1.89	12 (41%) 0 0	76, 94, 102, 104	0
10	J	156/167 (93%)	0.20	3 (1%) 66 37	35, 58, 85, 93	0
11	K	142/145 (97%)	-0.12	0 100 100	36, 50, 76, 84	0
12	L	132/132 (100%)	0.01	0 100 100	35, 56, 78, 82	0
13	M	145/164 (88%)	0.52	12 (8%) 11 3	31, 74, 108, 117	0
14	N	194/194 (100%)	0.22	16 (8%) 11 3	37, 55, 91, 98	0
15	O	186/186 (100%)	0.71	24 (12%) 3 1	48, 74, 112, 122	0
16	P	115/115 (100%)	-0.04	0 100 100	39, 59, 75, 79	0
17	Q	143/148 (96%)	0.17	2 (1%) 75 49	38, 60, 76, 84	0
18	R	95/95 (100%)	-0.11	1 (1%) 80 56	38, 51, 64, 79	0
19	S	150/154 (97%)	-0.17	0 100 100	32, 45, 66, 75	0
20	T	81/84 (96%)	0.05	1 (1%) 79 54	47, 65, 84, 89	0
21	U	119/119 (100%)	0.41	7 (5%) 22 7	44, 62, 86, 97	0
22	V	53/66 (80%)	3.20	37 (69%) 0 0	85, 94, 102, 110	0
23	W	65/70 (92%)	1.12	9 (13%) 2 1	55, 81, 112, 118	0
24	X	154/154 (100%)	-0.18	0 100 100	32, 49, 66, 76	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	Y	82/91 (90%)	0.28	4 (4%) 29 11	42, 58, 84, 99	0
26	Z	142/240 (59%)	-0.09	5 (3%) 44 18	25, 46, 70, 85	0
27	1	73/73 (100%)	3.54	47 (64%) 0 0	79, 98, 103, 104	0
28	2	56/56 (100%)	-0.41	0 100 100	30, 39, 45, 49	0
29	3	46/48 (95%)	0.06	1 (2%) 62 33	40, 66, 90, 102	0
30	4	92/92 (100%)	6.54	92 (100%) 0 0	91, 103, 108, 111	0
All	All	6577/7279 (90%)	0.24	402 (6%) 21 7	23, 57, 102, 150	0

All (402) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
30	4	37	ASP	15.8
30	4	65	THR	13.4
30	4	82	GLY	13.1
30	4	84	ARG	12.4
30	4	83	TRP	12.0
30	4	62	THR	11.7
30	4	11	CYS	10.9
30	4	38	ARG	10.8
14	N	71	SER	10.7
27	1	11	THR	9.9
30	4	59	ASP	9.7
30	4	14	CYS	9.6
27	1	30	GLU	9.5
30	4	1	MET	9.4
23	W	1	THR	9.3
30	4	35	TRP	9.3
30	4	33	MET	9.0
30	4	56	PRO	8.7
30	4	91	GLN	8.5
27	1	31	ILE	8.5
30	4	8	ASN	8.4
30	4	71	CYS	8.4
30	4	85	ALA	8.3
30	4	39	GLN	8.3
30	4	34	LYS	8.3
30	4	76	LYS	8.3
30	4	58	GLY	8.1
27	1	26	VAL	8.0
27	1	20	LEU	7.9

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Mol	Chain	Res	Type	RSRZ
30	4	31	THR	7.8
27	1	16	PRO	7.8
30	4	77	ALA	7.7
14	N	89	ASN	7.6
22	V	51	TRP	7.6
14	N	70	GLY	7.5
30	4	53	SER	7.4
27	1	12	GLY	7.4
30	4	20	HIS	7.4
30	4	75	GLY	7.4
27	1	44	PHE	7.3
27	1	34	LYS	7.3
30	4	81	GLU	7.1
30	4	22	VAL	7.1
27	1	15	GLY	7.1
30	4	42	ARG	7.1
30	4	9	THR	7.1
30	4	2	GLN	7.0
2	B	3001	U	7.0
30	4	10	TYR	6.9
30	4	3	MET	6.9
30	4	32	GLY	6.9
30	4	4	PRO	6.8
27	1	19	GLY	6.7
27	1	35	LYS	6.7
30	4	27	SER	6.6
