Full wwPDB X-ray Structure Validation Report (i)

Sep 16, 2023 – 01:52 PM EDT

PDB ID	:	4OX9
Title	:	Crystal structure of the aminoglycoside resistance methyltransferase NpmA bound to the 30S ribosomal subunit
Authors	:	Dunkle, J.A.; Conn, G.L.; Dunham, C.M.
Deposited on	:	2014-02-04
Resolution	:	3.80 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

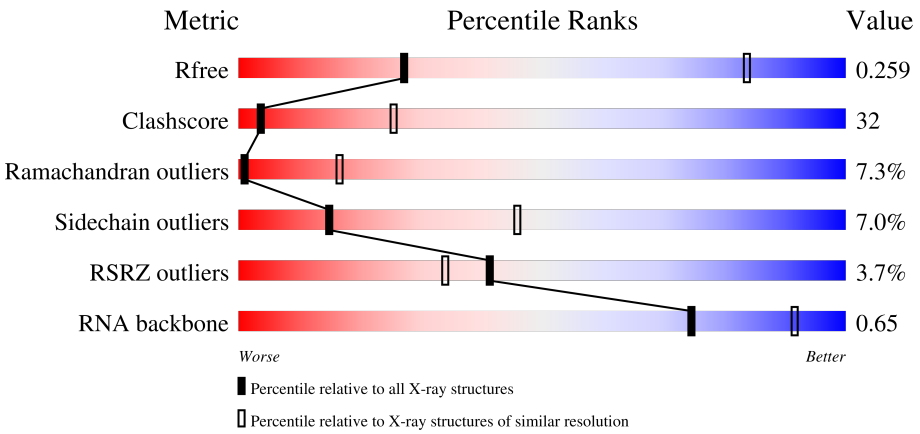
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1212 (4.00-3.60)
Clashscore	141614	1288 (4.00-3.60)
Ramachandran outliers	138981	1243 (4.00-3.60)
Sidechain outliers	138945	1237 (4.00-3.60)
RSRZ outliers	127900	1121 (4.00-3.60)
RNA backbone	3102	1036 (4.60-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	1513	2%, 32%, 52%, 13%, •
2	B	256	3%, 25%, 52%, 12%, •, 9%
3	C	239	4%, 26%, 46%, 14%, •, 14%
4	D	208	%, 43%, 52%, •

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Mol	Chain	Length	Quality of chain
5	E	161	44% 40% 9% 7%
6	F	101	% 45% 52%
7	G	155	2% 45% 52%
8	H	138	% 45% 46% 8%
9	I	128	12% 30% 61% 8%
10	J	104	12% 16% 56% 21% 6%
11	K	129	2% 29% 55% 7% 8%
12	L	131	3% 40% 45% 10% 5%
13	M	126	18% 25% 65% 9%
14	N	60	3% 28% 58% 13%
15	O	88	2% 36% 52% 11%
16	P	88	% 38% 53% 6%
17	Q	104	5% 45% 46% 8%
18	R	88	5% 23% 57% 17%
19	S	92	9% 22% 53% 12% 13%
20	T	106	2% 34% 47% 11% 7%
21	V	26	12% 31% 58% 8%
22	Y	222	8% 71% 24%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	MG	A	1601	-	-	-	X
23	MG	A	1602	-	-	-	X
23	MG	A	1603	-	-	-	X
23	MG	A	1604	-	-	-	X
23	MG	A	1606	-	-	-	X
23	MG	A	1607	-	-	-	X
23	MG	A	1613	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	MG	A	1616	-	-	-	X
23	MG	A	1620	-	-	-	X
23	MG	A	1621	-	-	-	X
23	MG	A	1624	-	-	-	X
23	MG	A	1626	-	-	-	X
23	MG	A	1627	-	-	-	X
23	MG	A	1630	-	-	-	X
23	MG	A	1646	-	-	-	X
23	MG	A	1647	-	-	-	X
23	MG	A	1649	-	-	-	X
23	MG	A	1650	-	-	-	X
23	MG	A	1652	-	-	-	X
23	MG	A	1654	-	-	-	X
23	MG	A	1656	-	-	-	X
23	MG	A	1658	-	-	-	X
23	MG	A	1662	-	-	-	X
23	MG	A	1665	-	-	-	X
23	MG	A	1667	-	-	-	X
23	MG	A	1669	-	-	-	X
23	MG	A	1674	-	-	-	X
23	MG	A	1677	-	-	-	X
23	MG	A	1684	-	-	-	X
23	MG	A	1688	-	-	-	X
23	MG	A	1693	-	-	-	X
23	MG	A	1694	-	-	-	X
23	MG	A	1695	-	-	-	X
23	MG	A	1696	-	-	-	X
23	MG	A	1697	-	-	-	X
23	MG	A	1698	-	-	-	X
23	MG	A	1699	-	-	-	X
23	MG	A	1705	-	-	-	X
23	MG	A	1708	-	-	-	X
23	MG	A	1711	-	-	-	X
23	MG	A	1713	-	-	-	X
23	MG	N	102	-	-	-	X

2 Entry composition (i)

There are 25 unique types of molecules in this entry. The entry contains 53527 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 16S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	A	1507	32394	14418	6002	10467	1507	0	0	0

- Molecule 2 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	234	1900	1213	341	341	5	0	0	0

- Molecule 3 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	206	1612	1016	314	281	1	0	0	0

- Molecule 4 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	208	1703	1066	339	291	7	0	0	0

- Molecule 5 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	E	150	1146	724	217	201	4	0	0	0

- Molecule 6 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	F	101	843	531	155	154	3	0	0	0

- Molecule 7 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
7	G	155	1257	781	252	218	6	0	0	0

- Molecule 8 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
8	H	138	1116	705	215	193	3	0	0	0

- Molecule 9 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
9	I	127	1010	639	197	174	0	0	0

- Molecule 10 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
10	J	98	785	494	153	137	1	0	0	0

- Molecule 11 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
11	K	119	885	549	168	165	3	0	0	0

- Molecule 12 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
12	L	124	970	611	195	163	1	0	0	0

- Molecule 13 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
13	M	125	997	617	207	171	2	0	0	0

- Molecule 14 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
14	N	60	492	312	104	72	4	0	0	0

- Molecule 15 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
15	O	88	734	459	147	126	2	0	0	0

- Molecule 16 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
16	P	83	700	443	139	117	1	0	0	0

- Molecule 17 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
17	Q	104	857	547	160	148	2	0	0	0

- Molecule 18 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
18	R	73	598	381	118	99	0	0	0

- Molecule 19 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
19	S	80	647	414	119	112	2	0	0	0

- Molecule 20 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
20	T	99	763	470	162	129	2	0	0	0

- Molecule 21 is a protein called 30S ribosomal protein Thx.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
21	V	24	208	128	50	30	0	0	0

- Molecule 22 is a protein called 16S rRNA (adenine(1408)-N(1))-methyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
22	Y	219	1761	1138	294	328	1	0	0	0

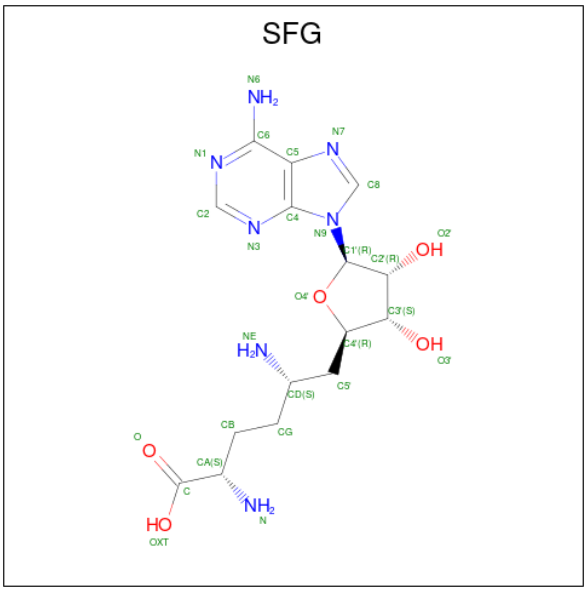
- Molecule 23 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
23	A	117	117	117	0	0
23	B	1	1	1	0	0
23	E	1	1	1	0	0
23	N	1	1	1	0	0

- Molecule 24 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
24	D	1	1	1	0	0
24	N	1	1	1	0	0

- Molecule 25 is SINEFUNGIN (three-letter code: SFG) (formula: $C_{15}H_{23}N_7O_5$).



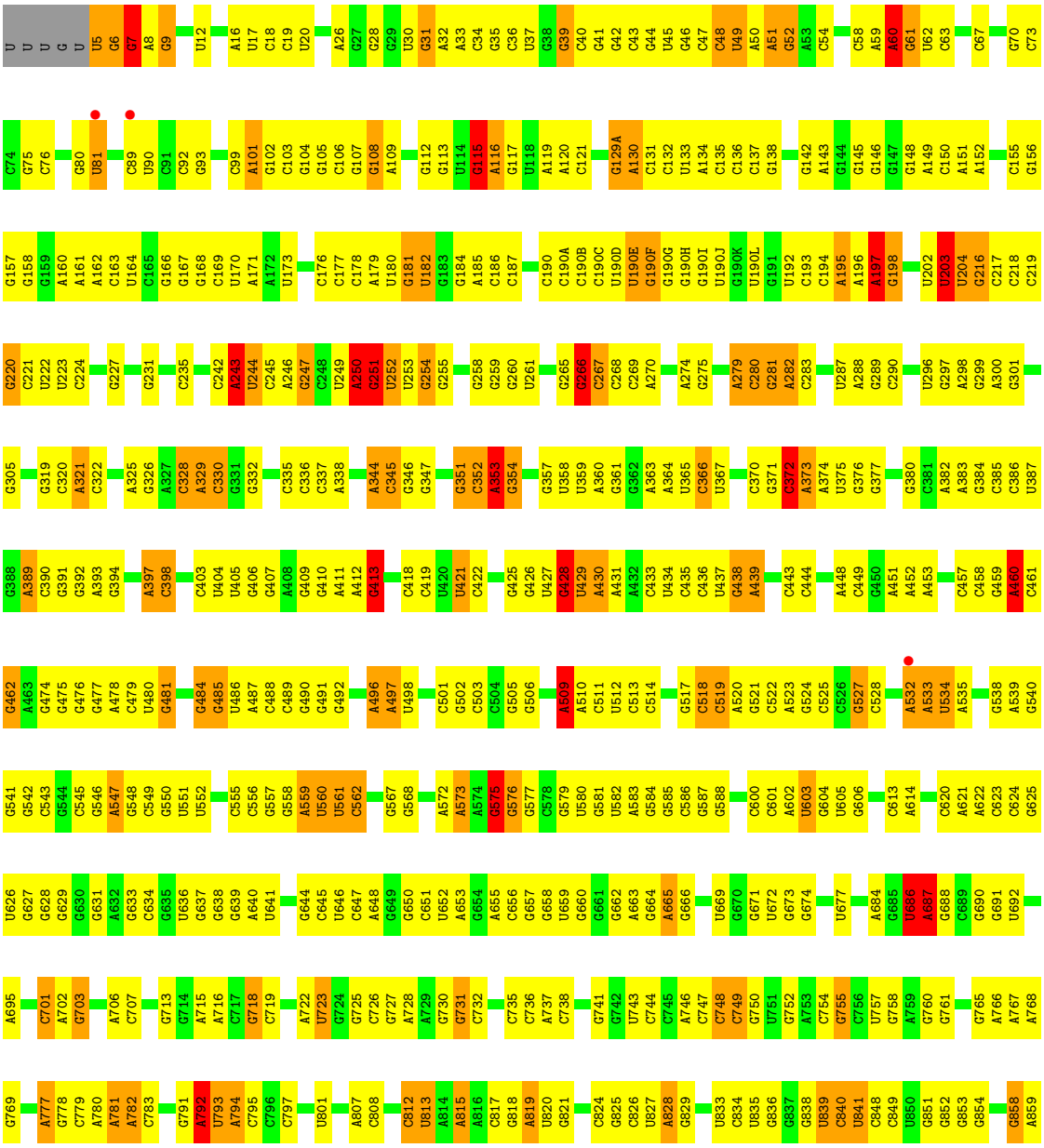
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
25	Y	1	27	15	7	5	0	0

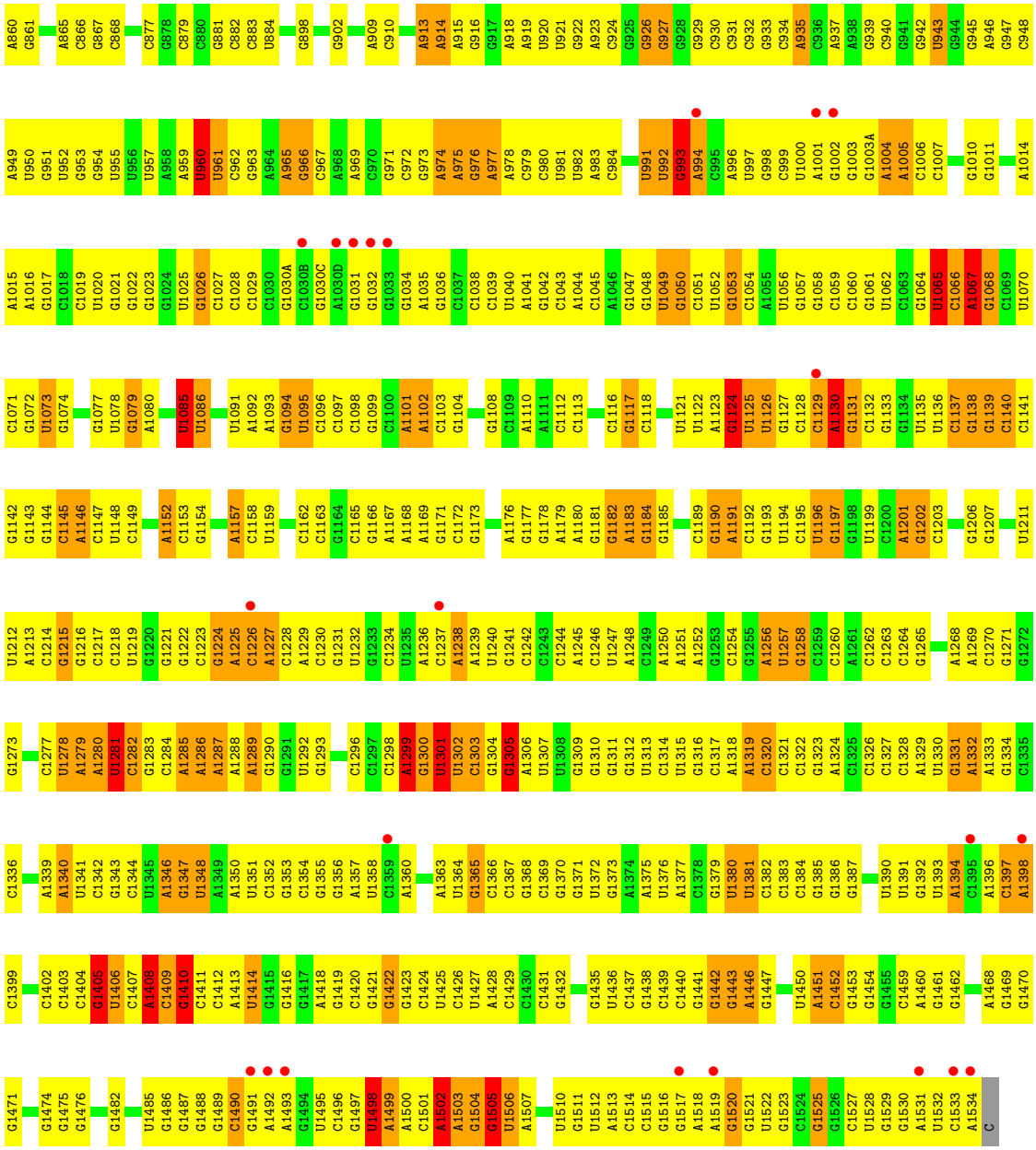
3 Residue-property plots (i)

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: 16S rRNA

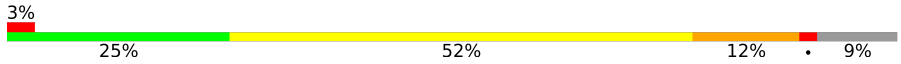
Chain A: 2% 32% 52% 13%

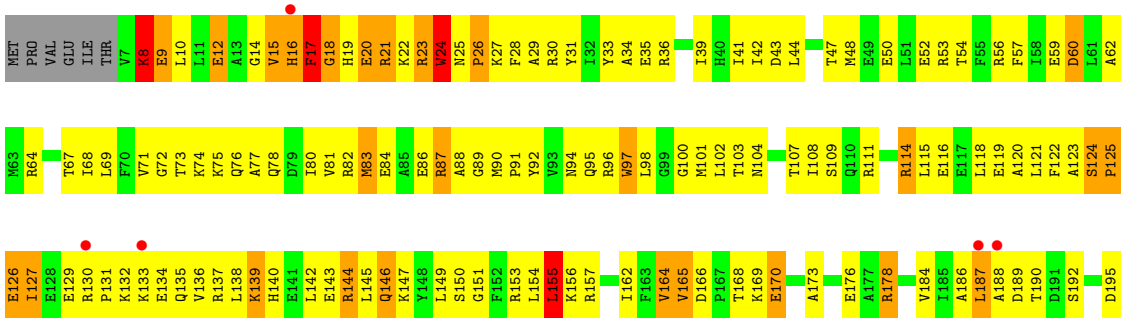


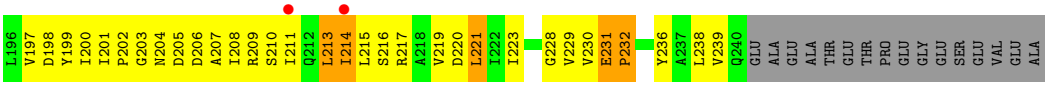


• Molecule 2: 30S ribosomal protein S2

Chain B:

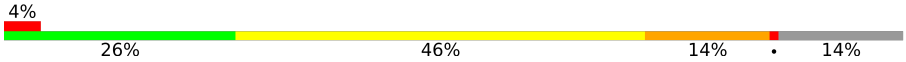


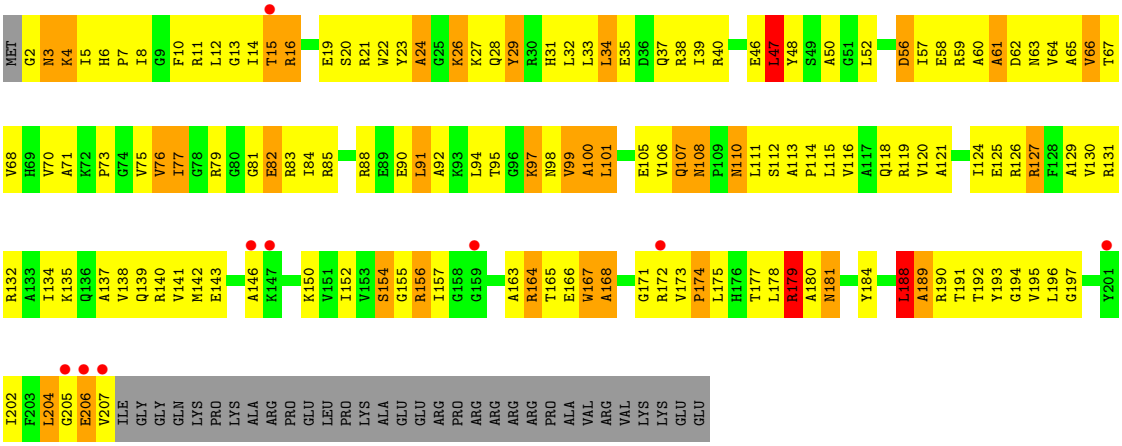




• Molecule 3: 30S ribosomal protein S3

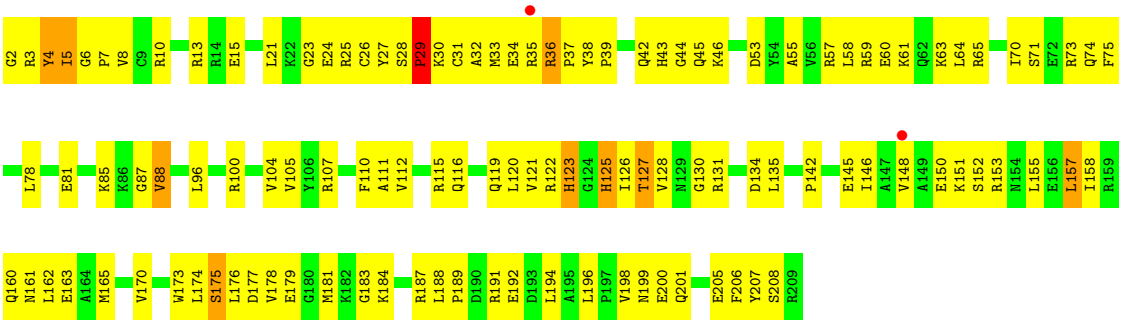
Chain C:





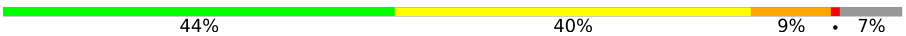
• Molecule 4: 30S ribosomal protein S4

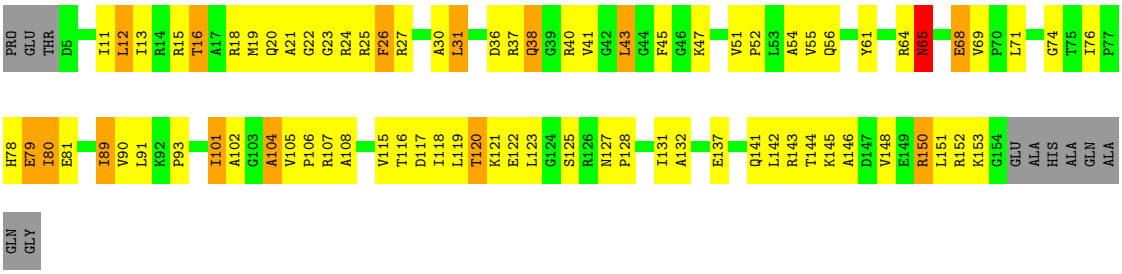
Chain D:



• Molecule 5: 30S ribosomal protein S5

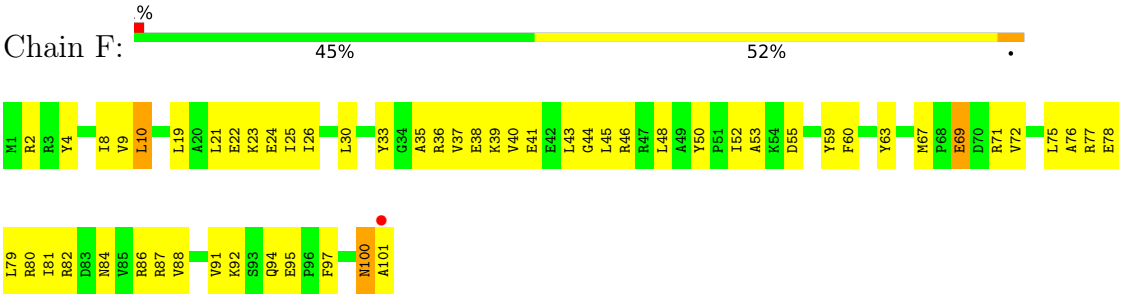
Chain E:





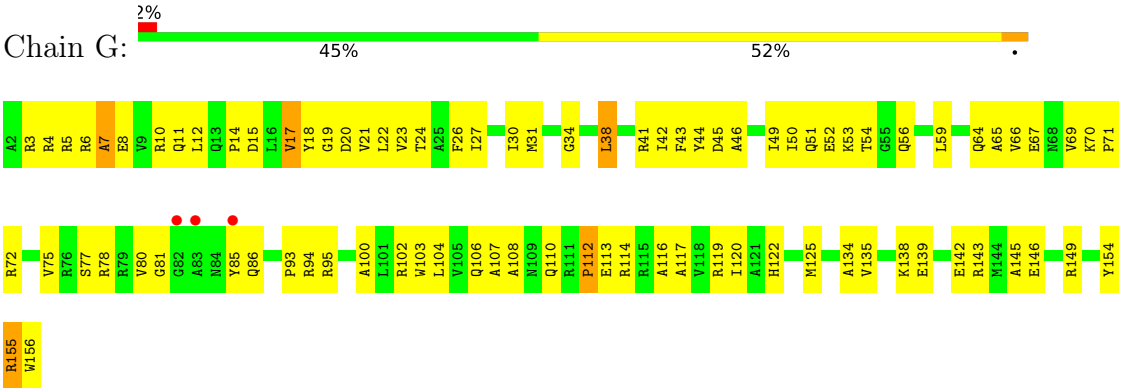
• Molecule 6: 30S ribosomal protein S6

Chain F:



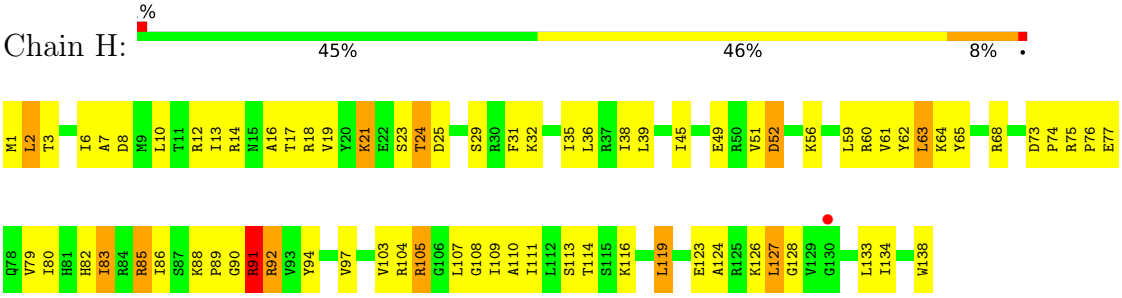
• Molecule 7: 30S ribosomal protein S7

Chain G:



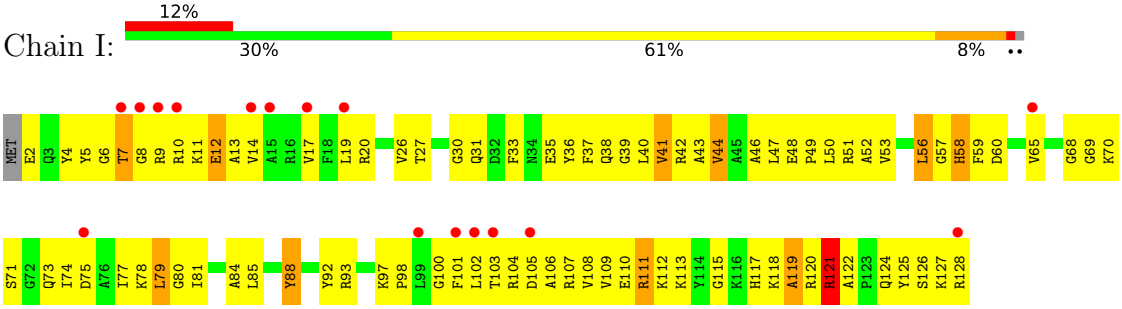
• Molecule 8: 30S ribosomal protein S8

Chain H:



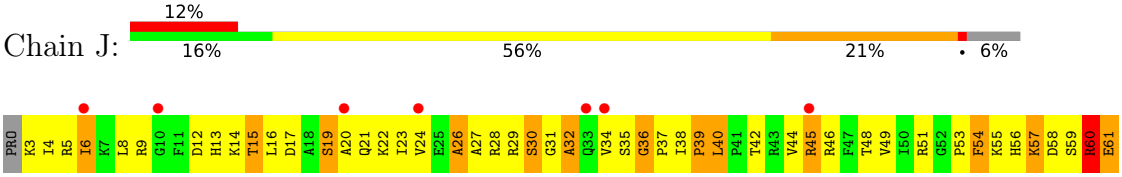
• Molecule 9: 30S ribosomal protein S9

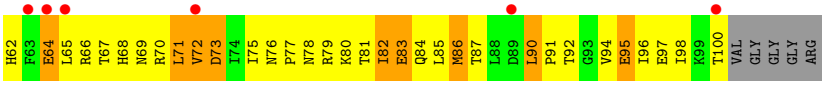
Chain I:



• Molecule 10: 30S ribosomal protein S10

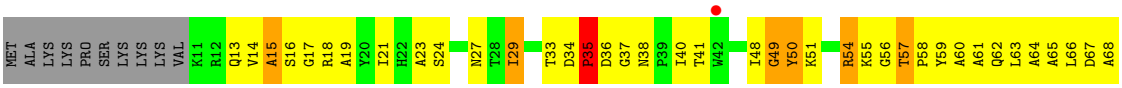
Chain J:

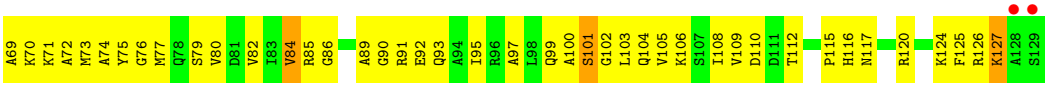




• Molecule 11: 30S ribosomal protein S11

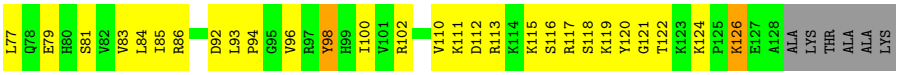
Chain K:





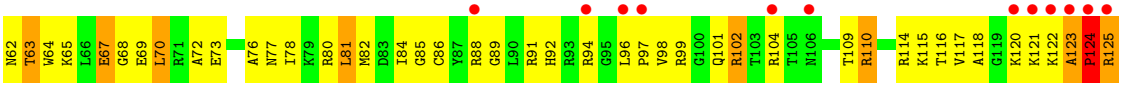
• Molecule 12: 30S ribosomal protein S12

Chain L:



• Molecule 13: 30S ribosomal protein S13

Chain M:

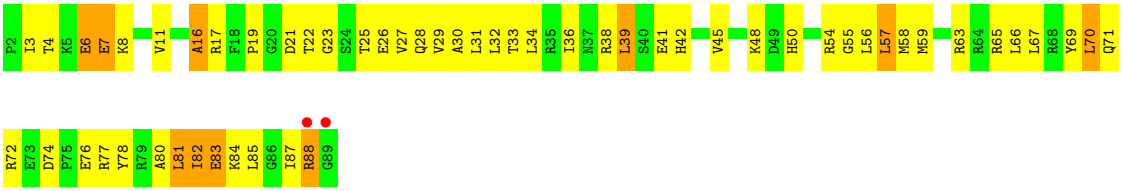


• Molecule 14: 30S ribosomal protein S14 type Z

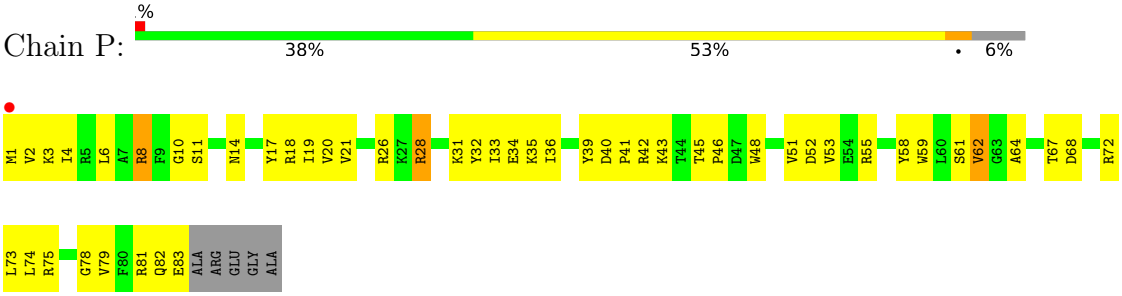
Chain N:

• Molecule 15: 30S ribosomal protein S15

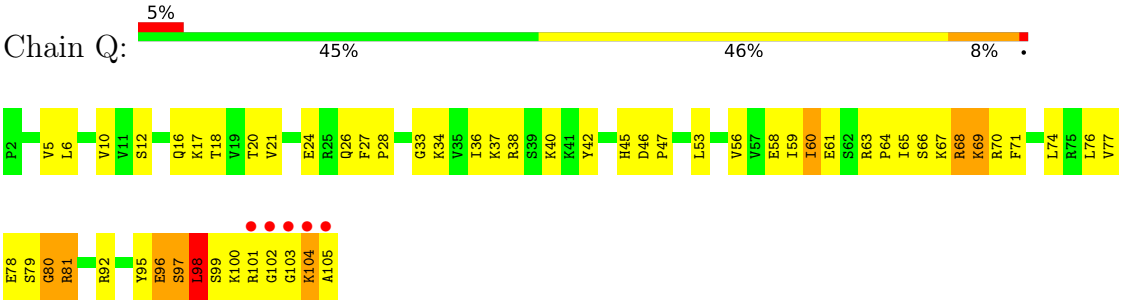
Chain O:



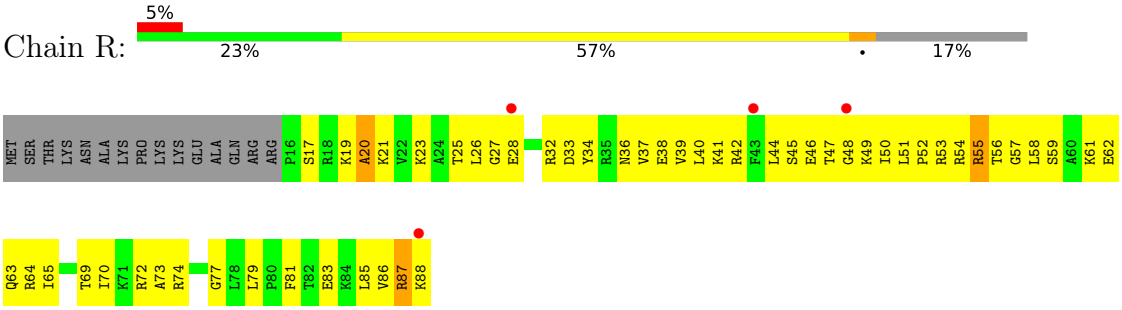
• Molecule 16: 30S ribosomal protein S16



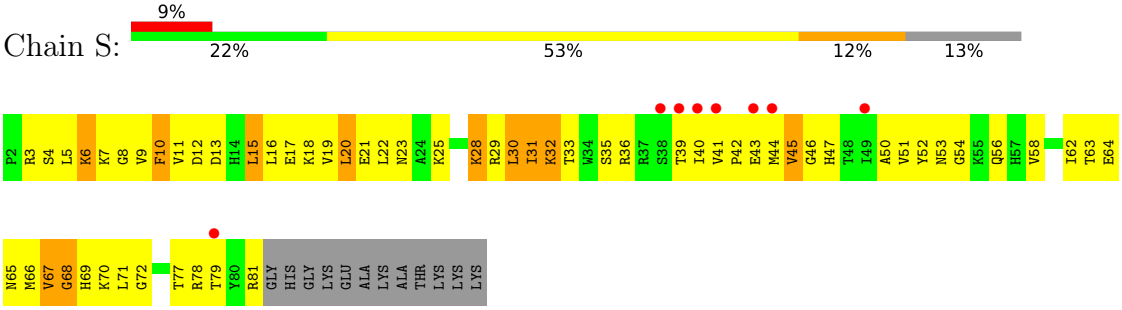
• Molecule 17: 30S ribosomal protein S17



• Molecule 18: 30S ribosomal protein S18

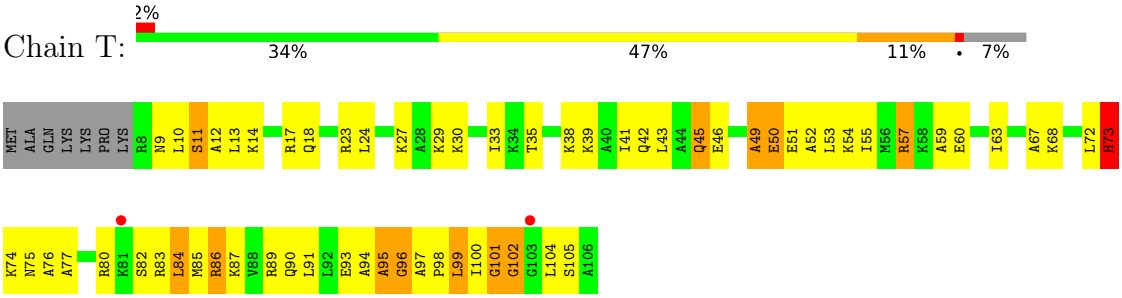


• Molecule 19: 30S ribosomal protein S19



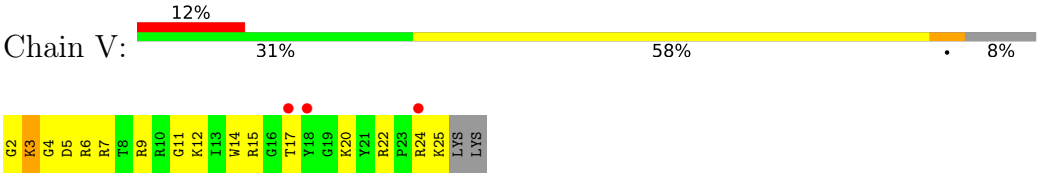
• Molecule 20: 30S ribosomal protein S20

Chain T:



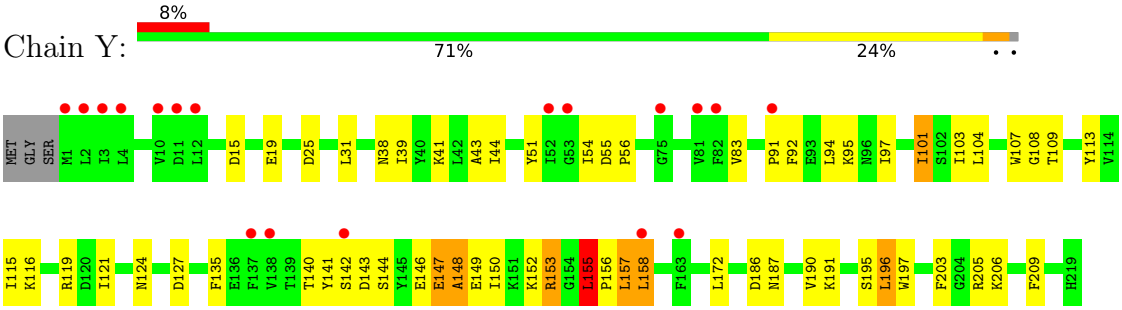
• Molecule 21: 30S ribosomal protein Thx

Chain V:



• Molecule 22: 16S rRNA (adenine(1408)-N(1))-methyltransferase

Chain Y:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	403.52Å 403.52Å 176.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.72 – 3.80 49.71 – 3.80	Depositor EDS
% Data completeness (in resolution range)	99.7 (49.72-3.80) 94.1 (49.71-3.80)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.48 (at 3.77Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.233 , 0.257 0.235 , 0.259	Depositor DCC
R_{free} test set	7034 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å^2)	132.9	Xtriage
Anisotropy	0.320	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 81.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	53527	wwPDB-VP
Average B, all atoms (Å^2)	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.52% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG, SFG

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	0.49	4/36262 (0.0%)	0.77	54/56597 (0.1%)
2	B	0.42	0/1935	0.69	1/2609 (0.0%)
3	C	0.43	0/1636	0.67	0/2205
4	D	0.44	0/1733	0.65	0/2318
5	E	0.69	2/1162 (0.2%)	0.83	2/1564 (0.1%)
6	F	0.43	0/856	0.64	0/1154
7	G	0.38	0/1276	0.62	0/1709
8	H	0.44	0/1136	0.74	0/1527
9	I	0.36	0/1029	0.62	0/1379
10	J	0.47	0/798	0.73	0/1073
11	K	0.39	0/900	0.70	0/1213
12	L	0.42	0/986	0.72	0/1320
13	M	0.40	0/1008	0.67	0/1347
14	N	0.40	0/501	0.78	0/664
15	O	0.36	0/745	0.63	1/992 (0.1%)
16	P	0.43	0/716	0.76	0/963
17	Q	0.48	0/870	0.75	0/1159
18	R	0.43	0/604	0.64	0/801
19	S	0.35	0/661	0.72	1/890 (0.1%)
20	T	0.45	0/765	0.74	0/1007
21	V	0.43	0/212	0.64	0/277
22	Y	0.49	0/1796	0.83	3/2418 (0.1%)
All	All	0.47	6/57587 (0.0%)	0.75	62/85186 (0.1%)

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	0	41

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Mol	Chain	#Chirality outliers	#Planarity outliers
22	Y	0	2
All	All	0	43

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	69	VAL	C-N	11.28	1.55	1.34
5	E	101	ILE	C-N	10.62	1.58	1.34
1	A	669	U	O3'-P	6.03	1.68	1.61
1	A	604	G	O3'-P	-5.28	1.54	1.61
1	A	1405	G	O3'-P	5.17	1.67	1.61
1	A	1410	G	C2-N3	5.08	1.36	1.32

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1406	U	O5'-P-OP2	-11.47	95.38	105.70
1	A	1498	U	C2'-C3'-O3'	9.91	131.29	109.50
1	A	1405	G	P-O3'-C3'	-9.56	108.22	119.70
1	A	243	A	C2'-C3'-O3'	9.46	130.32	109.50
1	A	559	A	C2'-C3'-O3'	9.15	129.63	109.50
1	A	1299	A	N9-C1'-C2'	8.59	125.17	114.00
1	A	1410	G	N3-C4-C5	-8.40	124.40	128.60
1	A	366	C	C2'-C3'-O3'	7.87	126.80	109.50
1	A	1410	G	C4-N9-C1'	7.84	136.69	126.50
1	A	197	A	N9-C1'-C2'	7.82	124.17	114.00
1	A	1410	G	C6-C5-N7	-7.80	125.72	130.40
1	A	687	A	C2'-C3'-O3'	7.73	126.51	109.50
1	A	575	G	C2'-C3'-O3'	7.72	126.48	109.50
1	A	266	G	C2'-C3'-O3'	7.57	126.14	109.50
1	A	1410	G	N3-C4-N9	7.55	130.53	126.00
1	A	60	A	C2'-C3'-O3'	7.54	126.09	109.50
22	Y	155	LEU	CA-CB-CG	7.20	131.87	115.30
1	A	792	A	C2'-C3'-O3'	7.20	125.34	109.50
1	A	1409	C	C6-N1-C2	-7.05	117.48	120.30
1	A	115	G	N9-C1'-C2'	6.92	123.00	114.00
1	A	1505	G	C2'-C3'-O3'	6.73	124.47	113.70
1	A	1067	A	C2'-C3'-O3'	6.60	124.25	113.70
1	A	1502	A	N9-C1'-C2'	6.58	122.56	114.00
1	A	1410	G	C4-C5-C6	6.45	122.67	118.80
1	A	115	G	C2'-C3'-O3'	6.41	123.96	113.70
1	A	7	G	C2'-C3'-O3'	6.38	123.91	113.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	372	C	C2'-C3'-O3'	6.36	123.88	113.70
1	A	509	A	C2'-C3'-O3'	6.32	123.81	113.70
1	A	1410	G	OP2-P-O3'	6.31	119.08	105.20
22	Y	155	LEU	N-CA-C	6.26	127.91	111.00
1	A	603	U	P-O3'-C3'	6.17	127.10	119.70
1	A	460	A	N9-C1'-C2'	6.13	121.97	114.00
1	A	1410	G	C8-N9-C4	-6.09	103.97	106.40
19	S	54	GLY	N-CA-C	-6.04	98.01	113.10
1	A	1410	G	C8-N9-C1'	-5.92	119.31	127.00
1	A	428	G	C2'-C3'-O3'	5.88	123.11	113.70
1	A	1410	G	N7-C8-N9	5.75	115.97	113.10
1	A	266	G	C5'-C4'-C3'	-5.70	106.88	116.00
1	A	63	C	C5'-C4'-C3'	-5.70	106.89	116.00
1	A	1124	G	N9-C1'-C2'	5.62	121.31	114.00
1	A	203	U	N1-C1'-C2'	5.59	121.27	114.00
22	Y	157	LEU	N-CA-C	5.51	125.87	111.00
1	A	353	A	C5'-C4'-O4'	-5.50	102.50	109.10
1	A	669	U	O3'-P-O5'	5.46	114.37	104.00
1	A	1380	U	C2'-C3'-O3'	5.46	122.43	113.70
1	A	1065	U	C1'-O4'-C4'	-5.42	105.57	109.90
1	A	1409	C	OP2-P-O3'	5.40	117.09	105.20
15	O	45	VAL	N-CA-C	-5.40	96.43	111.00
2	B	187	LEU	N-CA-C	-5.38	96.47	111.00
1	A	1405	G	OP2-P-O3'	5.36	117.00	105.20
1	A	1085	U	N1-C1'-C2'	5.32	120.92	114.00
1	A	484	G	C2'-C3'-O3'	5.30	122.17	113.70
1	A	389	A	C5'-C4'-C3'	5.28	124.45	116.00
5	E	101	ILE	O-C-N	5.27	131.14	122.70
1	A	108	G	O4'-C1'-N9	5.21	112.36	108.20
1	A	1409	C	C3'-C2'-C1'	5.19	105.65	101.50
1	A	686	U	C5'-C4'-C3'	-5.15	107.76	116.00
1	A	960	U	C2'-C3'-O3'	5.11	121.87	113.70
1	A	1408	A	N1-C6-N6	-5.06	115.56	118.60
5	E	101	ILE	CA-C-N	-5.02	106.17	117.20
1	A	993	G	N9-C1'-C2'	5.01	120.51	114.00
1	A	49	U	C5'-C4'-C3'	-5.00	108.00	116.00

There are no chirality outliers.