27	1	22	ILE	6.6
30	4	60	LYS	6.6
30	4	41	GLU	6.5
1	A	1198	U	6.5
30	4	18	GLN	6.5
30	4	43	ASN	6.5
30	4	78	HIS	6.5
30	4	48	ASN	6.5
30	4	88	LEU	6.4
27	1	45	LYS	6.4
30	4	74	CYS	6.3
27	1	25	ARG	6.3
30	4	68	LYS	6.3
1	A	1173	A	6.3
30	4	16	GLU	6.3
30	4	30	GLN	6.2

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Mol	Chain	Res	Type	RSRZ
22	V	9	CYS	6.2
30	4	67	LEU	6.2
30	4	86	GLY	6.1
30	4	15	ASN	6.1
30	4	61	PRO	6.1
14	N	80	GLY	6.1
30	4	44	SER	6.0
27	1	28	ASP	5.8
27	1	21	LYS	5.8
27	1	23	ARG	5.8
27	1	32	LYS	5.7
22	V	11	THR	5.7
1	A	735	C	5.6
22	V	39	ASN	5.6
22	V	52	THR	5.5
30	4	57	GLY	5.5
30	4	21	GLU	5.4
6	F	57	THR	5.4
9	I	27	ILE	5.4
30	4	80	ARG	5.4
30	4	55	VAL	5.3
22	V	54	THR	5.3
30	4	17	HIS	5.3
15	O	160	SER	5.3
22	V	55	ALA	5.3
9	I	23	ILE	5.3
27	1	39	CYS	5.3
30	4	36	ILE	5.3
6	F	69	ILE	5.3
6	F	88	LEU	5.3
30	4	12	PRO	5.2
22	V	6	CYS	5.2
27	1	13	ARG	5.2
30	4	40	ARG	5.2
27	1	24	VAL	5.1
27	1	18	TYR	5.1
22	V	53	ASP	5.1
30	4	72	GLY	5.0
30	4	24	LYS	5.0
27	1	33	HIS	5.0
1	A	1175	G	4.9
30	4	23	GLU	4.9

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Mol	Chain	Res	Type	RSRZ
27	1	14	PHE	4.9
30	4	6	ARG	4.8
30	4	19	GLU	4.8
15	O	179	LEU	4.8
30	4	66	ASP	4.8
30	4	26	ARG	4.7
30	4	51	LYS	4.7
30	4	52	PHE	4.7
27	1	27	ALA	4.7
30	4	47	GLY	4.7
30	4	49	ASP	4.7
1	A	1172	G	4.7
30	4	87	ARG	4.6
3	C	64	ASP	4.6
30	4	63	LYS	4.5
14	N	83	SER	4.5
22	V	48	ASN	4.5
15	O	186	LEU	4.5
27	1	40	PRO	4.5
22	V	40	ALA	4.5
27	1	29	VAL	4.5
27	1	36	LYS	4.5
30	4	89	GLU	4.4
30	4	64	LYS	4.4
27	1	42	CYS	4.4
27	1	37	HIS	4.4
30	4	45	GLY	4.3
22	V	36	CYS	4.3
30	4	13	HIS	4.3
1	A	1171	A	4.3
22	V	12	ASP	4.3
1	A	1177	A	4.3
23	W	40	PRO	4.3
30	4	79	LEU	4.2
6	F	18	ILE	4.2
14	N	74	ARG	4.2
30	4	5	ARG	4.2
22	V	4	ARG	4.1
30	4	25	VAL	4.1
6	F	89	PRO	4.1
2	B	3024	U	4.1
30	4	92	GLU	4.1

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Mol	Chain	Res	Type	RSRZ
6	F	63	ILE	4.1
27	1	10	ARG	4.0
30	4	69	TYR	4.0
1	A	1199	A	4.0
14	N	81	ARG	4.0
22	V	10	GLY	4.0
22	V	25	ASP	4.0
22	V	29	THR	4.0
22	V	50	GLU	3.9
15	O	162	ASP	3.9
27	1	41	VAL	3.9
27	1	17	ARG	3.9
27	1	58	GLY	3.9
1	A	2237	G	3.9
27	1	57	CYS	3.9
22	V	43	GLY	3.8
22	V	41	ASP	3.8
22	V	49	LEU	3.7
23	W	39	ALA	3.7
14	N	77	PHE	3.7
14	N	90	ARG	3.7
6	F	10	PHE	3.7
1	A	1168	C	3.7
6	F	102	GLY	3.6
6	F	75	LEU	3.6
14	N	73	ARG	3.6
30	4	7	PHE	3.6
21	U	112	LEU	3.6
21	U	119	ALA	3.6
15	O	147	ILE	3.6