All (43) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1048	G	Sidechain

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Mol	Chain	Res	Type	Group
1	A	1073	U	Sidechain
1	A	1079	G	Sidechain
1	A	1085	U	Sidechain
1	A	1092	A	Sidechain
1	A	1130	A	Sidechain
1	A	1139	G	Sidechain
1	A	12	U	Sidechain
1	A	1281	U	Sidechain
1	A	1289	A	Sidechain
1	A	1293	G	Sidechain
1	A	1299	A	Sidechain
1	A	1301	U	Sidechain
1	A	1305	G	Sidechain
1	A	1340	A	Sidechain
1	A	1360	A	Sidechain
1	A	1506	U	Sidechain
1	A	1525	G	Sidechain
1	A	197	A	Sidechain
1	A	203	U	Sidechain
1	A	220	G	Sidechain
1	A	231	G	Sidechain
1	A	249	U	Sidechain
1	A	250	A	Sidechain
1	A	251	G	Sidechain
1	A	254	G	Sidechain
1	A	266	G	Sidechain
1	A	274	A	Sidechain
1	A	290	C	Sidechain
1	A	297	G	Sidechain
1	A	305	G	Sidechain
1	A	380	G	Sidechain
1	A	413	G	Sidechain
1	A	481	G	Sidechain
1	A	573	A	Sidechain
1	A	575	G	Sidechain
1	A	603	U	Sidechain
1	A	727	G	Sidechain
1	A	879	C	Sidechain
1	A	898	G	Sidechain
1	A	982	U	Sidechain
22	Y	147	GLU	Peptide
22	Y	157	LEU	Peptide

5.2 Too-close contacts (i)

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	32394	0	16349	1169	0
2	B	1900	0	1951	206	0
3	C	1612	0	1677	212	0
4	D	1703	0	1764	134	0
5	E	1146	0	1207	101	0
6	F	843	0	857	65	0
7	G	1257	0	1296	91	0
8	H	1116	0	1177	66	0
9	I	1010	0	1037	114	0
10	J	785	0	823	123	0
11	K	885	0	904	82	0
12	L	970	0	1057	106	0
13	M	997	0	1072	119	0
14	N	492	0	529	74	0
15	O	734	0	771	58	0
16	P	700	0	720	56	0
17	Q	857	0	928	85	0
18	R	598	0	670	61	0
19	S	647	0	673	83	0
20	T	763	0	860	88	0
21	V	208	0	221	26	0
22	Y	1761	0	1792	47	0
23	A	117	0	0	0	0
23	B	1	0	0	0	0
23	E	1	0	0	0	0
23	N	1	0	0	0	0
24	D	1	0	0	0	0
24	N	1	0	0	0	0
25	Y	27	0	22	3	0
All	All	53527	0	38357	2882	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 32.

All (2882) 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)
9:I:57:GLY:O	9:I:58:HIS:HD2	1.22	1.18
20:T:54:LYS:HG3	20:T:100:ILE:CD1	1.73	1.18
12:L:41:ARG:HG2	12:L:42:THR:H	1.03	1.15
9:I:57:GLY:O	9:I:58:HIS:CD2	2.00	1.14
2:B:77:ALA:HB2	2:B:211:ILE:HD13	1.22	1.14
1:A:1443:G:H5"	1:A:1446:A:H5'	1.28	1.10
9:I:8:GLY:HA2	9:I:79:LEU:HD12	1.32	1.09
4:D:36:ARG:H	4:D:37:PRO:HD3	1.19	1.07
11:K:110:ASP:HB2	18:R:88:LYS:HD2	1.35	1.07
1:A:243:A:H4'	1:A:244:U:H5'	1.36	1.05
4:D:150:GLU:HG3	4:D:153:ARG:HH21	1.19	1.04
10:J:51:ARG:HB2	10:J:59:SER:HB3	1.33	1.04
12:L:60:LEU:HD11	12:L:85:ILE:HD12	1.39	1.03
12:L:27:LEU:O	12:L:29:GLY:N	1.94	1.01
13:M:49:THR:HG22	13:M:51:ALA:H	1.26	1.00
1:A:664:G:H22	1:A:741:G:H1	1.08	0.99
2:B:178:ARG:HH11	2:B:178:ARG:HG3	1.21	0.99
3:C:52:LEU:HD23	3:C:52:LEU:H	1.26	0.99
8:H:113:SER:HB2	8:H:134:ILE:HD11	1.43	0.99
11:K:54:ARG:HB3	11:K:54:ARG:HH11	1.26	0.99
19:S:28:LYS:HG2	19:S:29:ARG:H	1.26	0.98
1:A:539:A:OP2	12:L:115:LYS:HE2	1.63	0.97
20:T:50:GLU:O	20:T:100:ILE:HD12	1.62	0.97
3:C:6:HIS:HE1	3:C:8:ILE:HD12	1.25	0.97
20:T:54:LYS:HG3	20:T:100:ILE:HD13	0.99	0.97
1:A:1116:C:H2'	1:A:1117:G:H5"	1.46	0.97
1:A:1057:G:H5"	3:C:154:SER:HB2	1.47	0.96
3:C:91:LEU:HD21	3:C:99:VAL:HG13	1.48	0.96
20:T:50:GLU:HG3	20:T:99:LEU:CD1	1.96	0.96
20:T:53:LEU:CD1	20:T:101:GLY:N	2.30	0.95
20:T:54:LYS:CG	20:T:100:ILE:HD13	1.95	0.95
11:K:54:ARG:O	11:K:57:THR:HG22	1.66	0.95
1:A:1190:G:OP1	3:C:4:LYS:HA	1.67	0.94
3:C:14:ILE:HG22	3:C:15:THR:H	1.32	0.93
1:A:187:C:H1'	20:T:85:MET:CE	1.98	0.93
12:L:41:ARG:HG2	12:L:42:THR:N	1.83	0.93
19:S:31:ILE:HG22	19:S:32:LYS:H	1.34	0.93
1:A:1256:A:H4'	1:A:1257:U:H5'	1.51	0.93
20:T:50:GLU:HG3	20:T:99:LEU:HD12	1.51	0.92
2:B:124:SER:HB2	2:B:125:PRO:HD2	1.49	0.92
16:P:58:TYR:O	16:P:61:SER:HB3	1.68	0.92
1:A:1137:C:H4'	1:A:1138:G:C2	2.05	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:131:ARG:HG2	3:C:135:LYS:HE3	1.50	0.92
1:A:35:G:O2'	12:L:118:SER:O	1.88	0.92
12:L:28:LYS:HD2	12:L:33:ARG:HH12	1.35	0.92
1:A:1086:U:H3	1:A:1099:G:H22	1.08	0.91
1:A:838:G:H2'	1:A:839:U:H5"	1.52	0.91
1:A:942:G:C2'	1:A:943:U:H5'	2.01	0.91
1:A:1101:A:H4'	1:A:1102:A:O5'	1.65	0.91
3:C:195:VAL:O	3:C:196:LEU:HD23	1.69	0.91
12:L:27:LEU:C	12:L:29:GLY:H	1.74	0.90
9:I:70:LYS:O	9:I:74:ILE:HG13	1.72	0.90
1:A:1502:A:H2	1:A:1505:G:H1	1.20	0.90
1:A:1394:A:C6	1:A:1501:C:H4'	2.06	0.90
3:C:58:GLU:HB3	10:J:92:THR:HG21	1.51	0.90
5:E:81:GLU:HG2	5:E:90:VAL:HG22	1.52	0.90
1:A:1497:G:O2'	1:A:1498:U:H5'	1.71	0.89
1:A:235:C:H5'	17:Q:70:ARG:HG2	1.51	0.89
1:A:187:C:H1'	20:T:85:MET:HE2	1.55	0.89
10:J:8:LEU:HD21	10:J:96:ILE:HG12	1.54	0.89
2:B:91:PRO:HG2	2:B:155:LEU:HD23	1.54	0.89
17:Q:97:SER:HB2	17:Q:102:GLY:C	1.94	0.88
6:F:67:MET:HE1	6:F:72:VAL:HA	1.55	0.88
2:B:59:GLU:HG2	2:B:221:LEU:HD11	1.51	0.88
1:A:186:C:O3'	20:T:82:SER:HB3	1.74	0.87
1:A:1125:U:H3	10:J:5:ARG:HH21	1.18	0.87
4:D:36:ARG:N	4:D:37:PRO:HD3	1.88	0.87
1:A:1435:G:H2'	1:A:1436:U:C6	2.10	0.86
4:D:150:GLU:HG3	4:D:153:ARG:NH2	1.90	0.86
13:M:10:PRO:HB2	13:M:18:ALA:HB1	1.57	0.86
3:C:70:VAL:HG21	3:C:76:VAL:HG21	1.58	0.86
2:B:116:GLU:HG2	2:B:153:ARG:HH12	1.39	0.86
6:F:30:LEU:HD23	6:F:75:LEU:HD21	1.57	0.86
5:E:115:VAL:HG11	5:E:118:ILE:HG13	1.57	0.86
5:E:51:VAL:HB	5:E:52:PRO:HD3	1.55	0.85
6:F:10:LEU:HD12	6:F:59:TYR:HB3	1.55	0.85
1:A:1305:G:O2'	1:A:1306:A:H8	1.58	0.85
1:A:1394:A:C5	1:A:1501:C:H4'	2.11	0.85
1:A:1489:G:H2'	1:A:1490:C:H5"	1.59	0.85
10:J:22:LYS:HE2	10:J:90:LEU:HD12	1.57	0.85
3:C:190:ARG:HB3	3:C:190:ARG:NH1	1.92	0.85
2:B:102:LEU:HD21	2:B:162:ILE:HD11	1.57	0.85
10:J:49:VAL:HG13	14:N:41:ARG:HB2	1.57	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:250:A:H4'	1:A:251:G:O5'	1.76	0.84
1:A:1131:G:H1	1:A:1143:G:H21	1.22	0.84
1:A:1064:G:H4'	1:A:1065:U:H5'	1.58	0.84
1:A:1497:G:C2'	1:A:1498:U:H5'	2.08	0.84
13:M:3:ARG:HG2	13:M:9:ILE:HG23	1.56	0.84
3:C:64:VAL:HB	3:C:99:VAL:HB	1.59	0.84
13:M:50:GLU:O	13:M:54:VAL:HG23	1.77	0.84
17:Q:27:PHE:CZ	17:Q:36:ILE:HD11	2.12	0.84
4:D:104:VAL:HG11	4:D:146:ILE:HD12	1.58	0.84
9:I:8:GLY:HA2	9:I:79:LEU:CD1	2.07	0.84
5:E:105:VAL:HB	5:E:106:PRO:HD3	1.60	0.83
6:F:36:ARG:HH12	6:F:38:GLU:HG2	1.43	0.83
1:A:1421:G:C2'	1:A:1422:G:H5'	2.08	0.83
3:C:190:ARG:HB3	3:C:190:ARG:HH11	1.44	0.83
1:A:1305:G:HO2'	1:A:1306:A:H8	0.87	0.83
3:C:172:ARG:HH12	3:C:174:PRO:HG3	1.43	0.83
4:D:61:LYS:HD2	4:D:207:TYR:OH	1.78	0.83
20:T:53:LEU:HD13	20:T:101:GLY:N	1.92	0.83
1:A:135:C:O2	16:P:1:MET:HB2	1.78	0.82
1:A:1281:U:H5'	1:A:1282:C:H5	1.44	0.82
1:A:1356:G:H2'	1:A:1357:A:C8	2.15	0.82
3:C:91:LEU:HD23	3:C:92:ALA:N	1.95	0.82
7:G:75:VAL:CG1	7:G:86:GLN:HB3	2.10	0.82
3:C:191:THR:HG22	3:C:193:TYR:H	1.44	0.82
12:L:25:PRO:C	12:L:27:LEU:H	1.79	0.82
3:C:8:ILE:HG23	3:C:16:ARG:HG2	1.60	0.82
15:O:78:TYR:CZ	15:O:82:ILE:HD11	2.15	0.81
13:M:78:ILE:HA	13:M:81:LEU:HD21	1.62	0.81
19:S:29:ARG:O	19:S:30:LEU:HB2	1.80	0.81
4:D:150:GLU:HA	4:D:153:ARG:HE	1.44	0.81
6:F:30:LEU:HB3	6:F:35:ALA:HB3	1.62	0.81
10:J:19:SER:HB2	10:J:91:PRO:HG3	1.60	0.81
12:L:41:ARG:CG	12:L:42:THR:H	1.88	0.81
13:M:22:ILE:HD12	13:M:25:ILE:HD12	1.61	0.81
2:B:101:MET:HA	2:B:108:ILE:HD12	1.63	0.81
1:A:1060:C:C5	3:C:2:GLY:HA3	2.14	0.81
12:L:70:ILE:HD13	12:L:77:LEU:HD12	1.63	0.81
2:B:27:LYS:HD3	2:B:195:ASP:OD2	1.81	0.80
1:A:1410:G:H2'	1:A:1411:C:H5'	1.62	0.80
18:R:55:ARG:NH1	18:R:55:ARG:HB3	1.94	0.80
1:A:1285:A:H4'	1:A:1286:A:O5'	1.82	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:95:GLU:CD	6:F:95:GLU:H	1.85	0.80
1:A:673:G:H2'	1:A:674:G:C8	2.17	0.80
7:G:75:VAL:HG11	7:G:86:GLN:HB3	1.64	0.80
10:J:8:LEU:CD2	10:J:96:ILE:HG12	2.11	0.79
20:T:53:LEU:HD13	20:T:101:GLY:CA	2.12	0.79
5:E:118:ILE:HG22	5:E:119:LEU:N	1.95	0.79
12:L:126:LYS:H	12:L:126:LYS:HD2	1.47	0.79
1:A:80:G:H3'	1:A:81:U:H5"	1.62	0.79
11:K:54:ARG:HB3	11:K:54:ARG:NH1	1.97	0.79
2:B:8:LYS:O	2:B:9:GLU:HB2	1.81	0.79
12:L:67:THR:HG22	12:L:96:VAL:HG13	1.63	0.79
12:L:120:TYR:O	12:L:122:THR:HG23	1.83	0.79
1:A:942:G:N1	1:A:1341:U:O2	2.13	0.79
4:D:25:ARG:C	4:D:27:TYR:H	1.85	0.78
1:A:1412:C:H42	1:A:1488:G:H1	1.31	0.78
2:B:132:LYS:HA	2:B:135:GLN:HB3	1.63	0.78
1:A:1116:C:C2'	1:A:1117:G:H5"	2.12	0.78
3:C:15:THR:O	3:C:16:ARG:HB2	1.82	0.78
2:B:84:GLU:OE1	2:B:216:SER:HA	1.83	0.78
1:A:838:G:C2'	1:A:839:U:H5"	2.14	0.78
22:Y:108:GLY:HA2	22:Y:153:ARG:HH21	1.48	0.78
19:S:31:ILE:HG22	19:S:32:LYS:N	1.99	0.78
1:A:187:C:C1'	20:T:85:MET:HE1	2.14	0.78
1:A:942:G:H2'	1:A:943:U:H5'	1.66	0.78
16:P:21:VAL:HG21	16:P:59:TRP:CD1	2.19	0.78
1:A:1226:C:H4'	1:A:1227:A:OP1	1.84	0.78
1:A:187:C:C1'	20:T:85:MET:CE	2.62	0.77
15:O:17:ARG:HG3	15:O:17:ARG:HH11	1.49	0.77
2:B:197:VAL:HB	2:B:200:ILE:HG12	1.66	0.77
5:E:64:ARG:O	5:E:65:ASN:HB3	1.84	0.77
7:G:66:VAL:HG12	7:G:70:LYS:HE3	1.65	0.77
1:A:761:G:H1'	17:Q:104:LYS:O	1.84	0.77
1:A:130:A:OP2	1:A:190(E):U:H2'	1.84	0.77
1:A:1250:A:H4'	9:I:68:GLY:H	1.47	0.77
1:A:1366:C:H2'	1:A:1367:C:H6	1.48	0.77
3:C:150:LYS:HE2	3:C:152:ILE:HD11	1.67	0.77
7:G:95:ARG:HG3	7:G:95:ARG:HH11	1.50	0.77
9:I:118:LYS:O	9:I:119:ALA:HB3	1.85	0.77
12:L:27:LEU:HG	12:L:28:LYS:H	1.49	0.77
15:O:16:ALA:HB1	15:O:21:ASP:HB3	1.64	0.77
4:D:150:GLU:H	4:D:150:GLU:CD	1.86	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:243:A:C4'	1:A:244:U:H5'	2.13	0.77
3:C:110:ASN:O	3:C:111:LEU:HD23	1.85	0.77
1:A:1152:A:H5"	10:J:13:HIS:CD2	2.19	0.77
6:F:86:ARG:O	6:F:87:ARG:HG2	1.85	0.77
13:M:4:ILE:HG22	13:M:5:ALA:N	2.00	0.77
1:A:839:U:H5'	1:A:840:C:H5	1.50	0.76
3:C:107:GLN:H	3:C:107:GLN:CD	1.87	0.76
8:H:90:GLY:O	8:H:91:ARG:HB2	1.82	0.76
1:A:1236:A:H4'	1:A:1304:G:H4'	1.67	0.76
2:B:57:PHE:O	2:B:60:ASP:HB3	1.85	0.76
3:C:6:HIS:CE1	3:C:8:ILE:HD12	2.17	0.76
12:L:126:LYS:H	12:L:126:LYS:CD	1.96	0.76
20:T:14:LYS:O	20:T:18:GLN:HG3	1.86	0.76
1:A:1256:A:N6	1:A:1278:U:H1'	2.00	0.76
21:V:5:ASP:O	21:V:11:GLY:HA3	1.85	0.76
17:Q:97:SER:OG	17:Q:103:GLY:HA2	1.85	0.76
2:B:139:LYS:O	2:B:143:GLU:HG2	1.86	0.76
16:P:74:LEU:O	16:P:79:VAL:HG23	1.85	0.76
3:C:19:GLU:HB3	3:C:40:ARG:HH21	1.50	0.76
17:Q:95:TYR:C	17:Q:97:SER:H	1.89	0.76
1:A:328:C:O2	1:A:328:C:H2'	1.85	0.76
1:A:657:G:H4'	15:O:28:GLN:HG2	1.68	0.76
1:A:1025:U:H2'	1:A:1026:G:C8	2.21	0.76
2:B:36:ARG:HD2	2:B:41:ILE:HD12	1.68	0.76
10:J:82:ILE:O	10:J:86:MET:HB2	1.86	0.75
22:Y:109:THR:OG1	25:Y:301:SFG:N6	2.19	0.75
3:C:50:ALA:HB1	3:C:70:VAL:HG11	1.68	0.75
22:Y:156:PRO:HB2	22:Y:158:LEU:HD23	1.69	0.75
14:N:14:PRO:C	14:N:16:PHE:H	1.86	0.75
1:A:80:G:H3'	1:A:81:U:C5'	2.16	0.75
1:A:839:U:H5'	1:A:840:C:C5	2.22	0.75
10:J:96:ILE:HG22	10:J:97:GLU:H	1.52	0.75
19:S:16:LEU:O	19:S:19:VAL:HG12	1.87	0.75
3:C:116:VAL:HG21	3:C:202:ILE:HD11	1.67	0.75
12:L:48:PRO:HG2	12:L:49:ASN:H	1.52	0.75
13:M:3:ARG:HA	13:M:8:GLU:O	1.86	0.75
1:A:840:C:H5"	1:A:841:U:OP1	1.85	0.75
2:B:130:ARG:HH22	3:C:179:ARG:HH12	1.35	0.75
1:A:351:G:H4'	1:A:352:C:OP1	1.85	0.75
12:L:28:LYS:CD	12:L:33:ARG:HH12	1.99	0.74
1:A:1234:C:H5'	1:A:1365:G:OP1	1.86	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:162:LEU:HD13	4:D:181:MET:HG2	1.68	0.74
1:A:579:G:H5'	1:A:728:A:H1'	1.69	0.74
1:A:1391:U:H2'	1:A:1392:G:C8	2.22	0.74
13:M:88:ARG:HD2	19:S:3:ARG:HH21	1.50	0.74
17:Q:95:TYR:O	17:Q:97:SER:N	2.19	0.74
12:L:28:LYS:HD2	12:L:33:ARG:NH1	2.02	0.74
19:S:40:ILE:HD13	19:S:62:ILE:HD13	1.68	0.74
19:S:17:GLU:O	19:S:21:GLU:HG3	1.87	0.74
20:T:53:LEU:CD1	20:T:101:GLY:H	1.97	0.74
1:A:1421:G:H2'	1:A:1422:G:H5'	1.70	0.74
2:B:16:HIS:NE2	2:B:214:ILE:HG12	2.02	0.74
2:B:72:GLY:HA3	2:B:81:VAL:HG21	1.69	0.74
2:B:77:ALA:HB2	2:B:211:ILE:CD1	2.11	0.74
2:B:178:ARG:HG3	2:B:178:ARG:NH1	1.92	0.74
15:O:33:THR:HG23	15:O:63:ARG:NH1	2.03	0.74
18:R:55:ARG:HB3	18:R:55:ARG:HH11	1.50	0.74
1:A:942:G:H2'	1:A:943:U:H6	1.51	0.74
1:A:1064:G:H4'	1:A:1065:U:C5'	2.18	0.74
1:A:1117:G:H4'	9:I:104:ARG:NH1	2.03	0.74
4:D:64:LEU:HD12	4:D:75:PHE:HZ	1.52	0.74
1:A:748:C:H1'	1:A:749:C:H5	1.53	0.74
1:A:792:A:H4'	1:A:793:U:H5"	1.68	0.74
6:F:69:GLU:HA	6:F:72:VAL:HG23	1.70	0.74
1:A:1125:U:H3	10:J:5:ARG:NH2	1.85	0.73
3:C:52:LEU:HD23	3:C:52:LEU:N	2.02	0.73
7:G:23:VAL:HG12	7:G:27:ILE:HD11	1.70	0.73
1:A:992:U:H4'	1:A:993:G:O5'	1.86	0.73
1:A:1279:A:H5"	1:A:1280:A:OP1	1.88	0.73
2:B:23:ARG:NH1	2:B:24:TRP:N	2.35	0.73
22:Y:147:GLU:HB2	22:Y:150:ILE:HG12	1.71	0.73
3:C:52:LEU:H	3:C:52:LEU:CD2	2.00	0.73
1:A:187:C:H1'	20:T:85:MET:HE1	1.71	0.73
2:B:95:GLN:O	2:B:96:ARG:HD2	1.88	0.73
21:V:6:ARG:HD3	21:V:15:ARG:HH12	1.52	0.73
2:B:91:PRO:HG3	2:B:154:LEU:HB2	1.69	0.73
3:C:13:GLY:HA3	14:N:57:ARG:HH21	1.54	0.73
12:L:59:ARG:HD3	12:L:65:GLU:HG3	1.68	0.73
6:F:26:ILE:HG21	6:F:63:TYR:HE2	1.54	0.73
9:I:44:VAL:HG13	9:I:51:ARG:HH22	1.53	0.73
2:B:23:ARG:HH11	2:B:24:TRP:N	1.86	0.72
2:B:116:GLU:HG2	2:B:153:ARG:NH1	2.04	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:1:MET:HG2	8:H:2:LEU:N	2.05	0.72
1:A:1407:C:O2'	1:A:1408:A:OP1	2.06	0.72
10:J:39:PRO:O	10:J:40:LEU:HB2	1.89	0.72
20:T:10:LEU:O	20:T:12:ALA:N	2.22	0.72
1:A:353:A:H5'	1:A:353:A:H8	1.53	0.72
1:A:434:U:H2'	1:A:435:C:C6	2.24	0.72
1:A:877:C:O2	8:H:3:THR:HG21	1.89	0.72
1:A:197:A:H4'	1:A:198:G:O5'	1.90	0.72
4:D:158:ILE:HG22	4:D:181:MET:HE2	1.70	0.72
8:H:1:MET:HG2	8:H:2:LEU:H	1.54	0.72
18:R:26:LEU:HD12	18:R:27:GLY:H	1.53	0.72
1:A:161:A:H2'	1:A:162:A:C8	2.23	0.72
1:A:1152:A:H5"	10:J:13:HIS:HD2	1.53	0.72
1:A:1250:A:H4'	9:I:68:GLY:N	2.05	0.72
11:K:84:VAL:HG11	11:K:95:ILE:HD11	1.71	0.72
1:A:1148:U:H2'	1:A:1149:C:O4'	1.90	0.72
10:J:35:SER:HB2	10:J:72:VAL:O	1.90	0.72
17:Q:59:ILE:HG23	17:Q:71:PHE:HB3	1.70	0.72
1:A:974:A:OP1	14:N:31:ARG:HG2	1.89	0.71
1:A:1065:U:H4'	1:A:1066:C:O5'	1.89	0.71
9:I:4:TYR:CE2	9:I:88:TYR:HA	2.24	0.71
1:A:501:C:H2'	1:A:502:G:H8	1.53	0.71
18:R:33:ASP:OD2	18:R:36:ASN:HB2	1.90	0.71
1:A:1343:G:H2'	1:A:1344:C:C6	2.26	0.71
9:I:111:ARG:HD3	9:I:112:LYS:N	2.06	0.71
1:A:344:A:H4'	1:A:345:C:OP2	1.91	0.71
1:A:954:G:H5"	13:M:120:LYS:HD3	1.73	0.71
10:J:45:ARG:HH22	14:N:36:PHE:HD2	1.36	0.71
12:L:27:LEU:C	12:L:29:GLY:N	2.37	0.71
1:A:1281:U:H5'	1:A:1282:C:C5	2.25	0.71
19:S:15:LEU:HD12	19:S:16:LEU:N	2.06	0.71
1:A:977:A:H2'	1:A:978:A:H5"	1.73	0.71
22:Y:115:ILE:HD12	22:Y:156:PRO:HD2	1.73	0.71
1:A:706:A:O4'	11:K:29:ILE:HD11	1.91	0.70
2:B:19:HIS:CE1	2:B:206:ASP:HB3	2.26	0.70
8:H:108:GLY:HA3	8:H:138:TRP:HB3	1.70	0.70
9:I:65:VAL:HG21	9:I:73:GLN:HB3	1.72	0.70
13:M:40:ASN:HB3	13:M:43:THR:HG23	1.72	0.70
14:N:22:THR:HB	14:N:33:VAL:HG21	1.73	0.70
19:S:70:LYS:O	19:S:72:GLY:N	2.24	0.70
1:A:107:G:C2'	1:A:108:G:H5'	2.21	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:706:A:C1'	11:K:29:ILE:HD11	2.21	0.70
1:A:818:G:C3'	1:A:819:A:H5"	2.21	0.70
3:C:7:PRO:HG2	3:C:184:TYR:HB2	1.73	0.70
3:C:180:ALA:O	3:C:181:ASN:HB3	1.92	0.70
4:D:36:ARG:H	4:D:37:PRO:CD	2.02	0.70
10:J:78:ASN:O	10:J:80:LYS:N	2.24	0.70
13:M:6:GLY:O	13:M:7:VAL:HG22	1.91	0.70
5:E:102:ALA:HB1	5:E:120:THR:HG21	1.73	0.70
6:F:10:LEU:HD11	6:F:59:TYR:HD2	1.54	0.70
1:A:496:A:H4'	1:A:497:A:OP1	1.92	0.70
2:B:124:SER:HB2	2:B:125:PRO:CD	2.22	0.70
15:O:17:ARG:NH1	15:O:77:ARG:NH1	2.40	0.70
1:A:1278:U:H5"	1:A:1279:A:C5'	2.21	0.70
1:A:1351:U:H2'	1:A:1352:C:H6	1.55	0.70
4:D:70:ILE:HD11	4:D:100:ARG:CZ	2.21	0.70
10:J:65:LEU:HD23	10:J:65:LEU:O	1.90	0.70
13:M:49:THR:HG22	13:M:51:ALA:N	2.02	0.70
4:D:28:SER:O	4:D:30:LYS:N	2.25	0.70
5:E:74:GLY:HA3	5:E:116:THR:HG22	1.73	0.70
9:I:97:LYS:CG	9:I:102:LEU:HD12	2.22	0.70
9:I:97:LYS:HG2	9:I:102:LEU:HD12	1.72	0.70
10:J:61:GLU:OE1	14:N:45:ARG:NH1	2.25	0.70
18:R:39:VAL:O	18:R:42:ARG:HB2	1.90	0.70
1:A:1399:C:C2	1:A:1502:A:N6	2.60	0.70
17:Q:45:HIS:HB2	17:Q:65:ILE:HD13	1.71	0.70
1:A:438:G:H4'	1:A:439:A:OP1	1.90	0.70
1:A:1394:A:C6	1:A:1501:C:C4'	2.74	0.70
10:J:30:SER:O	10:J:78:ASN:HB2	1.92	0.70
1:A:1168:A:H2'	1:A:1169:A:C8	2.27	0.69
4:D:150:GLU:CG	4:D:153:ARG:HH21	2.02	0.69
1:A:254:G:OP1	17:Q:67:LYS:O	2.10	0.69
12:L:55:VAL:HG12	12:L:56:ALA:H	1.57	0.69
15:O:39:LEU:HD13	15:O:56:LEU:HB2	1.74	0.69
20:T:50:GLU:HG3	20:T:99:LEU:HD13	1.72	0.69
1:A:954:G:C5'	13:M:120:LYS:HD3	2.23	0.69
10:J:46:ARG:HH11	10:J:64:GLU:CB	2.05	0.69
13:M:81:LEU:O	13:M:86:CYS:HB3	1.92	0.69
1:A:352:C:H4'	1:A:354:G:OP1	1.91	0.69
1:A:1281:U:H4'	1:A:1282:C:OP2	1.92	0.69
10:J:30:SER:HB2	10:J:80:LYS:HB3	1.74	0.69
19:S:62:ILE:HD12	19:S:66:MET:HG3	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:28:LYS:HD2	12:L:33:ARG:HH22	1.57	0.69
1:A:1137:C:H4'	1:A:1138:G:N2	2.06	0.69
13:M:11:ARG:HG2	13:M:12:ASN:N	2.07	0.69
1:A:17:U:H2'	1:A:18:C:C6	2.28	0.69
1:A:392:G:H2'	1:A:393:A:H8	1.55	0.69
1:A:1418:A:H61	1:A:1482:G:H1'	1.56	0.69
11:K:108:ILE:HB	18:R:87:ARG:O	1.92	0.69
13:M:81:LEU:HD23	13:M:81:LEU:H	1.56	0.69
16:P:34:GLU:OE2	16:P:55:ARG:HD3	1.93	0.69
17:Q:24:GLU:OE2	17:Q:37:LYS:HD3	1.91	0.69
2:B:187:LEU:HD12	2:B:205:ASP:HA	1.74	0.69
6:F:36:ARG:NH1	6:F:38:GLU:HG2	2.08	0.69
12:L:47:LYS:CB	12:L:48:PRO:CD	2.71	0.69
17:Q:66:SER:O	17:Q:70:ARG:NH1	2.26	0.69
21:V:6:ARG:CD	21:V:15:ARG:HH12	2.06	0.69
4:D:64:LEU:HD12	4:D:75:PHE:CZ	2.28	0.69
10:J:42:THR:HG23	10:J:67:THR:O	1.92	0.69
4:D:64:LEU:HD23	4:D:198:VAL:HG21	1.75	0.68
9:I:93:ARG:HD3	9:I:97:LYS:HE3	1.75	0.68
1:A:477:G:H2'	1:A:478:A:H8	1.56	0.68
1:A:1443:G:C5'	1:A:1446:A:H5'	2.15	0.68
19:S:41:VAL:HG23	19:S:43:GLU:HG2	1.75	0.68
1:A:1141:C:H2'	1:A:1142:G:H8	1.57	0.68
19:S:5:LEU:O	19:S:6:LYS:HB2	1.92	0.68
1:A:701:C:H5'	1:A:703:G:O4'	1.93	0.68
13:M:81:LEU:HD12	13:M:88:ARG:HD3	1.74	0.68
1:A:731:G:OP1	1:A:766:A:H1'	1.94	0.68
4:D:151:LYS:N	4:D:151:LYS:HD2	2.08	0.68
12:L:126:LYS:HD2	12:L:126:LYS:N	2.07	0.68
1:A:948:C:OP1	13:M:109:THR:HG22	1.94	0.68
3:C:38:ARG:HH11	3:C:38:ARG:HG3	1.58	0.68
5:E:51:VAL:O	5:E:55:VAL:HG23	1.94	0.68
6:F:75:LEU:O	6:F:79:LEU:HG	1.94	0.68
1:A:382:A:H2'	1:A:383:A:C8	2.28	0.68
1:A:1016:A:H2'	1:A:1017:G:O4'	1.93	0.68
2:B:22:LYS:HD2	2:B:35:GLU:OE1	1.93	0.68
1:A:99:C:H2'	1:A:101:A:C8	2.28	0.68
1:A:1064:G:C4'	1:A:1065:U:H5'	2.23	0.68
1:A:1411:C:H2'	1:A:1412:C:C6	2.29	0.68
1:A:376:G:OP2	16:P:67:THR:HG21	1.94	0.68
4:D:3:ARG:HH22	4:D:74:GLN:CD	1.97	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:151:LEU:HD11	8:H:77:GLU:OE2	1.94	0.68
18:R:45:SER:OG	18:R:49:LYS:HB2	1.94	0.68
1:A:173:U:H5'	1:A:197:A:O4'	1.94	0.67
1:A:942:G:O2'	1:A:943:U:H5'	1.94	0.67
15:O:55:GLY:O	15:O:59:MET:HG3	1.95	0.67
1:A:652:U:O4	1:A:752:G:O2'	2.09	0.67
1:A:939:G:H2'	1:A:940:C:C6	2.28	0.67
2:B:18:GLY:HA2	2:B:42:ILE:H	1.59	0.67
9:I:26:VAL:HB	9:I:33:PHE:HB2	1.76	0.67
12:L:47:LYS:HB2	12:L:48:PRO:CD	2.23	0.67
1:A:105:G:H2'	1:A:106:C:C6	2.29	0.67
1:A:1366:C:H2'	1:A:1367:C:C6	2.30	0.67
4:D:151:LYS:HD2	4:D:151:LYS:H	1.60	0.67
1:A:31:G:N1	1:A:48:C:H5"	2.09	0.67
1:A:760:G:N1	17:Q:104:LYS:O	2.28	0.67
3:C:82:GLU:O	3:C:85:ARG:HB3	1.94	0.67
16:P:20:VAL:HG11	16:P:32:TYR:HB3	1.74	0.67
17:Q:96:GLU:O	17:Q:96:GLU:HG2	1.94	0.67
3:C:179:ARG:HD3	3:C:206:GLU:HG2	1.76	0.67
8:H:91:ARG:HG3	12:L:7:ILE:HG13	1.77	0.67
18:R:26:LEU:HD21	18:R:39:VAL:CG2	2.25	0.67
1:A:328:C:H4'	1:A:329:A:O5'	1.94	0.67
1:A:1057:G:O2'	1:A:1058:G:H5'	1.95	0.67
1:A:1112:C:O2	3:C:179:ARG:HB3	1.95	0.67
1:A:1368:G:O2'	1:A:1369:C:H5'	1.95	0.67
1:A:1502:A:H2	1:A:1505:G:N1	1.90	0.67
3:C:26:LYS:H	3:C:26:LYS:HD3	1.58	0.67
3:C:190:ARG:HH11	3:C:190:ARG:CB	2.08	0.67
4:D:187:ARG:HH21	4:D:188:LEU:HD12	1.60	0.67
1:A:371:G:O2'	1:A:372:C:H5'	1.95	0.67
1:A:521:G:OP1	12:L:73:GLU:O	2.13	0.67
3:C:130:VAL:HG21	3:C:157:ILE:HG23	1.75	0.67
1:A:915:A:H2'	1:A:916:G:H5'	1.76	0.67
3:C:195:VAL:C	3:C:196:LEU:HD23	2.15	0.67
1:A:942:G:H2'	1:A:943:U:C6	2.30	0.67
13:M:33:ALA:HA	13:M:59:TYR:HE2	1.60	0.67
1:A:748:C:H1'	1:A:749:C:C5	2.30	0.66
1:A:967:C:H4'	9:I:128:ARG:HG3	1.75	0.66
1:A:1410:G:C2'	1:A:1411:C:H5'	2.25	0.66
5:E:12:LEU:HD13	5:E:31:LEU:HB2	1.77	0.66
10:J:94:VAL:HG12	10:J:95:GLU:N	2.10	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:14:VAL:O	11:K:15:ALA:HB3	1.95	0.66
18:R:47:THR:HG23	18:R:83:GLU:H	1.60	0.66
1:A:129(A):G:N3	1:A:190(E):U:H5'	2.10	0.66
1:A:686:U:HO2'	1:A:687:A:H8	1.40	0.66
4:D:30:LYS:C	4:D:32:ALA:H	1.98	0.66
10:J:49:VAL:O	10:J:60:ARG:HA	1.95	0.66
13:M:65:LYS:HG3	13:M:69:GLU:OE2	1.96	0.66
15:O:33:THR:HG23	15:O:63:ARG:HH12	1.59	0.66
1:A:80:G:C3'	1:A:81:U:H5"	2.25	0.66
11:K:66:LEU:HB3	11:K:70:LYS:HE3	1.78	0.66
1:A:650:G:O2'	1:A:651:C:H5'	1.94	0.66
1:A:662:G:H2'	1:A:663:A:C8	2.30	0.66
3:C:155:GLY:O	3:C:156:ARG:HB2	1.96	0.66
10:J:60:ARG:O	10:J:61:GLU:HB3	1.95	0.66
20:T:87:LYS:O	20:T:91:LEU:HD12	1.96	0.66
2:B:71:VAL:O	2:B:165:VAL:HG23	1.96	0.66
18:R:45:SER:C	18:R:47:THR:H	1.97	0.66
1:A:427:U:OP1	4:D:13:ARG:NH2	2.29	0.66
1:A:1403:C:H1'	1:A:1500:A:N1	2.11	0.66
1:A:1405:G:O2'	1:A:1519:A:O4'	2.13	0.66
3:C:107:GLN:H	3:C:107:GLN:NE2	1.94	0.66
5:E:150:ARG:HG3	5:E:150:ARG:HH11	1.60	0.66
8:H:6:ILE:HD11	8:H:31:PHE:CD2	2.30	0.66
13:M:81:LEU:H	13:M:81:LEU:CD2	2.08	0.66
17:Q:97:SER:OG	17:Q:103:GLY:CA	2.44	0.66
1:A:353:A:H5'	1:A:353:A:C8	2.31	0.66
17:Q:67:LYS:HA	17:Q:70:ARG:HH12	1.60	0.66
1:A:266:G:O3'	17:Q:67:LYS:HB2	1.95	0.65
1:A:1216:G:H5"	14:N:5:ALA:CB	2.26	0.65
11:K:14:VAL:HG21	11:K:40:ILE:HD11	1.77	0.65
13:M:34:LEU:HD13	13:M:41:PRO:HA	1.77	0.65
19:S:33:THR:HG22	19:S:35:SER:H	1.60	0.65
22:Y:187:ASN:HD21	22:Y:206:LYS:HA	1.60	0.65
1:A:195:A:H4'	20:T:68:LYS:HE2	1.77	0.65
2:B:15:VAL:CG2	2:B:209:ARG:HG3	2.26	0.65
10:J:38:ILE:CG1	10:J:71:LEU:HB3	2.26	0.65
20:T:54:LYS:CG	20:T:100:ILE:CD1	2.65	0.65
1:A:443:C:H2'	1:A:444:C:H6	1.61	0.65
1:A:524:G:H2'	1:A:525:C:C6	2.31	0.65
1:A:1278:U:H5"	1:A:1279:A:H5'	1.77	0.65
1:A:1475:G:H2'	1:A:1476:G:H8	1.62	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:80:ILE:HD11	5:E:91:LEU:HD12	1.76	0.65
7:G:85:TYR:HD1	7:G:154:TYR:HE1	1.42	0.65
9:I:10:ARG:HG2	9:I:75:ASP:HB2	1.77	0.65
12:L:86:ARG:HH11	12:L:86:ARG:HG3	1.61	0.65
19:S:28:LYS:HG2	19:S:29:ARG:N	2.06	0.65
1:A:1224:G:H2'	19:S:78:ARG:HH22	1.62	0.65
12:L:33:ARG:HD3	12:L:62:SER:HB3	1.77	0.65
14:N:14:PRO:HB2	14:N:16:PHE:O	1.95	0.65
19:S:17:GLU:HA	19:S:20:LEU:HD11	1.78	0.65
2:B:18:GLY:HA3	2:B:41:ILE:HA	1.79	0.65
3:C:172:ARG:HB3	3:C:172:ARG:HH11	1.61	0.65
5:E:40:ARG:HG2	5:E:68:GLU:OE2	1.96	0.65
11:K:18:ARG:HB2	11:K:33:THR:HG23	1.78	0.65
1:A:1402:C:H2'	1:A:1403:C:O4'	1.97	0.65
2:B:74:LYS:HZ1	2:B:206:ASP:HA	1.60	0.65
10:J:96:ILE:HG22	10:J:97:GLU:N	2.10	0.65
21:V:6:ARG:HD3	21:V:15:ARG:NH1	2.12	0.65
1:A:1425:U:H2'	1:A:1426:C:C6	2.31	0.65
1:A:1522:U:O2'	1:A:1523:G:H5'	1.96	0.65
13:M:36:LYS:HD2	13:M:59:TYR:CZ	2.32	0.65
1:A:287:U:O2'	1:A:288:A:H5'	1.97	0.65
1:A:403:C:O2'	1:A:404:U:H5'	1.97	0.65
3:C:172:ARG:HB3	3:C:172:ARG:NH1	2.11	0.65
5:E:15:ARG:HD2	5:E:15:ARG:O	1.96	0.65
15:O:29:VAL:HG12	15:O:85:LEU:CD1	2.27	0.65
1:A:562:C:O2'	12:L:17:LYS:HE3	1.95	0.65
13:M:33:ALA:HA	13:M:59:TYR:CE2	2.32	0.65
3:C:188:LEU:O	3:C:189:ALA:HB2	1.96	0.65
13:M:81:LEU:O	13:M:89:GLY:HA3	1.97	0.65
14:N:22:THR:CB	14:N:33:VAL:HG21	2.27	0.65
1:A:677:U:H3	1:A:713:G:H22	1.45	0.64
1:A:168:G:O2'	1:A:169:C:H5'	1.97	0.64
1:A:392:G:H2'	1:A:393:A:C8	2.32	0.64
1:A:922:G:C2	1:A:1396:A:C6	2.86	0.64
4:D:187:ARG:NH2	4:D:188:LEU:HD12	2.10	0.64
7:G:50:ILE:O	7:G:54:THR:HB	1.96	0.64
19:S:64:GLU:O	19:S:67:VAL:HG23	1.97	0.64
1:A:203:U:H5"	1:A:204:U:OP1	1.97	0.64
1:A:397:A:H5'	1:A:398:C:OP1	1.98	0.64
1:A:738:C:OP2	6:F:92:LYS:HE3	1.97	0.64
9:I:49:PRO:O	9:I:52:ALA:HB3	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:118:LYS:O	9:I:119:ALA:CB	2.45	0.64
11:K:18:ARG:HB2	11:K:33:THR:CG2	2.28	0.64
1:A:281:G:O2'	1:A:282:A:OP2	2.12	0.64
1:A:393:A:O2'	1:A:394:G:H5'	1.98	0.64
6:F:21:LEU:O	6:F:24:GLU:HB3	1.97	0.64
11:K:77:MET:HE3	11:K:80:VAL:HG22	1.80	0.64
20:T:53:LEU:CD1	20:T:101:GLY:CA	2.75	0.64
1:A:765:G:H1	1:A:812:C:H2'	1.62	0.64
1:A:818:G:H3'	1:A:819:A:C5'	2.27	0.64
1:A:918:A:H2'	1:A:919:A:C8	2.32	0.64
1:A:1489:G:C2'	1:A:1490:C:H5"	2.26	0.64
10:J:90:LEU:H	10:J:91:PRO:HD2	1.60	0.64
16:P:18:ARG:HD3	16:P:35:LYS:HE3	1.79	0.64
16:P:45:THR:HB	16:P:46:PRO:HD2	1.80	0.64
1:A:1040:U:H2'	1:A:1041:A:C8	2.33	0.64
5:E:115:VAL:CG1	5:E:118:ILE:HG13	2.25	0.64
12:L:110:VAL:O	12:L:122:THR:HG21	1.97	0.64
19:S:44:MET:O	19:S:47:HIS:HB2	1.97	0.64
3:C:177:THR:CG2	3:C:180:ALA:HB2	2.28	0.64
7:G:26:PHE:CE2	7:G:30:ILE:HD11	2.33	0.64
19:S:40:ILE:HB	19:S:67:VAL:O	1.98	0.64
1:A:1142:G:H2'	1:A:1143:G:O4'	1.97	0.64
1:A:1492:A:H2'	1:A:1493:A:O4'	1.97	0.64
3:C:64:VAL:HB	3:C:99:VAL:CB	2.27	0.64
5:E:120:THR:CG2	5:E:121:LYS:N	2.60	0.64
17:Q:101:ARG:HA	17:Q:101:ARG:HE	1.62	0.64
1:A:922:G:H2'	1:A:923:A:C8	2.33	0.64
1:A:1347:G:O2'	1:A:1348:U:OP2	2.16	0.64
1:A:1497:G:H2'	1:A:1498:U:H5'	1.78	0.64
2:B:215:LEU:O	2:B:219:VAL:HG23	1.97	0.64
1:A:1346:A:H2'	7:G:10:ARG:HH22	1.63	0.64
3:C:112:SER:HB2	3:C:115:LEU:HD12	1.79	0.64
11:K:40:ILE:HG22	11:K:41:THR:HG23	1.80	0.64
11:K:48:ILE:HG22	11:K:49:GLY:H	1.61	0.64
12:L:25:PRO:C	12:L:27:LEU:N	2.52	0.64
12:L:55:VAL:HG12	12:L:56:ALA:N	2.13	0.64
21:V:6:ARG:CD	21:V:15:ARG:NH1	2.61	0.64
1:A:1422:G:O2'	1:A:1423:G:H5'	1.97	0.63
1:A:1442:G:N3	1:A:1442:G:H2'	2.12	0.63
9:I:48:GLU:N	9:I:49:PRO:HD2	2.13	0.63
1:A:255:G:H1'	17:Q:16:GLN:OE1	1.97	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:74:LYS:NZ	2:B:206:ASP:HA	2.13	0.63
3:C:120:VAL:O	3:C:124:ILE:HG13	1.99	0.63
4:D:70:ILE:HD11	4:D:100:ARG:NE	2.13	0.63
7:G:42:ILE:HG22	7:G:120:ILE:HD12	1.80	0.63
14:N:27:CYS:SG	14:N:29:ARG:HB2	2.37	0.63
1:A:1141:C:H2'	1:A:1142:G:C8	2.32	0.63
1:A:1153:C:H2'	1:A:1154:G:H8	1.62	0.63
2:B:84:GLU:HB3	2:B:219:VAL:HG21	1.79	0.63
3:C:64:VAL:CB	3:C:99:VAL:HB	2.27	0.63
4:D:131:ARG:H	4:D:131:ARG:HD2	1.62	0.63
4:D:152:SER:HB3	4:D:155:LEU:HD12	1.80	0.63
5:E:79:GLU:HG3	5:E:93:PRO:HD2	1.79	0.63
7:G:114:ARG:HG2	7:G:114:ARG:HH11	1.63	0.63
20:T:53:LEU:HD13	20:T:102:GLY:N	2.12	0.63
1:A:1316:G:H4'	14:N:18:VAL:CG1	2.29	0.63
1:A:1020:U:H2'	1:A:1021:G:H8	1.63	0.63
1:A:1131:G:H1	1:A:1143:G:N2	1.95	0.63
2:B:82:ARG:O	2:B:86:GLU:HG3	1.98	0.63
3:C:155:GLY:O	3:C:196:LEU:HD22	1.98	0.63
1:A:1026:G:H2'	1:A:1027:C:H5'	1.80	0.63
2:B:95:GLN:OE1	2:B:95:GLN:HA	1.96	0.63
3:C:29:TYR:OH	14:N:54:PRO:HG2	1.97	0.63
3:C:91:LEU:CD2	3:C:99:VAL:HG13	2.27	0.63
19:S:39:THR:HA	19:S:70:LYS:HG2	1.81	0.63
1:A:243:A:H4'	1:A:244:U:C5'	2.22	0.63
1:A:1053:G:C3'	1:A:1054:C:H5'	2.29	0.63
1:A:1407:C:HO2'	1:A:1408:A:P	2.22	0.63
1:A:1422:G:H2'	1:A:1423:G:O4'	1.98	0.63
2:B:130:ARG:NH2	3:C:207:VAL:HG22	2.14	0.63
5:E:150:ARG:HG3	5:E:150:ARG:NH1	2.14	0.63
1:A:1189:C:OP1	10:J:51:ARG:NH2	2.29	0.63
1:A:1238:A:H5'	1:A:1336:C:H41	1.64	0.63
2:B:20:GLU:HG2	2:B:189:ASP:OD2	1.99	0.63
2:B:132:LYS:HG2	2:B:135:GLN:OE1	1.99	0.63
5:E:102:ALA:CB	5:E:120:THR:HG21	2.29	0.63
5:E:116:THR:HG23	5:E:117:ASP:OD2	1.98	0.63
12:L:43:VAL:HG12	12:L:44:THR:N	2.14	0.63
1:A:1132:C:H2'	1:A:1133:G:H8	1.64	0.63
1:A:1229:A:OP2	13:M:114:ARG:HD3	1.99	0.63
1:A:1343:G:H1'	9:I:121:ARG:HH12	1.64	0.63
1:A:1405:G:O2'	1:A:1518:A:O2'	2.13	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:184:VAL:N	2:B:198:ASP:OD2	2.32	0.63
3:C:50:ALA:O	3:C:70:VAL:HG12	1.99	0.63
1:A:448:A:H2'	1:A:449:C:H6	1.64	0.62
1:A:556:C:O2'	1:A:557:G:H5'	1.99	0.62
1:A:1347:G:O2'	1:A:1348:U:P	2.57	0.62
1:A:1347:G:C4	9:I:107:ARG:NH1	2.67	0.62
2:B:73:THR:HB	2:B:170:GLU:OE2	1.99	0.62
6:F:9:VAL:HB	6:F:87:ARG:HB2	1.80	0.62
15:O:17:ARG:CZ	15:O:77:ARG:HH11	2.11	0.62
19:S:43:GLU:H	19:S:43:GLU:CD	2.00	0.62
1:A:405:U:H3'	1:A:406:G:H5'	1.81	0.62
1:A:924:C:H5'	1:A:1399:C:OP2	1.98	0.62
1:A:1307:U:H5'	13:M:109:THR:HG21	1.81	0.62
3:C:177:THR:HG23	3:C:180:ALA:HB2	1.81	0.62
16:P:8:ARG:HB2	16:P:28:ARG:NH1	2.14	0.62
1:A:475:G:H2'	1:A:476:G:H8	1.63	0.62
1:A:1132:C:H2'	1:A:1133:G:C8	2.35	0.62
3:C:60:ALA:O	3:C:61:ALA:HB2	2.00	0.62
7:G:71:PRO:HD3	7:G:103:TRP:CZ3	2.33	0.62
1:A:1225:A:H2'	1:A:1225:A:N3	2.14	0.62
13:M:84:ILE:O	13:M:86:CYS:N	2.33	0.62
1:A:113:G:H1'	1:A:354:G:H5'	1.80	0.62
1:A:216:G:H2'	1:A:217:C:C6	2.35	0.62
1:A:501:C:H2'	1:A:502:G:C8	2.34	0.62
1:A:1260:C:O5'	1:A:1284:C:H4'	1.99	0.62
2:B:69:LEU:HD12	2:B:155:LEU:HD11	1.82	0.62
1:A:760:G:C6	17:Q:105:ALA:HB2	2.35	0.62
1:A:976:G:OP1	14:N:32:SER:HA	1.98	0.62
2:B:186:ALA:HB3	2:B:197:VAL:HG11	1.81	0.62
7:G:23:VAL:O	7:G:27:ILE:HG13	2.00	0.62
20:T:53:LEU:HD12	20:T:101:GLY:N	2.13	0.62
22:Y:147:GLU:HG3	22:Y:150:ILE:HB	1.82	0.62
1:A:1370:G:O2'	1:A:1371:G:H5'	2.00	0.62
2:B:130:ARG:NH2	3:C:179:ARG:HH12	1.97	0.62
5:E:120:THR:HG23	5:E:121:LYS:N	2.15	0.62
1:A:542:G:OP1	4:D:10:ARG:NH2	2.33	0.62
7:G:155:ARG:O	7:G:156:TRP:HB3	1.99	0.62
9:I:93:ARG:NH1	9:I:97:LYS:HZ1	1.97	0.62
12:L:33:ARG:CD	12:L:62:SER:HB3	2.29	0.62
20:T:96:GLY:O	20:T:97:ALA:HB3	2.00	0.62
1:A:1425:U:H2'	1:A:1426:C:H6	1.65	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:115:LEU:HG	2:B:153:ARG:NH2	2.14	0.62
3:C:129:ALA:HB3	3:C:132:ARG:HD2	1.82	0.62
9:I:19:LEU:O	9:I:20:ARG:HG3	1.99	0.62
10:J:62:HIS:HB3	14:N:59:ALA:HB3	1.81	0.62
1:A:434:U:H2'	1:A:435:C:H6	1.64	0.62
1:A:1148:U:H4'	9:I:14:VAL:HG11	1.81	0.62
1:A:1182:G:H4'	1:A:1183:A:O5'	1.99	0.62
1:A:1440:C:H2'	1:A:1441:G:H5'	1.82	0.62
4:D:148:VAL:CG1	4:D:158:ILE:HD13	2.30	0.62
5:E:71:LEU:HD21	5:E:115:VAL:HG22	1.80	0.62
1:A:476:G:O2'	1:A:477:G:H5'	2.00	0.61
1:A:706:A:H1'	11:K:29:ILE:HD11	1.81	0.61
1:A:1176:A:H2'	1:A:1177:G:C8	2.35	0.61
7:G:139:GLU:O	7:G:143:ARG:HG3	2.00	0.61
14:N:53:LEU:HB3	14:N:56:VAL:HG21	1.82	0.61
19:S:52:TYR:HA	19:S:56:GLN:O	1.99	0.61
1:A:37:U:OP1	12:L:124:LYS:N	2.26	0.61
1:A:812:C:O2'	1:A:813:U:OP2	2.17	0.61
1:A:959:A:H3'	1:A:960:U:H5"	1.82	0.61
2:B:80:ILE:HD11	2:B:208:ILE:HG23	1.81	0.61
17:Q:21:VAL:HG21	17:Q:59:ILE:HD11	1.82	0.61
17:Q:76:LEU:C	17:Q:76:LEU:HD23	2.20	0.61
19:S:31:ILE:CG2	19:S:32:LYS:H	2.10	0.61
1:A:193:C:H2'	1:A:194:C:C6	2.36	0.61
1:A:575:G:C5	1:A:881:G:C2	2.89	0.61
1:A:664:G:N2	1:A:741:G:H1	1.89	0.61
1:A:954:G:H21	1:A:1227:A:H62	1.49	0.61
4:D:25:ARG:O	4:D:27:TYR:N	2.34	0.61
4:D:32:ALA:C	4:D:34:GLU:H	2.04	0.61
5:E:80:ILE:CD1	5:E:91:LEU:HB2	2.30	0.61
7:G:78:ARG:HB2	7:G:156:TRP:CZ3	2.36	0.61
3:C:191:THR:HG22	3:C:192:THR:N	2.15	0.61
9:I:4:TYR:CZ	9:I:88:TYR:HD1	2.17	0.61
10:J:30:SER:OG	10:J:81:THR:HA	1.99	0.61
1:A:551:U:H2'	1:A:552:U:H6	1.64	0.61
1:A:1147:C:H4'	9:I:5:TYR:HE1	1.65	0.61
4:D:191:ARG:O	4:D:191:ARG:HD2	2.00	0.61
5:E:115:VAL:HG11	5:E:118:ILE:CG1	2.28	0.61
11:K:84:VAL:CG1	11:K:95:ILE:HD11	2.31	0.61
1:A:386:C:O2'	1:A:387:U:H5'	2.00	0.61
1:A:1420:C:H2'	1:A:1421:G:H8	1.66	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:13:GLY:HA3	14:N:57:ARG:NH2	2.14	0.61
9:I:44:VAL:HG12	9:I:51:ARG:HH12	1.66	0.61
1:A:195:A:H4'	20:T:68:LYS:CE	2.30	0.61
2:B:34:ALA:O	2:B:41:ILE:N	2.31	0.61
4:D:23:GLY:HA3	4:D:112:VAL:CG1	2.30	0.61
7:G:38:LEU:HD12	7:G:38:LEU:O	2.01	0.61
16:P:4:ILE:HG13	16:P:64:ALA:HB1	1.83	0.61
16:P:67:THR:HG22	16:P:68:ASP:N	2.15	0.61
1:A:107:G:H2'	1:A:108:G:H5'	1.83	0.61
1:A:1003:G:H2'	1:A:1003(A):G:C8	2.36	0.61
1:A:1053:G:C4'	1:A:1054:C:H5'	2.31	0.61
1:A:1091:U:O2	1:A:1093:A:C8	2.54	0.61
1:A:1226:C:N4	13:M:104:ARG:HD2	2.16	0.61
3:C:83:ARG:C	3:C:85:ARG:H	2.04	0.61
17:Q:101:ARG:HA	17:Q:101:ARG:NE	2.16	0.61
1:A:1316:G:H4'	14:N:18:VAL:HG11	1.83	0.61
1:A:1475:G:H2'	1:A:1476:G:C8	2.36	0.61
2:B:115:LEU:O	2:B:119:GLU:HG3	2.00	0.61
3:C:191:THR:CG2	3:C:192:THR:N	2.64	0.61
5:E:80:ILE:HD11	5:E:91:LEU:HB2	1.83	0.61
13:M:54:VAL:O	13:M:58:GLU:HG2	2.01	0.61
1:A:1329:A:P	13:M:28:ALA:HB3	2.41	0.61
2:B:98:LEU:O	2:B:101:MET:HG3	2.01	0.61
10:J:46:ARG:HH11	10:J:64:GLU:HB3	1.64	0.61
11:K:48:ILE:HG22	11:K:49:GLY:N	2.16	0.61
1:A:104:G:N7	20:T:14:LYS:NZ	2.46	0.60
1:A:1495:U:H2'	1:A:1496:C:C6	2.36	0.60
4:D:148:VAL:HG11	4:D:158:ILE:HG21	1.81	0.60
12:L:40:VAL:O	12:L:40:VAL:HG12	1.99	0.60
18:R:52:PRO:O	18:R:56:THR:HG23	2.00	0.60
2:B:33:TYR:O	2:B:34:ALA:HB2	2.02	0.60
2:B:143:GLU:O	2:B:147:LYS:HG3	2.00	0.60
17:Q:76:LEU:HD23	17:Q:77:VAL:N	2.15	0.60
17:Q:104:LYS:O	17:Q:105:ALA:HB2	2.02	0.60
8:H:64:LYS:HG2	8:H:79:VAL:HG21	1.84	0.60
19:S:13:ASP:HA	19:S:16:LEU:HB3	1.83	0.60
1:A:390:C:H2'	1:A:391:G:H8	1.66	0.60
1:A:425:G:O2'	1:A:426:G:H5'	2.02	0.60
3:C:20:SER:HB3	3:C:22:TRP:HE1	1.67	0.60
5:E:43:LEU:HD11	5:E:132:ALA:HB1	1.84	0.60
7:G:72:ARG:HG2	7:G:142:GLU:OE1	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:71:LEU:O	10:J:72:VAL:HB	2.00	0.60
15:O:29:VAL:HG12	15:O:85:LEU:HD11	1.82	0.60
1:A:390:C:O3'	16:P:28:ARG:NH2	2.34	0.60
1:A:686:U:O2'	1:A:687:A:H8	1.84	0.60
1:A:953:G:H1'	13:M:125:ARG:CB	2.31	0.60
1:A:1381:U:O2'	1:A:1382:C:H5'	2.02	0.60
5:E:24:ARG:HG2	5:E:24:ARG:HH11	1.66	0.60
11:K:19:ALA:HB2	11:K:80:VAL:HG11	1.82	0.60
16:P:52:ASP:OD2	16:P:55:ARG:HG3	2.00	0.60
1:A:112:G:H21	1:A:354:G:H5'	1.65	0.60
1:A:112:G:N2	1:A:354:G:H5'	2.16	0.60
1:A:1147:C:H4'	9:I:5:TYR:CE1	2.36	0.60
14:N:24:CYS:HB3	14:N:28:GLY:H	1.66	0.60
20:T:53:LEU:HD12	20:T:101:GLY:H	1.66	0.60
1:A:1305:G:H5'	21:V:4:GLY:HA3	1.84	0.60
2:B:114:ARG:NH1	2:B:118:LEU:HD21	2.15	0.60
3:C:33:LEU:HD11	14:N:53:LEU:CD2	2.32	0.60
3:C:47:LEU:HD23	3:C:68:VAL:HG11	1.83	0.60
7:G:78:ARG:HB2	7:G:156:TRP:HZ3	1.65	0.60
11:K:69:ALA:O	11:K:73:MET:HG2	2.02	0.60
1:A:449:C:O2	16:P:42:ARG:HD2	2.01	0.60
2:B:122:PHE:HE2	2:B:139:LYS:HG2	1.65	0.60
2:B:140:HIS:O	2:B:143:GLU:HB2	2.01	0.60
3:C:26:LYS:HD3	3:C:26:LYS:N	2.17	0.60
5:E:65:ASN:CG	5:E:65:ASN:O	2.41	0.60
6:F:10:LEU:CD1	6:F:59:TYR:HB3	2.29	0.60
16:P:81:ARG:HG3	16:P:83:GLU:HG2	1.84	0.60
1:A:996:A:H2'	1:A:997:U:C6	2.37	0.60
1:A:1376:U:H2'	1:A:1377:A:C8	2.36	0.60
1:A:1470:G:O2'	1:A:1471:G:H5'	2.02	0.60
3:C:46:GLU:O	3:C:48:TYR:N	2.33	0.60
7:G:42:ILE:HG23	7:G:117:ALA:HA	1.84	0.60
13:M:10:PRO:O	13:M:45:VAL:HG11	2.01	0.60
1:A:435:C:H2'	1:A:436:C:H6	1.67	0.59
1:A:1306:A:N6	1:A:1331:G:H1'	2.17	0.59
3:C:47:LEU:H	3:C:47:LEU:CD1	2.15	0.59
12:L:46:LYS:HG2	12:L:47:LYS:N	2.16	0.59
14:N:11:LYS:O	14:N:13:THR:N	2.34	0.59
1:A:502:G:H4'	1:A:550:G:H4'	1.83	0.59
1:A:505:G:H2'	1:A:506:G:C8	2.37	0.59
1:A:1231:G:H5"	9:I:126:SER:CB	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:79:ARG:HE	3:C:82:GLU:HG2	1.67	0.59
9:I:93:ARG:NH1	9:I:97:LYS:NZ	2.51	0.59
11:K:84:VAL:HG21	18:R:88:LYS:HD3	1.83	0.59
15:O:11:VAL:HG21	15:O:34:LEU:HD12	1.83	0.59
1:A:457:C:H2'	1:A:458:C:H6	1.67	0.59
1:A:839:U:O2	1:A:839:U:H2'	2.01	0.59
1:A:923:A:O4'	1:A:1398:A:C2	2.56	0.59
1:A:1130:A:H3'	1:A:1130:A:OP2	2.02	0.59
1:A:1405:G:C2'	1:A:1518:A:HO2'	2.14	0.59
5:E:118:ILE:CG2	5:E:119:LEU:N	2.65	0.59
9:I:5:TYR:CD2	9:I:6:GLY:N	2.71	0.59
11:K:110:ASP:HB2	18:R:88:LYS:CD	2.20	0.59
1:A:1352:C:H2'	1:A:1353:G:C8	2.37	0.59
2:B:97:TRP:HZ2	2:B:102:LEU:HD13	1.66	0.59
4:D:33:MET:O	4:D:37:PRO:HG3	2.02	0.59
7:G:95:ARG:HG3	7:G:95:ARG:NH1	2.17	0.59
11:K:74:ALA:C	11:K:76:GLY:H	2.05	0.59
1:A:972:C:OP1	10:J:57:LYS:NZ	2.28	0.59
2:B:101:MET:CA	2:B:108:ILE:HD12	2.33	0.59
4:D:151:LYS:H	4:D:151:LYS:CD	2.16	0.59
1:A:103:C:P	20:T:17:ARG:HH11	2.26	0.59
1:A:109:A:H2'	1:A:326:G:N2	2.17	0.59
1:A:1086:U:H3	1:A:1099:G:N2	1.91	0.59
4:D:25:ARG:C	4:D:27:TYR:N	2.55	0.59
8:H:83:ILE:HG23	8:H:83:ILE:O	2.03	0.59
13:M:94:ARG:HH22	19:S:81:ARG:NH1	2.00	0.59
1:A:1247:U:O2'	1:A:1248:A:H5'	2.02	0.59
1:A:1420:C:O2'	1:A:1421:G:H5'	2.02	0.59
2:B:97:TRP:HH2	2:B:176:GLU:CD	2.06	0.59
22:Y:147:GLU:HA	22:Y:149:GLU:N	2.18	0.59
3:C:14:ILE:O	3:C:16:ARG:N	2.35	0.59
7:G:51:GLN:OE1	7:G:51:GLN:HA	2.02	0.59
10:J:3:LYS:N	10:J:77:PRO:HD3	2.18	0.59
10:J:46:ARG:NH1	10:J:64:GLU:HG2	2.18	0.59
12:L:55:VAL:CG1	12:L:67:THR:HG23	2.33	0.59
1:A:390:C:H2'	1:A:391:G:C8	2.38	0.59
1:A:457:C:H2'	1:A:458:C:C6	2.38	0.59
1:A:513:C:O2'	1:A:514:C:H5'	2.03	0.59
1:A:560:U:H4'	1:A:561:U:H5"	1.83	0.59
1:A:736:C:H2'	1:A:737:A:C8	2.38	0.59
1:A:1412:C:H2'	1:A:1413:A:O4'	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:120:ALA:O	2:B:124:SER:HB3	2.02	0.59
22:Y:147:GLU:HA	22:Y:149:GLU:H	1.67	0.59
7:G:122:HIS:HA	7:G:125:MET:HE3	1.85	0.59
10:J:60:ARG:HD2	10:J:60:ARG:N	2.17	0.59
10:J:82:ILE:O	10:J:82:ILE:HG22	2.03	0.59
13:M:81:LEU:HD23	13:M:81:LEU:N	2.17	0.59
16:P:51:VAL:O	16:P:51:VAL:HG12	2.02	0.59
18:R:86:VAL:O	18:R:87:ARG:HB2	2.02	0.59
1:A:39:G:O2'	1:A:40:C:H5'	2.03	0.58
1:A:1521:G:H2'	1:A:1522:U:C6	2.38	0.58
2:B:130:ARG:HD2	2:B:131:PRO:HD2	1.85	0.58
3:C:3:ASN:C	3:C:4:LYS:HG2	2.23	0.58
1:A:991:U:O2'	1:A:992:U:H5'	2.02	0.58
1:A:1182:G:O2'	1:A:1183:A:OP2	2.20	0.58
1:A:1251:A:H4'	9:I:12:GLU:OE2	2.02	0.58
2:B:144:ARG:HG3	2:B:145:LEU:N	2.18	0.58
3:C:10:PHE:CZ	3:C:178:LEU:HD13	2.38	0.58
4:D:23:GLY:HA3	4:D:112:VAL:HG12	1.84	0.58
12:L:24:VAL:O	12:L:24:VAL:HG12	2.03	0.58
12:L:28:LYS:HD2	12:L:33:ARG:NH2	2.17	0.58
14:N:14:PRO:C	14:N:16:PHE:N	2.56	0.58
1:A:760:G:C2	17:Q:103:GLY:O	2.57	0.58
1:A:1410:G:H2'	1:A:1411:C:C5'	2.34	0.58
1:A:1441:G:H4'	1:A:1442:G:N7	2.19	0.58
3:C:64:VAL:HB	3:C:99:VAL:CG2	2.33	0.58
10:J:45:ARG:O	10:J:64:GLU:HA	2.03	0.58
14:N:8:GLU:O	14:N:11:LYS:HB2	2.02	0.58
1:A:518:C:H5"	1:A:519:C:C6	2.37	0.58
1:A:1003(A):G:C2	1:A:1004:A:H1'	2.39	0.58
1:A:1072:G:H2'	1:A:1073:U:C6	2.38	0.58
2:B:115:LEU:HG	2:B:153:ARG:HH21	1.68	0.58
2:B:133:LYS:O	2:B:137:ARG:HG3	2.03	0.58
1:A:60:A:H4'	1:A:61:G:O5'	2.03	0.58
1:A:1152:A:H5'	10:J:70:ARG:HH22	1.68	0.58
1:A:1316:G:N2	1:A:1318:A:H3'	2.18	0.58
1:A:1487:G:O2'	1:A:1488:G:H5'	2.03	0.58
8:H:17:THR:HG22	8:H:63:LEU:HG	1.86	0.58
9:I:5:TYR:O	9:I:84:ALA:HA	2.03	0.58
9:I:11:LYS:O	9:I:11:LYS:HG2	2.03	0.58
9:I:79:LEU:HD23	9:I:101:PHE:O	2.02	0.58
15:O:17:ARG:NH1	15:O:77:ARG:HH11	2.01	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:812:C:O2'	1:A:813:U:P	2.62	0.58
1:A:1117:G:H5'	1:A:1117:G:H8	1.66	0.58
2:B:10:LEU:HD23	2:B:48:MET:HG3	1.86	0.58
10:J:24:VAL:HG12	10:J:28:ARG:HE	1.68	0.58
13:M:94:ARG:NH2	19:S:81:ARG:HD3	2.19	0.58
15:O:87:ILE:O	15:O:88:ARG:HB2	2.04	0.58
1:A:1498:U:H4'	1:A:1519:A:H2	1.69	0.58
2:B:156:LYS:O	2:B:156:LYS:HD3	2.03	0.58
10:J:15:THR:HG23	10:J:94:VAL:HG22	1.85	0.58
10:J:51:ARG:HB2	10:J:59:SER:CB	2.23	0.58
20:T:50:GLU:CG	20:T:99:LEU:HD12	2.30	0.58
20:T:53:LEU:O	20:T:57:ARG:HD2	2.04	0.58
1:A:376:G:P	16:P:67:THR:HG21	2.44	0.58
1:A:1054:C:OP1	1:A:1197:G:OP1	2.21	0.58
2:B:76:GLN:HG3	2:B:206:ASP:OD1	2.04	0.58
5:E:122:GLU:O	5:E:123:LEU:HD23	2.03	0.58
9:I:46:ALA:HB1	9:I:77:ILE:HG22	1.86	0.58
12:L:85:ILE:HG23	12:L:98:TYR:HB3	1.86	0.58
13:M:120:LYS:HE2	13:M:123:ALA:HB2	1.86	0.58
1:A:411:A:N9	1:A:413:G:H1'	2.19	0.58
1:A:723:U:O2	1:A:723:U:H2'	2.04	0.58
1:A:818:G:C2'	1:A:819:A:H5"	2.34	0.58
1:A:976:G:OP2	1:A:1358:U:H1'	2.03	0.58
2:B:16:HIS:NE2	2:B:214:ILE:CG1	2.66	0.58
3:C:191:THR:HG21	3:C:193:TYR:CZ	2.39	0.58
9:I:111:ARG:HD3	9:I:112:LYS:C	2.24	0.58
12:L:92:ASP:O	12:L:94:PRO:HD3	2.04	0.58
14:N:12:ARG:O	14:N:14:PRO:N	2.36	0.58
1:A:375:U:H4'	16:P:17:TYR:CE2	2.39	0.58
1:A:1228:C:OP1	13:M:115:LYS:HG3	2.03	0.58
3:C:10:PHE:CE2	3:C:178:LEU:HD13	2.38	0.58
7:G:15:ASP:OD1	7:G:17:VAL:N	2.37	0.58
13:M:13:LYS:O	13:M:45:VAL:HG23	2.04	0.58
13:M:84:ILE:CG2	19:S:65:ASN:HD22	2.17	0.58
20:T:53:LEU:HD13	20:T:102:GLY:H	1.68	0.58
11:K:109:VAL:HG13	18:R:85:LEU:O	2.04	0.57
12:L:26:ALA:O	12:L:27:LEU:O	2.22	0.57
1:A:1014:A:H2'	1:A:1015:A:C8	2.39	0.57
6:F:97:PHE:HB2	18:R:32:ARG:CZ	2.34	0.57
9:I:7:THR:HG21	9:I:9:ARG:NH1	2.19	0.57
9:I:17:VAL:HG21	9:I:80:GLY:HA3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:40:ILE:HG23	11:K:75:TYR:CD2	2.38	0.57
13:M:84:ILE:C	13:M:86:CYS:H	2.08	0.57
14:N:24:CYS:HB3	14:N:28:GLY:N	2.19	0.57
16:P:17:TYR:HE1	16:P:41:PRO:HG2	1.69	0.57
17:Q:69:LYS:C	17:Q:70:ARG:HD2	2.24	0.57
1:A:1095:U:H2'	1:A:1096:C:C6	2.39	0.57
1:A:1504:G:H3'	1:A:1504:G:OP2	2.04	0.57
14:N:29:ARG:HG2	14:N:29:ARG:HH11	1.69	0.57
1:A:346:G:C2'	1:A:347:G:H5'	2.35	0.57
2:B:23:ARG:NH1	2:B:23:ARG:C	2.58	0.57
13:M:31:LYS:O	13:M:35:GLU:HB2	2.05	0.57
19:S:40:ILE:HG21	19:S:62:ILE:CD1	2.33	0.57
1:A:1298:C:C4	7:G:114:ARG:HD3	2.40	0.57
4:D:30:LYS:C	4:D:32:ALA:N	2.58	0.57
8:H:29:SER:OG	8:H:32:LYS:HB2	2.04	0.57
14:N:3:ARG:NH1	14:N:6:LEU:HD11	2.20	0.57
20:T:10:LEU:HD12	20:T:12:ALA:HB3	1.85	0.57
1:A:757:U:H2'	1:A:758:G:O4'	2.03	0.57
1:A:835:U:OP1	18:R:64:ARG:NH2	2.34	0.57
1:A:860:A:H2'	1:A:861:G:O4'	2.03	0.57
1:A:1015:A:H2'	1:A:1016:A:C8	2.40	0.57
1:A:1044:A:C2'	1:A:1045:C:H5'	2.34	0.57
1:A:1305:G:N2	1:A:1331:G:O2'	2.38	0.57
3:C:121:ALA:O	3:C:125:GLU:HG3	2.04	0.57
4:D:7:PRO:HG2	4:D:10:ARG:HD2	1.87	0.57
8:H:19:VAL:HG23	8:H:21:LYS:HD3	1.86	0.57
13:M:49:THR:HB	13:M:52:GLU:HG3	1.86	0.57
1:A:1347:G:N2	1:A:1373:G:H2'	2.19	0.57
2:B:223:ILE:HG21	2:B:230:VAL:CG2	2.35	0.57
19:S:25:LYS:H	19:S:25:LYS:HD2	1.68	0.57
1:A:1004:A:H5"	1:A:1025:U:C5	2.40	0.57
1:A:1230:C:H1'	13:M:126:LYS:HA	1.86	0.57
1:A:1241:G:H2'	1:A:1242:C:C6	2.39	0.57
4:D:35:ARG:O	4:D:36:ARG:HB2	2.04	0.57
6:F:80:ARG:NH1	6:F:88:VAL:HB	2.19	0.57
8:H:103:VAL:HG21	8:H:110:ALA:HB2	1.87	0.57
9:I:9:ARG:HA	9:I:13:ALA:O	2.05	0.57
13:M:13:LYS:HD3	13:M:17:VAL:HG11	1.86	0.57
1:A:192:U:O2'	1:A:193:C:H5'	2.05	0.57
2:B:209:ARG:HE	2:B:239:VAL:HG11	1.68	0.57
12:L:47:LYS:CB	12:L:48:PRO:HD3	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:25:THR:O	18:R:26:LEU:HB2	2.04	0.57
18:R:47:THR:HG22	18:R:48:GLY:N	2.18	0.57
19:S:5:LEU:O	19:S:6:LYS:CB	2.52	0.57
19:S:7:LYS:HG3	19:S:7:LYS:O	2.03	0.57
1:A:1152:A:H5'	10:J:70:ARG:NH2	2.19	0.57
1:A:1372:U:OP1	9:I:71:SER:HB3	2.04	0.57
1:A:1491:G:H2'	1:A:1492:A:C8	2.40	0.57
1:A:1499:A:H1'	1:A:1520:G:H5'	1.87	0.57
3:C:84:ILE:O	3:C:88:ARG:HB2	2.05	0.57
3:C:91:LEU:HD11	3:C:99:VAL:HG13	1.87	0.57
3:C:188:LEU:HD13	3:C:195:VAL:HG13	1.86	0.57
5:E:80:ILE:HD12	5:E:80:ILE:O	2.05	0.57
8:H:123:GLU:O	8:H:127:LEU:HD23	2.05	0.57
12:L:6:THR:OG1	12:L:9:GLN:HG3	2.05	0.57
15:O:41:GLU:OE2	15:O:41:GLU:HA	2.05	0.57
20:T:67:ALA:HA	20:T:73:HIS:H	1.70	0.57
1:A:946:A:H2'	1:A:947:G:C8	2.40	0.56
1:A:1317:C:H2'	1:A:1318:A:O4'	2.04	0.56
2:B:12:GLU:C	2:B:14:GLY:H	2.07	0.56
3:C:29:TYR:CZ	14:N:54:PRO:HG2	2.40	0.56
17:Q:59:ILE:HG22	17:Q:71:PHE:CD1	2.39	0.56
1:A:129(A):G:O2'	1:A:190(E):U:H2'	2.05	0.56
1:A:780:A:O2'	1:A:781:A:H5"	2.05	0.56
1:A:1278:U:H5"	1:A:1279:A:O4'	2.04	0.56
2:B:88:ALA:C	2:B:90:MET:H	2.09	0.56
17:Q:5:VAL:HG22	17:Q:60:ILE:HG12	1.87	0.56
20:T:82:SER:C	20:T:84:LEU:H	2.08	0.56
1:A:760:G:O6	17:Q:105:ALA:HB2	2.05	0.56
1:A:818:G:H3'	1:A:819:A:H5"	1.87	0.56
1:A:1040:U:H2'	1:A:1041:A:H8	1.70	0.56
1:A:1256:A:H61	1:A:1278:U:H1'	1.70	0.56
2:B:126:GLU:HG2	2:B:129:GLU:OE1	2.05	0.56
3:C:32:LEU:HD23	3:C:32:LEU:O	2.05	0.56
5:E:101:ILE:O	5:E:120:THR:HB	2.05	0.56
8:H:60:ARG:HH11	8:H:60:ARG:HG3	1.70	0.56
13:M:17:VAL:O	13:M:20:THR:HB	2.05	0.56
15:O:3:ILE:HG22	15:O:7:GLU:HB3	1.86	0.56
19:S:28:LYS:CG	19:S:29:ARG:H	2.09	0.56
22:Y:156:PRO:HB2	22:Y:158:LEU:HB3	1.87	0.56
1:A:448:A:H2'	1:A:449:C:C6	2.40	0.56
1:A:915:A:C2'	1:A:916:G:H5'	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1195:C:H3'	1:A:1196:U:C5'	2.35	0.56
1:A:1223:C:OP1	1:A:1224:G:H3'	2.05	0.56
1:A:1346:A:H4'	1:A:1347:G:O5'	2.06	0.56
2:B:47:THR:HA	2:B:202:PRO:HG2	1.87	0.56
3:C:33:LEU:HD23	3:C:33:LEU:O	2.04	0.56
6:F:2:ARG:CD	6:F:69:GLU:HG2	2.35	0.56
10:J:4:ILE:HA	10:J:100:THR:HA	1.88	0.56
13:M:8:GLU:OE1	13:M:22:ILE:HG12	2.06	0.56
13:M:15:VAL:HG23	13:M:43:THR:O	2.04	0.56
17:Q:59:ILE:CG2	17:Q:71:PHE:HB3	2.36	0.56
19:S:63:THR:HG22	19:S:64:GLU:H	1.71	0.56
7:G:146:GLU:HA	7:G:149:ARG:HB2	1.87	0.56
9:I:39:GLY:O	9:I:40:LEU:HD23	2.06	0.56