14	N	72	SER	3.5
20	T	81	ILE	3.5
22	V	28	THR	3.5
6	F	66	GLY	3.5
30	4	29	ARG	3.5
6	F	85	GLN	3.5
27	1	38	LYS	3.5
6	F	27	ILE	3.4
6	F	128	LEU	3.4
30	4	54	LYS	3.4
1	A	1192	A	3.4
22	V	19	THR	3.4

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Mol	Chain	Res	Type	RSRZ
15	O	184	ILE	3.3
22	V	13	ILE	3.3
22	V	23	HIS	3.3
30	4	70	ARG	3.3
22	V	5	GLU	3.3
15	O	157	PRO	3.3
6	F	16	PRO	3.3
22	V	22	VAL	3.3
14	N	78	ASN	3.2
1	A	736	A	3.2
22	V	27	ALA	3.2
27	1	43	GLY	3.2
13	M	80	ASP	3.2
1	A	1176	C	3.1
17	Q	1	THR	3.1
10	J	135	TRP	3.1
30	4	73	GLU	3.1
1	A	1167	G	3.1
23	W	8	ILE	3.1
1	A	284	C	3.1
9	I	24	VAL	3.1
1	A	285	A	3.1
30	4	50	GLY	3.0
22	V	24	LYS	3.0
15	O	178	THR	3.0
6	F	170	TYR	3.0
30	4	28	GLY	3.0
6	F	90	LEU	3.0
27	1	79	VAL	3.0
22	V	8	TYR	3.0
1	A	1169	U	3.0
6	F	26	GLY	3.0
1	A	2344	G	3.0
2	B	3002	U	3.0
6	F	62	ASP	2.9
6	F	23	VAL	2.9
27	1	82	ALA	2.9
2	B	3023	U	2.9
4	D	1	PRO	2.9
13	M	73	VAL	2.9
3	C	83	GLY	2.9
15	O	161	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
22	V	47	ARG	2.8
9	I	71	LEU	2.8
1	A	1913	C	2.8
30	4	46	ILE	2.8
8	H	106	THR	2.8
9	I	65	THR	2.8
1	A	1948	G	2.8
9	I	17	GLN	2.8
22	V	46	ALA	2.8
3	C	85	ASP	2.8
6	F	56	ARG	2.8
1	A	1166	A	2.7
13	M	60	GLU	2.7
27	1	47	LEU	2.7
1	A	1181	A	2.7
6	F	134	LEU	2.7
22	V	7	ASP	2.7
6	F	130	VAL	2.7
15	O	148	ALA	2.7
1	A	1190	G	2.7
10	J	32	ASP	2.7
3	C	36	ASP	2.7
15	O	159	TYR	2.6
3	C	62	ASP	2.6
27	1	80	MET	2.6
25	Y	41	PHE	2.6
6	F	58	VAL	2.6
1	A	2345	A	2.6
15	O	127	LEU	2.6
1	A	2433	A	2.6
6	F	17	ARG	2.6
30	4	90	PHE	2.6
1	A	960	G	2.6
1	A	1197	G	2.6
8	H	26	THR	2.6
7	G	10	ASP	2.6
13	M	89	PHE	2.6
1	A	2238	A	2.6
1	A	1180	U	2.6
6	F	132	VAL	2.6
5	E	135	GLU	2.6
15	O	138	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	362	G	2.6
17	Q	116	SER	2.6
6	F	103	ASN	2.6
2	B	3122	C	2.5
7	G	108	LEU	2.5
9	I	15	TRP	2.5
14	N	82	ARG	2.5
15	O	150	TYR	2.5
6	F	15	GLU	2.5
9	I	64	ASN	2.5
1	A	1951	G	2.5
6	F	171	ASP	2.5
15	O	183	ASP	2.5
15	O	166	ALA	2.5
6	F	104	PHE	2.5
23	W	7	GLU	2.5
26	Z	108	ASP	2.5
1	A	2436	U	2.5
6	F	84	LEU	2.5
9	I	26	MET	2.5
14	N	69	LYS	2.5
1	A	1193	A	2.5
6	F	106	PHE	2.5
1	A	970	U	2.5
6	F	44	ILE	2.5
22	V	33	SER	2.5
6	F	28	GLY	2.4
13	M	81	VAL	2.4
27	1	59	HIS	2.4
6	F	166	ILE	2.4
3	C	237	GLY	2.4
13	M	118	LEU	2.4
15	O	175	LEU	2.4
6	F	98	PHE	2.4
9	I	16	LYS	2.4
13	M	59	GLU	2.4
26	Z	103	THR	2.4
6	F	24	HIS	2.4
6	F	172	VAL	2.4
1	A	1182	C	2.4
23	W	52	ALA	2.4