13:M:12:ASN:O	13:M:12:ASN:ND2	2.39	0.56
14:N:36:PHE:O	14:N:36:PHE:CD1	2.58	0.56
17:Q:67:LYS:O	17:Q:68:ARG:HB3	2.05	0.56
1:A:1053:G:H4'	1:A:1054:C:H5'	1.88	0.56
1:A:1257:U:H4'	1:A:1258:G:O5'	2.06	0.56
1:A:1443:G:H5"	1:A:1446:A:C5'	2.19	0.56
4:D:6:GLY:O	4:D:8:VAL:HG23	2.06	0.56
4:D:57:ARG:HB3	4:D:206:PHE:HB2	1.88	0.56
10:J:12:ASP:HB3	10:J:15:THR:HB	1.88	0.56
10:J:22:LYS:CE	10:J:90:LEU:HD12	2.33	0.56
19:S:10:PHE:CD2	19:S:11:VAL:N	2.73	0.56
22:Y:55:ASP:OD1	22:Y:56:PRO:HD2	2.06	0.56
22:Y:141:TYR:HB2	22:Y:142:SER:C	2.26	0.56
1:A:438:G:C4'	1:A:439:A:OP1	2.53	0.56
1:A:477:G:H2'	1:A:478:A:C8	2.40	0.56
1:A:1028:C:H2'	1:A:1029:C:C6	2.40	0.56
1:A:1339:A:H2'	1:A:1340:A:O4'	2.06	0.56
3:C:7:PRO:CG	3:C:184:TYR:HB2	2.35	0.56
8:H:105:ARG:HG3	8:H:105:ARG:HH11	1.71	0.56
1:A:1326:C:OP1	21:V:12:LYS:NZ	2.37	0.56
4:D:24:GLU:HG2	4:D:25:ARG:N	2.21	0.56
4:D:176:LEU:HA	4:D:183:GLY:HA2	1.87	0.56
18:R:53:ARG:HD3	18:R:63:GLN:CB	2.36	0.56
19:S:40:ILE:HG21	19:S:62:ILE:HD11	1.88	0.56
1:A:665:A:H2'	1:A:725:G:N2	2.21	0.56
4:D:148:VAL:HG11	4:D:158:ILE:HD13	1.88	0.56
13:M:117:VAL:HG12	13:M:118:ALA:H	1.70	0.56
17:Q:103:GLY:O	17:Q:104:LYS:O	2.24	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:411:A:C4	1:A:413:G:H1'	2.41	0.56
1:A:933:G:OP2	7:G:3:ARG:HB2	2.06	0.56
1:A:1044:A:H2'	1:A:1045:C:C5'	2.36	0.56
1:A:1202:G:O2'	1:A:1203:C:H5'	2.06	0.56
10:J:81:THR:O	10:J:85:LEU:HG	2.06	0.56
15:O:36:ILE:HA	15:O:59:MET:HE3	1.87	0.56
1:A:166:G:O2'	1:A:167:G:H5'	2.06	0.55
1:A:652:U:H2'	1:A:752:G:N1	2.21	0.55
1:A:1216:G:H5"	14:N:5:ALA:HB1	1.88	0.55
1:A:1257:U:O2'	1:A:1258:G:OP2	2.21	0.55
4:D:24:GLU:H	4:D:112:VAL:CG1	2.19	0.55
5:E:118:ILE:HG22	5:E:119:LEU:H	1.67	0.55
16:P:26:ARG:HD2	16:P:31:LYS:O	2.06	0.55
1:A:1042:G:O2'	1:A:1043:C:H5'	2.06	0.55
1:A:1405:G:C2	1:A:1497:G:C2	2.94	0.55
2:B:21:ARG:HG3	2:B:23:ARG:HD2	1.88	0.55
13:M:65:LYS:HE3	13:M:69:GLU:OE2	2.07	0.55
1:A:103:C:P	20:T:17:ARG:NH1	2.79	0.55
1:A:505:G:H2'	1:A:506:G:H8	1.69	0.55
1:A:1193:G:O2'	1:A:1194:U:H5'	2.07	0.55
2:B:15:VAL:HG22	2:B:209:ARG:HG3	1.88	0.55
20:T:86:ARG:O	20:T:90:GLN:HG3	2.06	0.55
2:B:23:ARG:HD3	2:B:23:ARG:N	2.22	0.55
10:J:24:VAL:HG21	10:J:37:PRO:HD3	1.88	0.55
16:P:81:ARG:CG	16:P:83:GLU:HG2	2.36	0.55
1:A:1236:A:H2'	1:A:1237:C:C6	2.41	0.55
1:A:1251:A:H2'	1:A:1252:A:C8	2.41	0.55
2:B:67:THR:HG22	2:B:68:ILE:N	2.21	0.55
3:C:33:LEU:HD11	14:N:53:LEU:HD22	1.87	0.55
6:F:69:GLU:HA	6:F:72:VAL:CG2	2.37	0.55
13:M:37:THR:HG22	13:M:37:THR:O	2.07	0.55
18:R:86:VAL:O	18:R:87:ARG:CB	2.55	0.55
1:A:18:C:H4'	1:A:1078:U:O2	2.07	0.55
1:A:490:G:H2'	1:A:491:G:H8	1.72	0.55
2:B:74:LYS:HZ1	2:B:206:ASP:CA	2.19	0.55
4:D:107:ARG:HH21	4:D:194:LEU:HD12	1.70	0.55
20:T:35:THR:O	20:T:39:LYS:HB2	2.06	0.55
20:T:94:ALA:O	20:T:95:ALA:HB3	2.06	0.55
1:A:227:G:O2'	16:P:62:VAL:HG11	2.05	0.55
1:A:620:C:H2'	1:A:621:A:O4'	2.07	0.55
1:A:1066:C:O2'	1:A:1067:A:H5'	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1268:A:H2'	1:A:1269:A:C8	2.41	0.55
1:A:1460:A:H2'	1:A:1461:G:O4'	2.07	0.55
4:D:177:ASP:OD1	4:D:179:GLU:HB2	2.07	0.55
7:G:116:ALA:HA	7:G:119:ARG:NH2	2.21	0.55
9:I:7:THR:HG22	9:I:8:GLY:N	2.22	0.55
10:J:49:VAL:HG11	14:N:41:ARG:O	2.07	0.55
1:A:551:U:H2'	1:A:552:U:C6	2.41	0.55
1:A:954:G:H2'	1:A:955:U:C6	2.42	0.55
1:A:1442:G:H21	1:A:1446:A:H5"	1.72	0.55
3:C:38:ARG:HB3	3:C:94:LEU:HD21	1.89	0.55
6:F:46:ARG:HB2	6:F:60:PHE:HE1	1.71	0.55
6:F:76:ALA:O	6:F:80:ARG:HG3	2.06	0.55
12:L:43:VAL:HG12	12:L:44:THR:H	1.72	0.55
12:L:50:SER:O	12:L:51:ALA:HB2	2.05	0.55
22:Y:43:ALA:HA	22:Y:51:TYR:CE2	2.42	0.55
1:A:818:G:C3'	1:A:819:A:C5'	2.83	0.55
1:A:1404:C:H1'	1:A:1499:A:C2	2.42	0.55
3:C:52:LEU:HD21	3:C:118:GLN:OE1	2.07	0.55
1:A:532:A:H2'	1:A:533:A:H5"	1.89	0.55
1:A:939:G:H2'	1:A:940:C:H6	1.71	0.55
1:A:1006:C:H2'	1:A:1007:C:H6	1.72	0.55
1:A:1333:A:H2'	1:A:1334:G:O4'	2.07	0.55
1:A:1404:C:C1'	1:A:1499:A:N1	2.70	0.55
2:B:75:LYS:O	2:B:75:LYS:HD3	2.07	0.55
5:E:21:ALA:O	5:E:23:GLY:N	2.40	0.55
12:L:47:LYS:HB2	12:L:48:PRO:HD2	1.88	0.55
20:T:67:ALA:HB2	20:T:77:ALA:HB2	1.88	0.55
1:A:26:A:N6	1:A:558:G:H1'	2.21	0.54
1:A:190(F):G:H4'	1:A:190(G):G:OP2	2.07	0.54
1:A:193:C:H2'	1:A:194:C:H6	1.72	0.54
1:A:1319:A:H5'	1:A:1320:C:OP1	2.06	0.54
3:C:138:VAL:HG21	3:C:168:ALA:HB1	1.89	0.54
15:O:87:ILE:O	15:O:88:ARG:CB	2.54	0.54
17:Q:68:ARG:N	17:Q:70:ARG:NH1	2.55	0.54
1:A:54:C:H2'	1:A:352:C:H41	1.71	0.54
2:B:17:PHE:CD1	2:B:18:GLY:N	2.75	0.54
2:B:33:TYR:HB3	2:B:41:ILE:O	2.08	0.54
3:C:37:GLN:NE2	14:N:52:GLN:OE1	2.40	0.54
3:C:58:GLU:H	3:C:65:ALA:HB3	1.72	0.54
3:C:112:SER:CB	3:C:115:LEU:HD12	2.36	0.54
6:F:25:ILE:HD12	6:F:82:ARG:HD2	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:125:ARG:HD2	13:M:125:ARG:C	2.27	0.54
15:O:32:LEU:O	15:O:36:ILE:HG13	2.06	0.54
1:A:967:C:C4'	9:I:128:ARG:HG3	2.38	0.54
1:A:1128:C:H2'	1:A:1129:C:H5"	1.89	0.54
2:B:12:GLU:C	2:B:14:GLY:N	2.59	0.54
7:G:69:VAL:HG12	7:G:100:ALA:HA	1.89	0.54
8:H:36:LEU:HD12	8:H:59:LEU:HD13	1.88	0.54
8:H:56:LYS:HD2	8:H:56:LYS:N	2.23	0.54
17:Q:79:SER:O	17:Q:80:GLY:O	2.25	0.54
1:A:130:A:C8	17:Q:63:ARG:HG3	2.42	0.54
1:A:977:A:C2'	1:A:978:A:H5"	2.38	0.54
2:B:33:TYR:HB2	2:B:43:ASP:HB2	1.89	0.54
5:E:15:ARG:O	5:E:27:ARG:O	2.25	0.54
7:G:116:ALA:HA	7:G:119:ARG:CZ	2.37	0.54
10:J:51:ARG:H	10:J:59:SER:HB2	1.72	0.54
20:T:72:LEU:HD21	20:T:80:ARG:CZ	2.38	0.54
1:A:743:U:H2'	1:A:744:C:C6	2.43	0.54
1:A:1351:U:H2'	1:A:1352:C:C6	2.40	0.54
6:F:4:TYR:OH	6:F:69:GLU:HB3	2.07	0.54
7:G:18:TYR:CE2	7:G:59:LEU:HB2	2.42	0.54
7:G:113:GLU:HG2	7:G:119:ARG:HG2	1.90	0.54
10:J:3:LYS:N	10:J:75:ILE:HA	2.22	0.54
13:M:60:VAL:O	13:M:63:THR:HG22	2.07	0.54
13:M:94:ARG:HH22	19:S:81:ARG:HH11	1.54	0.54
1:A:195:A:H4'	20:T:68:LYS:NZ	2.22	0.54
1:A:1030(A):G:N2	1:A:1030(C):G:H3'	2.23	0.54
1:A:1320:C:N3	19:S:36:ARG:HG3	2.22	0.54
2:B:17:PHE:HD1	2:B:18:GLY:N	2.05	0.54
5:E:137:GLU:O	5:E:141:GLN:HG3	2.08	0.54
13:M:29:ARG:HB3	13:M:64:TRP:CH2	2.42	0.54
16:P:21:VAL:O	16:P:33:ILE:HB	2.07	0.54
17:Q:67:LYS:CA	17:Q:70:ARG:HH12	2.21	0.54
1:A:190:C:H2'	1:A:190(A):C:C6	2.43	0.54
1:A:960:U:H5'	1:A:960:U:O2	2.08	0.54
1:A:1459:C:OP1	20:T:27:LYS:HE2	2.08	0.54
2:B:187:LEU:HD23	2:B:214:ILE:HG21	1.90	0.54
3:C:77:ILE:HG22	3:C:81:GLY:HA2	1.90	0.54
3:C:150:LYS:CE	3:C:152:ILE:HD11	2.38	0.54
3:C:174:PRO:HB2	3:C:177:THR:HG22	1.89	0.54
6:F:26:ILE:HG21	6:F:63:TYR:CE2	2.40	0.54
9:I:85:LEU:O	9:I:92:TYR:HD1	1.91	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:27:VAL:O	15:O:31:LEU:HD13	2.07	0.54
17:Q:18:THR:HG23	17:Q:69:LYS:HE3	1.88	0.54
22:Y:41:LYS:O	22:Y:44:ILE:HG22	2.08	0.54
1:A:429:U:H2'	4:D:25:ARG:HH12	1.73	0.54
3:C:14:ILE:HG22	3:C:15:THR:N	2.12	0.54
4:D:160:GLN:O	4:D:163:GLU:HB3	2.08	0.54
4:D:199:ASN:OD1	4:D:201:GLN:HB2	2.08	0.54
5:E:76:ILE:O	5:E:93:PRO:HB3	2.07	0.54
7:G:138:LYS:HE2	7:G:142:GLU:OE1	2.08	0.54
17:Q:95:TYR:C	17:Q:97:SER:N	2.58	0.54
20:T:53:LEU:HB2	20:T:100:ILE:HB	1.89	0.54
1:A:281:G:O2'	1:A:282:A:P	2.65	0.54
1:A:429:U:H2'	4:D:25:ARG:NH1	2.22	0.54
1:A:750:G:H1'	15:O:22:THR:OG1	2.08	0.54
4:D:126:ILE:HG22	4:D:127:THR:N	2.23	0.54
1:A:475:G:H2'	1:A:476:G:C8	2.43	0.54
1:A:1222:G:P	19:S:77:THR:HG21	2.48	0.54
1:A:1318:A:H4'	19:S:10:PHE:CE1	2.42	0.54
1:A:1516:G:H2'	1:A:1518:A:OP2	2.08	0.54
2:B:10:LEU:C	2:B:12:GLU:H	2.12	0.54
3:C:116:VAL:O	3:C:120:VAL:HG23	2.07	0.54
8:H:119:LEU:HD12	8:H:124:ALA:HA	1.89	0.54
9:I:81:ILE:O	9:I:85:LEU:HB2	2.08	0.54
19:S:51:VAL:HG12	19:S:52:TYR:N	2.23	0.54
1:A:299:G:H2'	1:A:300:A:C8	2.43	0.53
1:A:933:G:C2	1:A:1385:G:C2	2.96	0.53
1:A:1218:C:H2'	1:A:1219:U:C6	2.42	0.53
1:A:1488:G:H2'	1:A:1489:G:C8	2.44	0.53
2:B:18:GLY:CA	2:B:42:ILE:H	2.20	0.53
6:F:100:ASN:OD1	18:R:23:LYS:HG2	2.08	0.53
7:G:44:TYR:HE1	9:I:41:VAL:HG11	1.72	0.53
15:O:70:LEU:HD11	15:O:77:ARG:HB2	1.89	0.53
16:P:11:SER:OG	16:P:14:ASN:HB3	2.08	0.53
1:A:35:G:H2'	1:A:36:C:C6	2.43	0.53
1:A:181:G:H4'	1:A:182:U:H5'	1.89	0.53
1:A:639:G:O2'	1:A:640:A:H5'	2.08	0.53
1:A:957:U:H4'	19:S:79:THR:HB	1.89	0.53
1:A:1347:G:C2'	1:A:1348:U:OP2	2.56	0.53
2:B:134:GLU:C	2:B:136:VAL:H	2.12	0.53
11:K:14:VAL:O	11:K:15:ALA:CB	2.57	0.53
13:M:53:VAL:O	13:M:57:ARG:HB2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:9:LYS:HD3	14:N:9:LYS:C	2.28	0.53
14:N:44:LEU:C	14:N:44:LEU:HD12	2.29	0.53
1:A:983:A:H5'	1:A:984:C:OP2	2.07	0.53
3:C:33:LEU:HD23	3:C:33:LEU:C	2.29	0.53
3:C:91:LEU:HD21	3:C:99:VAL:CG1	2.30	0.53
3:C:113:ALA:HB3	3:C:114:PRO:HD3	1.90	0.53
5:E:79:GLU:OE1	8:H:105:ARG:HD3	2.08	0.53
7:G:42:ILE:CG2	7:G:120:ILE:HD12	2.38	0.53
16:P:43:LYS:HB3	16:P:48:TRP:CD1	2.43	0.53
20:T:93:GLU:HA	20:T:93:GLU:OE2	2.09	0.53
1:A:101:A:O2'	1:A:102:G:H5'	2.07	0.53
1:A:1003:G:C2	1:A:1003(A):G:C6	2.96	0.53
1:A:1121:U:H2'	1:A:1122:U:H6	1.73	0.53
1:A:1157:A:H4'	1:A:1158:C:O5'	2.08	0.53
9:I:17:VAL:HG11	9:I:81:ILE:HA	1.90	0.53
10:J:81:THR:C	10:J:83:GLU:H	2.10	0.53
13:M:8:GLU:OE1	13:M:22:ILE:HA	2.08	0.53
14:N:44:LEU:HD12	14:N:44:LEU:O	2.08	0.53
20:T:76:ALA:O	20:T:80:ARG:HG2	2.09	0.53
1:A:382:A:H2'	1:A:383:A:H8	1.70	0.53
1:A:407:G:O2'	4:D:116:GLN:HG3	2.08	0.53
10:J:38:ILE:HG13	10:J:71:LEU:HB3	1.90	0.53
12:L:46:LYS:CG	12:L:47:LYS:N	2.71	0.53
16:P:19:ILE:HG22	16:P:36:ILE:HG13	1.90	0.53
1:A:300:A:H2'	1:A:301:G:O4'	2.08	0.53
1:A:386:C:C2'	1:A:387:U:H5'	2.39	0.53
1:A:1003:G:N2	1:A:1039:C:C2	2.77	0.53
3:C:32:LEU:HD21	3:C:59:ARG:HD2	1.91	0.53
5:E:78:HIS:HD2	8:H:107:LEU:HD12	1.74	0.53
8:H:80:ILE:O	8:H:80:ILE:HG22	2.08	0.53
9:I:97:LYS:O	9:I:100:GLY:N	2.36	0.53
19:S:42:PRO:O	19:S:45:VAL:HG23	2.09	0.53
22:Y:141:TYR:N	22:Y:141:TYR:CD1	2.77	0.53
1:A:33:A:H2'	1:A:34:C:H6	1.73	0.53
1:A:818:G:O2'	1:A:819:A:H5"	2.08	0.53
1:A:959:A:C2	1:A:1222:G:O4'	2.61	0.53
1:A:979:C:H2'	1:A:980:C:H5'	1.91	0.53
5:E:18:ARG:HG2	5:E:19:MET:N	2.23	0.53
8:H:8:ASP:O	8:H:12:ARG:HG3	2.08	0.53
12:L:55:VAL:HG11	12:L:67:THR:HG23	1.91	0.53
17:Q:27:PHE:CE1	17:Q:36:ILE:HD11	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:A:H2'	1:A:34:C:C6	2.44	0.53
1:A:148:G:H2'	1:A:149:A:H8	1.74	0.53
1:A:1300:G:HO2'	1:A:1301:U:H6	1.55	0.53
1:A:1426:C:H2'	1:A:1427:U:C6	2.44	0.53
3:C:130:VAL:O	3:C:134:ILE:HG13	2.07	0.53
9:I:48:GLU:OE1	9:I:51:ARG:HD2	2.09	0.53
13:M:102:ARG:NH1	13:M:102:ARG:HB2	2.24	0.53
18:R:61:LYS:O	18:R:65:ILE:HG13	2.08	0.53
21:V:9:ARG:NH1	21:V:22:ARG:HA	2.23	0.53
1:A:179:A:H2'	1:A:180:U:C6	2.43	0.53
1:A:623:C:O2'	1:A:624:C:H5'	2.09	0.53
1:A:1117:G:H4'	9:I:104:ARG:HH11	1.72	0.53
1:A:1408:A:C6	22:Y:107:TRP:CE3	2.96	0.53
2:B:166:ASP:OD2	2:B:169:LYS:HB2	2.09	0.53
7:G:71:PRO:HD3	7:G:103:TRP:HZ3	1.74	0.53
10:J:44:VAL:HG22	10:J:66:ARG:HB3	1.91	0.53
12:L:47:LYS:HB3	12:L:48:PRO:HD3	1.91	0.53
12:L:53:ARG:HG2	12:L:69:TYR:HE1	1.73	0.53
13:M:11:ARG:CG	13:M:12:ASN:N	2.72	0.53
1:A:252:U:H2'	1:A:253:U:C6	2.44	0.53
1:A:370:C:O2'	1:A:371:G:H5'	2.09	0.53
1:A:373:A:O2'	1:A:374:A:H5'	2.09	0.53
1:A:656:C:O2'	15:O:28:GLN:OE1	2.23	0.53
1:A:666:G:H5'	1:A:726:C:H1'	1.90	0.53
1:A:937:A:C2	1:A:1379:G:C6	2.97	0.53
1:A:1184:G:H2'	1:A:1185:G:H8	1.74	0.53
2:B:23:ARG:O	2:B:24:TRP:O	2.27	0.53
9:I:31:GLN:HB3	9:I:35:GLU:HB3	1.91	0.53
22:Y:109:THR:HG1	25:Y:301:SFG:HN61	1.53	0.53
1:A:101:A:H2'	1:A:102:G:H8	1.74	0.52
1:A:1068:G:OP2	1:A:1068:G:H8	1.91	0.52
2:B:124:SER:O	2:B:127:ILE:HG13	2.08	0.52
4:D:32:ALA:C	4:D:34:GLU:N	2.60	0.52
14:N:33:VAL:HA	14:N:40:CYS:HA	1.91	0.52
22:Y:39:ILE:HD12	22:Y:51:TYR:HB3	1.91	0.52
1:A:246:A:N6	1:A:281:G:H1'	2.24	0.52
1:A:1513:A:H2'	1:A:1514:C:C6	2.44	0.52
5:E:12:LEU:CD1	5:E:31:LEU:HB2	2.39	0.52
22:Y:38:ASN:OD1	22:Y:195:SER:HB3	2.08	0.52
1:A:760:G:N1	17:Q:105:ALA:HB2	2.24	0.52
1:A:1006:C:H2'	1:A:1007:C:C6	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:23:TYR:CD2	3:C:24:ALA:N	2.78	0.52
3:C:70:VAL:O	3:C:106:VAL:HG23	2.09	0.52
6:F:43:LEU:H	6:F:43:LEU:CD2	2.22	0.52
6:F:94:GLN:OE1	18:R:32:ARG:HD3	2.09	0.52
7:G:69:VAL:HG21	7:G:104:LEU:HD21	1.90	0.52
11:K:13:GLN:HA	11:K:75:TYR:O	2.08	0.52
1:A:115:G:O2'	1:A:116:A:OP2	2.22	0.52
1:A:621:A:H2'	1:A:622:A:C8	2.44	0.52
1:A:657:G:C4'	15:O:28:GLN:HG2	2.36	0.52
1:A:953:G:H2'	1:A:954:G:O4'	2.09	0.52
1:A:1038:C:H2'	1:A:1039:C:C6	2.43	0.52
1:A:1038:C:H2'	1:A:1039:C:H6	1.74	0.52
1:A:1305:G:OP1	21:V:2:GLY:N	2.42	0.52
1:A:1397:C:H4'	1:A:1398:A:OP2	2.08	0.52
1:A:1423:G:O2'	1:A:1424:C:H5'	2.09	0.52
4:D:104:VAL:HG11	4:D:146:ILE:CD1	2.37	0.52
13:M:102:ARG:HB2	13:M:102:ARG:HH11	1.75	0.52
18:R:73:ALA:HB3	18:R:79:LEU:HD12	1.91	0.52
21:V:17:THR:O	21:V:22:ARG:HD3	2.10	0.52
1:A:684:A:H1'	11:K:38:ASN:HB3	1.91	0.52
1:A:1128:C:H1'	1:A:1146:A:H61	1.75	0.52
5:E:31:LEU:HD22	5:E:43:LEU:CD2	2.39	0.52
6:F:10:LEU:HD11	6:F:59:TYR:CD2	2.41	0.52
12:L:55:VAL:HG11	12:L:67:THR:CG2	2.39	0.52
13:M:117:VAL:HG12	13:M:118:ALA:N	2.24	0.52
14:N:3:ARG:O	14:N:4:LYS:C	2.48	0.52
19:S:13:ASP:O	19:S:17:GLU:HG2	2.10	0.52
3:C:83:ARG:C	3:C:85:ARG:N	2.63	0.52
4:D:65:ARG:HB2	4:D:75:PHE:CE1	2.45	0.52
8:H:14:ARG:O	8:H:18:ARG:HD3	2.10	0.52
13:M:86:CYS:SG	13:M:88:ARG:HB3	2.49	0.52
19:S:50:ALA:HA	19:S:58:VAL:O	2.10	0.52
21:V:24:ARG:O	21:V:25:LYS:HB2	2.10	0.52
1:A:142:G:O2'	1:A:196:A:N1	2.40	0.52
1:A:1405:G:O2'	1:A:1519:A:C4'	2.58	0.52
3:C:130:VAL:HG12	3:C:134:ILE:HD11	1.91	0.52
8:H:25:ASP:OD1	8:H:60:ARG:HD3	2.09	0.52
1:A:115:G:H1'	1:A:116:A:N7	2.24	0.52
1:A:148:G:H2'	1:A:149:A:C8	2.45	0.52
1:A:582:U:H1'	17:Q:105:ALA:HA	1.92	0.52
1:A:605:U:O2'	1:A:606:G:H5'	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:791:G:H2'	1:A:792:A:H5'	1.91	0.52
1:A:1021:G:C2'	1:A:1022:G:H5'	2.40	0.52
1:A:1167:A:H2'	1:A:1168:A:C8	2.45	0.52
1:A:1428:A:H2'	1:A:1429:C:C6	2.44	0.52
2:B:73:THR:HG23	2:B:95:GLN:O	2.09	0.52
2:B:130:ARG:HH22	3:C:179:ARG:NH1	2.05	0.52
3:C:22:TRP:CZ2	14:N:54:PRO:HG3	2.44	0.52
3:C:108:ASN:C	3:C:110:ASN:H	2.12	0.52
3:C:154:SER:O	3:C:165:THR:HA	2.09	0.52
11:K:17:GLY:O	11:K:80:VAL:HA	2.09	0.52
11:K:27:ASN:HA	11:K:56:GLY:HA2	1.92	0.52
1:A:190(E):U:O2'	17:Q:63:ARG:NH2	2.43	0.52
1:A:923:A:O2'	1:A:1398:A:H2'	2.10	0.52
1:A:935:A:O2'	1:A:1383:C:N3	2.39	0.52
1:A:1202:G:H2'	1:A:1203:C:O4'	2.10	0.52
1:A:1451:A:O2'	1:A:1452:C:OP1	2.26	0.52
4:D:170:VAL:CG1	4:D:174:LEU:HB2	2.39	0.52
6:F:8:ILE:HD11	6:F:79:LEU:HD13	1.91	0.52
9:I:9:ARG:HG2	9:I:14:VAL:HG22	1.92	0.52
10:J:39:PRO:O	10:J:40:LEU:CB	2.57	0.52
16:P:20:VAL:CG1	16:P:32:TYR:HB3	2.40	0.52
18:R:19:LYS:O	18:R:20:ALA:HB2	2.10	0.52
21:V:24:ARG:O	21:V:25:LYS:CB	2.58	0.52
3:C:20:SER:HB3	3:C:22:TRP:NE1	2.24	0.52
5:E:12:LEU:HD22	5:E:12:LEU:C	2.29	0.52
5:E:79:GLU:CD	8:H:105:ARG:HD3	2.30	0.52
11:K:62:GLN:HG3	11:K:97:ALA:HB2	1.92	0.52
22:Y:31:LEU:HB3	22:Y:103:ILE:HG12	1.91	0.52
1:A:1094:G:H5"	1:A:1095:U:H5	1.75	0.51
1:A:1424:C:O2'	1:A:1425:U:H5'	2.09	0.51
13:M:73:GLU:O	13:M:76:ALA:HB3	2.09	0.51
1:A:163:C:O2'	1:A:164:U:H5'	2.10	0.51
1:A:357:G:O2'	1:A:358:U:H5'	2.09	0.51
1:A:443:C:H2'	1:A:444:C:C6	2.43	0.51
1:A:452:A:H4'	16:P:72:ARG:NH2	2.25	0.51
1:A:1416:G:N2	1:A:1485:U:H1'	2.24	0.51
1:A:1511:G:H2'	1:A:1512:U:O4'	2.09	0.51
3:C:134:ILE:HG21	3:C:167:TRP:O	2.11	0.51
9:I:44:VAL:HG13	9:I:51:ARG:NH2	2.24	0.51
10:J:22:LYS:NZ	10:J:91:PRO:HD3	2.25	0.51
10:J:26:ALA:O	10:J:84:GLN:NE2	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:126:ARG:O	11:K:127:LYS:C	2.48	0.51
12:L:119:LYS:O	12:L:120:TYR:HB2	2.10	0.51
13:M:88:ARG:HG3	13:M:98:VAL:CG1	2.40	0.51
18:R:88:LYS:OXT	18:R:88:LYS:HG2	2.10	0.51
1:A:502:G:H1'	1:A:550:G:H5'	1.91	0.51
1:A:560:U:O2'	1:A:561:U:OP2	2.27	0.51
1:A:738:C:P	6:F:92:LYS:HE3	2.50	0.51
1:A:794:A:H2'	1:A:795:C:C6	2.45	0.51
1:A:1329:A:O2'	1:A:1330:U:H5'	2.11	0.51
2:B:126:GLU:O	2:B:129:GLU:HB2	2.11	0.51
5:E:40:ARG:HG2	5:E:40:ARG:HH11	1.76	0.51
8:H:24:THR:HG23	8:H:61:VAL:HB	1.92	0.51
8:H:91:ARG:HG2	12:L:7:ILE:HG21	1.92	0.51
14:N:21:TYR:HE2	14:N:23:ARG:NE	2.09	0.51
14:N:57:ARG:HG2	14:N:58:LYS:H	1.75	0.51
18:R:46:GLU:H	18:R:46:GLU:CD	2.14	0.51
1:A:828:A:H2'	1:A:829:G:O4'	2.10	0.51
3:C:94:LEU:HD22	3:C:95:THR:HG23	1.92	0.51
4:D:24:GLU:O	4:D:25:ARG:HB3	2.10	0.51
5:E:13:ILE:HG22	5:E:30:ALA:CB	2.40	0.51
7:G:102:ARG:O	7:G:106:GLN:HG3	2.11	0.51
9:I:115:GLY:HA2	10:J:58:ASP:OD1	2.10	0.51
10:J:20:ALA:O	10:J:24:VAL:HG23	2.11	0.51
10:J:23:ILE:N	10:J:23:ILE:HD12	2.26	0.51
12:L:42:THR:HG21	12:L:52:LEU:HB3	1.91	0.51
13:M:82:MET:HE2	13:M:92:HIS:HB3	1.92	0.51
1:A:992:U:O2'	1:A:993:G:OP2	2.26	0.51
1:A:1059:C:O2'	1:A:1060:C:H5'	2.11	0.51
1:A:1191:A:H2'	1:A:1192:C:C6	2.45	0.51
1:A:1221:G:O3'	19:S:77:THR:HG21	2.10	0.51
1:A:1468:A:H2'	1:A:1469:G:O4'	2.09	0.51
3:C:84:ILE:O	3:C:84:ILE:HG12	2.10	0.51
3:C:137:ALA:HA	3:C:140:ARG:NH1	2.26	0.51
6:F:69:GLU:OE1	6:F:69:GLU:N	2.44	0.51
7:G:156:TRP:OXT	7:G:156:TRP:HD1	1.93	0.51
20:T:41:ILE:O	20:T:45:GLN:HB2	2.10	0.51
1:A:478:A:O2'	1:A:479:C:H5'	2.11	0.51
1:A:922:G:N2	1:A:1396:A:C4	2.79	0.51
1:A:1021:G:H2'	1:A:1022:G:O4'	2.11	0.51
1:A:1021:G:C2	1:A:1022:G:H1'	2.45	0.51
1:A:1241:G:H2'	1:A:1242:C:H6	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1277:C:HO2'	1:A:1279:A:H8	1.54	0.51
1:A:1496:C:H2'	1:A:1497:G:O4'	2.11	0.51
1:A:1518:A:H2'	1:A:1519:A:C8	2.46	0.51
3:C:61:ALA:O	3:C:63:ASN:N	2.44	0.51
3:C:97:LYS:O	3:C:98:ASN:HB3	2.10	0.51
5:E:15:ARG:O	5:E:16:THR:O	2.28	0.51
5:E:89:ILE:HD13	5:E:90:VAL:H	1.75	0.51
9:I:125:TYR:CD2	9:I:125:TYR:N	2.79	0.51
9:I:127:LYS:N	9:I:127:LYS:HD2	2.24	0.51
12:L:27:LEU:HG	12:L:28:LYS:N	2.22	0.51
17:Q:45:HIS:CB	17:Q:65:ILE:HD13	2.39	0.51
19:S:10:PHE:CD2	19:S:10:PHE:C	2.83	0.51
19:S:45:VAL:HG12	19:S:46:GLY:N	2.26	0.51
19:S:53:ASN:HB2	19:S:56:GLN:H	1.74	0.51
19:S:81:ARG:O	19:S:81:ARG:HG2	2.11	0.51
1:A:1003(A):G:N1	1:A:1004:A:H1'	2.25	0.51
1:A:1152:A:H2'	1:A:1153:C:C6	2.45	0.51
1:A:1346:A:C4	7:G:10:ARG:NH2	2.78	0.51
1:A:1486:G:H2'	1:A:1487:G:O4'	2.10	0.51
2:B:15:VAL:HG11	2:B:209:ARG:C	2.30	0.51
2:B:26:PRO:O	2:B:29:ALA:HB2	2.10	0.51
8:H:49:GLU:HG2	8:H:62:TYR:HE2	1.75	0.51
17:Q:45:HIS:HB2	17:Q:65:ILE:CD1	2.37	0.51
18:R:45:SER:C	18:R:47:THR:N	2.64	0.51
22:Y:115:ILE:HD12	22:Y:156:PRO:CD	2.41	0.51
1:A:580:U:H2'	1:A:581:G:O4'	2.11	0.51
1:A:791:G:H2'	1:A:792:A:C5'	2.40	0.51
1:A:808:C:OP1	15:O:48:LYS:HE3	2.11	0.51
1:A:931:C:C2	1:A:1387:G:N1	2.79	0.51
1:A:1085:U:O3'	1:A:1086:U:C6	2.64	0.51
1:A:1126:U:OP2	1:A:1281:U:O2	2.29	0.51
1:A:1496:C:H6	1:A:1496:C:O5'	1.94	0.51
2:B:96:ARG:O	2:B:98:LEU:HD23	2.11	0.51
3:C:34:LEU:HD23	3:C:34:LEU:O	2.10	0.51
3:C:188:LEU:CD1	3:C:195:VAL:HG13	2.41	0.51
6:F:9:VAL:HG22	6:F:60:PHE:CE2	2.46	0.51
10:J:69:ASN:O	10:J:70:ARG:HD3	2.11	0.51
1:A:7:G:H5'	1:A:298:A:O4'	2.11	0.51
1:A:1162:C:H2'	1:A:1163:C:C6	2.46	0.51
1:A:1396:A:H4'	1:A:1397:C:H5"	1.93	0.51
1:A:1495:U:H2'	1:A:1496:C:C5	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:17:PHE:CD1	2:B:17:PHE:C	2.85	0.51
2:B:53:ARG:NH1	2:B:53:ARG:HG2	2.26	0.51
4:D:81:GLU:O	4:D:85:LYS:HG3	2.11	0.51
5:E:61:TYR:O	5:E:64:ARG:O	2.29	0.51
5:E:115:VAL:HG12	5:E:116:THR:N	2.25	0.51
6:F:43:LEU:H	6:F:43:LEU:HD22	1.76	0.51
9:I:93:ARG:HH11	9:I:97:LYS:HZ1	1.58	0.51
14:N:28:GLY:O	14:N:30:ALA:N	2.44	0.51
1:A:650:G:C2'	1:A:651:C:H5'	2.40	0.51
1:A:1097:C:H2'	1:A:1098:C:C6	2.45	0.51
1:A:1440:C:C2'	1:A:1441:G:H5'	2.41	0.51
2:B:97:TRP:CZ2	2:B:102:LEU:HD13	2.45	0.51
2:B:144:ARG:O	2:B:147:LYS:N	2.42	0.51
5:E:11:ILE:HB	5:E:31:LEU:HB3	1.93	0.51
9:I:27:THR:HG23	9:I:30:GLY:O	2.11	0.51
9:I:44:VAL:CG1	9:I:51:ARG:HH12	2.23	0.51
12:L:53:ARG:NH1	12:L:92:ASP:OD2	2.42	0.51
1:A:112:G:H21	1:A:354:G:C5'	2.24	0.50
1:A:160:A:H1'	1:A:344:A:C5	2.47	0.50
1:A:620:C:N1	4:D:135:LEU:HD13	2.26	0.50
1:A:1262:C:H42	1:A:1273:G:H1	1.59	0.50
1:A:1408:A:OP1	22:Y:205:ARG:NH1	2.44	0.50
2:B:124:SER:CB	2:B:125:PRO:HD2	2.32	0.50
3:C:47:LEU:CD1	3:C:47:LEU:N	2.74	0.50
8:H:126:LYS:C	8:H:128:GLY:H	2.14	0.50
9:I:17:VAL:CG2	9:I:80:GLY:HA3	2.41	0.50
1:A:149:A:O2'	1:A:150:C:H5'	2.12	0.50
1:A:853:G:O2'	1:A:854:G:H5'	2.11	0.50
1:A:942:G:C4	1:A:943:U:C5	2.99	0.50
1:A:1190:G:O2'	1:A:1191:A:P	2.69	0.50
3:C:112:SER:O	3:C:116:VAL:HG23	2.11	0.50
9:I:47:LEU:C	9:I:49:PRO:HD2	2.32	0.50
14:N:29:ARG:O	14:N:33:VAL:HG13	2.11	0.50
1:A:1035:A:H2'	1:A:1036:G:H8	1.76	0.50
1:A:1283:G:O2'	1:A:1284:C:H5'	2.11	0.50
2:B:33:TYR:HB3	2:B:41:ILE:HG22	1.93	0.50
2:B:53:ARG:HG2	2:B:53:ARG:HH11	1.76	0.50
2:B:88:ALA:O	2:B:90:MET:N	2.44	0.50
2:B:121:LEU:O	2:B:127:ILE:HG12	2.11	0.50
3:C:58:GLU:O	3:C:59:ARG:HG2	2.11	0.50
4:D:7:PRO:HB2	4:D:10:ARG:HD2	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:22:THR:OG1	14:N:33:VAL:HG21	2.11	0.50
21:V:6:ARG:HD2	21:V:15:ARG:NH1	2.25	0.50
1:A:659:U:O2'	1:A:660:G:H5'	2.11	0.50
1:A:824:C:H2'	1:A:825:G:H8	1.76	0.50
1:A:960:U:H1'	1:A:1223:C:H5'	1.93	0.50
1:A:1278:U:C5'	1:A:1279:A:O4'	2.59	0.50
1:A:1305:G:C8	1:A:1305:G:OP2	2.64	0.50
1:A:1310:G:O2'	1:A:1311:G:H5'	2.12	0.50
1:A:1392:G:O2'	1:A:1502:A:H5"	2.11	0.50
7:G:69:VAL:HG12	7:G:69:VAL:O	2.12	0.50
10:J:71:LEU:O	10:J:72:VAL:CB	2.60	0.50
12:L:46:LYS:HG2	12:L:47:LYS:HG3	1.93	0.50
13:M:78:ILE:HA	13:M:81:LEU:CD2	2.38	0.50
17:Q:27:PHE:HB2	17:Q:28:PRO:HD2	1.94	0.50
1:A:222:U:H2'	1:A:223:U:C6	2.47	0.50
1:A:576:G:N7	1:A:881:G:H1'	2.27	0.50
1:A:792:A:H4'	1:A:793:U:C5'	2.40	0.50
1:A:839:U:O2	1:A:839:U:C2'	2.59	0.50
1:A:999:C:H2'	1:A:1000:U:C6	2.46	0.50
1:A:1136:U:H5"	1:A:1137:C:OP2	2.12	0.50
1:A:1393:U:O4'	1:A:1502:A:H5'	2.11	0.50
1:A:1498:U:H4'	1:A:1519:A:C2	2.45	0.50
4:D:151:LYS:N	4:D:151:LYS:CD	2.75	0.50
10:J:3:LYS:HA	10:J:75:ILE:HA	1.94	0.50
13:M:77:ASN:O	13:M:80:ARG:HB3	2.10	0.50
1:A:187:C:N1	20:T:85:MET:HE1	2.25	0.50
1:A:325:A:H2'	1:A:326:G:O4'	2.12	0.50
1:A:1096:C:H2'	1:A:1097:C:H6	1.77	0.50
1:A:1179:A:H2'	1:A:1180:A:O4'	2.11	0.50
1:A:1305:G:C5'	21:V:4:GLY:HA3	2.41	0.50
2:B:44:LEU:HA	2:B:47:THR:OG1	2.12	0.50
2:B:186:ALA:HB3	2:B:197:VAL:CG1	2.41	0.50
2:B:221:LEU:O	2:B:221:LEU:HD13	2.11	0.50
3:C:79:ARG:HG2	3:C:82:GLU:HG2	1.92	0.50
3:C:178:LEU:O	3:C:179:ARG:CB	2.60	0.50
5:E:121:LYS:HE3	5:E:123:LEU:HD21	1.93	0.50
6:F:38:GLU:O	6:F:39:LYS:HB3	2.12	0.50
10:J:27:ALA:HB1	10:J:81:THR:HG23	1.92	0.50
12:L:45:PRO:HD3	12:L:51:ALA:O	2.11	0.50
1:A:556:C:C2'	1:A:557:G:H5'	2.40	0.50
1:A:746:A:O2'	1:A:747:C:H5'	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:177:THR:HG23	3:C:177:THR:O	2.10	0.50
4:D:3:ARG:NH2	4:D:74:GLN:OE1	2.43	0.50
4:D:126:ILE:CG2	4:D:127:THR:N	2.75	0.50
7:G:102:ARG:HG2	7:G:106:GLN:NE2	2.27	0.50
17:Q:45:HIS:NE2	17:Q:47:PRO:HG3	2.27	0.50
17:Q:97:SER:HB2	17:Q:103:GLY:N	2.26	0.50
1:A:217:C:O2'	1:A:218:C:H5'	2.12	0.50
1:A:933:G:N2	1:A:1385:G:C4	2.80	0.50
1:A:1057:G:H5"	3:C:154:SER:CB	2.30	0.50
1:A:1306:A:H2'	1:A:1307:U:O4'	2.12	0.50
2:B:132:LYS:O	2:B:136:VAL:HG23	2.12	0.50
8:H:113:SER:HB2	8:H:134:ILE:CD1	2.29	0.50
9:I:46:ALA:HA	9:I:78:LYS:HB2	1.93	0.50
20:T:101:GLY:O	20:T:102:GLY:O	2.30	0.50
1:A:136:C:H2'	1:A:137:C:H6	1.77	0.50
1:A:664:G:OP1	18:R:64:ARG:HD2	2.12	0.50
1:A:1025:U:OP1	1:A:1025:U:H4'	2.11	0.50
1:A:1044:A:H2'	1:A:1045:C:H5'	1.92	0.50
1:A:1256:A:C4'	1:A:1257:U:H5'	2.35	0.50
4:D:8:VAL:HG11	4:D:21:LEU:HB3	1.94	0.50
4:D:8:VAL:HG13	4:D:21:LEU:HD13	1.93	0.50
7:G:18:TYR:HD2	7:G:59:LEU:HD22	1.76	0.50
7:G:38:LEU:O	7:G:42:ILE:HG13	2.12	0.50
9:I:10:ARG:HG2	9:I:75:ASP:CB	2.41	0.50
11:K:23:ALA:CB	11:K:91:ARG:HB2	2.42	0.50
11:K:51:LYS:O	11:K:55:LYS:HE3	2.11	0.50
11:K:65:ALA:HB3	11:K:97:ALA:HB3	1.93	0.50
11:K:82:VAL:HG23	11:K:105:VAL:HG13	1.93	0.50
17:Q:10:VAL:O	17:Q:53:LEU:HD12	2.12	0.50
1:A:89:C:H2'	1:A:90:U:O4'	2.12	0.49
1:A:255:G:O6	1:A:266:G:O6	2.29	0.49
1:A:430:A:C2'	1:A:431:A:H5'	2.42	0.49
1:A:575:G:C4	1:A:881:G:C2	3.00	0.49
1:A:959:A:H2'	1:A:960:U:O4'	2.12	0.49
1:A:1074:G:O3'	2:B:103:THR:HG22	2.12	0.49
1:A:1181:G:O2'	1:A:1184:G:H5'	2.11	0.49
1:A:1499:A:O2'	1:A:1500:A:H5'	2.12	0.49
2:B:17:PHE:HD1	2:B:17:PHE:C	2.14	0.49
3:C:171:GLY:O	3:C:173:VAL:HG23	2.12	0.49
5:E:31:LEU:HD22	5:E:43:LEU:HD21	1.94	0.49
11:K:48:ILE:HD13	11:K:63:LEU:HB3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:28:LYS:HD2	12:L:33:ARG:CZ	2.42	0.49
14:N:15:LYS:HB3	14:N:16:PHE:CD1	2.47	0.49
15:O:3:ILE:CG2	15:O:7:GLU:HB3	2.41	0.49
1:A:204:U:H4'	1:A:216:G:O5'	2.12	0.49
1:A:625:G:H2'	1:A:626:U:C6	2.47	0.49
1:A:1085:U:O3'	1:A:1086:U:H6	1.95	0.49
1:A:1165:C:O2'	1:A:1166:G:H5'	2.13	0.49
3:C:6:HIS:ND1	3:C:8:ILE:HB	2.27	0.49
3:C:47:LEU:N	3:C:47:LEU:HD12	2.27	0.49
7:G:108:ALA:O	7:G:119:ARG:HB3	2.12	0.49
9:I:36:TYR:HD2	9:I:37:PHE:CE2	2.30	0.49
11:K:124:LYS:HD2	11:K:125:PHE:CE1	2.47	0.49
13:M:5:ALA:O	13:M:6:GLY:C	2.51	0.49
17:Q:26:GLN:O	17:Q:27:PHE:HB3	2.12	0.49
18:R:87:ARG:HG2	18:R:87:ARG:HH11	1.76	0.49
1:A:245:C:O2	1:A:283:C:N3	2.46	0.49
1:A:647:C:H2'	1:A:648:A:H8	1.78	0.49
1:A:665:A:H2'	1:A:732:C:O2	2.12	0.49
1:A:1172:C:O2'	1:A:1173:G:H5'	2.11	0.49
1:A:1301:U:O2'	1:A:1302:U:OP1	2.30	0.49
2:B:30:ARG:HG3	2:B:31:TYR:CD2	2.48	0.49
3:C:14:ILE:CG2	3:C:15:THR:H	2.11	0.49
3:C:38:ARG:HG3	3:C:38:ARG:NH1	2.26	0.49
3:C:172:ARG:HH12	3:C:174:PRO:CG	2.22	0.49
4:D:127:THR:CG2	4:D:128:VAL:N	2.75	0.49
8:H:38:ILE:N	8:H:38:ILE:HD12	2.27	0.49
10:J:60:ARG:O	10:J:61:GLU:CB	2.61	0.49
12:L:48:PRO:HG2	12:L:49:ASN:N	2.26	0.49
15:O:36:ILE:HA	15:O:59:MET:CE	2.42	0.49
1:A:521:G:O2'	1:A:522:C:H5'	2.12	0.49
1:A:1323:G:H2'	1:A:1324:A:C8	2.47	0.49
2:B:124:SER:CB	2:B:125:PRO:CD	2.90	0.49
3:C:167:TRP:O	3:C:168:ALA:HB3	2.11	0.49
1:A:129(A):G:O2'	1:A:130:A:OP2	2.28	0.49
1:A:190:C:H2'	1:A:190(A):C:H6	1.75	0.49
1:A:218:C:H2'	1:A:219:C:C6	2.47	0.49
1:A:761:G:H5"	17:Q:102:GLY:HA3	1.95	0.49
1:A:1102:A:H2'	1:A:1103:C:C6	2.47	0.49
1:A:1365:G:O2'	1:A:1366:C:H5'	2.12	0.49
3:C:180:ALA:O	3:C:181:ASN:CB	2.61	0.49
6:F:43:LEU:HD22	6:F:43:LEU:N	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:85:TYR:CD1	7:G:154:TYR:HE1	2.28	0.49
9:I:36:TYR:HE2	9:I:73:GLN:NE2	2.10	0.49
12:L:45:PRO:HB2	12:L:49:ASN:O	2.13	0.49
15:O:4:THR:HB	15:O:6:GLU:HG2	1.94	0.49
15:O:17:ARG:HG3	15:O:17:ARG:NH1	2.23	0.49
15:O:34:LEU:O	15:O:34:LEU:HD23	2.12	0.49
1:A:218:C:H2'	1:A:219:C:H6	1.76	0.49
1:A:489:C:H2'	1:A:490:G:H8	1.77	0.49
1:A:659:U:H2'	1:A:660:G:O4'	2.13	0.49
1:A:834:C:H2'	1:A:835:U:C6	2.48	0.49
1:A:1194:U:O2'	1:A:1195:C:H5'	2.12	0.49
1:A:1250:A:H2'	1:A:1251:A:C8	2.47	0.49
1:A:1366:C:C2	1:A:1367:C:C5	3.00	0.49
2:B:102:LEU:CD2	2:B:162:ILE:HD11	2.37	0.49
2:B:206:ASP:O	2:B:207:ALA:HB3	2.11	0.49
4:D:7:PRO:CG	4:D:10:ARG:HD2	2.43	0.49
13:M:94:ARG:CZ	19:S:81:ARG:HD3	2.43	0.49
16:P:42:ARG:O	16:P:43:LYS:C	2.51	0.49
1:A:149:A:H2'	1:A:150:C:C6	2.48	0.49
1:A:491:G:H2'	1:A:492:G:H8	1.77	0.49
1:A:1153:C:H2'	1:A:1154:G:C8	2.46	0.49
1:A:1503:A:O2'	1:A:1504:G:OP1	2.29	0.49
2:B:97:TRP:CH2	2:B:173:ALA:HA	2.47	0.49
4:D:38:TYR:CE1	4:D:45:GLN:HG3	2.48	0.49
4:D:78:LEU:HD22	4:D:96:LEU:HB3	1.94	0.49
5:E:36:ASP:O	5:E:37:ARG:HB2	2.13	0.49
6:F:100:ASN:O	18:R:28:GLU:HG3	2.13	0.49
7:G:85:TYR:HD1	7:G:154:TYR:CE1	2.27	0.49
17:Q:78:GLU:HG3	17:Q:78:GLU:O	2.12	0.49
18:R:34:TYR:HA	18:R:69:THR:HG23	1.93	0.49
1:A:1121:U:H2'	1:A:1122:U:C6	2.48	0.49
1:A:1162:C:H2'	1:A:1163:C:H6	1.78	0.49
1:A:1181:G:H4'	1:A:1184:G:H5'	1.94	0.49
1:A:1222:G:OP1	19:S:77:THR:HG21	2.13	0.49
1:A:1238:A:N7	1:A:1303:C:H1'	2.28	0.49
1:A:1279:A:O2'	1:A:1282:C:N4	2.46	0.49
2:B:168:THR:OG1	2:B:192:SER:HB3	2.12	0.49
4:D:119:GLN:CG	4:D:123:HIS:CE1	2.95	0.49
5:E:13:ILE:HG13	5:E:13:ILE:O	2.12	0.49
5:E:104:ALA:O	5:E:105:VAL:C	2.49	0.49
10:J:31:GLY:HA2	10:J:78:ASN:OD1	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:79:SER:OG	11:K:106:LYS:HG2	2.12	0.49
11:K:85:ARG:HH11	11:K:85:ARG:HG3	1.77	0.49
13:M:78:ILE:O	13:M:82:MET:HB2	2.12	0.49
20:T:54:LYS:HE3	20:T:100:ILE:HD11	1.94	0.49
1:A:346:G:H2'	1:A:347:G:H5'	1.94	0.49
1:A:393:A:C2	1:A:394:G:C8	3.00	0.49
1:A:586:C:O2'	1:A:587:G:H5'	2.13	0.49
1:A:760:G:C2	17:Q:104:LYS:O	2.66	0.49
1:A:760:G:O6	17:Q:105:ALA:CB	2.61	0.49
1:A:922:G:N2	1:A:1396:A:C5	2.80	0.49
1:A:1346:A:H1'	1:A:1348:U:C5	2.47	0.49
1:A:1404:C:C1'	1:A:1499:A:C2	2.96	0.49
3:C:116:VAL:O	3:C:119:ARG:HB3	2.13	0.49
3:C:139:GLN:O	3:C:143:GLU:N	2.37	0.49
3:C:191:THR:HG22	3:C:193:TYR:N	2.23	0.49
8:H:13:ILE:O	8:H:17:THR:HG23	2.13	0.49
8:H:65:TYR:HA	8:H:79:VAL:HG23	1.95	0.49
10:J:16:LEU:HD23	10:J:94:VAL:HG22	1.95	0.49
11:K:48:ILE:HD11	11:K:64:ALA:HA	1.95	0.49
16:P:51:VAL:O	16:P:51:VAL:CG1	2.60	0.49
18:R:41:LYS:O	18:R:41:LYS:HG2	2.13	0.49
25:Y:301:SFG:HB2	25:Y:301:SFG:H4'	1.95	0.49
1:A:178:C:O2'	1:A:179:A:H5'	2.13	0.49
1:A:220:G:O2'	1:A:221:C:H5'	2.12	0.49
1:A:265:G:O2'	1:A:266:G:H5'	2.13	0.49
1:A:1305:G:H22	1:A:1331:G:H2'	1.78	0.49
2:B:35:GLU:HA	2:B:39:ILE:O	2.13	0.49
8:H:60:ARG:HG3	8:H:60:ARG:NH1	2.28	0.49
8:H:103:VAL:CG2	8:H:110:ALA:HB2	2.43	0.49
15:O:30:ALA:HA	15:O:85:LEU:HD21	1.95	0.49
19:S:5:LEU:HD11	19:S:70:LYS:NZ	2.28	0.49
1:A:269:C:H2'	1:A:270:A:C8	2.48	0.48
1:A:722:A:H4'	1:A:723:U:C5	2.48	0.48
1:A:1505:G:C8	1:A:1505:G:H3'	2.48	0.48
10:J:38:ILE:HG13	10:J:71:LEU:CB	2.42	0.48
16:P:52:ASP:OD2	16:P:55:ARG:HB2	2.13	0.48
1:A:407:G:H5"	4:D:115:ARG:HB3	1.96	0.48
1:A:602:A:C2	1:A:637:G:C2	3.01	0.48
1:A:960:U:O2'	1:A:1223:C:H4'	2.13	0.48
1:A:974:A:OP2	14:N:41:ARG:NH1	2.45	0.48
1:A:1070:U:O2'	1:A:1071:C:H5'	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1230:C:O2'	1:A:1231:G:H5'	2.13	0.48
1:A:1369:C:H2'	1:A:1370:G:C8	2.48	0.48
2:B:97:TRP:CH2	2:B:176:GLU:CD	2.85	0.48
2:B:144:ARG:HG3	2:B:145:LEU:H	1.77	0.48
7:G:156:TRP:OXT	7:G:156:TRP:CD1	2.66	0.48
9:I:65:VAL:HG13	9:I:65:VAL:O	2.13	0.48
10:J:65:LEU:O	10:J:65:LEU:CD2	2.59	0.48
17:Q:68:ARG:O	17:Q:69:LYS:HB2	2.13	0.48
18:R:36:ASN:CG	18:R:39:VAL:HG12	2.34	0.48
1:A:279:A:H5"	1:A:280:C:H3'	1.94	0.48
1:A:624:C:O2'	1:A:625:G:H5'	2.13	0.48
1:A:1490:C:N4	1:A:1491:G:O6	2.45	0.48
2:B:25:ASN:O	2:B:27:LYS:N	2.47	0.48
2:B:188:ALA:O	2:B:202:PRO:HA	2.13	0.48
3:C:173:VAL:N	3:C:174:PRO:CD	2.76	0.48
10:J:27:ALA:C	10:J:29:ARG:H	2.15	0.48
10:J:32:ALA:HB2	10:J:76:ASN:HB2	1.94	0.48
1:A:61:G:H2'	1:A:62:U:O4'	2.12	0.48
1:A:1102:A:H2'	1:A:1103:C:H6	1.77	0.48
1:A:1129:C:O2'	1:A:1130:A:OP2	2.24	0.48
1:A:1298:C:C5	7:G:114:ARG:HD3	2.48	0.48
1:A:1347:G:N7	9:I:10:ARG:NH2	2.61	0.48
1:A:1407:C:O2'	1:A:1408:A:P	2.69	0.48
1:A:1410:G:OP1	22:Y:148:ALA:HB2	2.13	0.48
2:B:17:PHE:HA	2:B:44:LEU:HD21	1.96	0.48
4:D:36:ARG:N	4:D:37:PRO:CD	2.65	0.48
6:F:48:LEU:HD13	6:F:52:ILE:HG13	1.95	0.48
10:J:6:ILE:HG23	10:J:98:ILE:HG12	1.94	0.48
10:J:45:ARG:NH2	14:N:36:PHE:CD2	2.81	0.48
12:L:42:THR:CG2	12:L:52:LEU:HB3	2.44	0.48
12:L:83:VAL:HG21	12:L:100:ILE:HD13	1.95	0.48
17:Q:12:SER:HB3	17:Q:20:THR:HB	1.95	0.48
19:S:39:THR:HG22	19:S:40:ILE:N	2.28	0.48
20:T:38:LYS:O	20:T:39:LYS:C	2.51	0.48
1:A:184:G:H2'	1:A:185:A:H8	1.77	0.48
3:C:23:TYR:O	3:C:24:ALA:HB2	2.14	0.48
7:G:6:ARG:O	7:G:7:ALA:C	2.52	0.48
12:L:83:VAL:HG22	12:L:84:LEU:N	2.28	0.48
12:L:119:LYS:O	12:L:120:TYR:CB	2.61	0.48
15:O:25:THR:HG21	15:O:70:LEU:HD23	1.94	0.48
1:A:31:G:H1	1:A:48:C:H5"	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1342:C:O2'	1:A:1343:G:H5'	2.13	0.48
1:A:1533:C:O2'	1:A:1534:A:H5'	2.14	0.48
2:B:230:VAL:HG13	2:B:231:GLU:OE2	2.13	0.48
3:C:138:VAL:O	3:C:142:MET:HB2	2.13	0.48
12:L:110:VAL:O	12:L:122:THR:CG2	2.62	0.48
20:T:43:LEU:HD13	20:T:51:GLU:HG3	1.96	0.48
1:A:337:C:H2'	1:A:338:A:C8	2.49	0.48
1:A:538:G:O2'	1:A:539:A:H5'	2.13	0.48
1:A:555:C:H2'	1:A:556:C:C6	2.48	0.48
1:A:954:G:H2'	1:A:955:U:H6	1.78	0.48
1:A:1195:C:H2'	1:A:1197:G:H5'	1.96	0.48
1:A:1256:A:H8	3:C:27:LYS:HZ1	1.60	0.48
2:B:187:LEU:CD2	2:B:214:ILE:HG13	2.44	0.48
4:D:57:ARG:NH2	4:D:205:GLU:OE2	2.46	0.48
5:E:76:ILE:HD13	5:E:142:LEU:HD11	1.95	0.48
11:K:86:GLY:H	11:K:112:THR:HG23	1.79	0.48
18:R:39:VAL:HG13	18:R:40:LEU:N	2.28	0.48
1:A:926:G:H2'	1:A:1505:G:N3	2.28	0.48
1:A:1056:U:O2'	1:A:1057:G:H5'	2.14	0.48
1:A:1394:A:C6	1:A:1501:C:C5'	2.97	0.48
1:A:1422:G:C2'	1:A:1423:G:H5'	2.43	0.48
3:C:92:ALA:C	3:C:94:LEU:H	2.17	0.48
4:D:6:GLY:O	4:D:7:PRO:C	2.50	0.48
4:D:111:ALA:HB2	4:D:120:LEU:HD12	1.96	0.48
5:E:51:VAL:O	5:E:54:ALA:HB3	2.13	0.48
5:E:71:LEU:HD21	5:E:115:VAL:CG2	2.43	0.48
6:F:75:LEU:C	6:F:75:LEU:HD13	2.34	0.48
16:P:6:LEU:HB3	16:P:17:TYR:CD2	2.49	0.48
17:Q:17:LYS:HA	17:Q:46:ASP:O	2.14	0.48
18:R:28:GLU:OE1	18:R:28:GLU:N	2.46	0.48
20:T:89:ARG:HE	20:T:104:LEU:HD22	1.78	0.48
1:A:421:U:H5'	1:A:422:C:C5	2.48	0.48
1:A:731:G:H5'	1:A:766:A:H4'	1.94	0.48
1:A:780:A:C2	1:A:801:U:C5	3.02	0.48
1:A:922:G:H5'	5:E:19:MET:O	2.14	0.48
1:A:1497:G:H2'	1:A:1498:U:C5'	2.42	0.48
2:B:12:GLU:HG2	2:B:213:LEU:HD11	1.95	0.48
2:B:23:ARG:HH11	2:B:23:ARG:C	2.16	0.48
2:B:111:ARG:HB3	2:B:149:LEU:HD11	1.95	0.48
6:F:46:ARG:HB2	6:F:60:PHE:CE1	2.48	0.48
11:K:58:PRO:HB2	11:K:93:GLN:HG3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:53:ARG:HB3	12:L:93:LEU:HD11	1.94	0.48
17:Q:56:VAL:HG12	17:Q:77:VAL:HB	1.95	0.48
18:R:53:ARG:HD3	18:R:63:GLN:HB3	1.95	0.48
19:S:32:LYS:HG3	19:S:32:LYS:O	2.13	0.48
1:A:600:C:OP1	8:H:97:VAL:HG12	2.14	0.48
1:A:657:G:O2'	1:A:658:G:H5'	2.13	0.48
1:A:848:C:H2'	1:A:849:C:C6	2.49	0.48
1:A:1051:C:O2'	1:A:1052:U:H5'	2.13	0.48
1:A:1181:G:H4'	1:A:1184:G:C4'	2.43	0.48
2:B:213:LEU:C	2:B:213:LEU:CD2	2.82	0.48
4:D:3:ARG:O	4:D:5:ILE:HG13	2.13	0.48
5:E:148:VAL:O	5:E:152:ARG:HG3	2.14	0.48
7:G:64:GLN:O	7:G:67:GLU:HB3	2.14	0.48
10:J:39:PRO:HA	10:J:70:ARG:HH11	1.78	0.48
10:J:94:VAL:HG12	10:J:95:GLU:H	1.76	0.48
1:A:190(I):G:O2'	1:A:190(J):U:H5'	2.14	0.47
1:A:513:C:H2'	1:A:514:C:C6	2.49	0.47
1:A:625:G:H2'	1:A:626:U:H6	1.79	0.47
1:A:825:G:H2'	1:A:826:C:H6	1.78	0.47
1:A:1047:G:H5"	14:N:4:LYS:HD2	1.96	0.47
1:A:1127:G:N2	1:A:1147:C:N4	2.62	0.47
1:A:1347:G:H3'	9:I:108:VAL:O	2.14	0.47
4:D:200:GLU:OE1	4:D:200:GLU:N	2.46	0.47
9:I:111:ARG:HG3	9:I:111:ARG:NH1	2.28	0.47
1:A:528:C:H5'	1:A:535:A:C6	2.49	0.47
1:A:655:A:C2	1:A:754:C:C4	3.01	0.47
1:A:761:G:O4'	17:Q:103:GLY:O	2.31	0.47
9:I:117:HIS:HB2	9:I:121:ARG:HD2	1.95	0.47
18:R:47:THR:HA	18:R:83:GLU:HB2	1.97	0.47
20:T:59:ALA:O	20:T:63:ILE:HG13	2.14	0.47
1:A:613:C:O2'	1:A:614:A:H5'	2.14	0.47
1:A:1329:A:C2'	1:A:1330:U:H5'	2.43	0.47
2:B:108:ILE:O	2:B:108:ILE:HG22	2.13	0.47
2:B:115:LEU:O	2:B:115:LEU:HD12	2.13	0.47
4:D:43:HIS:CE1	4:D:46:LYS:HZ2	2.31	0.47
4:D:105:VAL:HG13	4:D:110:PHE:HB2	1.95	0.47
12:L:53:ARG:HG2	12:L:93:LEU:HD11	1.95	0.47
19:S:10:PHE:HE2	19:S:12:ASP:OD1	1.97	0.47
22:Y:196:LEU:O	22:Y:197:TRP:HB2	2.14	0.47
1:A:155:C:H2'	1:A:156:G:H8	1.79	0.47
1:A:1057:G:C2'	1:A:1058:G:H5'	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:75:LYS:HE3	2:B:78:GLN:OE1	2.14	0.47
3:C:8:ILE:O	3:C:11:ARG:N	2.47	0.47
3:C:35:GLU:O	3:C:38:ARG:N	2.47	0.47
3:C:100:ALA:O	3:C:101:LEU:HB2	2.14	0.47
4:D:174:LEU:O	4:D:175:SER:HB3	2.13	0.47
7:G:54:THR:HG22	7:G:56:GLN:H	1.79	0.47
12:L:34:ARG:HG3	12:L:34:ARG:O	2.13	0.47
12:L:86:ARG:HG3	12:L:86:ARG:NH1	2.28	0.47
14:N:12:ARG:O	14:N:13:THR:C	2.52	0.47
1:A:19:C:H2'	1:A:20:U:H6	1.80	0.47
1:A:41:G:H2'	1:A:42:G:C8	2.49	0.47
2:B:15:VAL:HG12	2:B:210:SER:HB2	1.97	0.47
7:G:21:VAL:HG23	7:G:22:LEU:N	2.29	0.47
7:G:77:SER:O	7:G:156:TRP:HZ3	1.98	0.47
10:J:27:ALA:HB2	10:J:85:LEU:HD21	1.96	0.47
10:J:30:SER:CB	10:J:80:LYS:HB3	2.45	0.47
13:M:39:ILE:CD1	13:M:56:LEU:HG	2.44	0.47
13:M:40:ASN:OD1	13:M:41:PRO:CD	2.62	0.47
1:A:51:A:H4'	1:A:52:G:C5'	2.45	0.47
1:A:518:C:HO2'	12:L:50:SER:HB3	1.79	0.47
1:A:560:U:O5'	1:A:560:U:H6	1.98	0.47
1:A:606:G:H2'	1:A:631:G:N2	2.30	0.47
1:A:768:A:H2'	1:A:769:G:O4'	2.14	0.47
1:A:927:G:H4'	1:A:1503:A:N7	2.29	0.47
1:A:1286:A:H5"	21:V:25:LYS:NZ	2.29	0.47
2:B:142:LEU:HD22	2:B:146:GLN:OE1	2.14	0.47
3:C:131:ARG:HA	3:C:134:ILE:HD12	1.96	0.47
3:C:167:TRP:HB3	3:C:168:ALA:H	1.32	0.47
5:E:127:ASN:O	5:E:128:PRO:C	2.53	0.47
6:F:4:TYR:CZ	6:F:72:VAL:HG21	2.49	0.47
6:F:53:ALA:C	6:F:55:ASP:H	2.18	0.47
7:G:23:VAL:HG12	7:G:27:ILE:CD1	2.41	0.47
9:I:111:ARG:HG3	9:I:111:ARG:HH11	1.80	0.47
1:A:51:A:H4'	1:A:52:G:O5'	2.15	0.47
1:A:435:C:O2'	1:A:436:C:H5'	2.15	0.47
1:A:998:G:O2'	1:A:999:C:H5'	2.15	0.47
1:A:1112:C:N3	3:C:178:LEU:N	2.62	0.47
1:A:1202:G:O4'	14:N:29:ARG:HD3	2.14	0.47
1:A:1231:G:H4'	9:I:126:SER:OG	2.14	0.47
1:A:1286:A:H2'	1:A:1287:A:H4'	1.96	0.47
1:A:1292:U:P	7:G:41:ARG:HH22	2.36	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1420:C:H2'	1:A:1421:G:C8	2.48	0.47
2:B:215:LEU:O	2:B:216:SER:C	2.52	0.47
3:C:79:ARG:HG2	3:C:82:GLU:CG	2.45	0.47
3:C:130:VAL:CG2	3:C:157:ILE:HG23	2.41	0.47
4:D:24:GLU:CG	4:D:25:ARG:N	2.77	0.47
7:G:46:ALA:O	7:G:50:ILE:HG13	2.15	0.47
10:J:94:VAL:CG1	10:J:95:GLU:N	2.77	0.47
11:K:72:ALA:HB1	11:K:77:MET:HG3	1.97	0.47
19:S:15:LEU:HD12	19:S:16:LEU:H	1.77	0.47
20:T:29:LYS:O	20:T:33:ILE:HG13	2.14	0.47
21:V:3:LYS:HB3	21:V:14:TRP:CD1	2.50	0.47
22:Y:141:TYR:N	22:Y:141:TYR:HD1	2.12	0.47
1:A:913:A:O2'	1:A:914:A:P	2.73	0.47
1:A:942:G:N3	1:A:943:U:C6	2.83	0.47
1:A:1123:A:O3'	10:J:36:GLY:HA3	2.14	0.47
1:A:1194:U:H2'	1:A:1195:C:C6	2.50	0.47
1:A:1367:C:H4'	10:J:48:THR:HG21	1.97	0.47
2:B:18:GLY:CA	2:B:41:ILE:HA	2.44	0.47
4:D:162:LEU:HD13	4:D:181:MET:CG	2.42	0.47
6:F:2:ARG:NE	6:F:69:GLU:HG2	2.29	0.47
14:N:53:LEU:HB3	14:N:56:VAL:CG2	2.45	0.47
19:S:15:LEU:O	19:S:19:VAL:N	2.48	0.47
22:Y:115:ILE:HB	22:Y:156:PRO:HG2	1.96	0.47
1:A:190(H):G:O2'	1:A:190(I):G:H5'	2.14	0.47
1:A:924:C:C4'	1:A:1399:C:OP2	2.63	0.47
1:A:1413:A:H2	1:A:1487:G:H22	1.63	0.47
1:A:1515:C:H2'	1:A:1516:G:C8	2.50	0.47
2:B:53:ARG:NH1	2:B:199:TYR:CD2	2.83	0.47
3:C:167:TRP:O	3:C:168:ALA:CB	2.63	0.47
6:F:2:ARG:HD2	6:F:69:GLU:HG2	1.96	0.47
10:J:22:LYS:HE2	10:J:90:LEU:HB2	1.97	0.47
11:K:80:VAL:HG21	11:K:103:LEU:HD13	1.97	0.47
15:O:77:ARG:O	15:O:80:ALA:HB3	2.15	0.47
16:P:43:LYS:HG2	16:P:48:TRP:CE2	2.50	0.47
22:Y:54:ILE:HG12	22:Y:83:VAL:HB	1.96	0.47
1:A:184:G:C4'	1:A:224:C:H4'	2.44	0.47
1:A:517:G:H5'	1:A:519:C:C2	2.50	0.47
1:A:951:G:O2'	1:A:952:U:H5'	2.15	0.47
1:A:1001:A:H2'	1:A:1002:G:H8	1.79	0.47
1:A:1245:A:H2'	1:A:1246:C:C6	2.50	0.47
2:B:50:GLU:HB3	2:B:200:ILE:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:74:GLY:CA	5:E:116:THR:HG22	2.43	0.47
11:K:110:ASP:OD2	18:R:88:LYS:NZ	2.45	0.47
12:L:54:LYS:N	12:L:54:LYS:HD2	2.30	0.47
17:Q:97:SER:O	17:Q:98:LEU:C	2.54	0.47
1:A:321:A:O2'	1:A:322:C:H5'	2.15	0.46
1:A:542:G:H2'	1:A:543:C:H6	1.80	0.46
1:A:633:G:H2'	1:A:634:C:C6	2.49	0.46
1:A:1232:U:H5"	9:I:124:GLN:O	2.14	0.46
1:A:1240:U:P	7:G:116:ALA:HB2	2.56	0.46
1:A:1326:C:H5"	21:V:12:LYS:NZ	2.30	0.46
1:A:1510:U:H2'	1:A:1511:G:C8	2.50	0.46
5:E:18:ARG:HG2	5:E:19:MET:H	1.81	0.46
5:E:107:ARG:HG2	5:E:108:ALA:N	2.29	0.46
13:M:82:MET:CE	13:M:92:HIS:HB3	2.44	0.46
17:Q:66:SER:OG	17:Q:69:LYS:HB3	2.15	0.46
1:A:538:G:P	12:L:115:LYS:HG3	2.55	0.46
1:A:781:A:H2'	1:A:782:A:H5'	1.98	0.46
1:A:952:U:O2'	1:A:953:G:H5'	2.14	0.46
1:A:1051:C:H2'	1:A:1052:U:H6	1.80	0.46
1:A:1238:A:H5'	1:A:1336:C:N4	2.29	0.46
1:A:1262:C:H2'	1:A:1263:C:H6	1.79	0.46
1:A:1277:C:C2'	1:A:1278:U:H5'	2.45	0.46
1:A:1320:C:H2'	1:A:1321:C:O4'	2.16	0.46
1:A:1490:C:C5'	1:A:1490:C:H6	2.28	0.46
2:B:15:VAL:CG1	2:B:209:ARG:HG3	2.46	0.46
3:C:173:VAL:O	3:C:173:VAL:HG12	2.14	0.46
4:D:111:ALA:HB1	4:D:116:GLN:HB3	1.96	0.46
9:I:48:GLU:N	9:I:49:PRO:CD	2.77	0.46
13:M:97:PRO:HB2	13:M:101:GLN:OE1	2.14	0.46
20:T:94:ALA:O	20:T:95:ALA:CB	2.63	0.46
1:A:582:U:C1'	17:Q:105:ALA:HA	2.44	0.46
1:A:976:G:C8	1:A:1358:U:C2	3.04	0.46
1:A:1404:C:O4'	1:A:1499:A:C2	2.69	0.46
1:A:1489:G:C3'	1:A:1490:C:H5"	2.45	0.46
2:B:129:GLU:O	2:B:130:ARG:HB2	2.15	0.46
3:C:64:VAL:CG2	3:C:99:VAL:HB	2.46	0.46
4:D:87:GLY:O	4:D:88:VAL:C	2.54	0.46
6:F:50:TYR:CE1	18:R:77:GLY:HA2	2.49	0.46
10:J:48:THR:OG1	10:J:62:HIS:CD2	2.68	0.46
10:J:96:ILE:CG2	10:J:97:GLU:H	2.25	0.46
12:L:48:PRO:CG	12:L:49:ASN:H	2.25	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:59:ARG:NH1	12:L:65:GLU:HG2	2.31	0.46
13:M:49:THR:CG2	13:M:51:ALA:H	2.13	0.46
13:M:62:ASN:O	13:M:63:THR:HB	2.16	0.46
15:O:66:LEU:O	15:O:69:TYR:HB3	2.15	0.46
1:A:41:G:H2'	1:A:42:G:H8	1.79	0.46
1:A:458:C:H2'	1:A:459:G:H8	1.80	0.46
1:A:1004:A:N6	1:A:1035:A:H62	2.13	0.46
1:A:1405:G:H1'	1:A:1519:A:O4'	2.16	0.46
2:B:42:ILE:HD12	2:B:203:GLY:HA2	1.98	0.46
4:D:39:PRO:HG2	4:D:44:GLY:HA2	1.97	0.46
7:G:15:ASP:O	7:G:19:GLY:HA2	2.16	0.46
7:G:135:VAL:O	7:G:139:GLU:HG3	2.15	0.46
12:L:60:LEU:HD21	12:L:66:VAL:HG22	1.97	0.46
17:Q:63:ARG:HG2	17:Q:64:PRO:HD2	1.97	0.46
1:A:5:U:O2'	1:A:6:G:P	2.73	0.46
1:A:92:C:O2'	1:A:93:G:H5'	2.15	0.46
1:A:518:C:H5"	1:A:519:C:H6	1.78	0.46
1:A:1301:U:O2'	1:A:1302:U:P	2.74	0.46
1:A:1442:G:N2	1:A:1446:A:C8	2.80	0.46
2:B:83:MET:HG3	2:B:238:LEU:CD1	2.46	0.46
5:E:144:THR:C	5:E:146:ALA:N	2.67	0.46
6:F:100:ASN:O	6:F:100:ASN:ND2	2.41	0.46
7:G:20:ASP:OD1	7:G:22:LEU:HB3	2.15	0.46
10:J:49:VAL:CG1	14:N:41:ARG:HB2	2.38	0.46
11:K:16:SER:O	11:K:35:PRO:HD3	2.16	0.46
11:K:50:TYR:HD1	11:K:60:ALA:HB2	1.80	0.46
11:K:59:TYR:O	11:K:62:GLN:HB3	2.15	0.46
12:L:37:CYS:O	12:L:79:GLU:O	2.34	0.46
16:P:20:VAL:CG1	16:P:21:VAL:N	2.76	0.46
18:R:59:SER:OG	18:R:62:GLU:HG3	2.15	0.46
19:S:22:LEU:CD1	19:S:31:ILE:HD11	2.46	0.46
20:T:67:ALA:O	20:T:73:HIS:ND1	2.47	0.46
1:A:129(A):G:O2'	1:A:190(E):U:H5"	2.16	0.46
1:A:377:G:P	16:P:3:LYS:HZ2	2.39	0.46
1:A:624:C:H2'	1:A:625:G:H8	1.81	0.46
1:A:707:C:OP1	11:K:85:ARG:NH1	2.49	0.46
1:A:1367:C:H5'	10:J:60:ARG:NH1	2.31	0.46
2:B:97:TRP:CH2	2:B:176:GLU:OE2	2.69	0.46
3:C:154:SER:OG	3:C:155:GLY:N	2.48	0.46
7:G:154:TYR:O	7:G:156:TRP:N	2.49	0.46
8:H:92:ARG:HG2	8:H:94:TYR:OH	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:33:PHE:CE2	9:I:47:LEU:HD11	2.51	0.46
11:K:34:ASP:O	11:K:36:ASP:N	2.48	0.46
11:K:84:VAL:HG23	11:K:109:VAL:O	2.16	0.46
12:L:46:LYS:O	12:L:47:LYS:C	2.54	0.46
13:M:40:ASN:OD1	13:M:41:PRO:HD2	2.15	0.46
13:M:46:LYS:HG3	13:M:47:ASP:N	2.30	0.46
19:S:18:LYS:HG2	19:S:18:LYS:O	2.15	0.46
1:A:279:A:C6	17:Q:98:LEU:HD13	2.51	0.46
1:A:390:C:H6	1:A:390:C:O5'	1.99	0.46
1:A:743:U:H2'	1:A:744:C:H6	1.79	0.46
1:A:828:A:H5"	1:A:859:A:C2	2.51	0.46
1:A:1171:G:H2'	1:A:1172:C:C6	2.51	0.46
1:A:1474:G:O2'	1:A:1475:G:H5'	2.16	0.46
2:B:16:HIS:CE1	2:B:210:SER:HG	2.34	0.46
2:B:78:GLN:O	2:B:94:ASN:OD1	2.33	0.46
4:D:162:LEU:HD13	4:D:181:MET:CE	2.46	0.46
4:D:173:TRP:CD2	4:D:189:PRO:HB3	2.51	0.46
5:E:78:HIS:CD2	8:H:107:LEU:HD12	2.51	0.46
6:F:44:GLY:HA2	6:F:59:TYR:CE1	2.50	0.46
10:J:24:VAL:CG1	10:J:28:ARG:HE	2.29	0.46
11:K:54:ARG:H	11:K:54:ARG:HG2	1.47	0.46
12:L:71:PRO:O	12:L:102:ARG:HD2	2.16	0.46
13:M:5:ALA:O	13:M:8:GLU:N	2.45	0.46
14:N:12:ARG:O	14:N:14:PRO:HD3	2.16	0.46
19:S:53:ASN:ND2	19:S:56:GLN:HB2	2.31	0.46
20:T:63:ILE:HG23	20:T:72:LEU:CD1	2.46	0.46
21:V:2:GLY:O	21:V:4:GLY:N	2.49	0.46
1:A:834:C:H2'	1:A:835:U:H6	1.79	0.46
1:A:1049:U:H4'	1:A:1050:G:OP2	2.16	0.46
1:A:1190:G:HO2'	1:A:1191:A:P	2.39	0.46
1:A:1221:G:O2'	1:A:1222:G:H5'	2.15	0.46
1:A:1238:A:OP1	1:A:1336:C:H5	1.98	0.46
1:A:1300:G:O2'	1:A:1301:U:P	2.73	0.46
3:C:21:ARG:NH2	3:C:56:ASP:OD2	2.48	0.46
3:C:23:TYR:CG	3:C:24:ALA:N	2.84	0.46
3:C:174:PRO:O	3:C:177:THR:HG22	2.15	0.46
5:E:121:LYS:HE3	5:E:123:LEU:CD2	2.46	0.46
8:H:23:SER:OG	8:H:60:ARG:HD2	2.15	0.46
9:I:50:LEU:C	9:I:52:ALA:N	2.69	0.46
9:I:97:LYS:HG3	9:I:102:LEU:HD12	1.96	0.46
10:J:62:HIS:CB	14:N:59:ALA:HB3	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:59:TYR:O	13:M:63:THR:HB	2.15	0.46
21:V:2:GLY:C	21:V:4:GLY:N	2.69	0.46
1:A:70:G:H2'	1:A:73:C:C6	2.51	0.46
1:A:132:C:O2'	1:A:133:U:H5'	2.15	0.46
1:A:458:C:H2'	1:A:459:G:O4'	2.16	0.46
1:A:1044:A:O2'	1:A:1045:C:H5'	2.15	0.46
1:A:1230:C:O2'	13:M:126:LYS:HA	2.16	0.46
1:A:1237:C:H2'	1:A:1336:C:C5	2.51	0.46
1:A:1309:G:N7	13:M:99:ARG:NH2	2.61	0.46
1:A:1405:G:H1'	1:A:1519:A:C1'	2.45	0.46
3:C:129:ALA:HB3	3:C:132:ARG:CD	2.45	0.46
3:C:164:ARG:HB3	3:C:164:ARG:HH11	1.81	0.46
4:D:145:GLU:HG2	4:D:184:LYS:HE2	1.96	0.46
7:G:107:ALA:O	7:G:110:GLN:HB2	2.16	0.46
8:H:116:LYS:NZ	8:H:127:LEU:HD12	2.31	0.46
9:I:48:GLU:OE1	9:I:48:GLU:HA	2.16	0.46
10:J:53:PRO:O	10:J:54:PHE:O	2.34	0.46
16:P:72:ARG:O	16:P:72:ARG:HG2	2.16	0.46
1:A:151:A:H2'	1:A:152:A:O4'	2.15	0.46
1:A:160:A:H1'	1:A:344:A:N7	2.32	0.46
1:A:421:U:H5'	1:A:422:C:H5	1.80	0.46
1:A:513:C:H2'	1:A:514:C:H6	1.80	0.46
1:A:1152:A:O2'	1:A:1153:C:H5'	2.16	0.46
1:A:1225:A:H5'	1:A:1226:C:OP2	2.16	0.46
1:A:1230:C:H2'	1:A:1231:G:H8	1.81	0.46
1:A:1390:U:H2'	1:A:1391:U:C6	2.51	0.46
1:A:1435:G:H2'	1:A:1436:U:H6	1.69	0.46
1:A:1461:G:O2'	1:A:1462:G:H5'	2.16	0.46
2:B:22:LYS:O	2:B:23:ARG:HG3	2.16	0.46
4:D:29:PRO:C	4:D:30:LYS:HG3	2.35	0.46
4:D:121:VAL:O	4:D:134:ASP:HA	2.16	0.46
4:D:152:SER:HA	4:D:155:LEU:HG	1.97	0.46
5:E:15:ARG:NE	5:E:26:PHE:CD2	2.84	0.46
6:F:19:LEU:C	6:F:19:LEU:HD23	2.36	0.46
8:H:6:ILE:HD12	8:H:35:ILE:HD12	1.97	0.46
1:A:690:G:H2'	1:A:691:G:O4'	2.15	0.45
1:A:909:A:H2'	1:A:910:C:O4'	2.16	0.45
1:A:975:A:H4'	1:A:976:G:H5'	1.97	0.45
1:A:1049:U:H1'	1:A:1201:A:N7	2.31	0.45
1:A:1515:C:H2'	1:A:1516:G:H8	1.81	0.45
1:A:1515:C:O2'	1:A:1516:G:H5'	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1532:U:O5'	1:A:1532:U:H6	1.99	0.45
2:B:52:GLU:O	2:B:56:ARG:HB2	2.17	0.45
3:C:131:ARG:O	3:C:135:LYS:HG3	2.16	0.45
5:E:21:ALA:C	5:E:23:GLY:H	2.19	0.45
8:H:45:ILE:O	8:H:45:ILE:HG13	2.16	0.45
9:I:85:LEU:O	9:I:92:TYR:CD1	2.69	0.45
12:L:38:THR:HG22	12:L:39:VAL:HG23	1.97	0.45
12:L:46:LYS:CG	12:L:47:LYS:H	2.29	0.45
13:M:37:THR:HG23	13:M:55:ARG:CB	2.46	0.45
17:Q:80:GLY:O	17:Q:81:ARG:HB3	2.15	0.45
1:A:877:C:H5"	8:H:88:LYS:HD3	1.97	0.45
1:A:882:C:O2'	1:A:883:C:H5'	2.16	0.45
1:A:947:G:H2'	1:A:948:C:O4'	2.15	0.45
1:A:1039:C:O2'	1:A:1040:U:H5'	2.16	0.45
1:A:1131:G:H2'	1:A:1132:C:C6	2.51	0.45
1:A:1256:A:O2'	1:A:1257:U:P	2.74	0.45
2:B:178:ARG:NH1	2:B:178:ARG:CG	2.67	0.45
3:C:99:VAL:CG2	3:C:100:ALA:N	2.80	0.45
4:D:157:LEU:HD22	4:D:161:ASN:OD1	2.16	0.45
9:I:112:LYS:C	9:I:112:LYS:HD3	2.37	0.45
10:J:4:ILE:HG12	10:J:100:THR:CB	2.47	0.45
13:M:49:THR:O	13:M:53:VAL:HG23	2.16	0.45
19:S:20:LEU:O	19:S:23:ASN:HB2	2.15	0.45
1:A:19:C:OP1	5:E:125:SER:OG	2.19	0.45
1:A:190(B):C:H2'	1:A:190(C):C:O4'	2.17	0.45
1:A:242:C:H2'	1:A:243:A:H5'	1.99	0.45
1:A:1019:C:O2'	1:A:1020:U:H5'	2.17	0.45
1:A:1202:G:C2'	1:A:1203:C:H5'	2.46	0.45
1:A:1216:G:H5"	14:N:5:ALA:HB2	1.99	0.45
1:A:1296:C:H4'	1:A:1302:U:C5	2.51	0.45
1:A:1300:G:O2'	1:A:1301:U:H6	1.98	0.45
5:E:15:ARG:CD	5:E:26:PHE:CD2	2.99	0.45
5:E:20:GLN:C	5:E:21:ALA:O	2.51	0.45
6:F:101:ALA:HB2	18:R:28:GLU:HB3	1.97	0.45
9:I:120:ARG:O	9:I:121:ARG:C	2.54	0.45
10:J:51:ARG:HG3	10:J:60:ARG:O	2.17	0.45
11:K:40:ILE:HG23	11:K:75:TYR:CE2	2.51	0.45
13:M:51:ALA:O	13:M:55:ARG:HG3	2.16	0.45
14:N:21:TYR:HE2	14:N:23:ARG:HE	1.63	0.45
14:N:39:LEU:CD1	14:N:47:LEU:HD12	2.47	0.45
19:S:63:THR:HG22	19:S:64:GLU:N	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:39:LYS:HD2	20:T:55:ILE:HD13	1.97	0.45
1:A:17:U:O2'	1:A:1079:G:H1'	2.16	0.45
1:A:28:G:O2'	1:A:296:U:OP1	2.33	0.45
1:A:58:C:O2'	1:A:59:A:H5'	2.16	0.45
1:A:575:G:C8	1:A:881:G:N2	2.85	0.45
1:A:686:U:O4	1:A:703:G:H1'	2.17	0.45
1:A:808:C:OP2	15:O:48:LYS:HE2	2.17	0.45
1:A:975:A:H4'	1:A:976:G:OP2	2.16	0.45
1:A:1158:C:N3	1:A:1181:G:N2	2.61	0.45
1:A:1250:A:H4'	9:I:68:GLY:CA	2.47	0.45
1:A:1318:A:H4'	19:S:10:PHE:CD1	2.51	0.45
1:A:1405:G:C2'	1:A:1518:A:O2'	2.65	0.45
5:E:102:ALA:HB2	5:E:120:THR:CB	2.46	0.45
5:E:115:VAL:HG11	5:E:118:ILE:CD1	2.46	0.45
7:G:77:SER:O	7:G:156:TRP:CZ3	2.69	0.45
10:J:8:LEU:HD12	10:J:20:ALA:HB2	1.97	0.45
10:J:54:PHE:O	10:J:55:LYS:HG2	2.17	0.45
12:L:117:ARG:HD2	12:L:122:THR:OG1	2.17	0.45
1:A:113:G:H1'	1:A:354:G:C5'	2.46	0.45
1:A:260:G:O2'	1:A:261:U:H5'	2.16	0.45
1:A:474:G:O2'	1:A:475:G:H5'	2.16	0.45
1:A:848:C:H2'	1:A:849:C:H6	1.80	0.45
1:A:920:U:H2'	1:A:921:U:C6	2.52	0.45
1:A:1196:U:H4'	1:A:1197:G:OP2	2.15	0.45
1:A:1206:G:C6	1:A:1207:G:C5	3.04	0.45
1:A:1501:C:OP2	1:A:1504:G:H2'	2.17	0.45
2:B:71:VAL:HB	2:B:164:VAL:HG23	1.99	0.45
2:B:137:ARG:O	2:B:140:HIS:HB2	2.16	0.45
2:B:223:ILE:HG21	2:B:230:VAL:HG23	1.99	0.45
3:C:157:ILE:HD11	3:C:166:GLU:HB2	1.97	0.45
3:C:188:LEU:O	3:C:189:ALA:CB	2.59	0.45
4:D:4:TYR:O	4:D:5:ILE:HB	2.17	0.45
4:D:142:PRO:HG2	4:D:187:ARG:NH1	2.32	0.45
9:I:19:LEU:C	9:I:20:ARG:HG3	2.37	0.45
13:M:84:ILE:C	13:M:86:CYS:N	2.70	0.45
14:N:26:ARG:NH1	14:N:47:LEU:HD21	2.32	0.45
18:R:74:ARG:HB3	18:R:81:PHE:CE1	2.51	0.45
19:S:67:VAL:O	19:S:69:HIS:N	2.49	0.45
1:A:411:A:C6	1:A:429:U:C4	3.04	0.45
1:A:533:A:O2'	1:A:534:U:P	2.75	0.45
1:A:820:U:H4'	1:A:821:G:OP2	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:826:C:H2'	1:A:827:U:H6	1.82	0.45
1:A:1044:A:H2'	1:A:1045:C:O4'	2.17	0.45
1:A:1254:C:OP1	10:J:45:ARG:HD3	2.16	0.45
2:B:100:GLY:O	2:B:104:ASN:N	2.45	0.45
5:E:45:PHE:CD2	5:E:47:LYS:HE3	2.52	0.45
6:F:33:TYR:HB2	6:F:75:LEU:HD23	1.98	0.45
9:I:36:TYR:CD2	9:I:37:PHE:CE2	3.04	0.45
14:N:25:VAL:O	14:N:25:VAL:HG13	2.16	0.45
20:T:50:GLU:C	20:T:100:ILE:HD12	2.36	0.45
1:A:319:G:O2'	1:A:320:C:H5'	2.16	0.45
1:A:439:A:C4	1:A:497:A:C2	3.05	0.45
1:A:627:G:O2'	1:A:628:G:H5'	2.17	0.45
1:A:797:C:OP1	11:K:124:LYS:HG3	2.17	0.45
1:A:976:G:C8	1:A:1358:U:O2	2.70	0.45
1:A:1108:G:H4'	1:A:1191:A:O4'	2.17	0.45
1:A:1305:G:N2	1:A:1331:G:C2'	2.79	0.45
1:A:1331:G:O2'	1:A:1332:A:OP2	2.31	0.45
2:B:69:LEU:C	2:B:69:LEU:HD23	2.36	0.45
3:C:12:LEU:HD23	3:C:12:LEU:HA	1.76	0.45
4:D:3:ARG:NE	4:D:71:SER:HB3	2.31	0.45
12:L:85:ILE:HG23	12:L:98:TYR:CB	2.46	0.45
14:N:12:ARG:O	14:N:14:PRO:CD	2.65	0.45
22:Y:150:ILE:HD13	22:Y:155:LEU:HD23	1.99	0.45
1:A:75:G:O2'	1:A:76:C:H5'	2.17	0.45
1:A:403:C:H2'	1:A:404:U:H6	1.81	0.45
1:A:1060:C:C4	3:C:2:GLY:HA3	2.52	0.45
1:A:1404:C:H2'	1:A:1405:G:C8	2.52	0.45
1:A:1408:A:C5	22:Y:107:TRP:CE3	3.05	0.45
1:A:1413:A:H2'	1:A:1414:U:O4'	2.16	0.45
2:B:23:ARG:CZ	2:B:23:ARG:HB2	2.47	0.45
3:C:108:ASN:OD1	3:C:110:ASN:HB2	2.16	0.45
5:E:102:ALA:HB2	5:E:120:THR:HB	1.97	0.45
7:G:18:TYR:CD2	7:G:59:LEU:HB2	2.52	0.45
9:I:40:LEU:O	9:I:42:ARG:N	2.50	0.45
9:I:121:ARG:HG2	9:I:121:ARG:HH11	1.81	0.45
17:Q:104:LYS:HB3	17:Q:105:ALA:H	1.48	0.45
18:R:47:THR:HG22	18:R:48:GLY:H	1.79	0.45
18:R:58:LEU:HD22	18:R:62:GLU:HB3	1.99	0.45
18:R:70:ILE:O	18:R:74:ARG:HG3	2.17	0.45
20:T:42:GLN:O	20:T:45:GLN:HB3	2.16	0.45
1:A:197:A:H1'	1:A:198:G:O4'	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:509:A:H5"	4:D:55:ALA:HB2	1.99	0.45
1:A:600:C:O2'	1:A:601:C:H5'	2.17	0.45
1:A:1044:A:H2'	1:A:1045:C:C4'	2.46	0.45
1:A:1450:U:H2'	1:A:1452:C:C5	2.52	0.45
2:B:195:ASP:O	8:H:74:PRO:HG3	2.16	0.45
3:C:60:ALA:O	3:C:61:ALA:CB	2.63	0.45
3:C:113:ALA:N	3:C:114:PRO:CD	2.80	0.45
7:G:38:LEU:HD11	7:G:42:ILE:HD11	1.99	0.45
9:I:103:THR:HG22	9:I:104:ARG:N	2.31	0.45
11:K:74:ALA:C	11:K:76:GLY:N	2.69	0.45
13:M:9:ILE:HD12	13:M:9:ILE:N	2.32	0.45
13:M:80:ARG:C	13:M:82:MET:H	2.20	0.45
14:N:29:ARG:HB3	14:N:40:CYS:HB3	1.99	0.45
15:O:48:LYS:O	15:O:50:HIS:N	2.50	0.45
17:Q:18:THR:HG23	17:Q:69:LYS:CE	2.47	0.45
1:A:258:G:H2'	1:A:259:G:H8	1.82	0.45
1:A:452:A:O2'	1:A:453:A:O4'	2.34	0.45
1:A:583:A:H2'	1:A:584:G:O4'	2.17	0.45
1:A:645:C:O2'	1:A:646:U:H5'	2.16	0.45
1:A:735:C:O2'	1:A:736:C:H5'	2.17	0.45
1:A:924:C:C5'	1:A:1399:C:OP2	2.63	0.45
1:A:1279:A:O2'	1:A:1281:U:OP2	2.33	0.45
1:A:1353:G:H2'	1:A:1354:C:H6	1.82	0.45
1:A:1391:U:H2'	1:A:1392:G:H8	1.74	0.45
4:D:78:LEU:HA	4:D:78:LEU:HD23	1.78	0.45
11:K:23:ALA:HB2	11:K:91:ARG:HB2	1.99	0.45
16:P:55:ARG:O	16:P:58:TYR:HB3	2.17	0.45
20:T:24:LEU:HD12	20:T:24:LEU:O	2.17	0.45
20:T:50:GLU:HG2	20:T:100:ILE:HG13	1.99	0.45
20:T:100:ILE:O	20:T:102:GLY:N	2.50	0.45
1:A:173:U:H5"	1:A:197:A:H5'	1.99	0.44
1:A:1074:G:O3'	2:B:103:THR:CG2	2.65	0.44
1:A:1372:U:O2'	1:A:1373:G:H5'	2.17	0.44
1:A:1408:A:H8	22:Y:146:GLU:OE2	2.00	0.44
1:A:1408:A:C8	22:Y:146:GLU:OE2	2.70	0.44
1:A:1503:A:O2'	1:A:1504:G:P	2.75	0.44
3:C:11:ARG:NH1	3:C:177:THR:O	2.50	0.44
5:E:13:ILE:HG22	5:E:30:ALA:HB2	1.99	0.44
6:F:40:VAL:CG2	6:F:41:GLU:N	2.80	0.44
10:J:27:ALA:CB	10:J:81:THR:HG23	2.48	0.44
13:M:84:ILE:HG21	19:S:65:ASN:HD22	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:81:ARG:HG3	17:Q:81:ARG:O	2.17	0.44
1:A:45:U:H2'	1:A:46:G:C8	2.53	0.44
1:A:384:G:H2'	1:A:385:C:C6	2.53	0.44
1:A:393:A:C2'	1:A:394:G:H5'	2.46	0.44
1:A:485:G:C2'	1:A:486:U:OP2	2.65	0.44
1:A:662:G:H2'	1:A:663:A:H8	1.79	0.44
1:A:691:G:O2'	1:A:797:C:H4'	2.17	0.44
1:A:865:A:H2'	1:A:866:C:C6	2.53	0.44
1:A:975:A:O5'	1:A:976:G:H5'	2.17	0.44
1:A:1128:C:O2'	1:A:1130:A:C8	2.62	0.44
1:A:1347:G:C5	9:I:107:ARG:NH1	2.86	0.44
2:B:92:TYR:CE1	2:B:151:GLY:HA3	2.51	0.44
4:D:8:VAL:HG21	4:D:115:ARG:CZ	2.46	0.44
7:G:12:LEU:HD12	7:G:12:LEU:N	2.32	0.44
10:J:8:LEU:CD1	10:J:20:ALA:HB2	2.48	0.44
12:L:28:LYS:C	12:L:30:ALA:N	2.70	0.44
13:M:34:LEU:HD13	13:M:41:PRO:CA	2.45	0.44
13:M:84:ILE:HG13	13:M:86:CYS:HB2	2.00	0.44
13:M:110:ARG:HG2	13:M:110:ARG:HH11	1.82	0.44
14:N:23:ARG:HD3	14:N:30:ALA:HB2	1.99	0.44
16:P:20:VAL:CG1	16:P:32:TYR:CB	2.95	0.44
22:Y:101:ILE:O	22:Y:135:PHE:HA	2.17	0.44
1:A:807:A:H2'	1:A:808:C:C6	2.52	0.44
1:A:981:U:H5'	14:N:21:TYR:CE1	2.53	0.44
1:A:1005:A:H2'	1:A:1006:C:O4'	2.17	0.44
1:A:1263:C:H2'	1:A:1264:C:H6	1.83	0.44
1:A:1319:A:H5"	19:S:5:LEU:HD21	1.98	0.44
2:B:54:THR:O	2:B:57:PHE:HB3	2.18	0.44
7:G:143:ARG:O	7:G:145:ALA:O	2.34	0.44
10:J:3:LYS:CA	10:J:75:ILE:HA	2.48	0.44
10:J:46:ARG:NH1	10:J:64:GLU:CG	2.80	0.44
10:J:68:HIS:N	10:J:68:HIS:CD2	2.85	0.44
14:N:9:LYS:HG3	14:N:21:TYR:O	2.17	0.44
15:O:87:ILE:CG2	15:O:88:ARG:N	2.80	0.44
20:T:30:LYS:O	20:T:33:ILE:HB	2.18	0.44
1:A:50:A:N6	1:A:361:G:H4'	2.33	0.44
1:A:129(A):G:C2	1:A:190(E):U:H5'	2.52	0.44
1:A:950:U:H2'	1:A:951:G:C8	2.52	0.44
3:C:28:GLN:O	3:C:31:HIS:N	2.46	0.44
4:D:24:GLU:CG	4:D:25:ARG:H	2.30	0.44
9:I:46:ALA:O	9:I:49:PRO:HD2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:6:ILE:O	10:J:71:LEU:O	2.35	0.44
11:K:51:LYS:O	11:K:55:LYS:CE	2.65	0.44
12:L:111:LYS:O	12:L:112:ASP:HB2	2.18	0.44
13:M:39:ILE:HD12	13:M:56:LEU:HG	1.98	0.44
16:P:20:VAL:HG13	16:P:21:VAL:N	2.32	0.44
1:A:321:A:H2'	1:A:322:C:C6	2.52	0.44
1:A:389:A:H2'	1:A:390:C:C5'	2.48	0.44
1:A:532:A:H2'	1:A:533:A:C5'	2.48	0.44
1:A:644:G:O2'	1:A:645:C:H5'	2.17	0.44
1:A:792:A:H1'	1:A:794:A:N7	2.31	0.44
1:A:1095:U:H2'	1:A:1096:C:H6	1.83	0.44
1:A:1152:A:H2'	1:A:1153:C:H6	1.82	0.44
1:A:1299:A:C8	1:A:1301:U:H1'	2.53	0.44
1:A:1404:C:C2	1:A:1499:A:N6	2.86	0.44
1:A:1421:G:O2'	1:A:1422:G:H5'	2.17	0.44
2:B:213:LEU:C	2:B:213:LEU:HD23	2.37	0.44
5:E:36:ASP:OD2	5:E:40:ARG:HD3	2.18	0.44
7:G:95:ARG:NH1	7:G:95:ARG:CG	2.79	0.44
8:H:91:ARG:CG	12:L:7:ILE:HG13	2.44	0.44
10:J:72:VAL:O	10:J:73:ASP:HB2	2.18	0.44
11:K:95:ILE:HD13	11:K:108:ILE:HG21	1.99	0.44
13:M:120:LYS:HE2	13:M:123:ALA:CB	2.47	0.44
17:Q:104:LYS:O	17:Q:105:ALA:CB	2.65	0.44
1:A:1178:G:P	9:I:97:LYS:HZ1	2.40	0.44
3:C:179:ARG:HD2	3:C:179:ARG:C	2.37	0.44
10:J:85:LEU:O	10:J:87:THR:N	2.50	0.44
16:P:43:LYS:HA	16:P:48:TRP:HB3	2.00	0.44
20:T:96:GLY:O	20:T:97:ALA:CB	2.66	0.44
22:Y:187:ASN:ND2	22:Y:206:LYS:HA	2.29	0.44
1:A:103:C:OP2	20:T:17:ARG:NH1	2.51	0.44
1:A:397:A:H3'	1:A:397:A:N3	2.32	0.44
1:A:460:A:N7	1:A:462:G:C6	2.86	0.44
1:A:755:G:OP2	15:O:65:ARG:HD2	2.17	0.44
1:A:962:C:H2'	1:A:963:G:O4'	2.18	0.44
1:A:1097:C:H2'	1:A:1098:C:H6	1.82	0.44
1:A:1288:A:O4'	1:A:1353:G:H4'	2.18	0.44
1:A:1289:A:H2'	1:A:1290:G:H5'	2.00	0.44
4:D:196:LEU:C	4:D:198:VAL:H	2.21	0.44
13:M:110:ARG:HH11	13:M:110:ARG:CG	2.31	0.44
20:T:42:GLN:HA	20:T:45:GLN:HB2	1.99	0.44
20:T:63:ILE:HD13	20:T:80:ARG:CB	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:540:G:H2'	1:A:541:G:O4'	2.18	0.44
1:A:677:U:O2	1:A:777:A:O2'	2.33	0.44
1:A:922:G:C2	1:A:1396:A:C5	3.05	0.44
1:A:922:G:O2'	1:A:1398:A:N1	2.45	0.44
1:A:953:G:H1'	13:M:125:ARG:HB3	1.99	0.44
1:A:1113:C:H1'	3:C:178:LEU:HD21	1.99	0.44
1:A:1440:C:H2'	1:A:1441:G:C5'	2.48	0.44
2:B:90:MET:HA	2:B:91:PRO:HD3	1.70	0.44
4:D:8:VAL:HG11	4:D:21:LEU:CB	2.47	0.44
7:G:78:ARG:HG2	7:G:80:VAL:HG23	1.99	0.44
7:G:108:ALA:O	7:G:119:ARG:HD2	2.18	0.44
8:H:7:ALA:HB2	8:H:85:ARG:HD2	1.99	0.44
8:H:73:ASP:OD2	8:H:75:ARG:HB2	2.18	0.44
8:H:103:VAL:HG21	8:H:109:ILE:O	2.18	0.44
9:I:93:ARG:CD	9:I:97:LYS:HE3	2.47	0.44
13:M:67:GLU:HB3	13:M:68:GLY:H	1.58	0.44
16:P:6:LEU:HB3	16:P:17:TYR:HD2	1.81	0.44
17:Q:68:ARG:H	17:Q:70:ARG:NH1	2.15	0.44
18:R:25:THR:O	18:R:25:THR:HG22	2.17	0.44
20:T:53:LEU:CD1	20:T:101:GLY:HA2	2.47	0.44
20:T:72:LEU:O	20:T:73:HIS:O	2.35	0.44
21:V:15:ARG:O	21:V:17:THR:HG23	2.18	0.44
22:Y:191:LYS:HE2	22:Y:203:PHE:CE1	2.53	0.44
1:A:116:A:H2'	1:A:117:G:O4'	2.18	0.44
1:A:1010:G:O2'	1:A:1011:G:H5'	2.18	0.44
1:A:1229:A:H2'	1:A:1230:C:H6	1.83	0.44
1:A:1314:C:OP2	19:S:6:LYS:CD	2.66	0.44
1:A:1533:C:O2	1:A:1533:C:H2'	2.17	0.44
3:C:79:ARG:C	3:C:81:GLY:H	2.21	0.44
7:G:138:LYS:HD3	7:G:138:LYS:C	2.38	0.44
16:P:39:TYR:CZ	16:P:41:PRO:HA	2.52	0.44
19:S:31:ILE:CG2	19:S:32:LYS:N	2.70	0.44
22:Y:155:LEU:HA	22:Y:156:PRO:HD3	1.53	0.44
1:A:253:U:H2'	1:A:254:G:C8	2.53	0.43
1:A:760:G:N2	17:Q:103:GLY:O	2.51	0.43
1:A:760:G:H1	17:Q:105:ALA:HB2	1.83	0.43
1:A:761:G:O2'	17:Q:104:LYS:HA	2.18	0.43
1:A:1314:C:H2'	1:A:1315:U:C6	2.52	0.43
2:B:92:TYR:CD1	2:B:151:GLY:HA3	2.53	0.43
4:D:31:CYS:C	4:D:33:MET:H	2.21	0.43
6:F:22:GLU:OE2	6:F:84:ASN:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:69:GLY:O	9:I:73:GLN:HG3	2.18	0.43
15:O:29:VAL:HG11	15:O:67:LEU:HD21	2.00	0.43
1:A:718:G:C8	11:K:116:HIS:HB3	2.53	0.43
1:A:1031:G:H2'	1:A:1032:G:H8	1.83	0.43
1:A:1131:G:H2'	1:A:1132:C:H6	1.82	0.43
1:A:1231:G:OP1	9:I:127:LYS:NZ	2.50	0.43
1:A:1525:G:P	11:K:120:ARG:HH22	2.40	0.43
4:D:10:ARG:HH11	4:D:10:ARG:HG3	1.83	0.43
4:D:24:GLU:HG2	4:D:25:ARG:H	1.81	0.43
4:D:55:ALA:O	4:D:59:ARG:HG2	2.19	0.43
9:I:78:LYS:HE2	9:I:78:LYS:HB3	1.87	0.43
10:J:75:ILE:HG22	10:J:76:ASN:N	2.33	0.43
11:K:85:ARG:HG3	11:K:85:ARG:NH1	2.33	0.43
11:K:100:ALA:O	11:K:102:GLY:N	2.51	0.43
12:L:115:LYS:O	12:L:117:ARG:N	2.37	0.43
15:O:54:ARG:O	15:O:58:MET:HG3	2.17	0.43
18:R:37:VAL:O	18:R:41:LYS:HB3	2.18	0.43
20:T:57:ARG:HE	20:T:100:ILE:CG2	2.31	0.43
1:A:409:G:OP1	4:D:24:GLU:O	2.36	0.43
1:A:1305:G:N2	1:A:1331:G:HO2'	2.16	0.43
2:B:83:MET:HG3	2:B:238:LEU:HD11	2.00	0.43
3:C:19:GLU:HB3	3:C:40:ARG:NH2	2.25	0.43
3:C:99:VAL:HG22	3:C:100:ALA:O	2.18	0.43
4:D:178:VAL:O	4:D:178:VAL:HG12	2.18	0.43
4:D:198:VAL:HG12	4:D:199:ASN:N	2.33	0.43
5:E:80:ILE:CD1	5:E:91:LEU:HD12	2.46	0.43
7:G:24:THR:HA	7:G:27:ILE:HD12	2.00	0.43
7:G:112:PRO:O	7:G:113:GLU:C	2.57	0.43
11:K:50:TYR:N	11:K:50:TYR:CD2	2.84	0.43
11:K:60:ALA:O	11:K:61:ALA:C	2.56	0.43
12:L:70:ILE:CD1	12:L:77:LEU:HD12	2.42	0.43
16:P:20:VAL:HG13	16:P:32:TYR:HB2	2.00	0.43
16:P:67:THR:CG2	16:P:68:ASP:N	2.81	0.43
18:R:26:LEU:HD21	18:R:39:VAL:HG23	2.00	0.43
1:A:16:A:O2'	1:A:17:U:H5'	2.18	0.43
1:A:80:G:C2'	1:A:81:U:H5"	2.48	0.43
1:A:143:A:H2	1:A:220:G:H22	1.66	0.43
1:A:267:C:H2'	1:A:268:C:C6	2.53	0.43
1:A:363:A:O2'	1:A:364:A:H5'	2.19	0.43
1:A:430:A:H2'	1:A:431:A:H5'	1.99	0.43
1:A:640:A:C2'	1:A:641:U:H5'	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:838:G:C3'	1:A:839:U:H5"	2.48	0.43
1:A:1051:C:H2'	1:A:1052:U:C6	2.53	0.43
1:A:1053:G:O2'	1:A:1199:U:H5	2.01	0.43
1:A:1497:G:C2'	1:A:1498:U:C5'	2.87	0.43
3:C:134:ILE:HG22	3:C:168:ALA:CB	2.48	0.43
3:C:188:LEU:HD22	3:C:188:LEU:HA	1.79	0.43
8:H:16:ALA:O	8:H:21:LYS:HG2	2.18	0.43
10:J:56:HIS:O	10:J:58:ASP:N	2.52	0.43
12:L:7:ILE:O	12:L:11:VAL:HG23	2.18	0.43
12:L:60:LEU:CD2	12:L:66:VAL:HG22	2.49	0.43
16:P:75:ARG:O	16:P:78:GLY:N	2.49	0.43
18:R:46:GLU:CD	18:R:46:GLU:N	2.72	0.43
22:Y:15:ASP:O	22:Y:19:GLU:HG2	2.17	0.43
22:Y:115:ILE:HG13	22:Y:116:LYS:N	2.33	0.43
1:A:383:A:H2'	1:A:384:G:H5'	1.99	0.43
1:A:436:C:H2'	1:A:437:U:C6	2.53	0.43
1:A:502:G:C1'	1:A:550:G:H5'	2.49	0.43
1:A:961:U:C2'	1:A:962:C:H5'	2.48	0.43
1:A:1286:A:H5"	21:V:25:LYS:HZ2	1.83	0.43
1:A:1286:A:H4'	21:V:25:LYS:HE3	2.01	0.43
2:B:74:LYS:HD2	2:B:166:ASP:HB2	2.00	0.43
2:B:134:GLU:C	2:B:136:VAL:N	2.71	0.43
3:C:7:PRO:HG2	3:C:184:TYR:CB	2.45	0.43
7:G:75:VAL:HG13	7:G:86:GLN:HB3	1.95	0.43
8:H:86:ILE:HD12	8:H:133:LEU:HD22	2.00	0.43
16:P:52:ASP:O	16:P:52:ASP:CG	2.57	0.43
19:S:12:ASP:HB2	19:S:35:SER:OG	2.19	0.43
1:A:254:G:O2'	1:A:255:G:H5'	2.18	0.43
1:A:718:G:H1'	11:K:116:HIS:HA	2.00	0.43
1:A:765:G:N2	1:A:812:C:O2'	2.51	0.43
1:A:851:G:H2'	1:A:852:G:H8	1.84	0.43
1:A:1152:A:OP1	10:J:13:HIS:HB2	2.18	0.43
1:A:1346:A:C4	7:G:10:ARG:CZ	3.02	0.43
2:B:17:PHE:H	2:B:44:LEU:HD21	1.83	0.43
2:B:41:ILE:O	2:B:41:ILE:HG22	2.19	0.43
3:C:116:VAL:HG11	3:C:141:VAL:HG21	2.01	0.43
3:C:188:LEU:HD13	3:C:189:ALA:H	1.84	0.43
9:I:106:ALA:O	9:I:108:VAL:HG23	2.19	0.43
10:J:46:ARG:HH11	10:J:64:GLU:CG	2.31	0.43
13:M:23:TYR:CE2	13:M:70:LEU:HD13	2.54	0.43
15:O:17:ARG:HH11	15:O:17:ARG:CG	2.25	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:41:GLU:O	15:O:42:HIS:C	2.57	0.43
17:Q:97:SER:O	17:Q:98:LEU:HD12	2.19	0.43
19:S:3:ARG:O	19:S:4:SER:HB3	2.18	0.43
19:S:41:VAL:HG22	19:S:44:MET:HE2	2.00	0.43
1:A:433:C:O2'	1:A:434:U:H5'	2.19	0.43
1:A:935:A:H1'	1:A:1384:C:N3	2.33	0.43
1:A:1460:A:P	20:T:27:LYS:HZ1	2.42	0.43
2:B:28:PHE:CD2	2:B:190:THR:HA	2.54	0.43
2:B:119:GLU:OE1	2:B:153:ARG:NH2	2.51	0.43
3:C:191:THR:HB	3:C:194:GLY:O	2.18	0.43
5:E:105:VAL:HB	5:E:106:PRO:CD	2.40	0.43
5:E:118:ILE:CG2	5:E:119:LEU:H	2.28	0.43
15:O:78:TYR:CE2	15:O:82:ILE:HD11	2.53	0.43
1:A:359:U:O2'	1:A:360:A:H5'	2.18	0.43
1:A:448:A:C4	1:A:487:A:C2	3.07	0.43
1:A:730:G:C5	1:A:731:G:H1'	2.54	0.43
1:A:913:A:O2'	1:A:914:A:OP2	2.36	0.43
1:A:1135:U:H6	1:A:1135:U:O5'	2.01	0.43
2:B:146:GLN:O	2:B:150:SER:HB3	2.18	0.43
4:D:25:ARG:HH21	4:D:30:LYS:HD3	1.82	0.43
4:D:127:THR:HG23	4:D:128:VAL:N	2.34	0.43
5:E:24:ARG:HG2	5:E:24:ARG:NH1	2.32	0.43
5:E:143:ARG:HD3	5:E:143:ARG:HA	1.71	0.43
6:F:77:ARG:O	6:F:81:ILE:HG13	2.18	0.43
15:O:39:LEU:HD12	15:O:59:MET:CE	2.48	0.43
16:P:40:ASP:HB3	16:P:48:TRP:HB2	2.00	0.43
19:S:40:ILE:HG23	19:S:44:MET:SD	2.59	0.43
20:T:63:ILE:HD13	20:T:80:ARG:HB3	2.01	0.43
1:A:137:C:O2'	1:A:138:G:H5'	2.18	0.43
1:A:157:G:O2'	1:A:158:G:H5'	2.18	0.43
1:A:487:A:H2'	1:A:488:C:O4'	2.19	0.43
1:A:628:G:H2'	1:A:629:G:H8	1.84	0.43
1:A:719:C:O2	18:R:50:ILE:HG13	2.19	0.43
1:A:1126:U:H2'	1:A:1127:G:O4'	2.18	0.43
1:A:1262:C:H2'	1:A:1263:C:C6	2.54	0.43
1:A:1394:A:N6	1:A:1501:C:C5'	2.82	0.43
1:A:1397:C:O2'	1:A:1398:A:P	2.77	0.43
1:A:1441:G:H4'	1:A:1442:G:C8	2.54	0.43
3:C:70:VAL:HG12	3:C:71:ALA:H	1.84	0.43
3:C:191:THR:HG21	3:C:193:TYR:CE1	2.53	0.43
3:C:193:TYR:HE1	3:C:196:LEU:HD11	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:120:LEU:HD23	4:D:125:HIS:CD2	2.54	0.43
6:F:75:LEU:O	6:F:75:LEU:HD13	2.18	0.43
8:H:68:ARG:HG2	8:H:68:ARG:HH11	1.84	0.43
9:I:97:LYS:HB2	9:I:98:PRO:HD3	2.01	0.43
13:M:33:ALA:HB2	13:M:64:TRP:CH2	2.54	0.43
14:N:14:PRO:O	14:N:16:PHE:N	2.44	0.43
16:P:4:ILE:HG23	16:P:36:ILE:HD11	2.01	0.43
16:P:39:TYR:CD2	16:P:73:LEU:HD11	2.54	0.43
17:Q:60:ILE:HD13	17:Q:61:GLU:N	2.34	0.43
19:S:25:LYS:HD2	19:S:25:LYS:N	2.34	0.43
19:S:41:VAL:HG22	19:S:44:MET:CE	2.49	0.43
20:T:84:LEU:O	20:T:84:LEU:HD22	2.18	0.43
1:A:247:G:OP2	17:Q:100:LYS:HG3	2.19	0.43
1:A:370:C:C2'	1:A:371:G:H5'	2.48	0.43
1:A:451:A:N6	1:A:480:U:H2'	2.33	0.43
1:A:522:C:O2'	1:A:523:A:H5'	2.19	0.43
1:A:647:C:H2'	1:A:648:A:C8	2.54	0.43
1:A:782:A:H2'	1:A:783:C:O4'	2.19	0.43
1:A:991:U:O2	1:A:993:G:H8	2.02	0.43
1:A:1064:G:H1'	1:A:1190:G:H21	1.84	0.43
1:A:1125:U:H5"	1:A:1126:U:H5	1.83	0.43
1:A:1270:C:H4'	1:A:1313:U:O2'	2.19	0.43
1:A:1331:G:O2'	1:A:1332:A:P	2.76	0.43
1:A:1504:G:OP1	1:A:1507:A:H4'	2.19	0.43
2:B:130:ARG:HH22	3:C:207:VAL:HG22	1.82	0.43
3:C:134:ILE:HD13	3:C:166:GLU:HB3	2.01	0.43
5:E:16:THR:HG23	5:E:27:ARG:O	2.18	0.43
5:E:80:ILE:HD12	5:E:80:ILE:H	1.84	0.43
12:L:33:ARG:HD2	12:L:62:SER:HB3	2.01	0.43
22:Y:124:ASN:O	22:Y:127:ASP:HB2	2.19	0.43
1:A:176:C:H2'	1:A:177:C:H6	1.83	0.42
1:A:518:C:O2'	12:L:50:SER:HB3	2.18	0.42
1:A:858:G:O2'	1:A:859:A:H5'	2.18	0.42
1:A:1230:C:H1'	13:M:125:ARG:O	2.19	0.42
1:A:1376:U:H2'	1:A:1377:A:H8	1.80	0.42
1:A:1404:C:O4'	1:A:1499:A:N1	2.52	0.42
1:A:1438:G:H2'	1:A:1439:C:C6	2.54	0.42
2:B:59:GLU:O	2:B:60:ASP:C	2.57	0.42
2:B:125:PRO:C	2:B:127:ILE:H	2.22	0.42
4:D:158:ILE:CG2	4:D:181:MET:HE2	2.45	0.42
10:J:55:LYS:O	10:J:56:HIS:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:45:HIS:CD2	17:Q:47:PRO:HG3	2.54	0.42
19:S:20:LEU:HD12	19:S:21:GLU:N	2.34	0.42
22:Y:140:THR:HG21	22:Y:209:PHE:CE1	2.54	0.42
1:A:160:A:H2'	1:A:161:A:O4'	2.18	0.42
1:A:418:C:H2'	1:A:419:C:H6	1.84	0.42
1:A:512:U:H1'	4:D:42:GLN:OE1	2.19	0.42
1:A:636:U:H2'	1:A:637:G:C8	2.54	0.42
1:A:1004:A:H5"	1:A:1025:U:C4	2.53	0.42
1:A:1305:G:H22	1:A:1331:G:C2'	2.33	0.42
5:E:40:ARG:NH1	5:E:68:GLU:OE1	2.51	0.42
5:E:115:VAL:CG1	5:E:116:THR:N	2.82	0.42
6:F:30:LEU:HB3	6:F:35:ALA:CB	2.41	0.42
9:I:78:LYS:HD3	9:I:101:PHE:CD2	2.54	0.42
17:Q:59:ILE:CG2	17:Q:71:PHE:CD1	3.02	0.42
20:T:53:LEU:HD13	20:T:101:GLY:C	2.39	0.42
1:A:413:G:N2	1:A:428:G:H1'	2.34	0.42
1:A:640:A:O2'	1:A:641:U:H5'	2.20	0.42
1:A:960:U:O2	1:A:960:U:H2'	2.18	0.42
1:A:994:A:N7	1:A:1216:G:H4'	2.35	0.42
1:A:1157:A:O4'	1:A:1158:C:C2	2.72	0.42
2:B:8:LYS:O	2:B:9:GLU:CB	2.60	0.42
3:C:11:ARG:O	3:C:14:ILE:O	2.36	0.42
5:E:80:ILE:HD12	5:E:91:LEU:HB2	2.00	0.42
7:G:31:MET:SD	7:G:34:GLY:HA2	2.60	0.42
7:G:65:ALA:O	7:G:66:VAL:C	2.58	0.42
10:J:17:ASP:O	10:J:21:GLN:HB2	2.19	0.42
11:K:21:ILE:HD12	11:K:95:ILE:HG12	2.00	0.42
11:K:104:GLN:OE1	11:K:106:LYS:HE2	2.19	0.42
12:L:26:ALA:C	12:L:27:LEU:O	2.58	0.42
13:M:96:LEU:HB3	13:M:97:PRO:HD2	2.00	0.42
22:Y:146:GLU:O	22:Y:149:GLU:HG2	2.20	0.42
1:A:173:U:C5'	1:A:197:A:O4'	2.65	0.42
1:A:243:A:N6	1:A:281:G:O2'	2.51	0.42
1:A:545:C:O2'	1:A:549:C:OP1	2.37	0.42
1:A:1057:G:H4'	3:C:197:GLY:H	1.85	0.42
1:A:1104:G:OP1	2:B:111:ARG:HD2	2.18	0.42
1:A:1126:U:H2'	1:A:1127:G:H8	1.84	0.42
1:A:1353:G:H2'	1:A:1354:C:C6	2.54	0.42
3:C:50:ALA:O	3:C:70:VAL:CG1	2.67	0.42
6:F:19:LEU:HD21	6:F:23:LYS:HD2	2.02	0.42
7:G:38:LEU:HD12	7:G:42:ILE:HG13	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:33:THR:OG1	11:K:37:GLY:C	2.58	0.42
15:O:39:LEU:HD12	15:O:59:MET:HE2	2.01	0.42
19:S:41:VAL:HB	19:S:43:GLU:OE2	2.20	0.42
22:Y:113:TYR:CD2	22:Y:121:ILE:HG21	2.55	0.42
1:A:409:G:H2'	1:A:410:G:O4'	2.18	0.42
1:A:833:U:H2'	1:A:834:C:C6	2.55	0.42
1:A:839:U:C5'	1:A:840:C:H5	2.27	0.42
1:A:932:C:C2	1:A:1386:G:C2	3.08	0.42
1:A:1060:C:O2'	1:A:1061:G:H5'	2.18	0.42
1:A:1091:U:O2	1:A:1093:A:H8	2.02	0.42
1:A:1181:G:O2'	1:A:1182:G:H5'	2.19	0.42
1:A:1217:C:O2'	1:A:1218:C:H5'	2.19	0.42
1:A:1244:C:O2'	1:A:1245:A:H5'	2.19	0.42
1:A:1288:A:H1'	1:A:1353:G:O4'	2.19	0.42
1:A:1487:G:C2'	1:A:1488:G:H5'	2.50	0.42
4:D:8:VAL:CG1	4:D:21:LEU:HD13	2.49	0.42
7:G:155:ARG:O	7:G:156:TRP:CB	2.64	0.42
10:J:32:ALA:HB2	10:J:75:ILE:O	2.19	0.42
11:K:57:THR:OG1	11:K:58:PRO:HD2	2.20	0.42
1:A:80:G:H2'	1:A:81:U:H5"	2.01	0.42
1:A:162:A:H2'	1:A:163:C:O4'	2.20	0.42
1:A:576:G:C6	1:A:881:G:O4'	2.73	0.42
1:A:815:A:N3	1:A:1527:C:O2'	2.44	0.42
1:A:1129:C:O2'	1:A:1130:A:P	2.78	0.42
1:A:1202:G:C2	14:N:42:ILE:HG21	2.55	0.42
1:A:1327:C:O2'	1:A:1328:C:H5'	2.19	0.42
1:A:1346:A:C8	7:G:10:ARG:NH2	2.87	0.42
2:B:187:LEU:HD21	2:B:214:ILE:HG13	2.00	0.42
3:C:64:VAL:HG12	3:C:65:ALA:H	1.84	0.42
4:D:25:ARG:HA	4:D:28:SER:OG	2.19	0.42
4:D:163:GLU:C	4:D:165:MET:N	2.72	0.42
6:F:40:VAL:HG22	6:F:41:GLU:N	2.34	0.42
8:H:75:ARG:HA	8:H:76:PRO:HD3	1.70	0.42
10:J:12:ASP:OD1	10:J:14:LYS:N	2.50	0.42
13:M:7:VAL:O	13:M:7:VAL:HG23	2.18	0.42
16:P:51:VAL:O	16:P:52:ASP:C	2.58	0.42
22:Y:92:PHE:CD1	22:Y:95:LYS:HD2	2.55	0.42
1:A:169:C:O2'	1:A:170:U:H5'	2.19	0.42
1:A:397:A:H5'	1:A:398:C:P	2.60	0.42
1:A:825:G:H2'	1:A:826:C:C6	2.53	0.42
2:B:17:PHE:CA	2:B:44:LEU:HD21	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:70:ILE:HD11	4:D:100:ARG:CD	2.49	0.42
8:H:114:THR:C	8:H:116:LYS:H	2.22	0.42
8:H:126:LYS:C	8:H:128:GLY:N	2.73	0.42
12:L:41:ARG:CB	12:L:41:ARG:NH1	2.82	0.42
13:M:80:ARG:C	13:M:82:MET:N	2.73	0.42
15:O:38:ARG:O	15:O:41:GLU:HB3	2.20	0.42
18:R:44:LEU:HD23	18:R:44:LEU:HA	1.89	0.42
20:T:11:SER:C	20:T:13:LEU:H	2.22	0.42
20:T:42:GLN:O	20:T:46:GLU:HG3	2.19	0.42
21:V:9:ARG:HH11	21:V:22:ARG:HA	1.85	0.42
1:A:418:C:H2'	1:A:419:C:C6	2.54	0.42
1:A:502:G:H2'	1:A:503:C:H6	1.84	0.42
1:A:974:A:P	14:N:41:ARG:HH12	2.42	0.42
1:A:1271:G:H5'	1:A:1314:C:OP1	2.20	0.42
1:A:1306:A:O2'	13:M:109:THR:HG21	2.19	0.42
3:C:23:TYR:OH	10:J:9:ARG:HD3	2.20	0.42
9:I:56:LEU:O	9:I:58:HIS:N	2.49	0.42
12:L:41:ARG:HB3	12:L:41:ARG:HH11	1.84	0.42
13:M:46:LYS:HB2	13:M:46:LYS:HE3	1.86	0.42
1:A:145:G:O2'	1:A:146:G:H5'	2.20	0.42
1:A:252:U:O2'	1:A:275:G:N2	2.53	0.42
1:A:584:G:H2'	1:A:585:G:C8	2.54	0.42
1:A:930:C:O2'	1:A:931:C:H5'	2.20	0.42
1:A:965:A:C2	13:M:124:PRO:HB2	2.55	0.42
1:A:974:A:OP1	1:A:974:A:H8	2.03	0.42
2:B:8:LYS:HB2	2:B:9:GLU:H	1.58	0.42
2:B:87:ARG:NH2	2:B:220:ASP:OD1	2.51	0.42
2:B:187:LEU:HA	2:B:201:ILE:HB	2.02	0.42
6:F:45:LEU:O	6:F:46:ARG:HG2	2.20	0.42
9:I:104:ARG:O	9:I:105:ASP:C	2.59	0.42
9:I:110:GLU:HG2	9:I:113:LYS:NZ	2.35	0.42
11:K:86:GLY:H	11:K:112:THR:CG2	2.32	0.42
18:R:17:SER:HB2	18:R:54:ARG:HH21	1.85	0.42
1:A:373:A:H2'	1:A:374:A:H8	1.85	0.42
1:A:413:G:H22	1:A:428:G:H1'	1.85	0.42
1:A:951:G:C6	1:A:1231:G:C6	3.08	0.42
1:A:961:U:O2'	1:A:962:C:H5'	2.20	0.42
1:A:1056:U:H5'	3:C:163:ALA:HB2	2.02	0.42
1:A:1060:C:OP1	14:N:45:ARG:NH2	2.53	0.42
1:A:1260:C:H4'	1:A:1284:C:H5'	2.01	0.42
1:A:1375:A:OP1	7:G:12:LEU:HD21	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1405:G:O2'	1:A:1519:A:C5'	2.68	0.42
1:A:1426:C:H2'	1:A:1427:U:H6	1.84	0.42
1:A:1505:G:H3'	1:A:1505:G:H8	1.85	0.42
3:C:38:ARG:CB	3:C:94:LEU:HD21	2.50	0.42
3:C:77:ILE:CG2	3:C:81:GLY:HA2	2.50	0.42
3:C:108:ASN:C	3:C:110:ASN:N	2.73	0.42
4:D:8:VAL:CG1	4:D:21:LEU:CD1	2.98	0.42
5:E:24:ARG:O	5:E:25:ARG:HG2	2.20	0.42
13:M:36:LYS:C	13:M:38:GLY:H	2.24	0.42
17:Q:40:LYS:HD3	17:Q:42:TYR:OH	2.20	0.42
18:R:48:GLY:O	18:R:74:ARG:NH2	2.41	0.42
20:T:54:LYS:HA	20:T:57:ARG:HD3	2.02	0.42
1:A:192:U:O2	20:T:60:GLU:OE1	2.38	0.41
1:A:490:G:H2'	1:A:491:G:C8	2.54	0.41
1:A:767:A:H2'	1:A:768:A:O4'	2.20	0.41
1:A:825:G:O2'	1:A:826:C:H5'	2.20	0.41
1:A:977:A:H2'	1:A:978:A:C5'	2.46	0.41
1:A:1061:G:C2'	1:A:1062:U:H5'	2.50	0.41
1:A:1277:C:H1'	1:A:1282:C:O2	2.20	0.41
2:B:10:LEU:C	2:B:12:GLU:N	2.72	0.41
4:D:60:GLU:OE1	4:D:60:GLU:HA	2.20	0.41
6:F:48:LEU:HD13	6:F:52:ILE:CG1	2.50	0.41
7:G:15:ASP:OD2	7:G:23:VAL:HG11	2.20	0.41
7:G:93:PRO:HG2	7:G:94:ARG:H	1.85	0.41
9:I:120:ARG:O	9:I:122:ALA:N	2.53	0.41
10:J:80:LYS:HA	10:J:83:GLU:HB2	2.02	0.41
17:Q:95:TYR:N	17:Q:95:TYR:CD1	2.88	0.41
18:R:51:LEU:HA	18:R:52:PRO:HD3	1.80	0.41
20:T:43:LEU:HD12	20:T:55:ILE:HD12	2.02	0.41
1:A:867:G:O2'	1:A:868:C:H5'	2.20	0.41
1:A:1034:G:O2'	1:A:1035:A:H5'	2.20	0.41
1:A:1213:A:N1	1:A:1215:G:H1'	2.35	0.41
1:A:1264:C:H2'	1:A:1265:G:H8	1.85	0.41
1:A:1264:C:H2'	1:A:1265:G:C8	2.54	0.41
1:A:1346:A:C5	7:G:10:ARG:CZ	3.02	0.41
3:C:134:ILE:HG22	3:C:168:ALA:HB3	2.01	0.41
4:D:205:GLU:O	4:D:208:SER:HB2	2.20	0.41
8:H:6:ILE:O	8:H:10:LEU:HG	2.20	0.41
13:M:32:GLU:O	13:M:35:GLU:N	2.53	0.41
16:P:19:ILE:HG22	16:P:36:ILE:CG1	2.51	0.41
1:A:47:C:C6	1:A:365:U:H2'	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:184:G:O4'	1:A:224:C:H4'	2.19	0.41
1:A:550:G:O2'	1:A:551:U:H5'	2.20	0.41
1:A:628:G:O2'	1:A:629:G:H5'	2.20	0.41
1:A:778:G:O2'	1:A:779:C:H5'	2.19	0.41
1:A:965:A:O2'	1:A:966:G:C5'	2.67	0.41
1:A:1127:G:N2	1:A:1144:G:N2	2.69	0.41
1:A:1531:A:O5'	1:A:1531:A:H8	2.03	0.41
2:B:165:VAL:O	2:B:187:LEU:O	2.38	0.41
4:D:24:GLU:H	4:D:112:VAL:HG11	1.85	0.41
5:E:51:VAL:HB	5:E:52:PRO:CD	2.37	0.41
8:H:51:VAL:CG1	8:H:52:ASP:N	2.82	0.41
11:K:48:ILE:O	11:K:49:GLY:C	2.59	0.41
15:O:83:GLU:C	15:O:83:GLU:OE1	2.58	0.41
1:A:547:A:H4'	1:A:548:G:O5'	2.19	0.41
1:A:655:A:C2	1:A:754:C:N4	2.88	0.41
1:A:1371:G:H2'	1:A:1372:U:H6	1.86	0.41
2:B:228:GLY:O	2:B:229:VAL:C	2.58	0.41
7:G:69:VAL:O	7:G:69:VAL:CG1	2.68	0.41
9:I:59:PHE:HB3	9:I:60:ASP:H	1.56	0.41
9:I:110:GLU:HG2	9:I:113:LYS:HZ2	1.85	0.41
10:J:3:LYS:HG3	10:J:75:ILE:HG23	2.01	0.41
15:O:34:LEU:HD23	15:O:34:LEU:C	2.40	0.41
20:T:82:SER:C	20:T:84:LEU:N	2.74	0.41
1:A:489:C:H2'	1:A:490:G:C8	2.54	0.41
1:A:546:G:OP1	4:D:73:ARG:HB2	2.21	0.41
1:A:866:C:H2'	1:A:867:G:O4'	2.20	0.41
1:A:1030(A):G:H21	1:A:1030(C):G:H3'	1.84	0.41
1:A:1094:G:OP2	1:A:1095:U:C5	2.74	0.41
1:A:1137:C:H4'	1:A:1138:G:N1	2.33	0.41
1:A:1322:C:OP1	19:S:78:ARG:NH2	2.54	0.41
1:A:1350:A:C6	1:A:1351:U:N3	2.89	0.41
1:A:1453:G:H2'	1:A:1454:G:O4'	2.21	0.41
2:B:62:ALA:C	2:B:64:ARG:H	2.23	0.41
3:C:112:SER:HB2	3:C:115:LEU:HB2	2.01	0.41
5:E:40:ARG:NH1	5:E:68:GLU:OE2	2.49	0.41
5:E:131:ILE:HD13	5:E:131:ILE:HA	1.93	0.41
8:H:108:GLY:CA	8:H:138:TRP:HB3	2.46	0.41
8:H:126:LYS:O	8:H:128:GLY:N	2.54	0.41
10:J:3:LYS:CG	10:J:75:ILE:HG23	2.51	0.41
11:K:77:MET:CE	11:K:80:VAL:HG22	2.48	0.41
15:O:70:LEU:HD12	15:O:78:TYR:HB2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:87:ILE:HG22	15:O:88:ARG:N	2.34	0.41
17:Q:95:TYR:N	17:Q:95:TYR:HD1	2.18	0.41
20:T:100:ILE:C	20:T:102:GLY:N	2.74	0.41
21:V:7:ARG:O	21:V:7:ARG:HG3	2.19	0.41
22:Y:38:ASN:ND2	22:Y:104:LEU:HD12	2.35	0.41
22:Y:94:LEU:O	22:Y:97:ILE:HG22	2.21	0.41
1:A:67:C:O2'	1:A:171:A:H1'	2.20	0.41
1:A:659:U:OP2	15:O:8:LYS:NZ	2.40	0.41
1:A:1126:U:P	1:A:1126:U:H6	2.43	0.41
1:A:1145:C:HO2'	1:A:1146:A:H8	1.63	0.41
1:A:1145:C:O2'	1:A:1146:A:O5'	2.39	0.41
1:A:1239:A:C4	1:A:1298:C:N4	2.88	0.41
1:A:1262:C:N4	1:A:1273:G:H1	2.18	0.41
1:A:1311:G:H2'	1:A:1312:G:O4'	2.20	0.41
1:A:1431:C:H2'	1:A:1432:G:O4'	2.21	0.41
3:C:73:PRO:HD3	3:C:105:GLU:HG3	2.03	0.41
9:I:110:GLU:OE2	9:I:113:LYS:NZ	2.53	0.41
11:K:86:GLY:N	11:K:112:THR:HG23	2.35	0.41
11:K:100:ALA:O	11:K:101:SER:C	2.57	0.41
11:K:127:LYS:HD3	11:K:127:LYS:HA	1.78	0.41
12:L:53:ARG:CB	12:L:93:LEU:HD11	2.50	0.41
12:L:83:VAL:HG22	12:L:84:LEU:H	1.85	0.41
13:M:78:ILE:CA	13:M:81:LEU:HD21	2.43	0.41
16:P:4:ILE:CG1	16:P:64:ALA:HB1	2.49	0.41
16:P:82:GLN:O	16:P:83:GLU:C	2.59	0.41
22:Y:186:ASP:O	22:Y:190:VAL:HG23	2.20	0.41
1:A:43:C:H2'	1:A:44:G:O4'	2.21	0.41
1:A:107:G:O2'	1:A:108:G:H5'	2.19	0.41
1:A:1228:C:H4'	13:M:116:THR:HA	2.02	0.41
1:A:1292:U:P	7:G:41:ARG:NH2	2.94	0.41
1:A:1390:U:H2'	1:A:1391:U:H6	1.86	0.41
4:D:148:VAL:HG13	4:D:158:ILE:HD13	2.01	0.41
7:G:45:ASP:O	7:G:49:ILE:HG13	2.20	0.41
8:H:82:HIS:O	8:H:83:ILE:HB	2.21	0.41
9:I:108:VAL:HG12	9:I:109:VAL:N	2.36	0.41
10:J:75:ILE:O	10:J:76:ASN:HB2	2.21	0.41
12:L:60:LEU:HD21	12:L:66:VAL:CG2	2.50	0.41
18:R:21:LYS:HG3	18:R:57:GLY:CA	2.51	0.41
19:S:5:LEU:HD23	19:S:5:LEU:HA	1.88	0.41
22:Y:91:PRO:HD2	22:Y:94:LEU:HD12	2.02	0.41
1:A:382:A:C2	1:A:383:A:C4	3.08	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:436:C:H2'	1:A:437:U:H6	1.86	0.41
1:A:439:A:N6	1:A:497:A:H1'	2.35	0.41
1:A:620:C:C2	4:D:135:LEU:HD13	2.56	0.41
1:A:625:G:O2'	1:A:626:U:H5'	2.20	0.41
1:A:665:A:H2'	1:A:725:G:H22	1.83	0.41
1:A:692:U:O2	1:A:695:A:C8	2.73	0.41
1:A:1077:G:N2	1:A:1080:A:OP2	2.50	0.41
1:A:1116:C:O2'	9:I:108:VAL:HG21	2.21	0.41
1:A:1352:C:OP1	21:V:3:LYS:NZ	2.51	0.41
1:A:1404:C:C2	1:A:1499:A:C6	3.08	0.41
2:B:95:GLN:C	2:B:96:ARG:HD2	2.40	0.41
2:B:116:GLU:CG	2:B:153:ARG:NH1	2.80	0.41
2:B:125:PRO:HG2	2:B:126:GLU:H	1.86	0.41
3:C:179:ARG:O	3:C:179:ARG:CG	2.69	0.41
4:D:23:GLY:HA3	4:D:112:VAL:HG13	2.02	0.41
5:E:144:THR:O	5:E:145:LYS:C	2.59	0.41
6:F:48:LEU:HD13	6:F:52:ILE:HD12	2.03	0.41
8:H:39:LEU:HD13	8:H:39:LEU:HA	1.86	0.41
11:K:99:GLN:HG2	11:K:105:VAL:HG21	2.02	0.41
16:P:43:LYS:HA	16:P:48:TRP:CB	2.51	0.41
22:Y:196:LEU:HD13	22:Y:196:LEU:HA	1.92	0.41
1:A:134:A:H1'	1:A:325:A:C5	2.56	0.41
1:A:335:C:H2'	1:A:336:C:H6	1.85	0.41
1:A:519:C:H2'	1:A:520:A:C8	2.56	0.41
1:A:736:C:H2'	1:A:737:A:H8	1.83	0.41
1:A:913:A:H1'	1:A:914:A:O4'	2.21	0.41
1:A:953:G:H1'	13:M:125:ARG:HA	2.03	0.41
1:A:976:G:OP1	14:N:31:ARG:O	2.39	0.41
1:A:1096:C:H2'	1:A:1097:C:C6	2.56	0.41
1:A:1195:C:H3'	1:A:1196:U:H5"	2.02	0.41
1:A:1203:C:OP1	14:N:2:ALA:HB3	2.20	0.41
1:A:1231:G:H5"	9:I:126:SER:HB3	2.01	0.41
1:A:1286:A:H2'	1:A:1287:A:O5'	2.21	0.41
1:A:1402:C:H2'	1:A:1403:C:H6	1.85	0.41
1:A:1404:C:H1'	1:A:1499:A:N1	2.35	0.41
2:B:15:VAL:HG11	2:B:210:SER:N	2.36	0.41
2:B:130:ARG:NH2	3:C:207:VAL:CG2	2.82	0.41
3:C:70:VAL:O	3:C:106:VAL:N	2.51	0.41
3:C:174:PRO:HB2	3:C:177:THR:CG2	2.50	0.41
3:C:191:THR:HG21	3:C:193:TYR:CE2	2.56	0.41
4:D:63:LYS:O	4:D:64:LEU:C	2.58	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:36:ASP:OD1	5:E:38:GLN:N	2.39	0.41
5:E:119:LEU:HD23	5:E:119:LEU:HA	1.84	0.41
6:F:33:TYR:HA	6:F:71:ARG:NH2	2.36	0.41
6:F:78:GLU:HA	6:F:81:ILE:CD1	2.51	0.41
6:F:91:VAL:HG13	18:R:72:ARG:NH2	2.36	0.41
7:G:23:VAL:HG13	7:G:43:PHE:CE2	2.56	0.41
10:J:15:THR:HG23	10:J:94:VAL:CG2	2.48	0.41
10:J:53:PRO:HA	14:N:41:ARG:HH21	1.85	0.41
11:K:65:ALA:O	11:K:68:ALA:HB3	2.20	0.41
12:L:46:LYS:NZ	12:L:47:LYS:HE3	2.36	0.41
13:M:4:ILE:HG22	13:M:5:ALA:H	1.83	0.41
17:Q:97:SER:O	17:Q:99:SER:N	2.53	0.41
19:S:16:LEU:O	19:S:20:LEU:HG	2.21	0.41
1:A:836:G:C6	1:A:851:G:C6	3.09	0.41
1:A:883:C:O2'	1:A:884:U:H5'	2.21	0.41
1:A:942:G:C4	1:A:943:U:C6	3.09	0.41
1:A:948:C:O2'	1:A:949:A:H5'	2.21	0.41
1:A:1057:G:H2'	1:A:1058:G:O4'	2.20	0.41
1:A:1110:A:O5'	1:A:1110:A:H8	2.04	0.41
1:A:1257:U:H4'	1:A:1258:G:C5'	2.50	0.41
2:B:134:GLU:HG2	2:B:137:ARG:HH21	1.86	0.41
3:C:67:THR:O	3:C:67:THR:HG22	2.21	0.41
3:C:79:ARG:NE	3:C:82:GLU:HG2	2.34	0.41
4:D:130:GLY:O	4:D:131:ARG:C	2.58	0.41
5:E:31:LEU:HD23	5:E:31:LEU:HA	1.74	0.41
7:G:104:LEU:HD23	7:G:134:ALA:HB1	2.03	0.41
11:K:67:ASP:OD2	11:K:71:LYS:HE3	2.21	0.41
12:L:55:VAL:CG1	12:L:67:THR:CG2	2.96	0.41
15:O:57:LEU:HD12	15:O:57:LEU:HA	1.86	0.41
15:O:74:ASP:OD1	15:O:76:GLU:HB3	2.21	0.41
15:O:81:LEU:HD22	15:O:85:LEU:HD12	2.02	0.41
1:A:19:C:O2'	1:A:20:U:H5'	2.20	0.40
1:A:190(L):U:H3	20:T:105:SER:HB2	1.87	0.40
1:A:502:G:H2'	1:A:503:C:C6	2.56	0.40
1:A:637:G:O2'	1:A:638:G:H5'	2.21	0.40
1:A:750:G:N3	15:O:23:GLY:HA3	2.37	0.40
1:A:913:A:O2'	1:A:914:A:O4'	2.27	0.40
1:A:919:A:O2'	1:A:920:U:H5'	2.22	0.40
1:A:1124:G:C8	1:A:1145:C:C5	3.09	0.40
1:A:1263:C:H2'	1:A:1264:C:C6	2.56	0.40
2:B:53:ARG:NH1	2:B:199:TYR:HD2	2.19	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:145:LEU:HA	2:B:145:LEU:HD23	1.84	0.40
3:C:57:ILE:O	3:C:57:ILE:HG22	2.20	0.40
3:C:65:ALA:O	3:C:66:VAL:HB	2.21	0.40
3:C:126:ARG:C	3:C:127:ARG:HG3	2.42	0.40
6:F:30:LEU:CB	6:F:35:ALA:HB3	2.41	0.40
10:J:23:ILE:N	10:J:23:ILE:CD1	2.85	0.40
11:K:95:ILE:O	11:K:95:ILE:HG22	2.20	0.40
15:O:26:GLU:HG3	15:O:81:LEU:HG	2.03	0.40
15:O:71:GLN:O	15:O:72:ARG:C	2.59	0.40
16:P:34:GLU:HG2	16:P:35:LYS:N	2.36	0.40
17:Q:6:LEU:O	17:Q:58:GLU:HA	2.21	0.40
20:T:49:ALA:O	20:T:52:ALA:HB3	2.21	0.40
1:A:527:G:O2'	1:A:535:A:N1	2.32	0.40
1:A:660:G:C2	1:A:746:A:C2	3.09	0.40
1:A:929:G:OP1	1:A:1533:C:N4	2.55	0.40
1:A:952:U:H2'	1:A:953:G:H8	1.85	0.40
1:A:973:G:H8	1:A:973:G:O5'	2.04	0.40
1:A:1138:G:N1	1:A:1140:C:C2	2.89	0.40
1:A:1331:G:HO2'	1:A:1332:A:P	2.44	0.40
1:A:1372:U:H5"	9:I:71:SER:CB	2.51	0.40
1:A:1428:A:H2'	1:A:1429:C:O4'	2.21	0.40
2:B:14:GLY:O	2:B:15:VAL:HG22	2.22	0.40
2:B:24:TRP:CG	2:B:25:ASN:N	2.89	0.40
2:B:60:ASP:O	2:B:64:ARG:HB2	2.20	0.40
3:C:47:LEU:H	3:C:47:LEU:HD13	1.83	0.40
3:C:77:ILE:O	3:C:83:ARG:HB3	2.21	0.40
4:D:194:LEU:HD22	4:D:194:LEU:N	2.37	0.40
5:E:118:ILE:HG21	5:E:118:ILE:HD13	1.74	0.40
8:H:19:VAL:CG2	8:H:21:LYS:HD3	2.52	0.40
8:H:89:PRO:HA	8:H:92:ARG:NH1	2.37	0.40
12:L:55:VAL:CG1	12:L:56:ALA:N	2.83	0.40
18:R:44:LEU:HD22	18:R:48:GLY:O	2.21	0.40
1:A:359:U:H2'	1:A:360:A:C8	2.57	0.40
1:A:547:A:OP2	4:D:2:GLY:N	2.54	0.40
1:A:567:G:H2'	1:A:568:G:O4'	2.21	0.40
1:A:818:G:H3'	1:A:819:A:H5'	2.01	0.40
1:A:1003(A):G:H2'	1:A:1004:A:H4'	2.03	0.40
1:A:1028:C:H2'	1:A:1029:C:H6	1.84	0.40
1:A:1118:C:H1'	1:A:1179:A:C4	2.56	0.40
1:A:1355:G:O2'	1:A:1356:G:H5'	2.21	0.40
1:A:1392:G:H2'	1:A:1393:U:H6	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:216:SER:OG	2:B:217:ARG:N	2.54	0.40
4:D:58:LEU:HD23	4:D:206:PHE:CE1	2.57	0.40
8:H:111:ILE:O	8:H:134:ILE:HB	2.20	0.40
10:J:44:VAL:HG11	10:J:46:ARG:NH1	2.37	0.40
10:J:65:LEU:HD12	14:N:56:VAL:HG22	2.04	0.40
17:Q:92:ARG:O	17:Q:95:TYR:HB2	2.21	0.40
18:R:26:LEU:CD1	18:R:27:GLY:H	2.29	0.40
19:S:77:THR:HG22	19:S:78:ARG:N	2.36	0.40
1:A:9:G:OP2	5:E:121:LYS:NZ	2.41	0.40
1:A:16:A:C2'	1:A:17:U:H5'	2.51	0.40
1:A:458:C:H2'	1:A:459:G:C8	2.57	0.40
1:A:671:G:H2'	1:A:672:U:O4'	2.22	0.40
1:A:715:A:H2'	1:A:716:A:C8	2.57	0.40
1:A:769:G:H4'	1:A:1513:A:H4'	2.03	0.40
1:A:939:G:C6	1:A:940:C:N4	2.89	0.40
1:A:965:A:O2'	1:A:966:G:P	2.80	0.40
1:A:1298:C:H2'	7:G:114:ARG:HH12	1.86	0.40
1:A:1327:C:H5"	21:V:20:LYS:HB3	2.04	0.40
2:B:14:GLY:O	2:B:15:VAL:CG2	2.69	0.40
2:B:68:ILE:HB	2:B:90:MET:HE3	2.02	0.40
2:B:134:GLU:O	2:B:138:LEU:HG	2.21	0.40
3:C:126:ARG:O	3:C:127:ARG:HB2	2.22	0.40
6:F:48:LEU:HD13	6:F:52:ILE:CD1	2.51	0.40
10:J:59:SER:O	10:J:60:ARG:HB2	2.21	0.40
11:K:115:PRO:C	11:K:117:ASN:H	2.25	0.40
12:L:43:VAL:CG1	12:L:44:THR:N	2.81	0.40
13:M:91:ARG:HD2	13:M:91:ARG:HA	1.85	0.40
13:M:96:LEU:O	13:M:110:ARG:NH1	2.54	0.40
14:N:39:LEU:HD11	14:N:47:LEU:HD12	2.02	0.40
19:S:67:VAL:HG12	19:S:68:GLY:N	2.35	0.40
1:A:155:C:H2'	1:A:156:G:C8	2.57	0.40
1:A:176:C:H2'	1:A:177:C:C6	2.56	0.40
1:A:330:C:H6	1:A:330:C:H5"	1.86	0.40
1:A:1116:C:H2'	1:A:1117:G:C5'	2.34	0.40
1:A:1312:G:N7	19:S:4:SER:HB3	2.36	0.40
1:A:1372:U:H5"	9:I:71:SER:HB2	2.04	0.40
1:A:1437:C:H2'	1:A:1438:G:H8	1.86	0.40
2:B:33:TYR:O	2:B:34:ALA:CB	2.67	0.40
2:B:107:THR:C	2:B:109:SER:N	2.75	0.40
2:B:130:ARG:HB3	2:B:134:GLU:OE1	2.20	0.40
3:C:110:ASN:OD1	3:C:140:ARG:HB3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:204:LEU:O	3:C:205:GLY:C	2.59	0.40
5:E:118:ILE:HG22	5:E:119:LEU:O	2.21	0.40
9:I:117:HIS:C	9:I:118:LYS:HG3	2.41	0.40
10:J:94:VAL:CG1	10:J:95:GLU:H	2.35	0.40
13:M:37:THR:HG23	13:M:55:ARG:HB2	2.04	0.40
13:M:63:THR:HG23	13:M:64:TRP:CD2	2.56	0.40
13:M:69:GLU:O	13:M:72:ALA:HB3	2.21	0.40
14:N:3:ARG:NH1	14:N:6:LEU:CD1	2.84	0.40
17:Q:97:SER:CB	17:Q:102:GLY:C	2.78	0.40
20:T:23:ARG:HG2	20:T:23:ARG:NH1	2.36	0.40
20:T:68:LYS:HD2	20:T:68:LYS:HA	1.92	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
2	B	232/256 (91%)	174 (75%)	34 (15%)	24 (10%)	0 9
3	C	204/239 (85%)	135 (66%)	41 (20%)	28 (14%)	0 4
4	D	206/208 (99%)	166 (81%)	31 (15%)	9 (4%)	2 25
5	E	148/161 (92%)	130 (88%)	13 (9%)	5 (3%)	3 31
6	F	99/101 (98%)	79 (80%)	19 (19%)	1 (1%)	15 52
7	G	153/155 (99%)	127 (83%)	16 (10%)	10 (6%)	1 19
8	H	136/138 (99%)	125 (92%)	7 (5%)	4 (3%)	4 34
9	I	125/128 (98%)	88 (70%)	27 (22%)	10 (8%)	1 14
10	J	96/104 (92%)	59 (62%)	20 (21%)	17 (18%)	0 2
11	K	117/129 (91%)	88 (75%)	20 (17%)	9 (8%)	1 15
12	L	122/131 (93%)	97 (80%)	16 (13%)	9 (7%)	1 16