6	F	11	HIS	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	1525	G	2.4
21	U	37	GLN	2.4
3	C	82	VAL	2.3
6	F	83	PHE	2.3
1	A	282	C	2.3
13	M	104	ASP	2.3
1	A	713	U	2.3
1	A	1170	U	2.3
10	J	83	PHE	2.3
22	V	26	GLY	2.3
6	F	25	MET	2.3
23	W	3	LEU	2.3
15	O	152	GLU	2.3
1	A	2239	C	2.3
7	G	95	VAL	2.3
8	H	90	GLU	2.3
15	O	74	PRO	2.3
26	Z	102	LEU	2.3
26	Z	98	GLN	2.3
21	U	117	ASP	2.2
27	1	46	LYS	2.2
6	F	45	THR	2.2
6	F	67	ASP	2.2
6	F	43	GLU	2.2
21	U	49	GLU	2.2
23	W	59	ILE	2.2
6	F	80	ALA	2.2
6	F	86	THR	2.2
1	A	2249	G	2.2
25	Y	40	HIS	2.2
25	Y	88	GLU	2.2
1	A	280	C	2.2
15	O	140	GLN	2.2
15	O	151	ASP	2.2
14	N	76	ARG	2.2
1	A	1174	A	2.2
1	A	1200	A	2.2
21	U	116	ASP	2.2
7	G	131	LEU	2.2
27	1	56	MET	2.2
6	F	73	VAL	2.1
7	G	100	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
22	V	30	HIS	2.1
7	G	124	VAL	2.1
4	D	117	GLU	2.1
7	G	129	GLU	2.1
13	M	58	GLN	2.1
9	I	20	VAL	2.1
1	A	1914	C	2.1
29	3	36	ASN	2.1
8	H	44	SER	2.1
23	W	33	VAL	2.1
15	O	94	GLU	2.1
15	O	167	ASP	2.1
22	V	14	GLU	2.1
3	C	96	LEU	2.1
14	N	75	THR	2.1
3	C	112	PRO	2.1
6	F	54	ALA	2.1
26	Z	235	GLU	2.1
1	A	130	C	2.1
13	M	106	VAL	2.1
7	G	87	PHE	2.1
9	I	68	GLU	2.1
18	R	95	GLU	2.1
1	A	1912	A	2.1
13	M	123	ASP	2.1
2	B	3025	G	2.0
13	M	91	VAL	2.0
21	U	82	THR	2.0
6	F	87	ALA	2.0
27	1	61	GLY	2.0
4	D	110	ASP	2.0
6	F	47	GLN	2.0
3	C	37	VAL	2.0
15	O	165	ALA	2.0
25	Y	74	ALA	2.0
27	1	53	GLY	2.0
6	F	137	PRO	2.0

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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
33	NA	T	8312	1/1	0.38	0.82	124,124,124,124	0
33	NA	A	8384	1/1	0.40	2.02	114,114,114,114	0
33	NA	A	8329	1/1	0.40	0.52	70,70,70,70	0
32	MG	A	8024	1/1	0.45	0.69	116,116,116,116	0
32	MG	A	8049	1/1	0.50	0.60	89,89,89,89	0
34	CL	M	8510	1/1	0.52	0.46	87,87,87,87	0
33	NA	A	8382	1/1	0.54	0.38	62,62,62,62	0
33	NA	A	8341	1/1	0.56	0.19	43,43,43,43	0
36	CD	4	8404	1/1	0.58	0.79	156,156,156,156	0
34	CL	4	8504	1/1	0.67	0.71	95,95,95,95	0
33	NA	A	8371	1/1	0.69	0.33	54,54,54,54	0
33	NA	S	8337	1/1	0.70	0.33	49,49,49,49	0
33	NA	B	8383	1/1	0.71	0.62	63,63,63,63	0
33	NA	A	8331	1/1	0.72	0.35	61,61,61,61	0
32	MG	A	8090	1/1	0.73	0.29	36,36,36,36	0
33	NA	A	8369	1/1	0.73	0.38	52,52,52,52	0
36	CD	P	8405	1/1	0.73	0.45	169,169,169,169	0
33	NA	A	8365	1/1	0.74	0.41	49,49,49,49	0
33	NA	A	8373	1/1	0.74	0.52	59,59,59,59	0
32	MG	A	8076	1/1	0.76	0.16	71,71,71,71	0