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
13	M	123/126 (98%)	88 (72%)	27 (22%)	8 (6%)	1 19
14	N	58/60 (97%)	40 (69%)	11 (19%)	7 (12%)	0 6
15	O	86/88 (98%)	70 (81%)	11 (13%)	5 (6%)	1 21
16	P	81/88 (92%)	65 (80%)	15 (18%)	1 (1%)	13 50
17	Q	102/104 (98%)	84 (82%)	10 (10%)	8 (8%)	1 15
18	R	71/88 (81%)	62 (87%)	7 (10%)	2 (3%)	5 35
19	S	78/92 (85%)	49 (63%)	18 (23%)	11 (14%)	0 4
20	T	97/106 (92%)	63 (65%)	21 (22%)	13 (13%)	0 4
21	V	22/26 (85%)	19 (86%)	2 (9%)	1 (4%)	2 25
22	Y	217/222 (98%)	206 (95%)	6 (3%)	5 (2%)	6 38
All	All	2573/2750 (94%)	2014 (78%)	372 (14%)	187 (7%)	1 16

All (187) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	9	GLU
2	B	15	VAL
2	B	16	HIS
2	B	17	PHE
2	B	21	ARG
2	B	24	TRP
3	C	4	LYS
3	C	15	THR
3	C	16	ARG
3	C	26	LYS
3	C	47	LEU
3	C	61	ALA
3	C	62	ASP
3	C	97	LYS
3	C	101	LEU
3	C	146	ALA
3	C	154	SER
3	C	179	ARG
3	C	189	ALA
4	D	29	PRO
4	D	36	ARG
5	E	16	THR
5	E	153	LYS