33	NA	B	8351	1/1	0.78	0.23	69,69,69,69	0
36	CD	V	8401	1/1	0.78	0.48	142,142,142,142	0
32	MG	A	8001	1/1	0.79	0.12	39,39,39,39	0
33	NA	A	8364	1/1	0.80	0.32	40,40,40,40	0
33	NA	A	8324	1/1	0.80	0.15	51,51,51,51	0
32	MG	A	8082	1/1	0.81	0.21	52,52,52,52	0
34	CL	R	8511	1/1	0.81	0.45	63,63,63,63	0
32	MG	A	8104	1/1	0.81	0.23	40,40,40,40	0
33	NA	A	8332	1/1	0.81	0.22	58,58,58,58	0
33	NA	A	8362	1/1	0.82	0.38	69,69,69,69	0
34	CL	N	8518	1/1	0.82	0.22	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
32	MG	B	8095	1/1	0.82	0.07	67,67,67,67	0
34	CL	A	8503	1/1	0.83	0.33	50,50,50,50	0
33	NA	A	8372	1/1	0.83	0.66	55,55,55,55	0
33	NA	S	8386	1/1	0.83	0.27	53,53,53,53	0
33	NA	A	8356	1/1	0.83	0.68	58,58,58,58	0
35	K	A	8602	1/1	0.83	0.28	68,68,68,68	0
31	SPR	A	9001	59/59	0.83	0.36	78,88,95,95	0
33	NA	A	8363	1/1	0.84	0.41	66,66,66,66	0
32	MG	A	8117	1/1	0.84	0.12	31,31,31,31	0
33	NA	A	8360	1/1	0.85	0.86	55,55,55,55	0
36	CD	1	8403	1/1	0.85	0.27	138,138,138,138	0
35	K	A	8603	1/1	0.85	0.36	88,88,88,88	0
33	NA	A	8377	1/1	0.85	0.25	60,60,60,60	0
33	NA	A	8355	1/1	0.85	0.36	55,55,55,55	0
33	NA	A	8352	1/1	0.86	0.43	52,52,52,52	0
32	MG	1	8105	1/1	0.86	0.28	44,44,44,44	0
33	NA	A	8370	1/1	0.86	0.34	49,49,49,49	0
32	MG	Z	8109	1/1	0.86	0.22	53,53,53,53	0
32	MG	A	8118	1/1	0.86	0.34	62,62,62,62	0
34	CL	A	8517	1/1	0.87	0.31	55,55,55,55	0
32	MG	A	8093	1/1	0.87	0.23	56,56,56,56	0
34	CL	A	8515	1/1	0.87	0.58	100,100,100,100	0
33	NA	E	8304	1/1	0.88	0.12	35,35,35,35	0
32	MG	A	8119	1/1	0.88	0.36	71,71,71,71	0
32	MG	A	8115	1/1	0.88	0.10	59,59,59,59	0
34	CL	O	8507	1/1	0.88	0.25	62,62,62,62	0
32	MG	A	8116	1/1	0.88	0.17	67,67,67,67	0
33	NA	A	8333	1/1	0.88	0.13	33,33,33,33	0
32	MG	A	8070	1/1	0.88	0.59	66,66,66,66	0
33	NA	A	8308	1/1	0.88	0.23	69,69,69,69	0
32	MG	A	8040	1/1	0.88	0.19	78,78,78,78	0
33	NA	A	8328	1/1	0.88	0.19	45,45,45,45	0
33	NA	A	8305	1/1	0.89	0.15	34,34,34,34	0
33	NA	A	8326	1/1	0.89	0.26	46,46,46,46	0
34	CL	K	8502	1/1	0.89	0.08	52,52,52,52	0
32	MG	A	8102	1/1	0.89	1.21	87,87,87,87	0
33	NA	A	8343	1/1	0.89	0.09	16,16,16,16	0
33	NA	A	8385	1/1	0.89	0.40	41,41,41,41	0
34	CL	A	8522	1/1	0.89	0.43	75,75,75,75	0
33	NA	A	8336	1/1	0.89	0.20	49,49,49,49	0
32	MG	A	8050	1/1	0.89	0.13	85,85,85,85	0
32	MG	A	8039	1/1	0.89	0.06	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
33	NA	A	8344	1/1	0.89	0.09	30,30,30,30	0