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Mol	Chain	Res	Type
7	G	7	ALA
7	G	155	ARG
8	H	24	THR
8	H	83	ILE
8	H	91	ARG
9	I	58	HIS
9	I	88	TYR
10	J	32	ALA
10	J	39	PRO
10	J	54	PHE
10	J	57	LYS
10	J	79	ARG
10	J	86	MET
11	K	57	THR
11	K	127	LYS
12	L	27	LEU
12	L	28	LYS
12	L	47	LYS
13	M	63	THR
13	M	67	GLU
13	M	121	LYS
13	M	122	LYS
13	M	124	PRO
14	N	22	THR
14	N	29	ARG
15	O	88	ARG
17	Q	69	LYS
17	Q	80	GLY
17	Q	81	ARG
17	Q	96	GLU
17	Q	98	LEU
17	Q	104	LYS
18	R	87	ARG
19	S	6	LYS
19	S	71	LEU
20	T	11	SER
20	T	73	HIS
22	Y	143	ASP
2	B	8	LYS
2	B	18	GLY
2	B	20	GLU
2	B	97	TRP

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Mol	Chain	Res	Type
2	B	123	ALA
2	B	232	PRO
3	C	29	TYR
3	C	156	ARG
3	C	168	ALA
3	C	181	ASN
3	C	206	GLU
4	D	4	TYR
4	D	26	CYS
4	D	88	VAL
4	D	125	HIS
4	D	175	SER
5	E	22	GLY
5	E	104	ALA
6	F	37	VAL
7	G	52	GLU
9	I	41	VAL
10	J	30	SER
10	J	34	VAL
10	J	40	LEU
10	J	72	VAL
11	K	15	ALA
11	K	49	GLY
11	K	50	TYR
11	K	89	ALA
12	L	41	ARG
12	L	48	PRO
12	L	51	ALA
12	L	116	SER
12	L	121	GLY
13	M	6	GLY
13	M	85	GLY
16	P	10	GLY
18	R	20	ALA
19	S	9	VAL
19	S	45	VAL
19	S	67	VAL
19	S	68	GLY
20	T	9	ASN
20	T	49	ALA
20	T	50	GLU
20	T	95	ALA