32	MG	A	8110	1/1	0.89	0.13	47,47,47,47	0
33	NA	A	8301	1/1	0.89	0.20	43,43,43,43	0
33	NA	A	8357	1/1	0.90	0.17	67,67,67,67	0
34	CL	Z	8520	1/1	0.90	0.18	35,35,35,35	0
32	MG	A	8103	1/1	0.90	0.30	55,55,55,55	0
32	MG	A	8088	1/1	0.90	0.15	45,45,45,45	0
32	MG	A	8023	1/1	0.90	0.07	42,42,42,42	0
33	NA	A	8313	1/1	0.90	0.22	63,63,63,63	0
32	MG	A	8062	1/1	0.90	0.11	72,72,72,72	0
33	NA	A	8374	1/1	0.90	0.60	63,63,63,63	0
32	MG	4	8078	1/1	0.90	0.25	74,74,74,74	0
33	NA	A	8366	1/1	0.90	0.26	49,49,49,49	0
32	MG	A	8113	1/1	0.90	0.10	45,45,45,45	0
34	CL	A	8516	1/1	0.90	0.18	44,44,44,44	0
33	NA	A	8375	1/1	0.91	0.34	53,53,53,53	0
33	NA	A	8378	1/1	0.91	0.42	37,37,37,37	0
34	CL	A	8512	1/1	0.91	0.20	32,32,32,32	0
32	MG	A	8085	1/1	0.91	0.13	72,72,72,72	0
32	MG	A	8089	1/1	0.91	0.19	84,84,84,84	0
33	NA	A	8310	1/1	0.91	0.22	29,29,29,29	0
33	NA	A	8354	1/1	0.91	0.16	40,40,40,40	0
32	MG	A	8092	1/1	0.91	0.20	91,91,91,91	0
33	NA	A	8321	1/1	0.91	0.43	39,39,39,39	0
33	NA	A	8323	1/1	0.91	0.25	50,50,50,50	0
32	MG	A	8045	1/1	0.92	0.08	54,54,54,54	0
34	CL	D	8519	1/1	0.92	0.51	65,65,65,65	0
33	NA	R	8348	1/1	0.92	0.11	37,37,37,37	0
33	NA	A	8367	1/1	0.92	0.20	52,52,52,52	0
32	MG	A	8061	1/1	0.92	0.09	44,44,44,44	0
33	NA	A	8306	1/1	0.92	0.50	56,56,56,56	0
32	MG	A	8096	1/1	0.92	0.08	53,53,53,53	0
32	MG	A	8041	1/1	0.92	0.07	46,46,46,46	0
32	MG	A	8081	1/1	0.92	0.18	58,58,58,58	0
34	CL	A	8505	1/1	0.92	0.67	88,88,88,88	0
32	MG	A	8015	1/1	0.93	0.10	57,57,57,57	0
33	NA	A	8322	1/1	0.93	0.42	46,46,46,46	0
33	NA	A	8330	1/1	0.93	0.18	43,43,43,43	0
35	K	A	8601	1/1	0.93	0.16	73,73,73,73	0
33	NA	A	8320	1/1	0.93	0.12	33,33,33,33	0
33	NA	A	8340	1/1	0.93	0.30	31,31,31,31	0
32	MG	U	8073	1/1	0.93	0.20	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
32	MG	A	8067	1/1	0.93	0.24	50,50,50,50	0
32	MG	A	8114	1/1	0.93	0.47	92,92,92,92	0
34	CL	A	8514	1/1	0.93	0.21	61,61,61,61	0
33	NA	A	8368	1/1	0.93	0.15	47,47,47,47	0
33	NA	A	8359	1/1	0.93	0.42	61,61,61,61	0
33	NA	A	8307	1/1	0.94	0.11	39,39,39,39	0
34	CL	K	8521	1/1	0.94	0.14	46,46,46,46	0
34	CL	A	8513	1/1	0.94	0.12	56,56,56,56	0
34	CL	C	8509	1/1	0.94	0.29	86,86,86,86	0
32	MG	A	8075	1/1	0.94	0.08	57,57,57,57	0
33	NA	A	8318	1/1	0.94	0.17	34,34,34,34	0
32	MG	A	8068	1/1	0.94	0.13	58,58,58,58	0
33	NA	A	8353	1/1	0.94	0.12	38,38,38,38	0
32	MG	A	8006	1/1	0.94	0.08	48,48,48,48	0
32	MG	A	8053	1/1	0.94	0.11	52,52,52,52	0
32	MG	A	8051	1/1	0.94	0.09	56,56,56,56	0
33	NA	A	8316	1/1	0.94	0.34	51,51,51,51	0
33	NA	A	8342	1/1	0.94	0.24	47,47,47,47	0
32	MG	A	8072	1/1	0.94	0.13	80,80,80,80	0
32	MG	A	8034	1/1	0.94	0.06	39,39,39,39	0
32	MG	C	8065	1/1	0.94	0.11	57,57,57,57	0
32	MG	A	8029	1/1	0.94	0.07	51,51,51,51	0
33	NA	A	8379	1/1	0.94	0.24	41,41,41,41	0
32	MG	A	8101	1/1	0.94	0.16	55,55,55,55	0
32	MG	A	8031	1/1	0.94	0.05	31,31,31,31	0
34	CL	K	8501	1/1	0.94	0.13	56,56,56,56	0
33	NA	A	8327	1/1	0.95	0.13	32,32,32,32	0
32	MG	A	8033	1/1	0.95	0.07	30,30,30,30	0
32	MG	A	8046	1/1	0.95	0.08	79,79,79,79	0
32	MG	A	8066	1/1	0.95	0.13	83,83,83,83	0
32	MG	A	8027	1/1	0.95	0.05	63,63,63,63	0
32	MG	A	8074	1/1	0.95	0.08	31,31,31,31	0
32	MG	A	8059	1/1	0.95	0.08	31,31,31,31	0
32	MG	A	8043	1/1	0.95	0.08	39,39,39,39	0
33	NA	A	8381	1/1	0.95	0.20	51,51,51,51	0
32	MG	A	8064	1/1	0.95	0.16	24,24,24,24	0
32	MG	A	8079	1/1	0.95	0.15	39,39,39,39	0
32	MG	A	8047	1/1	0.95	0.18	62,62,62,62	0
33	NA	J	8309	1/1	0.95	0.14	21,21,21,21	0
33	NA	A	8317	1/1	0.95	0.12	27,27,27,27	0
32	MG	A	8057	1/1	0.95	0.11	49,49,49,49	0
32	MG	L	8069	1/1	0.95	0.06	50,50,50,50	0

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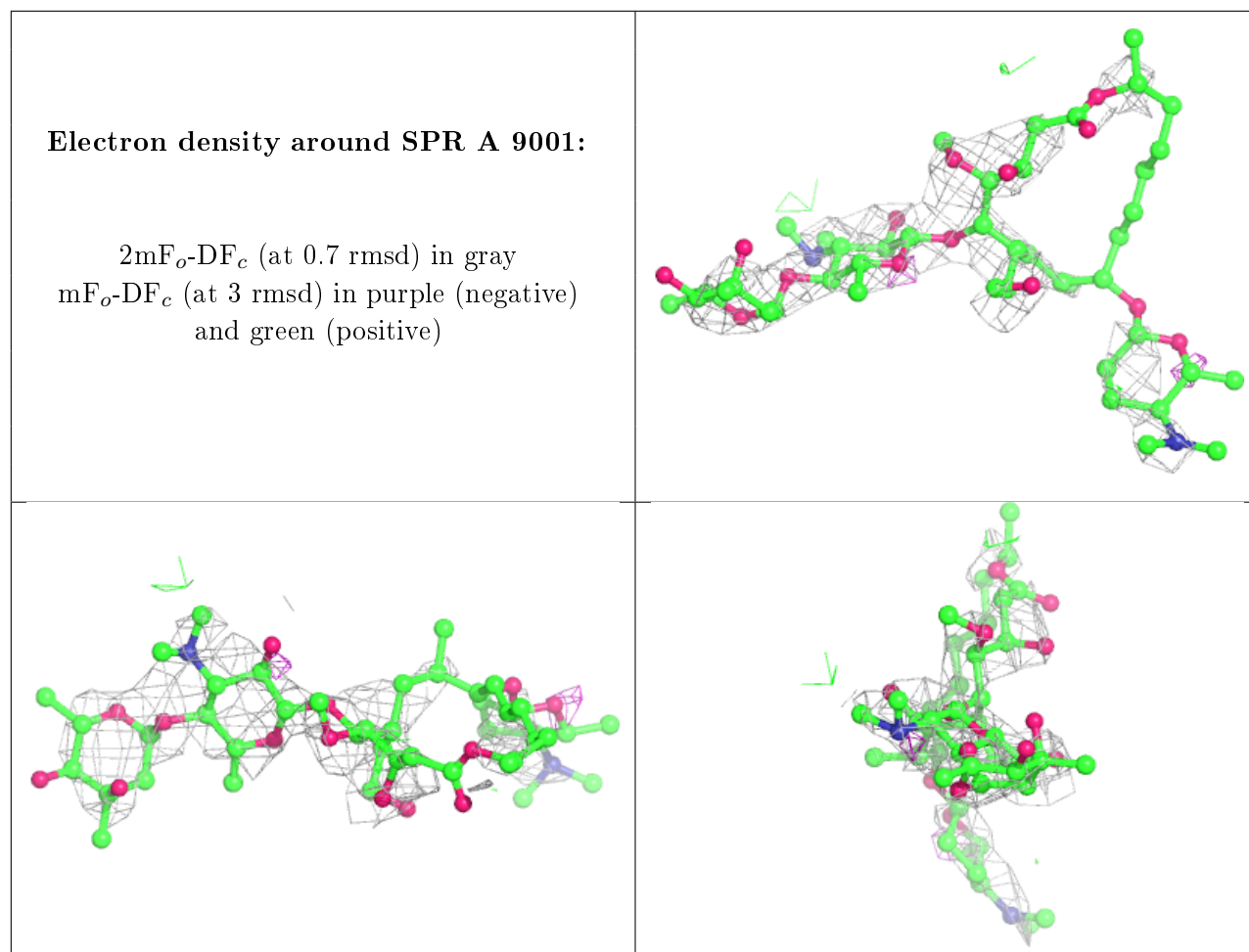
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
32	MG	A	8018	1/1	0.95	0.11	61,61,61,61	0
34	CL	P	8508	1/1	0.95	0.18	93,93,93,93	0
32	MG	A	8055	1/1	0.96	0.08	71,71,71,71	0
32	MG	A	8099	1/1	0.96	0.08	38,38,38,38	0
32	MG	A	8106	1/1	0.96	0.08	47,47,47,47	0
33	NA	A	8350	1/1	0.96	0.15	34,34,34,34	0
33	NA	A	8311	1/1	0.96	0.09	42,42,42,42	0
33	NA	A	8319	1/1	0.96	0.11	52,52,52,52	0
32	MG	A	8016	1/1	0.96	0.09	41,41,41,41	0
33	NA	A	8303	1/1	0.96	0.20	51,51,51,51	0
34	CL	S	8506	1/1	0.96	0.18	46,46,46,46	0
32	MG	A	8022	1/1	0.96	0.09	41,41,41,41	0
32	MG	A	8087	1/1	0.96	0.06	48,48,48,48	0
33	NA	A	8376	1/1	0.96	0.28	78,78,78,78	0
32	MG	A	8071	1/1	0.96	0.14	91,91,91,91	0
32	MG	A	8042	1/1	0.96	0.09	44,44,44,44	0
33	NA	K	8346	1/1	0.96	0.08	27,27,27,27	0
32	MG	A	8014	1/1	0.96	0.06	30,30,30,30	0
32	MG	A	8091	1/1	0.96	0.07	48,48,48,48	0
32	MG	A	8060	1/1	0.96	0.12	45,45,45,45	0
32	MG	A	8084	1/1	0.97	0.08	48,48,48,48	0
32	MG	A	8108	1/1	0.97	0.09	88,88,88,88	0
32	MG	A	8004	1/1	0.97	0.07	48,48,48,48	0
32	MG	A	8010	1/1	0.97	0.05	40,40,40,40	0