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Mol	Chain	Res	Type
20	T	99	LEU
20	T	102	GLY
2	B	26	PRO
2	B	60	ASP
2	B	83	MET
2	B	89	GLY
2	B	204	ASN
5	E	65	ASN
7	G	5	ARG
8	H	127	LEU
9	I	56	LEU
10	J	19	SER
10	J	60	ARG
10	J	61	GLU
10	J	90	LEU
11	K	35	PRO
11	K	101	SER
12	L	49	ASN
14	N	13	THR
14	N	23	ARG
17	Q	97	SER
19	S	28	LYS
19	S	30	LEU
19	S	32	LYS
20	T	74	LYS
20	T	83	ARG
22	Y	144	SER
22	Y	155	LEU
2	B	126	GLU
2	B	165	VAL
3	C	39	ILE
3	C	100	ALA
3	C	188	LEU
7	G	4	ARG
7	G	81	GLY
7	G	112	PRO
9	I	7	THR
9	I	12	GLU
9	I	119	ALA
13	M	123	ALA
14	N	12	ARG
14	N	60	SER

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Mol	Chain	Res	Type
15	O	16	ALA
17	Q	33	GLY
21	V	3	LYS
22	Y	148	ALA
2	B	155	LEU
3	C	24	ALA
3	C	66	VAL
3	C	127	ARG
4	D	123	HIS
7	G	53	LYS
9	I	121	ARG
14	N	36	PHE
15	O	84	LYS
19	S	31	ILE
2	B	127	ILE
3	C	108	ASN
3	C	174	PRO
4	D	5	ILE
9	I	43	ALA
10	J	26	ALA
22	Y	152	LYS
2	B	124	SER
2	B	214	ILE
7	G	14	PRO
10	J	82	ILE
20	T	98	PRO
2	B	125	PRO
3	C	76	VAL
3	C	77	ILE
7	G	17	VAL
10	J	36	GLY
15	O	82	ILE
19	S	8	GLY
9	I	44	VAL
15	O	19	PRO
20	T	96	GLY
20	T	101	GLY
11	K	90	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	202/220 (92%)	182 (90%)	20 (10%)	8	32
3	C	160/188 (85%)	142 (89%)	18 (11%)	6	28
4	D	180/180 (100%)	173 (96%)	7 (4%)	32	60
5	E	115/122 (94%)	101 (88%)	14 (12%)	5	25
6	F	90/90 (100%)	87 (97%)	3 (3%)	38	65
7	G	126/126 (100%)	123 (98%)	3 (2%)	49	71
8	H	119/119 (100%)	109 (92%)	10 (8%)	11	40
9	I	98/99 (99%)	92 (94%)	6 (6%)	18	50
10	J	86/91 (94%)	77 (90%)	9 (10%)	7	30
11	K	90/99 (91%)	84 (93%)	6 (7%)	16	47
12	L	104/108 (96%)	96 (92%)	8 (8%)	13	43
13	M	100/101 (99%)	90 (90%)	10 (10%)	7	32
14	N	49/49 (100%)	47 (96%)	2 (4%)	30	59
15	O	79/79 (100%)	72 (91%)	7 (9%)	9	38
16	P	72/74 (97%)	67 (93%)	5 (7%)	15	46
17	Q	96/96 (100%)	90 (94%)	6 (6%)	18	49
18	R	64/77 (83%)	62 (97%)	2 (3%)	40	65
19	S	71/79 (90%)	68 (96%)	3 (4%)	30	58
20	T	76/82 (93%)	70 (92%)	6 (8%)	12	42
21	V	19/21 (90%)	19 (100%)	0	100	100
22	Y	193/195 (99%)	185 (96%)	8 (4%)	30	59
All	All	2189/2295 (95%)	2036 (93%)	153 (7%)	15	46

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

Mol	Chain	Res	Type
2	B	8	LYS

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Mol	Chain	Res	Type
2	B	12	GLU
2	B	17	PHE
2	B	23	ARG
2	B	24	TRP
2	B	87	ARG
2	B	114	ARG
2	B	139	LYS
2	B	144	ARG
2	B	146	GLN
2	B	155	LEU
2	B	157	ARG
2	B	164	VAL
2	B	170	GLU
2	B	178	ARG
2	B	213	LEU
2	B	221	LEU
2	B	231	GLU
2	B	232	PRO
2	B	236	TYR
3	C	3	ASN
3	C	5	ILE
3	C	34	LEU
3	C	47	LEU
3	C	56	ASP
3	C	75	VAL
3	C	82	GLU
3	C	90	GLU
3	C	91	LEU
3	C	99	VAL
3	C	107	GLN
3	C	110	ASN
3	C	164	ARG
3	C	167	TRP
3	C	175	LEU
3	C	179	ARG
3	C	188	LEU
3	C	204	LEU
4	D	15	GLU
4	D	29	PRO
4	D	53	ASP
4	D	122	ARG
4	D	127	THR

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Mol	Chain	Res	Type
4	D	157	LEU
4	D	192	GLU
5	E	12	LEU
5	E	26	PHE
5	E	31	LEU
5	E	38	GLN
5	E	41	VAL
5	E	43	LEU
5	E	56	GLN
5	E	65	ASN
5	E	68	GLU
5	E	79	GLU
5	E	80	ILE
5	E	89	ILE
5	E	120	THR
5	E	150	ARG
6	F	10	LEU
6	F	69	GLU
6	F	100	ASN
7	G	8	GLU
7	G	11	GLN
7	G	38	LEU
8	H	2	LEU
8	H	21	LYS
8	H	52	ASP
8	H	63	LEU
8	H	85	ARG
8	H	91	ARG
8	H	92	ARG
8	H	104	ARG
8	H	105	ARG
8	H	119	LEU
9	I	2	GLU
9	I	38	GLN
9	I	53	VAL
9	I	79	LEU
9	I	111	ARG
9	I	121	ARG
10	J	6	ILE
10	J	15	THR
10	J	45	ARG
10	J	60	ARG

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Mol	Chain	Res	Type
10	J	64	GLU
10	J	71	LEU
10	J	73	ASP
10	J	83	GLU
10	J	95	GLU
11	K	24	SER
11	K	29	ILE
11	K	35	PRO
11	K	54	ARG
11	K	84	VAL
11	K	92	GLU
12	L	17	LYS
12	L	33	ARG
12	L	53	ARG
12	L	60	LEU
12	L	81	SER
12	L	98	TYR
12	L	113	ARG
12	L	126	LYS
13	M	9	ILE
13	M	12	ASN
13	M	16	ASP
13	M	44	ARG
13	M	70	LEU
13	M	81	LEU
13	M	102	ARG
13	M	110	ARG
13	M	124	PRO
13	M	125	ARG
14	N	41	ARG
14	N	44	LEU
15	O	6	GLU
15	O	7	GLU
15	O	39	LEU
15	O	57	LEU
15	O	70	LEU
15	O	81	LEU
15	O	83	GLU
16	P	2	VAL
16	P	8	ARG
16	P	28	ARG
16	P	53	VAL

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Mol	Chain	Res	Type
16	P	62	VAL
17	Q	34	LYS
17	Q	38	ARG
17	Q	60	ILE
17	Q	68	ARG
17	Q	74	LEU
17	Q	98	LEU
18	R	38	GLU
18	R	55	ARG
19	S	10	PHE
19	S	15	LEU
19	S	20	LEU
20	T	45	GLN
20	T	57	ARG
20	T	73	HIS
20	T	75	ASN
20	T	84	LEU
20	T	86	ARG
22	Y	25	ASP
22	Y	101	ILE
22	Y	119	ARG
22	Y	153	ARG
22	Y	155	LEU
22	Y	158	LEU
22	Y	172	LEU
22	Y	196	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
9	I	58	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1507/1513 (99%)	229 (15%)	90 (5%)

All (229) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	6	G
1	A	8	A
1	A	9	G
1	A	31	G
1	A	32	A
1	A	39	G
1	A	48	C
1	A	49	U
1	A	51	A
1	A	52	G
1	A	61	G
1	A	81	U
1	A	101	A
1	A	116	A
1	A	120	A
1	A	121	C
1	A	129(A)	G
1	A	130	A
1	A	131	C
1	A	182	U
1	A	190(D)	U
1	A	190(E)	U
1	A	190(F)	G
1	A	195	A
1	A	197	A
1	A	198	G
1	A	202	U
1	A	203	U
1	A	204	U
1	A	216	G
1	A	244	U
1	A	247	G
1	A	251	G
1	A	252	U
1	A	266	G
1	A	267	C
1	A	280	C
1	A	282	A
1	A	289	G
1	A	321	A
1	A	328	C
1	A	329	A
1	A	330	C

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Mol	Chain	Res	Type
1	A	332	G
1	A	344	A
1	A	345	C
1	A	352	C
1	A	353	A
1	A	354	G
1	A	367	U
1	A	373	A
1	A	397	A
1	A	398	C
1	A	412	A
1	A	413	G
1	A	421	U
1	A	428	G
1	A	429	U
1	A	430	A
1	A	439	A
1	A	460	A
1	A	461	C
1	A	462	G
1	A	481	G
1	A	484	G
1	A	485	G
1	A	497	A
1	A	498	U
1	A	509	A
1	A	510	A
1	A	511	C
1	A	518	C
1	A	519	C
1	A	527	G
1	A	532	A
1	A	533	A
1	A	534	U
1	A	547	A
1	A	559	A
1	A	560	U
1	A	561	U
1	A	562	C
1	A	572	A
1	A	573	A
1	A	575	G

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Mol	Chain	Res	Type
1	A	576	G
1	A	577	G
1	A	588	G
1	A	653	A
1	A	665	A
1	A	686	U
1	A	687	A
1	A	688	G
1	A	702	A
1	A	703	G
1	A	718	G
1	A	723	U
1	A	731	G
1	A	749	C
1	A	755	G
1	A	777	A
1	A	781	A
1	A	782	A
1	A	793	U
1	A	794	A
1	A	813	U
1	A	815	A
1	A	817	C
1	A	819	A
1	A	828	A
1	A	839	U
1	A	840	C
1	A	841	U
1	A	858	G
1	A	902	G
1	A	913	A
1	A	914	A
1	A	926	G
1	A	927	G
1	A	934	C
1	A	935	A
1	A	943	U
1	A	945	G
1	A	960	U
1	A	961	U
1	A	966	G
1	A	969	A

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Mol	Chain	Res	Type
1	A	971	G
1	A	974	A
1	A	975	A
1	A	976	G
1	A	977	A
1	A	991	U
1	A	992	U
1	A	993	G
1	A	994	A
1	A	1004	A
1	A	1005	A
1	A	1023	G
1	A	1026	G
1	A	1050	G
1	A	1053	G
1	A	1065	U
1	A	1066	C
1	A	1068	G
1	A	1085	U
1	A	1086	U
1	A	1094	G
1	A	1095	U
1	A	1101	A
1	A	1102	A
1	A	1117	G
1	A	1124	G
1	A	1125	U
1	A	1126	U
1	A	1129	C
1	A	1130	A
1	A	1131	G
1	A	1137	C
1	A	1138	G
1	A	1139	G
1	A	1140	C
1	A	1145	C
1	A	1146	A
1	A	1152	A
1	A	1157	A
1	A	1159	U
1	A	1183	A
1	A	1184	G

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Mol	Chain	Res	Type
1	A	1191	A
1	A	1196	U
1	A	1197	G
1	A	1201	A
1	A	1202	G
1	A	1211	U
1	A	1212	U
1	A	1215	G
1	A	1225	A
1	A	1226	C
1	A	1227	A
1	A	1238	A
1	A	1257	U
1	A	1258	G
1	A	1279	A
1	A	1280	A
1	A	1281	U
1	A	1282	C
1	A	1285	A
1	A	1286	A
1	A	1287	A
1	A	1299	A
1	A	1300	G
1	A	1301	U
1	A	1302	U
1	A	1303	C
1	A	1305	G
1	A	1320	C
1	A	1332	A
1	A	1347	G
1	A	1348	U
1	A	1363	A
1	A	1364	U
1	A	1365	G
1	A	1381	U
1	A	1394	A
1	A	1398	A
1	A	1405	G
1	A	1406	U
1	A	1408	A
1	A	1409	C
1	A	1410	G

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Mol	Chain	Res	Type
1	A	1414	U
1	A	1419	G
1	A	1422	G
1	A	1442	G
1	A	1443	G
1	A	1446	A
1	A	1447	G
1	A	1452	C
1	A	1490	C
1	A	1499	A
1	A	1502	A
1	A	1504	G
1	A	1505	G
1	A	1506	U
1	A	1517	G
1	A	1520	G
1	A	1529	G
1	A	1530	G

All (90) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	5	U
1	A	7	G
1	A	30	U
1	A	48	C
1	A	51	A
1	A	60	A
1	A	115	G
1	A	119	A
1	A	129(A)	G
1	A	181	G
1	A	197	A
1	A	202	U
1	A	203	U
1	A	204	U
1	A	243	A
1	A	250	A
1	A	251	G
1	A	266	G
1	A	279	A
1	A	281	G

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Mol	Chain	Res	Type
1	A	328	C
1	A	329	A
1	A	344	A
1	A	351	G
1	A	353	A
1	A	366	C
1	A	372	C
1	A	428	G
1	A	429	U
1	A	438	G
1	A	484	G
1	A	496	A
1	A	497	A
1	A	509	A
1	A	518	C
1	A	533	A
1	A	559	A
1	A	560	U
1	A	575	G
1	A	576	G
1	A	687	A
1	A	701	C
1	A	748	C
1	A	792	A
1	A	812	C
1	A	840	C
1	A	913	A
1	A	960	U
1	A	965	A
1	A	975	A
1	A	976	G
1	A	992	U
1	A	993	G
1	A	1049	U
1	A	1065	U
1	A	1067	A
1	A	1085	U
1	A	1101	A
1	A	1129	C
1	A	1145	C
1	A	1182	G
1	A	1183	A

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Mol	Chain	Res	Type
1	A	1190	G
1	A	1196	U
1	A	1201	A
1	A	1214	C
1	A	1224	G
1	A	1226	C
1	A	1256	A
1	A	1257	U
1	A	1278	U
1	A	1281	U
1	A	1285	A
1	A	1300	G
1	A	1301	U
1	A	1302	U
1	A	1319	A
1	A	1331	G
1	A	1346	A
1	A	1347	G
1	A	1364	U
1	A	1380	U
1	A	1397	C
1	A	1409	C
1	A	1451	A
1	A	1498	U
1	A	1503	A
1	A	1504	G
1	A	1505	G
1	A	1528	U

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 123 ligands modelled in this entry, 122 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	$\#\|Z\| > 2$
25	SFG	Y	301	-	25,29,29	1.04	2 (8%)	23,42,42	1.34	3 (13%)

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
25	SFG	Y	301	-	-	3/13/33/33	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	Y	301	SFG	O4'-C1'	2.78	1.45	1.41
25	Y	301	SFG	C8-N7	-2.25	1.30	1.34

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	Y	301	SFG	N3-C2-N1	-3.99	122.44	128.68
25	Y	301	SFG	O4'-C1'-C2'	-2.39	103.44	106.93
25	Y	301	SFG	C4-C5-N7	-2.20	107.11	109.40

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
25	Y	301	SFG	C5'-CD-CG-CB
25	Y	301	SFG	N-CA-CB-CG
25	Y	301	SFG	C-CA-CB-CG

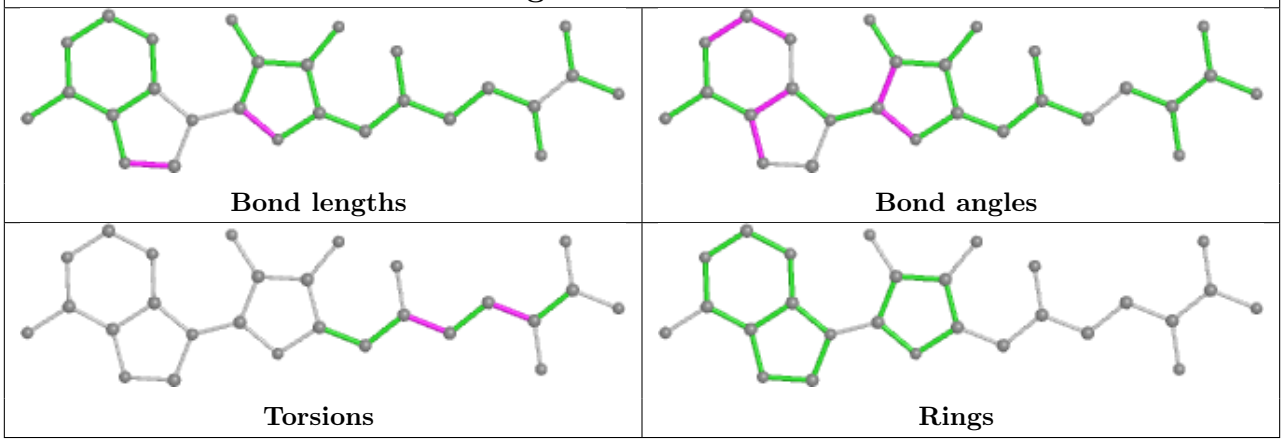
There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	Y	301	SFG	3	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 then 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.

Ligand SFG Y 301



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	1507/1513 (99%)	0.04	25 (1%)	70	62	18, 71, 170, 260	0
2	B	234/256 (91%)	0.14	7 (2%)	50	40	29, 94, 152, 190	0
3	C	206/239 (86%)	0.06	9 (4%)	34	29	44, 104, 145, 171	0
4	D	208/208 (100%)	0.02	2 (0%)	82	76	25, 79, 127, 182	0
5	E	150/161 (93%)	-0.18	0	100	100	18, 56, 106, 148	0
6	F	101/101 (100%)	-0.11	1 (0%)	82	76	48, 103, 142, 156	0
7	G	155/155 (100%)	-0.18	3 (1%)	66	59	40, 96, 148, 172	0
8	H	138/138 (100%)	-0.01	1 (0%)	87	83	11, 41, 81, 116	0
9	I	127/128 (99%)	0.59	16 (12%)	3	4	40, 105, 144, 165	0
10	J	98/104 (94%)	0.81	13 (13%)	3	3	55, 123, 165, 188	0
11	K	119/129 (92%)	0.14	3 (2%)	57	49	36, 81, 129, 171	0
12	L	124/131 (94%)	0.28	4 (3%)	47	38	18, 74, 120, 165	0
13	M	125/126 (99%)	1.08	23 (18%)	1	1	56, 97, 137, 185	0
14	N	60/60 (100%)	0.32	2 (3%)	46	38	44, 102, 136, 160	0
15	O	88/88 (100%)	0.15	2 (2%)	60	52	17, 63, 122, 167	0
16	P	83/88 (94%)	0.36	1 (1%)	79	72	21, 56, 95, 122	0
17	Q	104/104 (100%)	0.39	5 (4%)	30	26	13, 56, 119, 198	0
18	R	73/88 (82%)	0.25	4 (5%)	25	21	35, 82, 143, 191	0
19	S	80/92 (86%)	0.49	8 (10%)	7	6	73, 124, 155, 197	0
20	T	99/106 (93%)	0.11	2 (2%)	65	58	38, 80, 118, 156	0
21	V	24/26 (92%)	0.62	3 (12%)	3	4	51, 88, 137, 141	0
22	Y	219/222 (98%)	0.32	18 (8%)	11	9	64, 119, 160, 196	0
All	All	4122/4263 (96%)	0.15	152 (3%)	41	34	11, 82, 153, 260	0

All (152) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
13	M	124	PRO	17.1
13	M	123	ALA	12.9
15	O	89	GLY	10.6
10	J	64	GLU	7.7
13	M	125	ARG	7.2
11	K	128	ALA	6.6
9	I	15	ALA	6.5
13	M	120	LYS	6.3
17	Q	102	GLY	6.1
1	A	1031	G	6.0
1	A	1492	A	5.8
17	Q	103	GLY	5.5
1	A	1030(D)	A	5.2
11	K	129	SER	4.7
22	Y	1	MET	4.5
13	M	122	LYS	4.4
1	A	1129	C	4.1
13	M	126	LYS	4.0
3	C	207	VAL	4.0
3	C	15	THR	4.0
13	M	43	THR	3.9
9	I	7	THR	3.8
12	L	33	ARG	3.7
22	Y	12	LEU	3.7
10	J	45	ARG	3.7
3	C	206	GLU	3.7
1	A	1534	A	3.7
13	M	121	LYS	3.6
9	I	8	GLY	3.6
10	J	63	PHE	3.6
19	S	49	ILE	3.6
22	Y	3	ILE	3.5
9	I	65	VAL	3.5
9	I	101	PHE	3.4
17	Q	104	LYS	3.4
1	A	1531	A	3.3
19	S	41	VAL	3.3
1	A	1493	A	3.2
13	M	41	PRO	3.2
22	Y	11	ASP	3.2
20	T	103	GLY	3.2
9	I	17	VAL	3.2
22	Y	53	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
10	J	34	VAL	3.1
19	S	39	THR	3.1
1	A	994	A	3.0
12	L	62	SER	3.0
1	A	1533	C	3.0
19	S	79	THR	3.0
17	Q	101	ARG	3.0
17	Q	105	ALA	3.0
3	C	159	GLY	2.9
9	I	99	LEU	2.9
10	J	65	LEU	2.9
22	Y	158	LEU	2.9
1	A	1032	G	2.9
22	Y	4	LEU	2.9
6	F	101	ALA	2.8
15	O	88	ARG	2.8
1	A	1517	G	2.7
18	R	28	GLU	2.7
9	I	19	LEU	2.7
22	Y	91	PRO	2.7
9	I	9	ARG	2.7
10	J	89	ASP	2.7
9	I	102	LEU	2.7
13	M	2	ALA	2.7
10	J	33	GLN	2.7
1	A	1491	G	2.7
4	D	35	ARG	2.6
9	I	128	ARG	2.6
1	A	1237	C	2.6
12	L	19	ARG	2.6
22	Y	82	PHE	2.6
13	M	96	LEU	2.6
13	M	6	GLY	2.6
19	S	38	SER	2.6
13	M	104	ARG	2.6
3	C	201	TYR	2.5
9	I	75	ASP	2.5
1	A	532	A	2.5
13	M	52	GLU	2.5
22	Y	10	VAL	2.5
1	A	81	U	2.5
3	C	147	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
13	M	15	VAL	2.5
19	S	40	ILE	2.5
21	V	18	TYR	2.4
1	A	1395	C	2.4
7	G	83	ALA	2.4
9	I	105	ASP	2.4
1	A	1359	C	2.4
18	R	48	GLY	2.4
22	Y	75	GLY	2.4
22	Y	52	ILE	2.3
11	K	42	TRP	2.3
10	J	6	ILE	2.3
2	B	130	ARG	2.3
13	M	42	ALA	2.3
18	R	88	LYS	2.3
1	A	1398	A	2.3
14	N	22	THR	2.3
2	B	188	ALA	2.3
22	Y	163	PHE	2.3
10	J	72	VAL	2.3
22	Y	81	VAL	2.3
21	V	17	THR	2.2
9	I	10	ARG	2.2
2	B	16	HIS	2.2
3	C	146	ALA	2.2
4	D	148	VAL	2.2
8	H	130	GLY	2.2
16	P	1	MET	2.2
13	M	8	GLU	2.2
7	G	82	GLY	2.2
10	J	100	THR	2.2
19	S	44	MET	2.2
1	A	1030(B)	C	2.2
22	Y	2	LEU	2.2
13	M	94	ARG	2.2
2	B	211	ILE	2.2
10	J	24	VAL	2.2
10	J	10	GLY	2.1
1	A	1001	A	2.1
9	I	14	VAL	2.1
2	B	214	ILE	2.1
3	C	205	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	1033	G	2.1
21	V	24	ARG	2.1
13	M	106	ASN	2.1
19	S	43	GLU	2.1
22	Y	142	SER	2.1
10	J	20	ALA	2.1
13	M	37	THR	2.1
22	Y	138	VAL	2.1
13	M	5	ALA	2.1
20	T	81	LYS	2.1
2	B	133	LYS	2.1
7	G	85	TYR	2.1
3	C	172	ARG	2.1
1	A	1519	A	2.1
1	A	1226	C	2.0
13	M	97	PRO	2.0
14	N	14	PRO	2.0
1	A	1002	G	2.0
1	A	89	C	2.0
2	B	187	LEU	2.0
9	I	103	THR	2.0
18	R	43	PHE	2.0
22	Y	137	PHE	2.0
12	L	61	THR	2.0
13	M	88	ARG	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
23	MG	A	1626	1/1	0.21	1.00	70,70,70,70	0
23	MG	A	1601	1/1	0.24	0.59	42,42,42,42	0
23	MG	A	1665	1/1	0.24	0.85	107,107,107,107	0
23	MG	A	1646	1/1	0.37	0.68	18,18,18,18	0
23	MG	A	1612	1/1	0.38	0.33	46,46,46,46	0
23	MG	A	1669	1/1	0.39	0.81	33,33,33,33	0
23	MG	A	1627	1/1	0.43	0.45	52,52,52,52	0
23	MG	A	1652	1/1	0.47	1.18	42,42,42,42	0
23	MG	A	1603	1/1	0.50	0.80	36,36,36,36	0
23	MG	A	1662	1/1	0.52	0.49	67,67,67,67	0
23	MG	A	1675	1/1	0.52	0.36	43,43,43,43	0
23	MG	A	1684	1/1	0.53	0.51	17,17,17,17	0
23	MG	A	1688	1/1	0.53	0.85	28,28,28,28	0
23	MG	A	1621	1/1	0.55	0.59	59,59,59,59	0
23	MG	N	102	1/1	0.56	1.20	24,24,24,24	0
23	MG	A	1711	1/1	0.57	0.61	9,9,9,9	0
23	MG	A	1631	1/1	0.58	0.22	46,46,46,46	0
23	MG	A	1661	1/1	0.60	0.39	93,93,93,93	0
23	MG	A	1604	1/1	0.60	1.98	70,70,70,70	0
23	MG	A	1658	1/1	0.60	0.59	40,40,40,40	0
23	MG	A	1696	1/1	0.61	0.73	27,27,27,27	0
23	MG	A	1656	1/1	0.65	0.79	33,33,33,33	0
23	MG	A	1645	1/1	0.66	0.35	12,12,12,12	0
23	MG	A	1624	1/1	0.66	0.88	70,70,70,70	0
23	MG	A	1620	1/1	0.66	1.90	15,15,15,15	0
23	MG	B	301	1/1	0.67	0.23	59,59,59,59	0
23	MG	A	1677	1/1	0.67	0.73	63,63,63,63	0
23	MG	A	1694	1/1	0.68	0.93	14,14,14,14	0
23	MG	A	1689	1/1	0.68	0.34	58,58,58,58	0
23	MG	A	1708	1/1	0.68	0.73	21,21,21,21	0
23	MG	A	1693	1/1	0.69	1.40	18,18,18,18	0
23	MG	A	1606	1/1	0.70	0.62	37,37,37,37	0
23	MG	A	1695	1/1	0.71	1.53	52,52,52,52	0
23	MG	A	1666	1/1	0.71	0.23	26,26,26,26	0
23	MG	A	1647	1/1	0.72	0.73	70,70,70,70	0
23	MG	A	1713	1/1	0.73	0.81	39,39,39,39	0
23	MG	A	1716	1/1	0.73	0.32	42,42,42,42	0
23	MG	A	1667	1/1	0.73	0.46	76,76,76,76	0
23	MG	A	1699	1/1	0.73	0.58	43,43,43,43	0
23	MG	A	1630	1/1	0.74	0.78	7,7,7,7	0
23	MG	A	1698	1/1	0.74	0.49	23,23,23,23	0
23	MG	A	1602	1/1	0.74	1.13	22,22,22,22	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
23	MG	A	1649	1/1	0.75	0.81	15,15,15,15	0
23	MG	A	1607	1/1	0.76	0.56	61,61,61,61	0
23	MG	A	1611	1/1	0.76	0.39	57,57,57,57	0
23	MG	A	1674	1/1	0.77	0.76	8,8,8,8	0
23	MG	A	1654	1/1	0.77	0.83	16,16,16,16	0
23	MG	A	1705	1/1	0.77	0.81	16,16,16,16	0
23	MG	A	1650	1/1	0.78	0.93	57,57,57,57	0
23	MG	A	1616	1/1	0.78	0.71	19,19,19,19	0
23	MG	A	1697	1/1	0.79	0.74	38,38,38,38	0
23	MG	A	1613	1/1	0.79	0.92	63,63,63,63	0
23	MG	A	1640	1/1	0.80	0.31	33,33,33,33	0
23	MG	A	1635	1/1	0.81	0.57	25,25,25,25	0
23	MG	A	1632	1/1	0.81	0.79	27,27,27,27	0
23	MG	A	1643	1/1	0.81	0.46	10,10,10,10	0
23	MG	A	1671	1/1	0.81	1.27	10,10,10,10	0
23	MG	A	1678	1/1	0.83	0.98	27,27,27,27	0
23	MG	A	1605	1/1	0.83	1.21	8,8,8,8	0
23	MG	A	1644	1/1	0.84	0.36	54,54,54,54	0
23	MG	A	1614	1/1	0.84	0.77	59,59,59,59	0
23	MG	A	1707	1/1	0.84	0.83	42,42,42,42	0
23	MG	A	1629	1/1	0.85	0.94	70,70,70,70	0
23	MG	A	1668	1/1	0.86	0.38	15,15,15,15	0
23	MG	A	1700	1/1	0.86	0.94	10,10,10,10	0
23	MG	A	1690	1/1	0.86	1.15	33,33,33,33	0
23	MG	A	1651	1/1	0.86	1.10	8,8,8,8	0
23	MG	A	1600	1/1	0.86	0.11	63,63,63,63	0
23	MG	A	1709	1/1	0.87	0.35	34,34,34,34	0
23	MG	A	1637	1/1	0.87	0.97	70,70,70,70	0
25	SFG	Y	301	27/27	0.87	0.36	110,110,110,110	0
23	MG	A	1680	1/1	0.88	0.69	22,22,22,22	0
23	MG	A	1692	1/1	0.88	0.40	23,23,23,23	0
23	MG	A	1686	1/1	0.89	0.30	62,62,62,62	0
23	MG	A	1704	1/1	0.89	0.36	29,29,29,29	0
23	MG	A	1609	1/1	0.89	0.52	33,33,33,33	0
23	MG	A	1622	1/1	0.90	0.35	29,29,29,29	0
23	MG	A	1617	1/1	0.90	0.20	76,76,76,76	0
23	MG	A	1706	1/1	0.90	0.46	30,30,30,30	0
23	MG	A	1623	1/1	0.91	1.39	30,30,30,30	0
23	MG	A	1670	1/1	0.91	0.39	34,34,34,34	0
23	MG	A	1653	1/1	0.91	1.27	11,11,11,11	0
23	MG	A	1712	1/1	0.91	0.51	36,36,36,36	0
23	MG	A	1702	1/1	0.91	0.45	32,32,32,32	0

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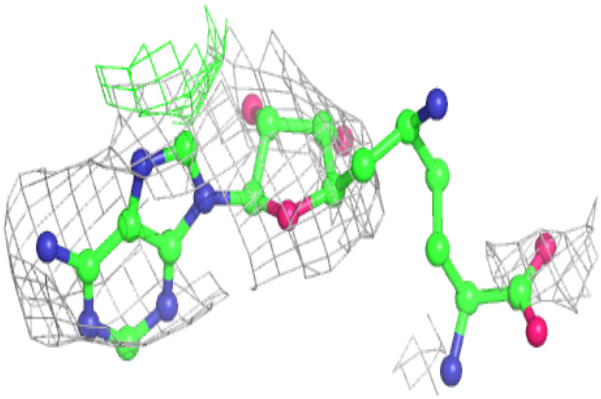
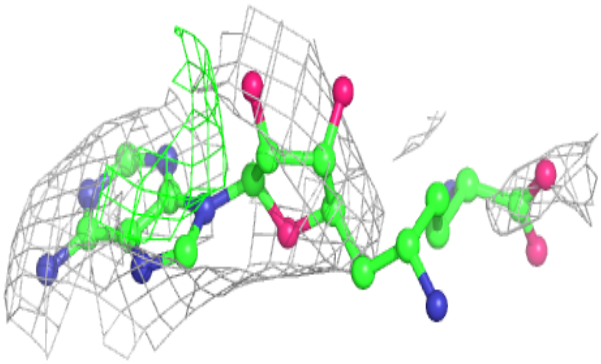
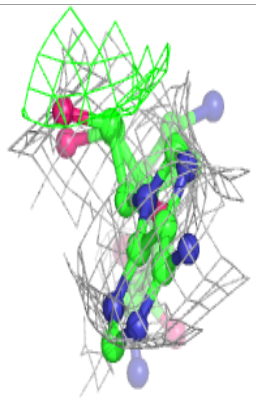
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
23	MG	A	1714	1/1	0.91	0.86	19,19,19,19	0
23	MG	A	1673	1/1	0.91	0.34	3,3,3,3	0
23	MG	A	1641	1/1	0.91	0.30	0,0,0,0	0
23	MG	A	1655	1/1	0.91	0.20	47,47,47,47	0
23	MG	A	1676	1/1	0.91	0.41	5,5,5,5	0
23	MG	A	1703	1/1	0.92	1.06	70,70,70,70	0
23	MG	A	1710	1/1	0.92	0.36	20,20,20,20	0
23	MG	A	1618	1/1	0.92	0.38	69,69,69,69	0
23	MG	A	1715	1/1	0.92	0.45	9,9,9,9	0
23	MG	A	1619	1/1	0.93	0.35	40,40,40,40	0
23	MG	A	1639	1/1	0.94	0.28	15,15,15,15	0
23	MG	A	1660	1/1	0.94	0.29	4,4,4,4	0
23	MG	A	1683	1/1	0.95	0.41	38,38,38,38	0
23	MG	E	201	1/1	0.95	1.24	21,21,21,21	0
23	MG	A	1663	1/1	0.95	0.41	16,16,16,16	0
23	MG	A	1681	1/1	0.95	0.38	41,41,41,41	0
23	MG	A	1634	1/1	0.96	0.55	3,3,3,3	0
23	MG	A	1685	1/1	0.96	0.90	36,36,36,36	0
23	MG	A	1679	1/1	0.96	0.19	27,27,27,27	0
23	MG	A	1608	1/1	0.96	0.09	56,56,56,56	0
23	MG	A	1648	1/1	0.96	0.52	4,4,4,4	0
23	MG	A	1625	1/1	0.96	0.78	0,0,0,0	0
23	MG	A	1691	1/1	0.96	0.22	2,2,2,2	0
23	MG	A	1642	1/1	0.97	0.38	33,33,33,33	0
23	MG	A	1682	1/1	0.97	0.88	36,36,36,36	0
23	MG	A	1638	1/1	0.97	0.15	47,47,47,47	0
23	MG	A	1628	1/1	0.97	0.30	54,54,54,54	0
23	MG	A	1701	1/1	0.97	0.28	6,6,6,6	0
24	ZN	N	101	1/1	0.97	0.17	108,108,108,108	0
23	MG	A	1672	1/1	0.97	0.08	15,15,15,15	0
23	MG	A	1687	1/1	0.98	0.69	17,17,17,17	0
23	MG	A	1636	1/1	0.98	0.47	1,1,1,1	0
23	MG	A	1664	1/1	0.98	0.25	7,7,7,7	0
23	MG	A	1659	1/1	0.98	0.23	12,12,12,12	0
23	MG	A	1615	1/1	0.98	0.57	27,27,27,27	0
23	MG	A	1610	1/1	0.98	0.23	63,63,63,63	0
23	MG	A	1657	1/1	0.98	0.73	0,0,0,0	0
23	MG	A	1633	1/1	0.99	0.52	27,27,27,27	0
24	ZN	D	301	1/1	0.99	0.35	34,34,34,34	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.

Electron density around SFG Y 301: 2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)	
	

6.5 Other polymers (i)

There are no such residues in this entry.