32	MG	A	8100	1/1	0.97	0.12	69,69,69,69	0
33	NA	A	8334	1/1	0.97	0.06	36,36,36,36	0
33	NA	A	8314	1/1	0.97	0.18	33,33,33,33	0
32	MG	A	8063	1/1	0.97	0.06	78,78,78,78	0
32	MG	A	8003	1/1	0.97	0.10	24,24,24,24	0
32	MG	A	8080	1/1	0.97	0.05	50,50,50,50	0
33	NA	A	8302	1/1	0.97	0.13	40,40,40,40	0
32	MG	A	8083	1/1	0.97	0.05	47,47,47,47	0
32	MG	A	8008	1/1	0.97	0.07	49,49,49,49	0
32	MG	A	8048	1/1	0.97	0.09	45,45,45,45	0
33	NA	A	8325	1/1	0.97	0.09	52,52,52,52	0
33	NA	A	8361	1/1	0.97	0.14	53,53,53,53	0
33	NA	A	8315	1/1	0.97	0.15	30,30,30,30	0
32	MG	A	8038	1/1	0.97	0.10	35,35,35,35	0
32	MG	A	8035	1/1	0.97	0.06	54,54,54,54	0
33	NA	C	8345	1/1	0.97	0.10	42,42,42,42	0
32	MG	A	8086	1/1	0.98	0.07	50,50,50,50	0
32	MG	A	8005	1/1	0.98	0.10	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
32	MG	A	8032	1/1	0.98	0.05	34,34,34,34	0
32	MG	A	8056	1/1	0.98	0.10	53,53,53,53	0
32	MG	A	8028	1/1	0.98	0.07	44,44,44,44	0
32	MG	A	8097	1/1	0.98	0.22	44,44,44,44	0
32	MG	A	8017	1/1	0.98	0.03	27,27,27,27	0
32	MG	A	8044	1/1	0.98	0.14	52,52,52,52	0
32	MG	A	8019	1/1	0.98	0.07	35,35,35,35	0
32	MG	A	8111	1/1	0.98	0.07	69,69,69,69	0
32	MG	A	8020	1/1	0.98	0.05	51,51,51,51	0
32	MG	A	8077	1/1	0.98	0.07	31,31,31,31	0
32	MG	A	8009	1/1	0.98	0.06	20,20,20,20	0
32	MG	A	8011	1/1	0.98	0.10	52,52,52,52	0
33	NA	M	8380	1/1	0.98	0.15	55,55,55,55	0
33	NA	A	8335	1/1	0.98	0.23	52,52,52,52	0
32	MG	A	8054	1/1	0.98	0.08	48,48,48,48	0
32	MG	A	8012	1/1	0.98	0.11	52,52,52,52	0
32	MG	A	8094	1/1	0.98	0.14	85,85,85,85	0
32	MG	A	8098	1/1	0.98	0.20	50,50,50,50	0
33	NA	A	8339	1/1	0.98	0.14	16,16,16,16	0
36	CD	2	8402	1/1	0.98	0.06	59,59,59,59	0
32	MG	A	8058	1/1	0.98	0.10	43,43,43,43	0
32	MG	A	8112	1/1	0.98	0.15	44,44,44,44	0
33	NA	A	8338	1/1	0.98	0.13	67,67,67,67	0
32	MG	A	8021	1/1	0.98	0.07	27,27,27,27	0
32	MG	A	8107	1/1	0.99	0.04	47,47,47,47	0
32	MG	A	8052	1/1	0.99	0.05	45,45,45,45	0
32	MG	A	8025	1/1	0.99	0.09	60,60,60,60	0
32	MG	A	8026	1/1	0.99	0.05	11,11,11,11	0
33	NA	N	8347	1/1	0.99	0.05	21,21,21,21	0
33	NA	A	8349	1/1	0.99	0.14	53,53,53,53	0
32	MG	A	8002	1/1	0.99	0.10	31,31,31,31	0
32	MG	A	8007	1/1	0.99	0.04	23,23,23,23	0
32	MG	A	8037	1/1	0.99	0.10	48,48,48,48	0
32	MG	A	8013	1/1	0.99	0.12	46,46,46,46	0
32	MG	A	8036	1/1	0.99	0.06	45,45,45,45	0
32	MG	A	8030	1/1	0.99	0.09	26,26,26,26	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.